

Finite element models for the study of hydrogen embrittlement of steel structures

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Thesis defense

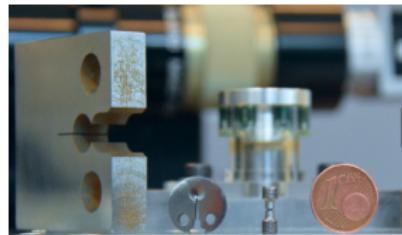
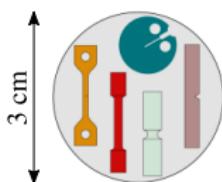
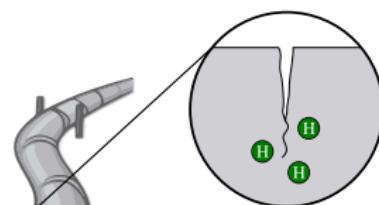
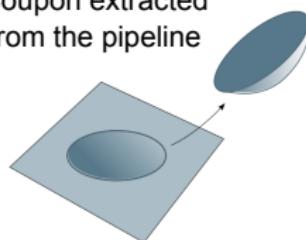
March 7th 2025

- ▶ In the context of **energy transition**, **hydrogen** plays an important role as an **energy vector**
- ▶ Hydrogen can be produced from other **renewable sources**, such as wind and solar
- ▶ Hydrogen transport using **existing natural gas pipelines** (40,000 km in France, 50 billion in assets, up to 80 years old) is a proposal for hydrogen transport



- ▶ The steels used in gas pipelines are typically susceptible to **hydrogen embrittlement**
- ▶ Hydrogen embrittlement: ductility and toughness reduction, premature failure
- ▶ **Measure material properties from small samples without service interruption**

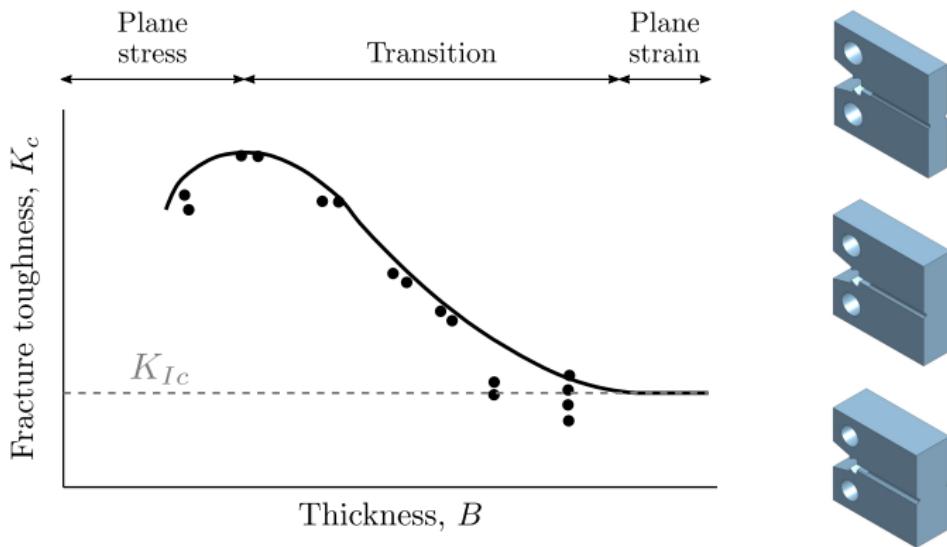
Coupon extracted
from the pipeline



MESSIAH
Chaire ANR industrielle

The logo for the MESSIAH industrial chair, featuring a stylized blue and white circular graphic next to the text "MESSIAH Chaire ANR industrielle".

- ▶ Experimental observations show that **toughness decreases with increasing specimen thickness** until reaching a plateau
- ▶ Beyond a critical thickness, toughness becomes relatively insensitive to further increases



Adapted from Barsom and Rolfe, 1987.

- ▶ Develop a model coupling **plasticity, damage, and hydrogen diffusion**
- ▶ Validate the model against experimental data
- ▶ Simulate size and thickness effects on toughness using sub-size specimens

