A NUMERICAL MODEL TO ANALYZE THE EFFECT OF HYDROGEN ON DUCTILE FRACTURE BEHAVIOUR

M.A.Astiz*, J.A.Álvarez† & F.Gutiérrez-Solana†

Hydrogen has an important influence on the ductile fracture behaviour of microalloyed steel. This paper presents an analytical/numerical model to be applied to this problem. The model consists of two parts. Ductile fracture is modelled by means of the finite element method in combination with a cohesive crack mechanism. A finite element based model which takes into account the influence of plastic deformation is used to study hydrogen diffusion. Both models are combined to build a numerical model of ductile fracture in hydrogen filled steel.

INTRODUCTION

Stress corrosion has traditionally been studied by means of experimental research and simple analytical models. Numerical methods are now a very well known tool which may also be used in the analysis of stress corrosion problems. This methodology is presented in this paper as a result of a CECA-sponsored project which has been developped by the Universities of Cantabria, Gijón and Madrid in Spain and the CNRS (Orsay) in France in cooperation with Creusot-Loire Industries (France) and Ensidesa (Spain) as industrial partners.

The tests which have been performed on the steel qualities which are the object of this study show that the presence of hydrogen is specially important in the ductile fracture behaviour of the material.Then a cracking model in the elastic-plastic range has been developped. As material behaviour is affected by the presence of hydrogen, specially in the process zone, a hydrogen diffusion model has also been developped. Both models are combined to build a single model which may be used to study crack propagation in hydrogen environment after measuring a set of fracture and corrosion-related material parameters.

* Department of Aerospace Vehicles, Polytechnic University of Madrid, Spain
† Laboratory of Materials Science, University of Cantabria, Santander, Spain

DUCTILE FRACTURE MODEL

The J integral is the best alternative we have to analyze crack propagation. Nevertheless we will not consider the original integral as defined by Eshelby (1) and Rice (2). As this definition is only valid for non-linear elastic materials (although it may be extended to deformation theory of plasticity), we will prefer the definition of J as an energy release rate after discounting from the work of external forces not only elastic energy but also plastic deformation dissipated energy as presented by Atkins&Mai (3).

It is well known that simple crack propagation models as, for instance, the EPRI (4) model give excellent results to predict the mechanical behaviour of the fracture specimens. The model we propose is based on the cohesive crack models of Dugdale and Barenblatt and on the more recent work on concrete cracking as the Hillerborg (5) model. The main idea consists in substituting the crack by a cohesive line which may absorb an energy J_R per unit area with a negligible deformation. Once this amount of energy has been absorbed, the line looses its stiffness and both crack faces are free to separate one from the other.

The main advantages of this model are:- it is a simple model with a single parameter, J_R; - it avoids the discussions about how to take into account the elastic recoverable energy in the ductile fracture tests; - it allows the description of crack propagation in the way it really happens by reproduciong the elastic unloading behind the crack front; - it allows the separation of the plastic deformation work which is dissipated in areas which are located far from the process zone (in the cases where generalized plasticity develops) and the plastic dissipation in the process zone which has to be accounted as part of the fracture energy; - it avoids the use of sophisticated numerical models to study the stress and strain fields in the neighbourhood of the crack tip (problems with very large deformations) since all the process zone straining is circumscribed to the crack line model; - it allows to model any J_R-Δa curve by changing the constitutive equations of the crack line. As a conclusion, it is an engineering model; this means that it is somewhat simplistic but it is effective since it allows a satisfactory description of ductile fracture.

This model is to be used in combination with the finite element method. Crack will be associated with a set of elastic supports with a non-linear load-displacement response which will be located along the supposed crack propagation path (the plane of symmetry in the case of mode I fracture).The load-displacement diagram at each support has to be defined by means of two parameters: a limit load and a limit displacement (the two dimensions of the rectangular block (fig. 1). The limit load is a function of the material flow stress (an intermediate value between the yield stress and the ultimate tensile stress) and of the fraction of the finite element which is associated with each node (some kind of element integration will be involved as we will see later). The limit displacement is defined to make the area of the diagram equal to the fracture energy. It will then depend on the value of J_R.

Finally, to avoid numerical instabilities, it is necessary to reduce as much as possible the inclination of the decreasing segments of the load displacement diagrams. Then the original rectangular diagram is substituted by a triangular diagram in which the overall enclosed area is preserved but the limit displacement is duplicated (fig. 1). The elastic positive stiffness is defined as a very high value to avoid noticeable crack node displacements before yielding (yielding displacement is taken as 1/100 of the rupture displacement).

