Application of classical finite element methods to environmentally assisted fracture modelling

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ABSTRACT

This paper shows the application of classical numerical methods to environmentally assisted fracture (EAF) modelling of metals. Three examples demonstrate the use of the finite element method to model these processes in different ways. The first approach is a chemical model on the basis of hydrogen diffusion. The second is a kinematic model based on the local strain rate computed at the notch tip. The third is a mechanical model of hydrogen damage as a crack or notch.

INTRODUCTION

Environmentally assisted fracture (EAF) of metals is a transient process which involves both mechanical and chemical phenomena, since the fracture itself depends on the stress level, and the chemical environment exerts an additional influence. In this context, classical numerical methods appear as very interesting possibilities in the computer modelling of EAF, since corrosion engineers are not usually familiar with more complicated numerical methods.

In this paper, three examples show the possibilities of standard finite element methods to model EAF phenomena. They are based on three variables of primary importance in environmental fracture: the chemical environment, the time (and consequently the strain rate), and the damage variable. The first approach is a chemical model based on diffusion of chemical aggressive species (hydrogen in this particular case). The second is a kinematic model based on the local strain rate computed at the notch tip, relevant variable which depends on time and should be used instead of the less realistic global strain rate. The third approach is a mechanical model of hydrogen damage as a crack or notch from the macroscopical point of view.
CHEMICAL MODELLING

This section illustrates chemical modelling of EAF, and describes a computer model to predict the life of prestressing steel wires in the standard ammonium thiocyanate solution [1]. The model allows the introduction of residual stresses which influence the hydrogen concentration at the wire surface and the hydrogen diffusion towards the inner points, thus conditioning the life of the wire in the solution.

The diffusion problem to solve is that of a cylinder of radius $a$ surrounded by hydrogen. The diffusion equation is:

$$\frac{\partial c}{\partial t} = D \left( \frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} \right) - \frac{DV^*}{RT} \frac{\partial c}{\partial s} \frac{\partial s}{\partial r} - \frac{DV^*}{RT} c \left( \frac{\partial^2 s}{\partial r^2} + \frac{1}{r} \frac{\partial s}{\partial r} \right), \quad (1)$$

where $c$ is the concentration, $s$ the hydrostatic stress, $D$ the diffusion coefficient, $V^*$ the molar partial volume of hydrogen, $R$ the ideal gas constant and $T$ the absolute temperature, with the initial condition $c = 0$ in $0 \leq r \leq a$ and the boundary conditions $\frac{\partial c}{\partial r} (0, t) = 0$ and $c (a, t) = c_0^*$ for $t \geq 0$. It was solved by a weighted residuals formulation [2].

Residual stress distributions generated in the vicinity of the wire surface during the manufacturing process can be introduced into the model, thus influencing the hydrogen entry. Six laws were considered (Fig. 1a). Distribution 1 is that of a material free of residual stresses; laws 2, 3, 4 and 5 correspond to materials with residual stresses associated with the manufacturing process. Plot 6 represents a material which has undergone a rolling process after manufacture, introducing strong compressive residual stresses.

Regarding fracture, it is assumed that a crack with depth $x_c$ is created when the hydrogen reaches a critical concentration $c_c$ over a distance $x_c$ (damaged zone or critical size for initiation). The critical depth (calculated on the basis of LEFM principles) and the critical concentration at the boundary (modified according to the levels of residual and applied stresses) are introduced into the diffusion results (hydrogen concentration at any point at any time). First of all, the hydrogen concentration at the $x_c$ depth point is calculated at any instant (from the nodal concentrations); later, the time for which such a concentration reaches the critical value is obtained.

Fig. 1b shows model predictions compared with experimental results (shaded area) taken from Ref [3]. The agreement is excellent, because curve 1 exactly fits the central tendency, and curves 2, 3, 4 and 5 cover the experimental band. Compressive residual stresses extend the life of the wires, while tensile residual stresses decrease it. Very strong residual stresses (Curve 6) extend the wire life even more. The importance of the externally applied stress in the scattering of the results (higher for lower stresses) is clear.
Figure 1. Chemical modelling: (a) residual stress distributions, (b) model predictions and experimental results (shaded area).
KINEMATIC MODELLING

This section deals with a kinematic modelling (strain-rate based) of EAF in round notched samples of high strength pearlitic steel. It is well known that EAF phenomena are localized and transient, the effect of strain rate being relevant [4]. However, when precracked or notched specimens are used, it is the local strain rate at the crack or notch tip—and not the externally applied testing displacement rate—that is the variable controlling the environmental process.

The present approach consists of the computation—by the finite element method in elastic-plastic regime—of local strain rate at a notch tip as a function of global strain rate in the specimen. Local or effective strain rate is the damage variable governing the EAF process, whereas global, nominal or applied strain rate is the control variable during a test. Their respective expressions are:

\[ \varepsilon_L = \frac{u_{l,i+1} - u_{l,i}}{B \Delta t} \]  
(2a)

\[ \varepsilon_G = \frac{u_{G,i+1} - u_{G,i}}{D \Delta t} \]  
(2b)

where \( u_L \) and \( u_G \) are respectively the local and global displacements; \( B \) is the local reference length; \( D \) the sample diameter; superscripts \( i \) and \( i+1 \) mean a loading step and the next one, respectively; the value \( \Delta t \) represents the time interval between two loading steps.