Introduction

Hydrogen inside metals

Finite element formulation

Numerical simulations

Pressurized disks tests

Hydrogen embrittlement modeling

Simulation of fracture toughness tests

Conclusions and perspectives

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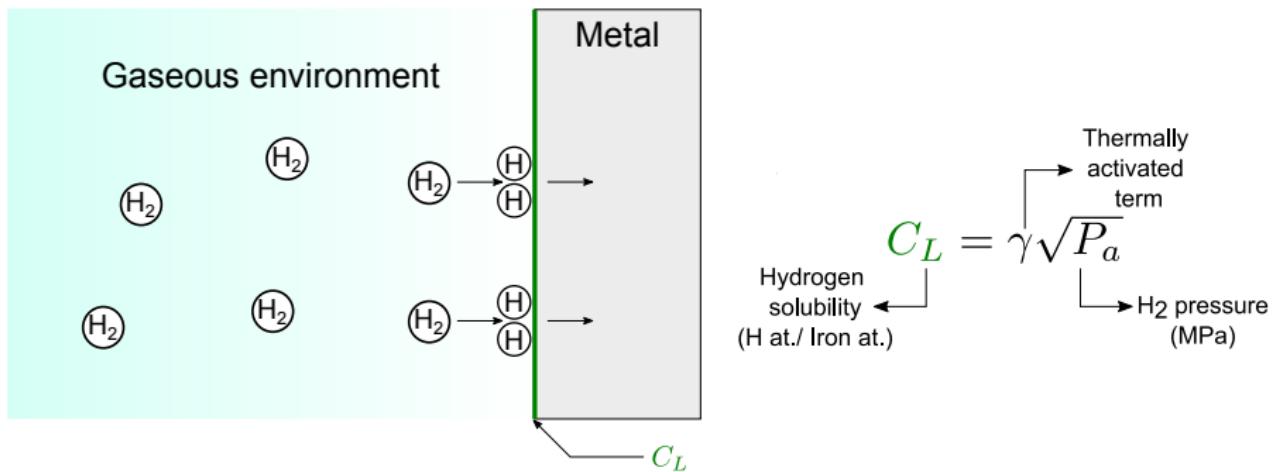
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- ▶ **Sieverts' law:** The solubility of a diatomic gas in a metal is proportional to the square root of the gas pressure

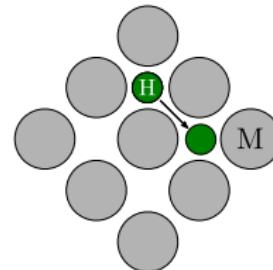


- Model from Sofronis and McMeeking (1989) and corrected by Krom *et al.* (1999)

- **Hydrogen concentration:** $C = C_L + C_T$

- Lattice concentration: $C_L = \beta N_L \theta_L$

- Trapped concentration: $C_T = \sum_i^N C_T^i = N_T^i(\kappa) \theta_T^i$



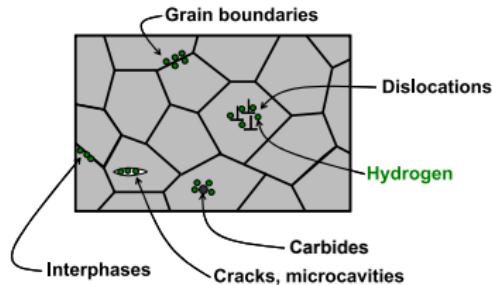
- **Hydrogen flux:**

$$J = -D_L \nabla C_L + \frac{D_L C_L V_H}{RT} \nabla p$$

- **Oriani's equilibrium:**

$$\frac{1 - \theta_L}{\theta_L} \frac{\theta_T^i}{1 - \theta_T^i} = K$$

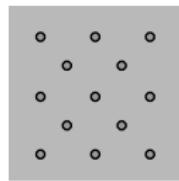
(Coupling terms)



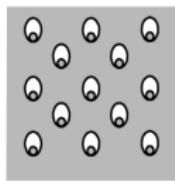
- The **ductile behavior** of the metal is described by the **GTN model** (Tvergaard *et al.* 1984):

$$\frac{\sigma_{eq}^2}{\sigma_F^2} + 2q_1 f_* \cosh \left(\frac{q_2}{2} \frac{\sigma_{ii}}{\sigma_F} \right) - 1 - q_1^2 f_*^2 = 0$$

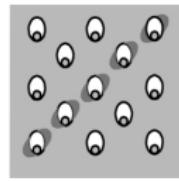
$$\dot{f} = \dot{f}_{nucleation} + \dot{f}_{growth}$$



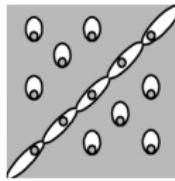
Impurities or second phase particles



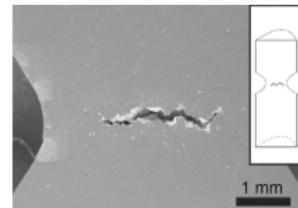
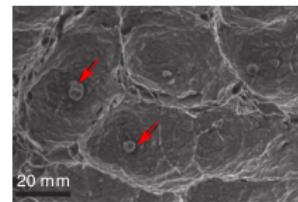
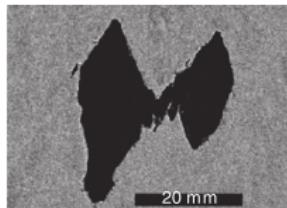
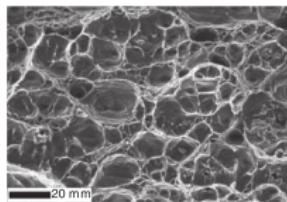
Void nucleation and growth