To evaluate the load which will be supported at each node in the crack plane, a stress integration has been performed along the finite element after supposing that the stress field is governed by the HRR singularity. Then the load at each node may be evaluated as

$$F_i = \lambda_i b h \sigma_{yy}(h) \qquad (1)$$

where $\sigma_{yy}(h)$ is the stress value at a distance h from the crack tip, h is the element size, b the specimen thickness and λ_i is a non-dimensional integration factor. These integration factors have been computed for corner (λ_1) and midside nodes (λ_2) and for different strain-hardening Ramberg-Osgood exponents, m (we suppose that the finite element model only uses quadratic elements). Results are plotted on fig. 2.

These analytical results have been compared to numerical results which have been obtained by computing the response of a compact cracked specimen with a stable crack. Although results are different from those which are represented on figure 2, the ratio between corner nodal forces and midside nodal forces tends to be similar to the analytical prediction. This is an important result since it only leaves the definition of the limit load value to adjust the model. The importance of this step may be checked by analyzing the same cracked specimen (in this case a CTS with B=25mm and W=100mm) with different limit loads in the crack non-linear springs. Material is an E-690 steel with J_R=300kJ/m^2. Results indicate that there are two extreme typical kinds of behaviour which should be avoided. For extremely high limit loads in the springs, crack stays stable and results are similar to what could be obtained by considering the crack plane nodes fixed. For extremely low limit load values the model does not develop plastic deformation; the overall displacements are only dependent on the non-linear springs; this is a bad approximation to the crack propagation process. for intermediate limit load values the model shows a maximum load which is roughly coincident with the moment when crack propagation begins. Results have been compared to the EPRI model prediction with very good results (fig. 3). Nevertheless the best fit has been obtained after reducing the fracture energy of the springs to 58% of J_R. This result is not surprising since the cohesive crack model is simplistic as applied to ductile fracture; then it becomes necessary to previously know what is the overall behaviour of the particular specimen under analysis (either through EPRI techniques or by means of experimental tests). In any case this is something which has to be done before undertaking any stress corrosion study. Once the fracture model has been adjusted, it may be used as a valuable tool to study the effects of hydrogen embrittlement.

HYDROGEN DIFFUSION MODEL

Although in previous hydrogen diffusion studies by the authors (6) only the hydrostatic stress influence was considered, there are many experimental data which indicate that plastic deformation is also an important factor which may govern hydrogen diffusion. On the basis of previous studies by van Leeuwen (7) and Kikuta *et al.* (8), we have assumed that hydrogen solubility, S, may be computed by means of the factorial expression

$$S = c_0 . \exp\left(\frac{V^* s}{RT}\right).(1 + \alpha\varepsilon_p) \tag{2}$$

where c0 is a reference concentration, V^* is the partial molar volume of hydrogen, R is the universal gas constant, T is the absolute temperature, s is hydrostatic stress, ε_p is plastic deformation and α is an experimentally measured non-dimensional factor. Hydrogen flux may be derived from previous expression as

$$\vec{q} = -D\left[\vec{\nabla}c - \frac{cV^*}{RT}\vec{\nabla}s - \alpha c_0 \exp\left(\frac{V^* s}{RT}\right)\vec{\nabla}\varepsilon_p\right] \tag{3}$$

This equation shows how hydrogen is driven to high hydrostatic stress regions and to high plastic deformation regions. The relative importance of these two competing mechanisms depends on parameter α since all the other constants have a fixed value.

Numerical solution of these equations is performed again by means of the finite element method. This methos has the advantage that it allows the use of the same model for the solid mechanics problem as for the hydrogen diffusion problem. Both problems are coupled through equation (3) and any node in the mesh will have three degrees of freedom: two displacements (for a 2D problem) and one concentration (for a model without hydrogen traps).

The parameters of this diffusion model have been adjusted to experimental results which were obtained during this research project. The relation between hydrogen solubility and plastic deformation was investigated by measuring hydrogen contents in saturated specimens with different plastic deformations. Results were found to be adequately described by a bi-linear relation as in fig. 4. Permeation tests on plastically deformed specimens showed that diffusivity is also somewhat dependent on plastic deformation. As our model does not take into account hydrogen traps, diffusion has to be made equal to the apparent diffusivity which has been obtained in these experiments. The best fit to these results is

$$D = D_0\, 10^{-1.25\varepsilon_p} \tag{4}$$

where the reference diffusivity, D_0, is taken to be 10^{-6}cm^2/s. The hydrostatic stress factor, V^*/RT, is computed from the theoretical values of its parameters to adopt a value equal to 8.10^{-4}mm^2/N.

