**Work package 4 --- Modeling**

We propose to develop a fully coupled diffusion-elastoplastic-stress-analysis model that accounts for possible damage development due to the effects of hydrogen on the mechanical behavior of pipeline steels. The proposed work builds on the original contribution of Sofronis and McMeeking (1989) who were the first to develop a detailed analysis of hydrogen transport near a blunting crack tip. The principle of mass conservation leads to the following diffusion-type equation

,

where  denotes the number of hydrogen atoms per unit lattice volume,  the number of trapped hydrogen atoms per unit lattice volume, and the vector  the hydrogen flux (hydrogen atoms per unit area per unit time). We treat  as the primary unknown and use the following equation (Sofronis and McMeeking, 1989) to define 

, ,

where  is the ratio of occupied sites to the total available,  denotes the number of traps per unit lattice volume,  is the equivalent plastic strain, and  is an appropriate constant resulting from Oriani’s (1970) theory of trap behavior. The hydrogen flux is related to  and the spatial gradient of the hydrostatic stress  with an equation of the form (Sofronis and McMeeking, 1989)

,

where  is the lattice diffusion constant,  the partial molar volume of hydrogen in solid solution,  the gas constant (8.3144 J mol-1K-1), and  the absolute temperature. ***The terms  and  couple the hydrogen transport problem to the corresponding problem of stress analysis***.

*Damage development and stress-state dependence*

A first attempt to account for hydrogen-induced damage was made by Sofronis *et al*. (2001) and Lian *et al*. (2003), who introduced a hydrogen-dependent flow stress and studied the effects of hydrogen on plastic instabilities in metals. We propose to use a similar approach by introducing in the model an appropriate damage parameter , in the spirit of *Damage Mechanics*. ***The damage parameter will depend on the total hydrogen concentration  and on the stress state***. In particular, it is proposed to build on the results of Lian *et al.* (2012) and Wu *et al*. (2017), who developed an extension of the well-known Bai-Wierzbicki (2008) damage model. The aforementioned extended model defines the equivalent plastic strain for failure as a function of the stress triaxiality and the Lode angle; we will be referring to it as the **M**odified **B**ai-**W**ierzbicki damage model (MBW model).

An attempt has already been made in this direction by the group of Dr. Lian (member of the proposing team) and preliminary results have been reported in Liu *et al*. (2022). In particular, it is proposed to carry out a series of uniaxial tests on specimens of different geometries that cover a wide range of triaxialities and Lode angles with and without in-situ electrochemical hydrogen charging to determine the effects of hydrogen on material failure. These experiments, combined with detailed finite element calculations, will be used to calibrate the developed damage model.

*Deliverables*: Report with model description

*Numerical implementation*

Sofronis and McMeeking (1989) were the first to present a detailed analysis of hydrogen diffusion in the region near a crack tip, where elastic plastic deformations take place. Their analysis involves “one-way-coupling”, in that the diffusion equation was influenced by the elastoplastic deformation and the hydrostatic stress in the crack-tip region, whereas the elastoplastic solution was not influenced by the presence of hydrogen. An improved numerical solution was presented by Krom *et al*. (1999), who accounted properly for the dependence of the solution of the *incremental* (rate) problem on the equivalent plastic strain increment .

We propose to develop a methodology for the numerical solution of the ***fully-coupled*** diffusion-stress-analysis problem including damage. The model to be developed will be implemented in the ABAQUS general purpose finite element program. It should be noted that all ABAQUS solutions available in the literature are based on the use of the \*COUPLED TEMPERATURE-DISPLACEMENT analysis option in ABAQUS/Standard together with appropriate user subroutines and the analogy introduced by Oh *et al*. (2010), in which  is identified with temperature in ABAQUS. It should be emphasized that the original analogy introduced by Oh *et al*. (2010) was later modified/improved by various authors (Moriconi *et al*. 2014, Barrera *et al*. 2016, Díaz *et al*. 2016, Charles *et al*. 2017, Fernández-Sousa *et al*. 2020) and used always in the context of ABAQUS/Standard (as opposed to Explicit). Since ABAQUS/Standard is an ***implicit*** code and is known to experience convergence difficulties when material damage develops and element elimination techniques are used (see Aravas and Papadioti, 2021).

To overcome this difficulty, we propose to develop the appropriate implementation in ABAQUS/Explicit, which has been successfully used by several member of the proposing group to model material failure at a structural level (Lian *et al*. 2012, Papadioti *et al*. 2019, Aravas and Papadioti 2021). In particular, the \*DYNAMIC TEMPERATURE-DISPLACEMENT analysis option will be used together with the analogy of Oh *et al*. (2010) and the appropriate used subroutines. The calculations require the determination of the spatial gradient of the hydrostatic stress , where  is the hydrostatic stress and  is the stress tensor. Most authors use second order (quadratic) elements (e.g., 8-node plane-strain elements) for an accurate determination of . It should be noted though that first order (linear) elements are i) more appropriate for capturing the discontinuities that may develop in elastoplastic solution and, more importantly, ii) are a lot easier to use in explicit codes with reduced integration and hourglass control, when “element vanish” techniques are required to study damage development due to hydrogen. The development of a methodology for the accurate evaluation of  with first order elements is part of the proposed work. In particular, we propose to define a continuous pressure field in the mesh by using an averaging technique to calculate the appropriate nodal pressure values and the then evaluate the required  from the resulting continuous pressure filed.

It should be also noted that the modification introduced by Krom *et al*. (1999) *is not an issue* in our formulation, as it affects only the *rate form* of the mass concentration equation and accounts for the appropriate implementation of the dependence of  on the equivalent plastic strain .

*Deliverables*: Report with detailed description of numerical implementation and “user subroutines”.

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