Coupled analysis of hydrogen transport using ABAQUS

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ON COUPLED ANALYSIS OF HYDROGEN TRANSPORT USING ABAQUS

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1. Background

The research group at University of Illinois implemented coupled hydrogen transport equations and published a number of papers related to hydrogen transport and embrittlement [1-6]. The developed code, however, is based on an in-house code, not on general purpose finite element (FE) programs. Considering possible needs of numerical simulations of hydrogen-related failure in the near future, implementation of hydrogen transport equations into general purpose FE programs would be desirable. This paper explains implementation of hydrogen transport equations into the general purpose FE program, ABAQUS [7]. To incorporate effects of the hydrostatic stress and plastic strain on hydrogen transport, two user subroutines are developed. To validate the developed subroutines, present results are compared with published ones in Ref. [3].

2. Hydrogen Diffusion Model

The governing equation for transient hydrogen diffusion accounting for trapping and hydrostatic drift are given by

$$\frac{D_L}{D_{eff}}\frac{\partial C_L}{\partial t} - D_L\nabla^2 C_L + \nabla\cdot\left(\frac{D_L C_L V_H}{3RT}\nabla\sigma_{kk}\right) + \alpha\theta_T\frac{dN_T}{d\varepsilon_p}\frac{\partial\varepsilon_p}{\partial t} = 0$$
$$D_{eff} = \frac{D_L}{\left[\frac{C_L + C_T(1-\theta_T)}{C_L}\right]} \tag{1}$$

where $\partial/\partial t$ is the time derivative. In Eq. (1), D_L is the hydrogen diffusion constant through NILS; D_{eff} is an effective diffusion constant that varies pointwise; C_T is the hydrogen concentration per unit volume in trapping sites; C_L is the hydrogen concentration per unit volume in normal interstitial lattice sites (NILS); θ_T denotes the occupancy of the trapping sites; N_T denotes the trap density which is a function of the local effective plastic strain ε_p, i.e., $N_T = N_T(\varepsilon_p)$, and is measured in number of traps per unit volume.

To incorporate the hydrogen induced lattice deformation, the deformation rate D_{ij} should be calculated from

$$D_{ij} = D_{ij}^e + D_{ij}^p + D_{ij}^t \tag{2}$$

with D_{ij}^e, D_{ij}^p and D_{ij}^t denote the elastic part, the plastic part and the part due to lattice straining by the solute hydrogen. The hydrogen induced deformation rate D_{ij}^t is purely dilatational and, in the context of the large strain formulation, is given by

$$D_{ij}^{t} = \frac{d}{dt}\left\{\ln\left[1+\frac{(C-C_o)\Delta\upsilon}{3\Omega}\right]\right\} \tag{3}$$

where C is total hydrogen concentration (in NILS and trapping sites) measured in hydrogen atoms per solvent atom; C_o is the initial hydrogen concentration in the absence of any straining; $\Delta\upsilon$ is the volume change per atom of hydrogen introduced into solution that is directly related to the partial molar volume of hydrogen $V_H = \Delta\upsilon N_A$ in solution; and Ω is the mean atomic volume of the host metal atom. Detailed explanations are given in Ref. [3].

3. Finite Element Implementation to ABAQUS

To implement constitutive equations for hydrogen diffusion, two user subroutines within ABAQUS are developed. The first one is UMATHT to define a material's thermal behaviour for the heat transfer analysis (in this paper hydrogen diffusion analysis), and the second one UMAT to define a material's mechanical behaviour to incorporate deformation rate induced due to lattice straining by the solute hydrogen.

ABAQUS provides the built-in program for the heat transfer analysis [7]. An interesting point is that the governing equation for the heat transfer analysis is similar to that for transient hydrogen diffusion given in Eq. (1). Table 1 summarizes equivalency of variables associated with two types of analyses.

Table 1 Analogy of variables between the heat transfer analysis within ABAQUS and the hydrogen diffusion analysis.