The approach was applied to the formulation of a kinematic fracture criterion for round notched samples of high strength pearlitic steel under hydrogen embrittlement [5]. Four notched geometries were used, as sketched in Fig. 2a. The relationship between local and global strain rates—numerically computed—is shown in Fig. 2b. It rises as the global strain increases and the plastic zone spreads, thus emphasizing the role of the constitutive equation of the material.

Experimental H-embrittlement results, represented as a function of global strain rate, were geometry-dependent. To unify the results, the average value of the equivalent stress over the microscopically affected (or critical) region was computed. In addition, local strain rate in the vicinity of the notch tip was averaged over the critical region (space average) and throughout the test duration (time average). The final operation was the change of variable from global to local strain rate. Fig. 2c shows the results according to this approach, where \( \sigma^* \) is the dimensionless equivalent stresses in hydrogen and \( \varepsilon^* \) is the dimensionless local strain rate. Most of results fit into the same universal curve (geometry-independent). The limit of applicability of this formulation is given by the asymptotic value (for quasi-static tests) of the equivalent stress for each geometry (horizontal dashed lines in the left part of Fig. 2c).
Figure 2. Kinematic modelling: (a) notched geometries, (b) relationship between local and global strain rates, (c) experimental results expressed as a function of local strain rate (universal curve).
MECHANICAL MODELLING

In this section, two mechanical models are presented to describe the failure behaviour of 316L austenitic stainless steel notched bars in hydrogen [6]. Tests had shown that hydrogen damage consisted of micro-cracking in the area surrounding the notch, thus suggesting two mechanical models [7], as depicted in Fig. 3a. The notch extension model (NEM) considers that hydrogen effect can be modelled as a geometric enlargement of the notch. In the notch cracking model (NCM), it is assumed that the embrittled area at the notch tip behaves as a macroscopic crack extending the original notch.

In both models the failure load was calculated as a function of damage depth \(c\), where the latter means notch depth increment in the NEM and extra-crack length in the NCM. The values for the NEM can be estimated by dimensional analysis, which gives the plastic-instability failure load for an axisymmetric notched bar as:

\[
F_m = \sigma_0 a^2 M (a/R,...) = \sigma_0 (a_0-c)^2 M (a/R,...)
\]  

where \(\sigma_0\) is any stress constant used to define the plastic behaviour of the material, \(a\) is a characteristic length of the cross sectional area of the bar, \(R\) is the notch tip radius and \(M\) is a dimensionless factor. Values for the NCM can be numerically computed by the finite element method with an elastic-plastic code. Then the load-elongation curves of notched specimens with cracks of different depths emanating from the notch tip were numerically obtained to determine the failure load corresponding to each crack length.

Two round notched samples were chosen: sharp notch specimen (SNS) and blunt notch specimen (BNS), corresponding to A and C in Fig. 2a. H-embrittlement results were given in terms of failure load decrease in hydrogen vs. embrittlement time (time to failure, up to the maximum load). Since model predictions were in the form of failure load decrease vs. damage depth, a data-fitting technique was used to obtain an evolution law of damage depth with time.

Fig. 3b shows model predictions and experimental results. By choosing the adequate time scale (second vertical axis) the experimental points cluster round the curve of the NEM. It is not possible to fit such results into the curve of the NCM even changing the scales of the second Y axis. For the NEM, it might be possible to obtain a similar clustering by assuming a different evolution law for damage depth in time and some kind of relationship between this variable and the ratio \(a/R\). However, this new damage NEM would be equivalent to the old one, but more complicated, in representing the hydrogen effect from a mechanical point of view. Only an exhaustive microscopical analysis of the shape and the evolution of the damaged zone would determine which is nearer to the physical reality.
Figure 3. Mechanical modelling: (a) notch extension model (NEM) and notch cracking model (NCM), (b) model predictions and experimental results.
SUMMARY

A chemical model is described to predict the life of high strength steel wires in ammonium thiocyanate. The model is formulated on the basis of hydrogen diffusion and a fracture criterion. Residual stresses generated at the wire surface during the manufacturing process can also be introduced into the model, thus influencing the hydrogen penetration and modifying the wire life. Tensile residual stresses shorten the wire life, whereas compressive ones extend it.

A kinematic model of hydrogen assisted fracture is formulated on high strength steel notched bars. It is based on the space and time average of the local strain rate in the vicinity of the notch tip, numerically computed from the global strain rate by the finite element method. Fracture criteria in aggressive environments must be formulated on the basis of local strain rate, which makes the experimental results objective, i.e., geometry-independent.

Two mechanical models are shown to represent hydrogen damage in austenitic stainless steel notched bars. The notch extension model (NEM) describes the action of hydrogen as a geometric enlargement of the notch. In the notch cracking model (NCM), the damaged zone is modelled as a macroscopic crack prolonging the original notch. The NEM agrees fairly well with the experimental results of hydrogen-embrittlement tests.

REFERENCES