Computational modeling of the mechanism of hydrogen embrittlement (HE) and stress corrosion cracking (SCC) in metals

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Abstract. In this article theoretical models and some existing data sets were examined in order to model the two main causes (hydrogen embrittlement and corrosion-cracking under stress) of the called environmentally assisted cracking phenomenon (EAC). Additionally, a computer simulation of flat metal plate subject to mechanical stress and cracking due both to hydrogen embrittlement and corrosion was developed. The computational simulation was oriented to evaluate the effect on the stress-strain behavior, elongation percent and the crack growth rate of AISI SAE 1040 steel due to three corrosive environments (H₂ @ 0.06MPa; HCl, pH=1.0; HCl, pH=2.5). From the computer simulation we conclude that cracking due to internal corrosion of the material near to the crack tip limits affects more the residual strength of the flat plate than hydrogen embrittlement and generates a failure condition almost imminent of the mechanical structural element.

1. Introducción

Many processes in the oil and gas industry involve the use of raw materials and environments rich in hydrogen, main cause of failure by embrittlement and stress corrosion cracking in pipes and pressure vessels manufactured usually with low carbon steel. The result is normally a catastrophic fragile fracture and occurs unexpectedly, in some cases after a long time in service [1]. In this industry the evaluation of the susceptibility to stress corrosion cracking is a basic aspect that is required for safe and economical operation of many types of equipments [2]. On the other hand, machines and structural components in permanent contact in hydrogen environment can fail prematurely. Due the effect of external loading or even internal stresses some damage can occur in materials through cracking, blistering, reduction of ductility, and/or by formation of brittle hydrides [3].

2. Model for hydrogen and acid diffusion due to mechanical stress

Duda et al. [4], developed a one-dimensional model in the context of the mechanics of the continuous media to simulate mechanical strain, degradation and hydrogen diffusion through free surfaces in elastic solids. Hyodo et al. [5], evaluated the growth of a crack in high strength steel subjected to environmental and mechanical effects by coupling numerical models of linear elastic fracture mechanics and continuous damage theory (see Equation 1).
\[ \rho \frac{\partial^2 [u]}{\partial t^2} - \nabla \cdot \sigma = F \cdot V \]  

(1)

Hydrogen is concentrated in a zone called fracture process zone which is near to the crack tip. Due to high stress triaxiality near the crack tip the crystal lattice expands, which increases the hydrogen solubility locally. The high local concentration of hydrogen causes embrittlement in both, the crack tip and the fracture process zone. Embrittlement along with the high local stresses, results in microcracking in the process zone. Within the metal, hydrogen atoms are dissolved at interstitial sites remain trapped at lattice vacancies and dislocations. Both, Hydrogen diffusion and thermal desorption measurements suggest the importance of trapping by vacancies and dislocations. The equilibrium distribution of hydrogen among traps is governed by the hydrogen chemical potential \( \mu_H \) or fugacity in the metal and the binding energy of H to a dislocation \( E_{bd} \). Additionally, the concentration of H trapped at dislocations is taken as \( C_{HD} = K_{DH} C_H \), where the dislocation trapping equilibrium constant is \( K_{DH} = \exp(-E_{bd}/RT) \) [6].

Hydrogen diffusion can be modeled through the term of effective diffusivity \( D_{\text{eff}} \) into the Equation 2, in which \( V_H \) is the partial molar volume of hydrogen in iron-based alloys, \( R \) is the gas constant, \( T \) the actual temperature, \( T_Z \) the absolute zero temperature both in Kelvin and \( \sigma_h \) is the hydrostatic stress [7].

\[ \frac{\partial C}{\partial t} = D_{\text{eff}} \nabla^2 C + \frac{V_H}{R \cdot (T - T_Z)} C \cdot \nabla^2 \sigma_h \]  

(2)