Strain localization



Void coalescence and fracture

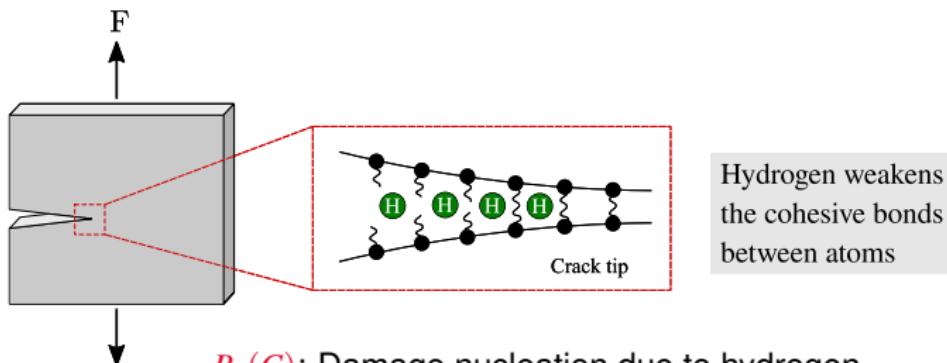


- **Void growth:** Unchanged due to mass conservation

$$\dot{f}_g = (1 - f_g) \text{trace}(\dot{\varepsilon}_p)$$

- **Void nucleation:** Proposed dependence on hydrogen concentration

$$\dot{f}_n = A_n(\kappa)\dot{\kappa} + B_n(C)\dot{\kappa} \quad (\text{Coupling terms})$$



Hydrogen weakens
the cohesive bonds
between atoms

$B_n(C)$: Damage nucleation due to hydrogen
HEDE (Hydrogen Enhanced Decohesion)

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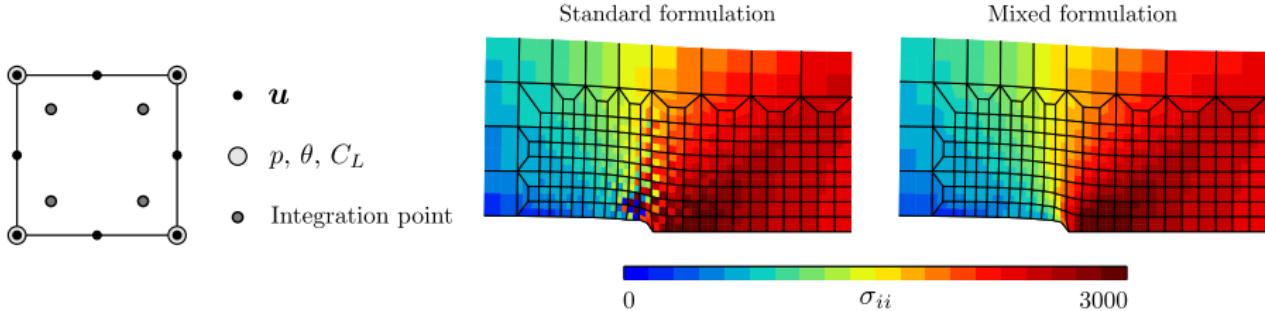
- ▶ Fully implicit finite strain framework
- ▶ Based on a mixed formulation: \underline{u}, P, θ (Zhang et al. 2017) and C_L
- ▶ Quadratic elements with reduced integration
- ▶ **Aim:** better pressure fields by avoiding volumetric locking



Advantage

∇p can be directly computed from nodal values

$$J = -D_L \nabla C_L + \frac{D_L C_L V_H}{RT} \nabla p$$



- ▶ The use of **quadratic elements** with additional dofs lead to **high simulation times**

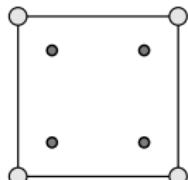


- B -bar (or \bar{B}) formulation (Hughes, 1980):

- ▶ Linear elements with full integration
 - ▶ Solves volumetric locking by modifying the strain-displacement matrix:

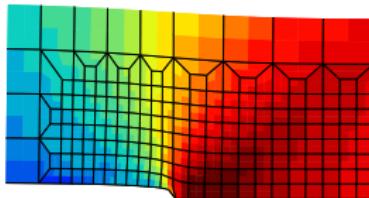
$$\bar{B} = B_d + \bar{B}_h$$

- To avoid extrapolating p to the nodes for ∇p computation, it is considered as a dof