The example which is presented here corresponds to the same CTS specimen as before which is stressed in such a way as to make its crack growing from 50 to 70 mm in 200 hours. This is a rather quick test since about 5000 hours would be necessary to get a uniform hydrogen distribution by charging the specimen through its surface. Figure 5 shows the solubility contours at two different moments and it can be observed that these contours are basically governed by the position of the crack tip. Corresponding hydrogen concentration contours (fig. 6) show that hydrogen travels at a lower speed in this case since the highest concentrations are localized close to the original crack tip.

CONCLUSIONS

A hydrogen diffusion model has been presented and applied in combination with a ductile fracture model. Both the ductile fracture model and the diffusion model need some experimental evidence to adjust their parameters. The combined model has a good potential for describing stress corrosion cracking as soon as a relation between J_R and hydrogen concentration will be added to it.

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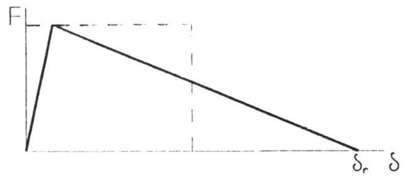

Figure 1. Load-displacement law for a crack plane spring.

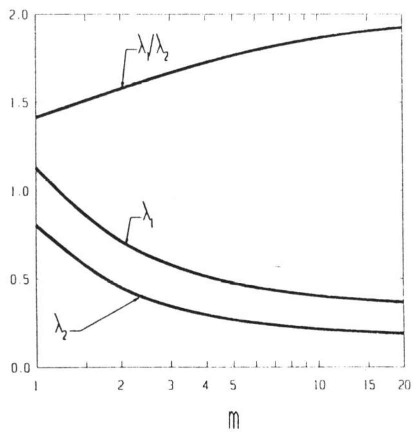

Figure 2. Integration factors.

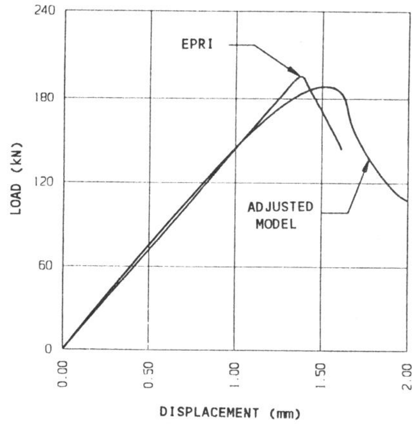

Figure 3. CTS load-displacement adjusted diagram.

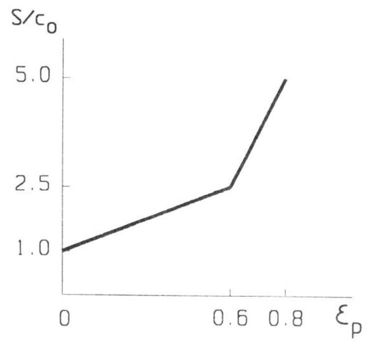

Figure 4. Hydrogen solubility as a function of plastic deformation.

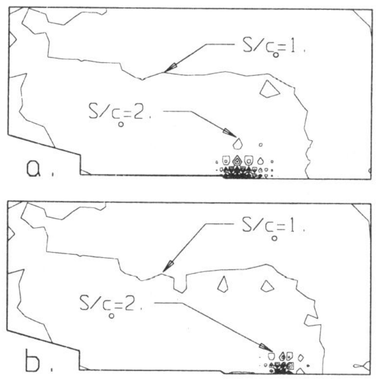

Figure 5. Solubility contours for a) t=108h and b) t=186h.

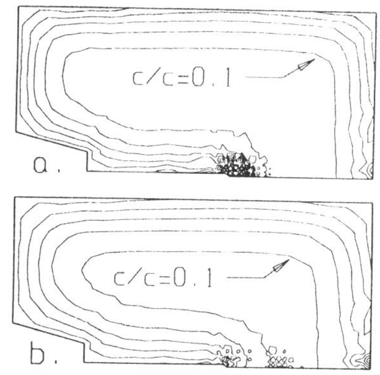

Figure 6. Hydrogen concentration contours for a) t=108h and b) t=186h.