3. Computational implementation

Tetrahedral elements were used for the construction of the mesh, because this type of elements coupling better to the geometry near to the tip of the crack, compared with hexahedral elements of similar sizes. On the crack tip, mesh refinement was performed. This refinement has the shape of circular rings, which permits to find more realistic values around the tip of the crack. All algorithms used in the mesh are available in the software Comsol Multiphysics, that was used to resolve the state of the stress in each node. Material properties of low carbon steel AISI SAE 1040 used in the simulation were taken from the software material database. However, some of these properties has been extracted from the literature available about the behavior of metals under the stress corrosion cracking and hydrogen fragilization conditions [8]. The computational simulation is oriented to evaluate the effect on the stress-strain behavior, elongation percent and the crack growth rate of the material under study due to three corrosive enviroments: (\( H_2 \) @ 0.06MPa; HCl, pH=1.0; HCl, pH=2.5).

4. Results and analysis

Figure 1 presents the results of simulations to evaluate the corrosion under stress and embrittlement due to the presence of hydrogen. These graphs illustrate schematically the behavior of the stress concentration factor about the remote applied stress on the plate as well as the first and second order for the stress \( \sigma_{xx} \) at the crack tip \( \theta = 0 \).

Figure 2(a) shows the behavior of the applied stress and strain based on the results obtained from the computational simulation for metallic material cracked in the presence of three corrosive environments at a rate strain of \( 3 \cdot 10^{-6}s^{-1} \). From the graph it can be inferred that under the condition of remote stress on the cracked flat plate with a crack that starts from one end, the presence of corrosive environment HCl (pH=1.0) presents the most unfavorable loading condition because according to the results of the simulation stress levels reached before the sudden failure of the material is lower than those obtained for other corrosive environments.

Figure 2(b) also presents the stress-strain relation for the same material under the same conditions of corrosion and embbrittlement, however, the strain process is developed to a higher
strain rate which is in the order of $6 \cdot 10^{-6} \text{s}^{-1}$. Based on the results shown in this graph, the load condition in presence of HCl (pH=1.0) again presents the lower stress values, before that material reaches the level of $K_{I,EAC}$.

![Figure 1](image1.jpg)

**Figure 1.** (a) Representation of normal stress in the plane of the crack and the curve of remote applied stress on the plate, and (b) Representation of the estimates of first and second order (elastic and plastic model) to the size of the plastic area at the tip of the crack in a flat plate.

![Figure 2](image2.jpg)

**Figure 2.** (a) Stress-strain relation in the presence of corrosive medium at a rate of $3 \cdot 10^{-6} \text{s}^{-1}$ and (b) at a rate of $6 \cdot 10^{-6} \text{s}^{-1}$.

The numerical model implemented allows the evaluation of the results for elongation at the tip of the crack in the presence of corrosive environments so the results illustrated in Figure 3(a) presents the elongation percentage evaluated to a load condition of $\sigma = 0.75 \sigma_y$. Based on the results for this load condition is established that HCl (pH=1.0) environment has the highest elongation percentage of the crack tip as a function of the time compared with others corrosive environments.
environments. This condition reaches values near to 4% in a few hours after started the process of degradation of the surface the crack.

Figure 3(b) shows the rate of crack growth as a function of the level of remote stress applied to the cracked flat plate. In this figure is evidenced that the highest crack growth rate is achieved under the condition of stress and corrosion for the environment HCl to pH=1.0, which reaches values of \(9 \cdot 10^{-7}\) cm/s.

5. Conclusion

In this study has been established the behavior of the strength of the material, crack tip plastic strain and crack growth rate considering the influence of hydrogen and corrosion damage. Finite element method has been implemented based closely on the stress intensity factors in Linear Elastic Fracture Mechanics theory. Two dimensional analytical solution of diffusion combined with FE analysis of crack growth permits evaluate experimental predictions as those determined by Scheider et al. [8], in the sense that values obtained in the present research through simulation for stress and strain of the material under stress corrosion cracking are similar to the values determined through the simulation developed in that research.

References

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