Modelling of cavity hydrogen pressure for a cast steel

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Introduction

Hydrogen is a harmful element for steels because it can easily embrittle them. This phenomenon is known as Hydrogen Embrittlement (H.E).
The hydrogen pressure theory is a H.E. mechanism in which atomic hydrogen H diffuses through the material and recombines to molecular hydrogen H2 inside the cavities. As a result, the internal pressure rises until reaching equilibrium. Consequently, the pressure can attain hundreds of MPa in some cases and it generates a stress field around the cavity, which can lead to rupture.

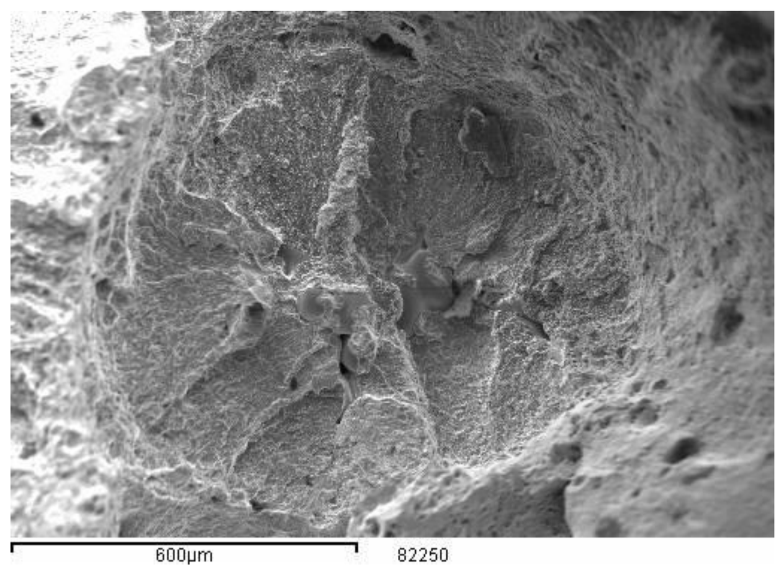

Figure 1. Fracture surface of a steel shown a particular feature related to H.E known as "fish-eyes".

Computational methods

The **internal pressure** cannot be measured experimentally, thus, in order to estimate it a finite element model was elaborated using COMSOL Multiphysics®.