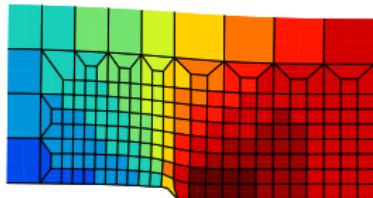


- \mathbf{u}, p, C_L
- Integration point

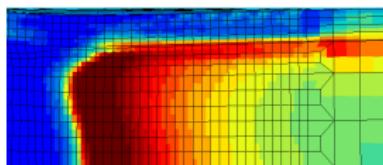
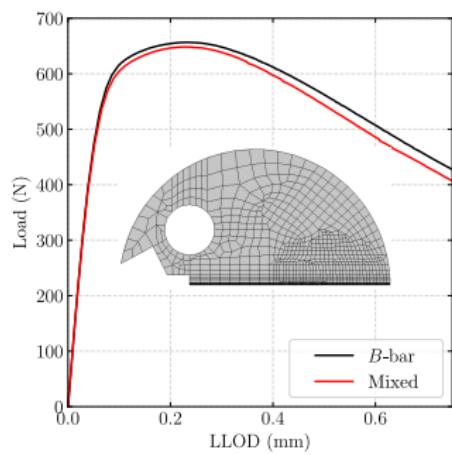
Mixed formulation



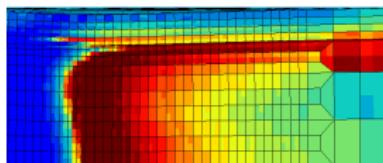
B-bar formulation



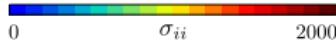
- ▶ Test on a Disk Compact Tension (DCT) specimen with 5200 elements:
 - ▶ **Mixed formulation:** 103,762 dofs, 1h 40 minutes to complete
 - ▶ **B-bar formulation:** 33,974 dofs, 18 minutes to complete
- ▶ Slightly higher force for the **B-bar** formulation → Linear elements are inherently stiffer since they have less nodes



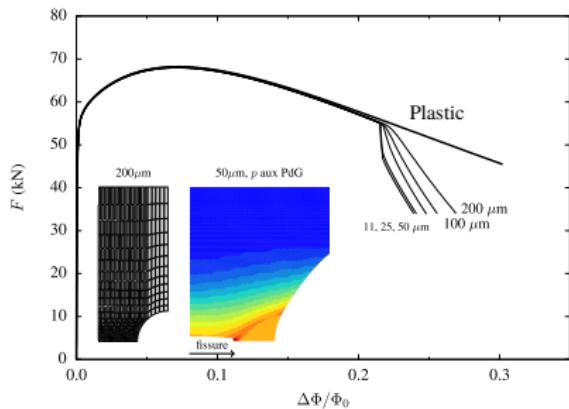
Mixed formulation



B-bar formulation

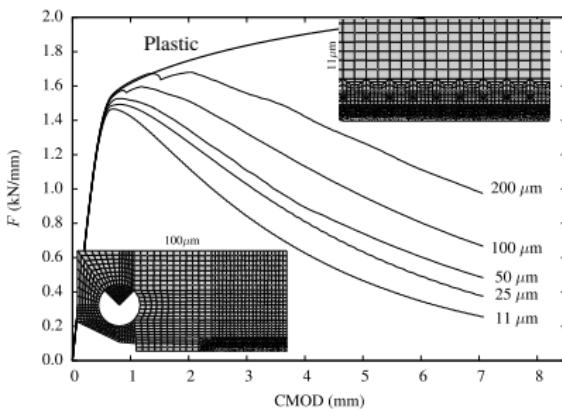


- ▶ Damage models such as the GTN model are known to induce **spurious mesh dependency** (element size, type and orientation)
- ▶ To solve this problem, it is proposed to use a **nonlocal damage model** based on the **implicit gradient** by Peerlings *et al.*, 1996



Notched tensile (NT) specimen

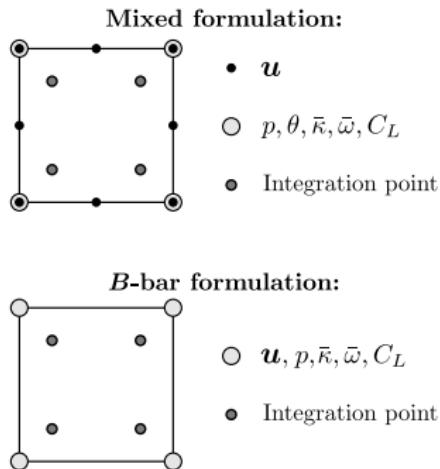
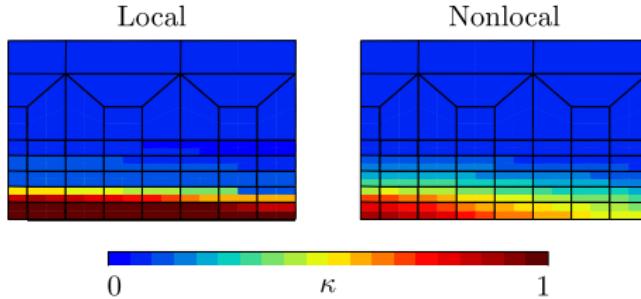
(Besson, 2021)