Heat transfer analysis (ABAQUS)		Hydrogen diffusion analysis	
Variable	Description	Variable	Description
$U(\theta)$	Thermal energy	$U(c)$	Chemical potential
T	Temperature	C_L	Interstitial hydrogen concentration
C_p	Specific heat	D_L/D_{eff}	Effective diffusion constant
ρ	Density	1	Unity
k	Conductivity	D_L	Diffusivity

4. Comparisons with Published Results

To validate user subroutines implemented into ABAQUS for hydrogen diffusion simulations, simulated results are compared with published results in Ref. [3]. The geometry was the boundary layer problem simulating small scale yielding under plane strain Mode I opening mode (see Fig. 1).

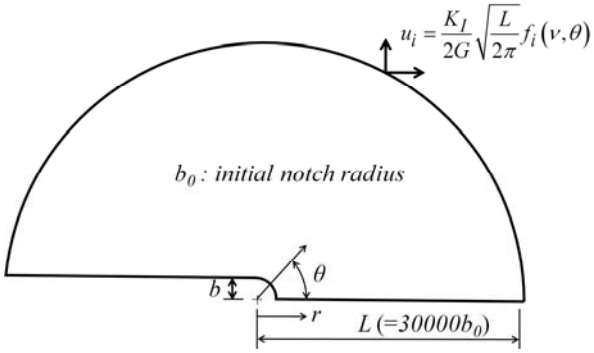

Figure 1 The boundary layer approach simulating small scale yielding under plane strain Mode I opening mode

Variations of the normalized concentration C_L/C_o in NILS with the normalized distance are shown in Fig. 2 for the boundary layer problem with the constant concentration condition. The distance r (from the notch root) is normalized with respect to the current crack opening displacement b (see Fig. 1 for the definition of r and b). In the figures, the results for $t=t_1$ indicate variations of C_L/C_o at time $t=t_1$, and the results for three different cases of t_1, t_1=1.3s, 13s, 130s, are shown. After sufficiently long times have elapsed, variations of C_L/C_o do not change with time anymore regardless of the choice of t_1, which are indicated as the steady state. Present FE results agree well with published ones in Ref. [3] for all cases considered.

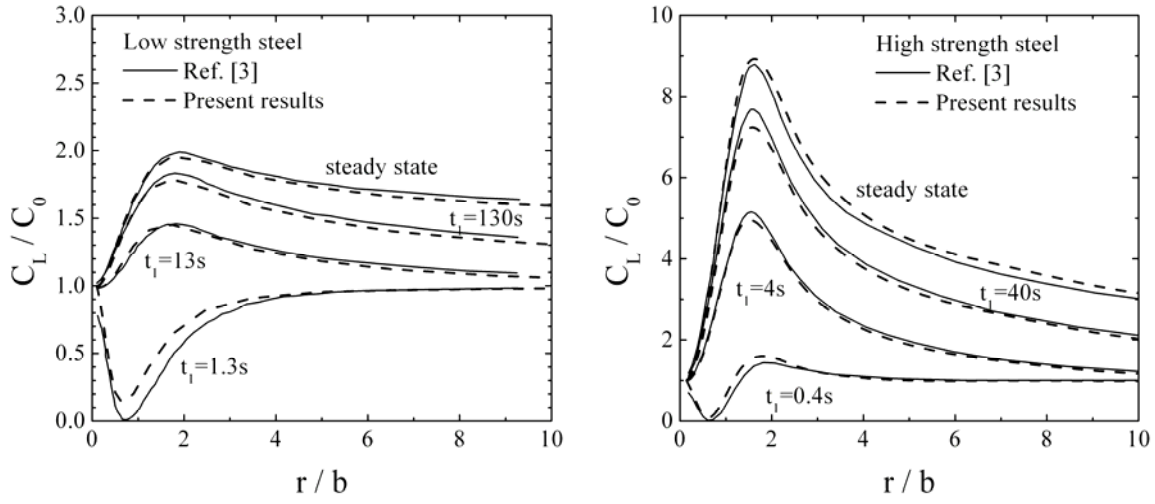

Figure 2 Variations of the normalized concentration C_L/C_o in NILS with the normalized distance for the boundary layer problem with the constant concentration condition: (a) the low strength steel and (b) the high strength steel.

5. Conclusions

This paper introduce a method to simulate coupled hydrogen transport equations via user-defined subroutines provided by the general purpose FE program, ABAQUS. Good agreement with published results in Ref. [3] gives confidence in the use of developed subroutines for simulating hydrogen transport with ABAQUS.

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