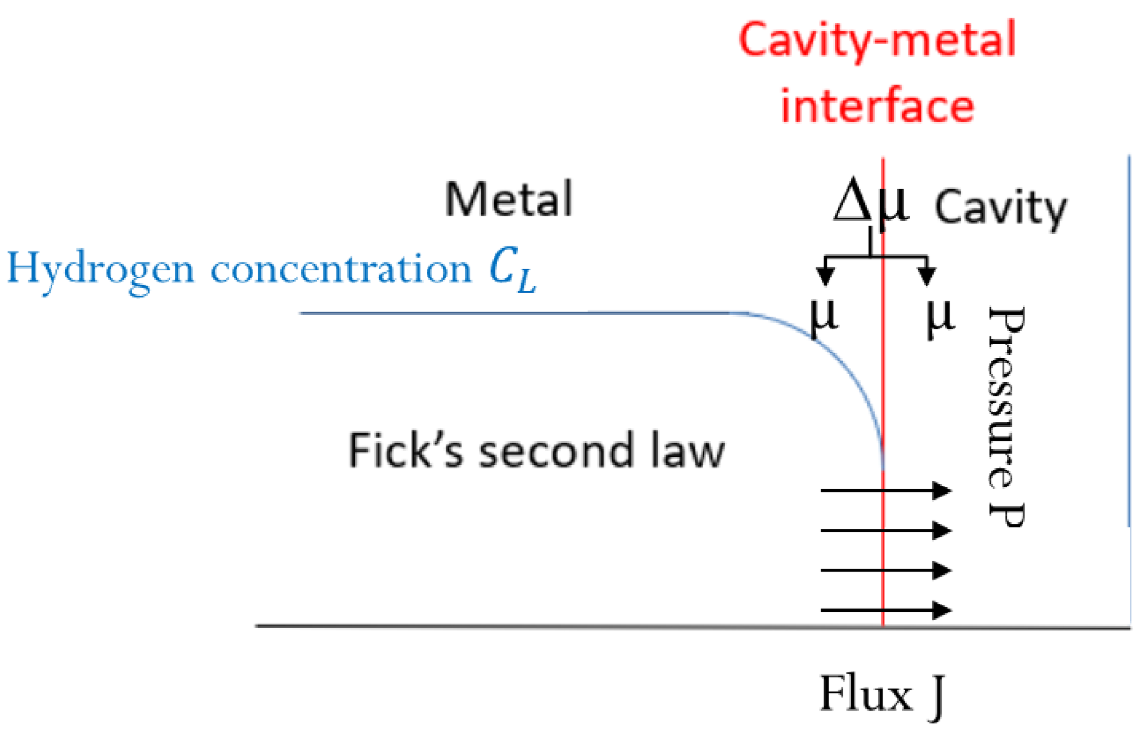

Figure 2. Simulation approach

Defining flux at cavity-metal interface

- $J = -CM\dfrac{\partial \mu}{\partial x} \quad \equiv \quad J = -CM'\Delta\mu$
- $2H \leftrightarrow H_2 \Rightarrow \frac{1}{2}(\mu^0_{H_2} + RT\ln f) = \mu^0_{H} + RT\ln c_L,$

$$\boxed{J = -C \times Q \times ln\frac{S \times \sqrt{f}}{C}}$$

- C : hydrogen concentration
- Q : constant
- S: hydrogen solubility
- f : fugacity

The pressure

$$\ln\left(\frac{f}{P}\right) = \int_0^P \left(\frac{V_m}{RT} - \frac{1}{P}\right) dP$$

- P : pressure
- R : gas constant
- T : temperature
- V_m : molar volume

The present model uses mainly two physics interfaces :

- The transport of diluted species
- Boundary ODEs and DAEs

Results

Simulation

The setup consists of a rectangular metal sample that contains 3 cavities with different dimensions.
Initially, hydrogen is located only in the matrix and no flux was applied on the box boundaries.

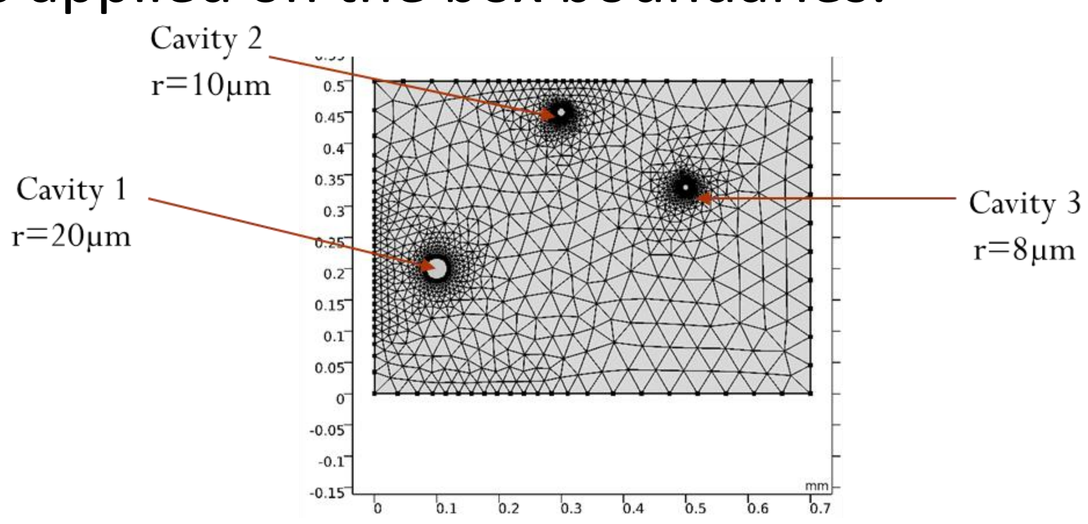

Figure 3. Simulation box

Pressure

The model is able to predict the equilibrium pressure inside a cavity and permits to follow the time-dependence of hydrogen pressure during diffusion.