Compact tension (CT) specimen

- ▶ Two variables are used (two associated internal lengths: $\bar{\omega}$ and $\bar{\kappa}$):
 - ▶ **Plastic volume variation:** $\bar{\omega} - \ell_{\omega}^2 \Delta \bar{\omega} = \omega$ where $\omega = \text{trace}(\dot{\varepsilon}_p)$
 - ▶ **Accumulated plastic strain:** $\bar{\kappa} - \ell_{\kappa}^2 \Delta \bar{\kappa} = \kappa$ - ▶ The modified evolution laws for the damage variables are now:

- ▶ **Void growth:** $\dot{f}_g = (1 - f_g) \dot{\bar{\omega}}$
 - ▶ **Void nucleation:** $\dot{f}_n = A_n \dot{\bar{\kappa}} + B_n(C) \dot{\bar{\kappa}}$



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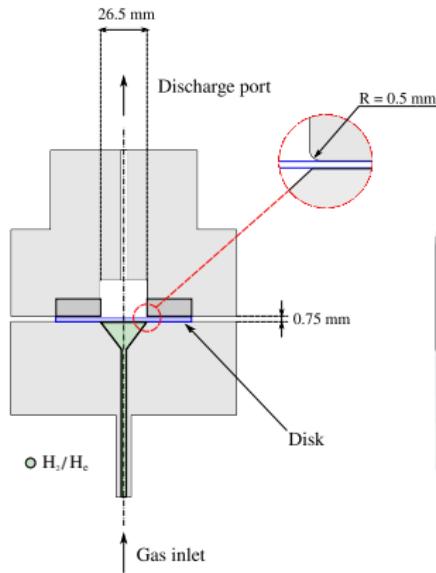
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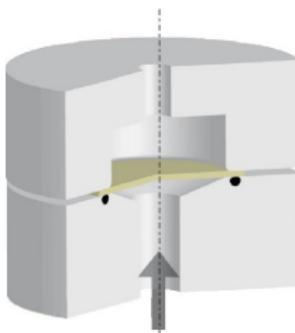
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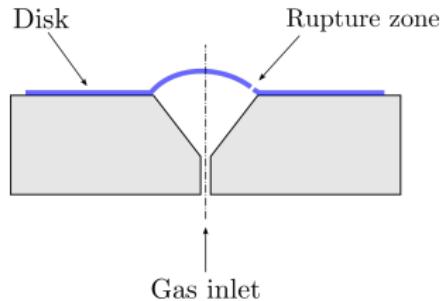
- ▶ **ISO 11114-4 standard:** uses pressurized disk tests for selecting metallic materials resistant to hydrogen embrittlement
- ▶ Disk often fails in the clamping zone
- ▶ **First step:** redesigning the disk geometry to control failure location



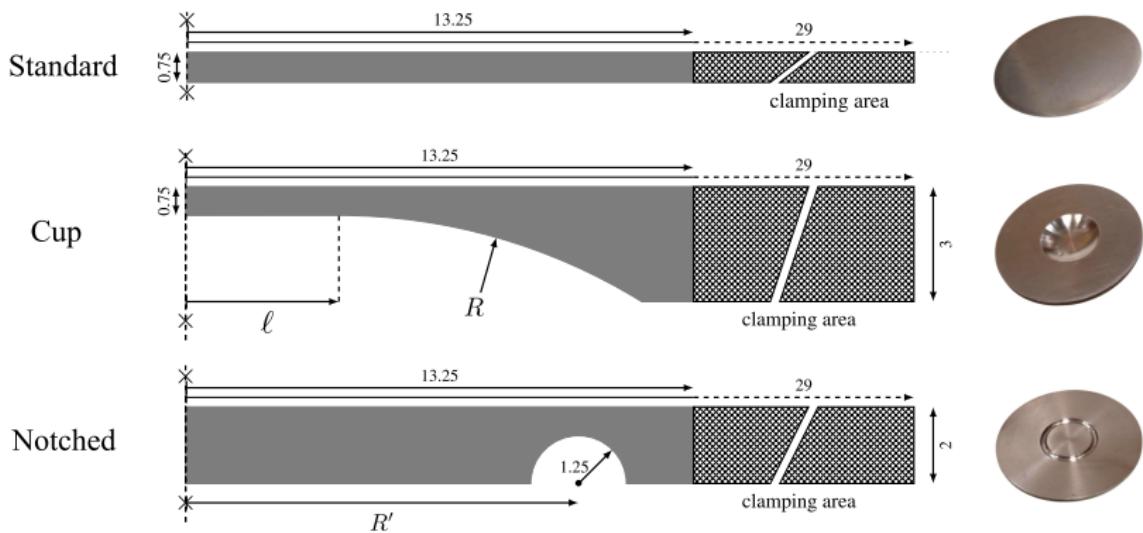
$$\text{HEI} = \frac{P_r(\text{He})}{P_r(\text{H}_2)}$$