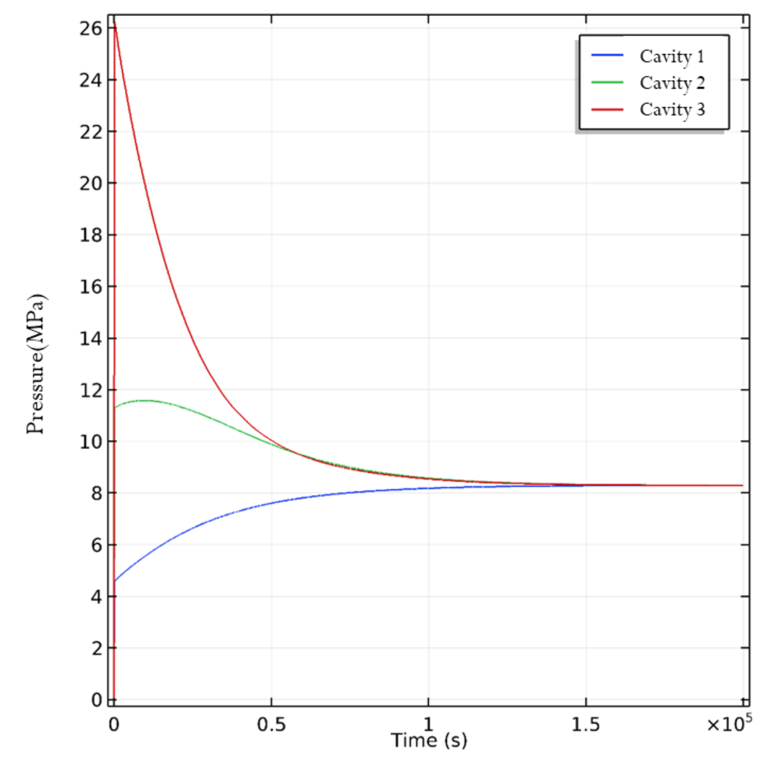

Figure 4. Simulation box

Mass balance

The following graph shows the evolution of hydrogen quantities between the matrix and cavities. The mass is conserved at every time step.

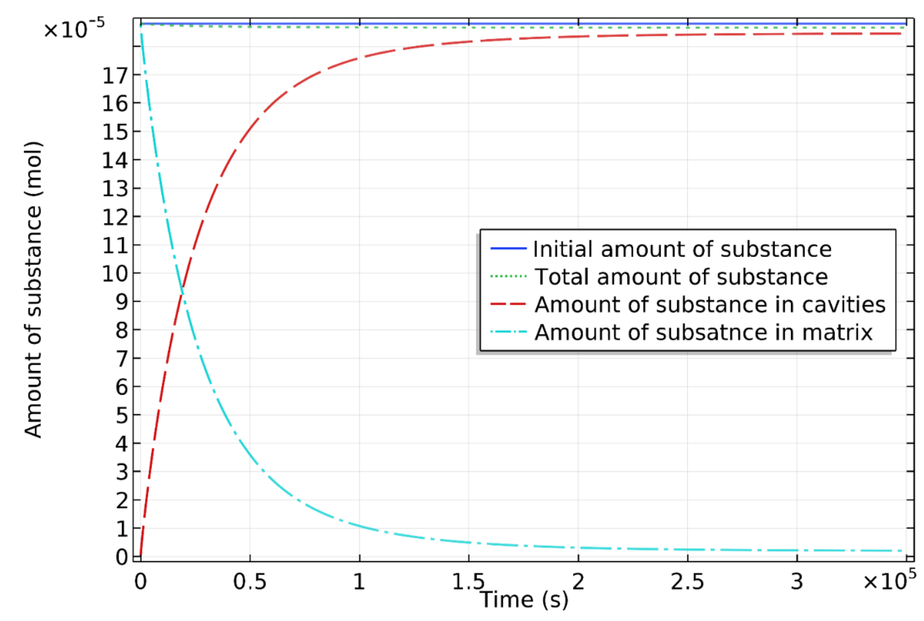

Figure 5. Simulation box

Conclusions

- A numerical model that predicts hydrogen pressure inside a cavity was created.
- The time dependence of hydrogen pressure during diffusion permits to have a better understanding of the problem.
- Results show that the maximum pressure can be reached before equilibrium.

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