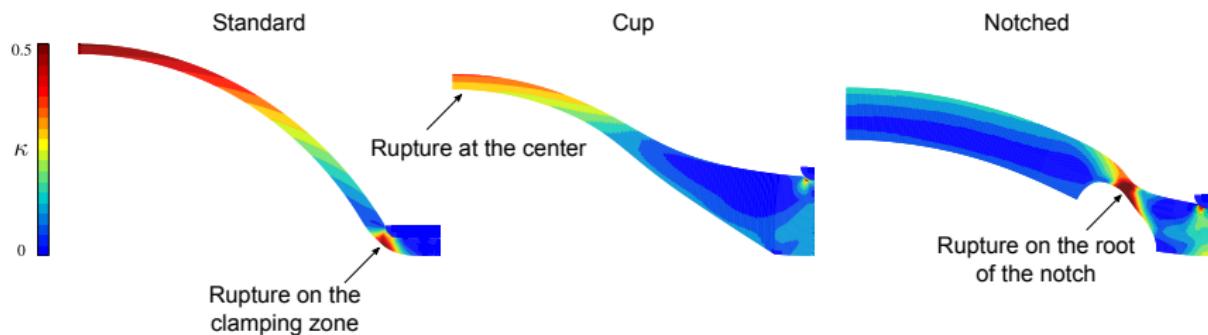
Disk specimen:



- ▶ New proposed geometries:
 - ▶ No need to modify the test setup
 - ▶ Keep the same minimum thickness of the standard (0.75 mm)
- ▶ Optimization with respect to ℓ , R and R' with FE simulations considering an elasto-plastic behavior



- ▶ The location of the maximum accumulated plastic strain (κ) corresponds to the failure location



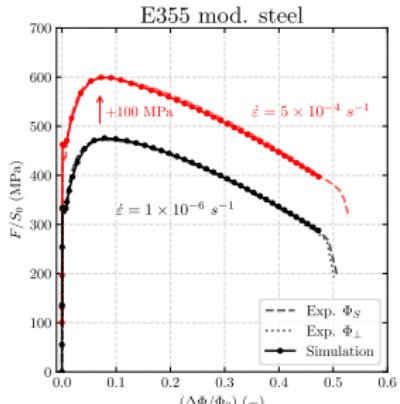
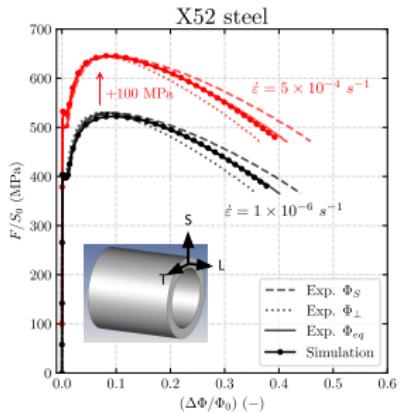
► X52 vintage steel:

- ▶ Yield strength: 400 MPa
- ▶ Different elongation at rupture in T and L directions

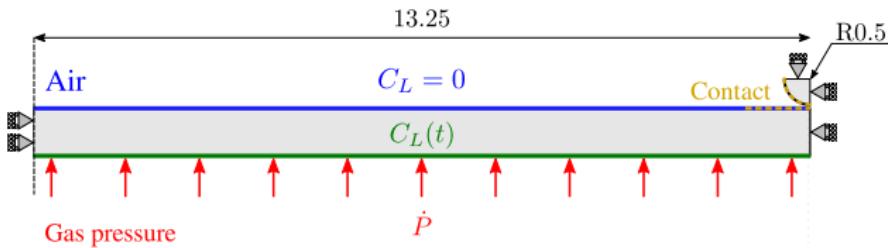
► E355 mod. steel:

- ▶ Yield strength: 330 MPa
 - ▶ Higher elongation at rupture and lower Ultimate Tensile Strength in relation with the vintage material
 - ▶ Similar elongation at rupture in both directions
- Elasto(visco)-plastic model coefficients' identified through optimization:

$$\sigma_F(p) = \max(\sigma_L, \sigma_0 + Q_1(1 - \exp(-b_1 p)) + Q_2(1 - \exp(-b_2 p)) + H p)$$

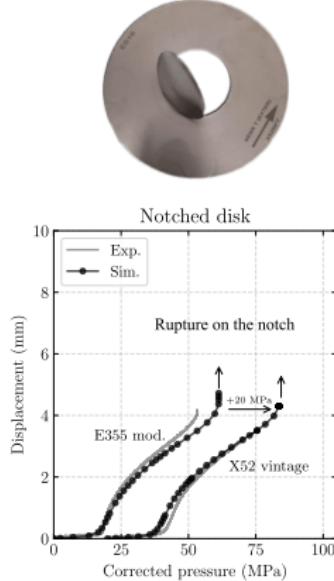
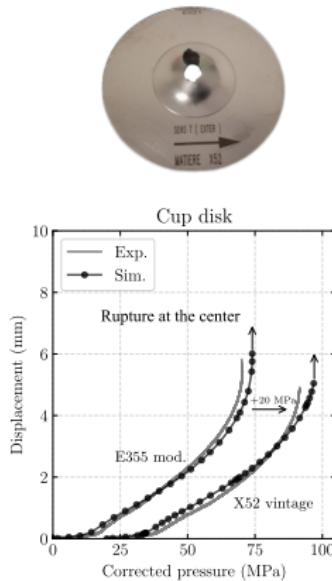
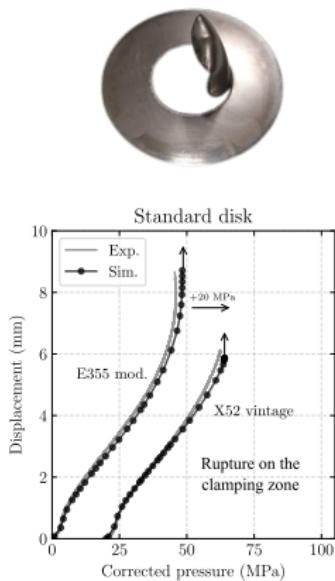
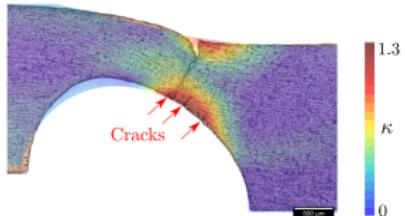


- ▶ Axisymmetric model, quadratic elements with reduced integration (mixed formulation)
- ▶ Hydrogen diffusion parameters taken from the literature
- ▶ Since damage is not considered into the numerical model, the simulations were stopped once they reached experimentally observed rupture pressure (P_r)
- ▶ Model's boundary conditions:



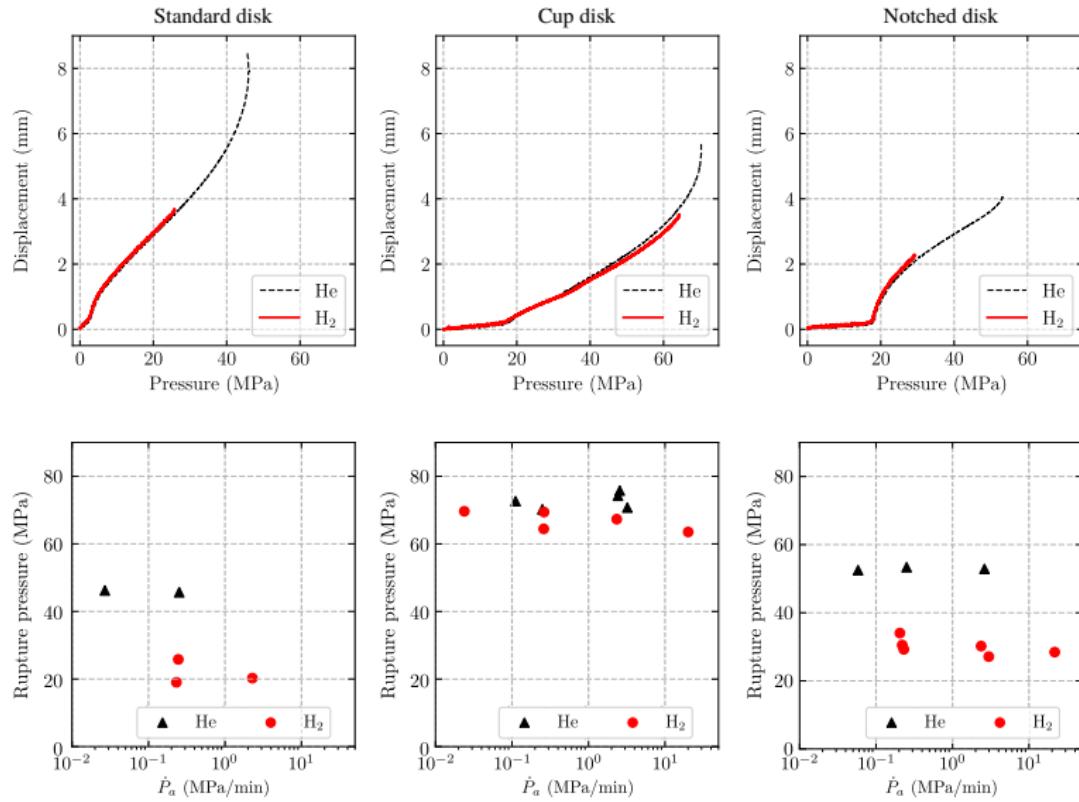
Results under helium

- ▶ Successfully modification of fracture location
- ▶ Failure is primarily driven by plasticity and occurs under a limit load scenario



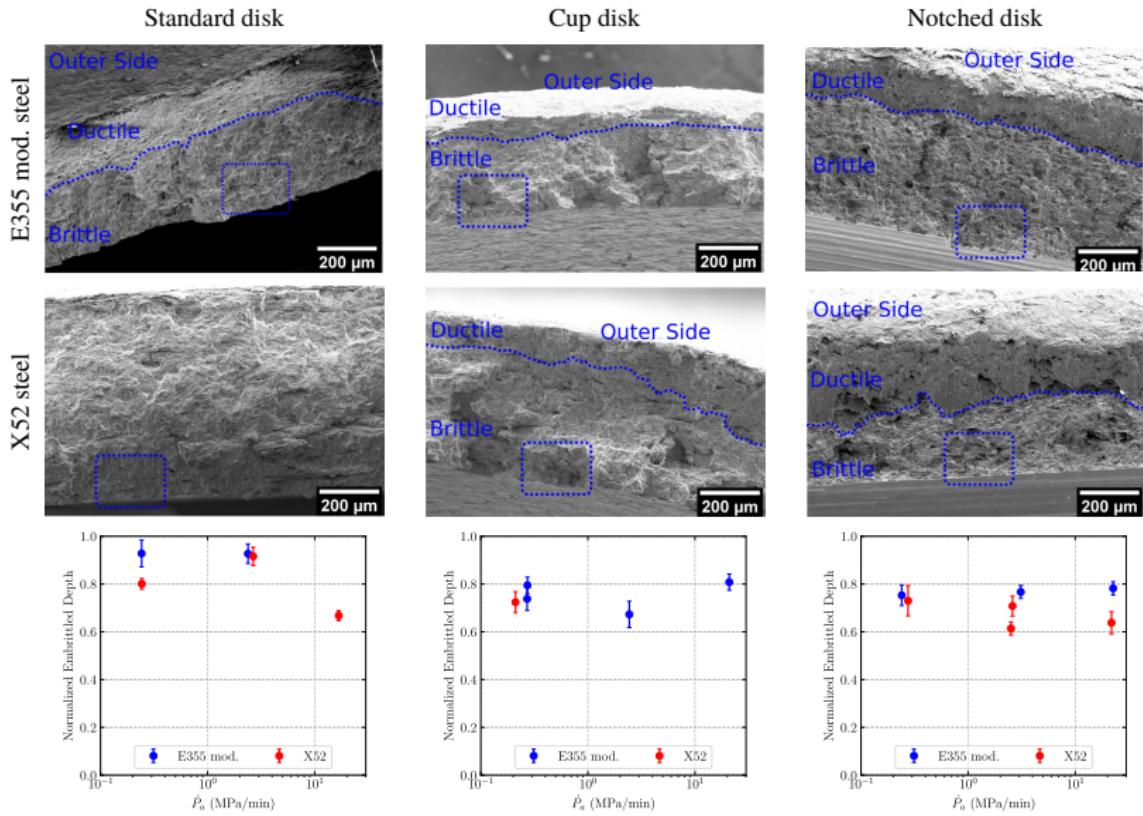
(Experimental data: Santana *et al.*, 2024)

Results under hydrogen (E355 mod. steel)



(Experimental data: Santana *et al.*, 2024)

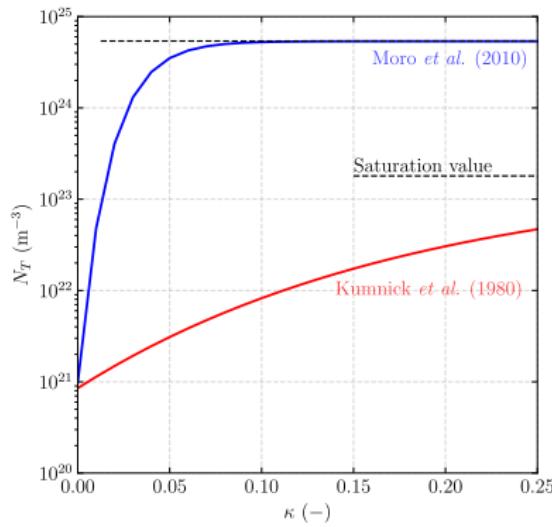
Hydrogen embrittled depth



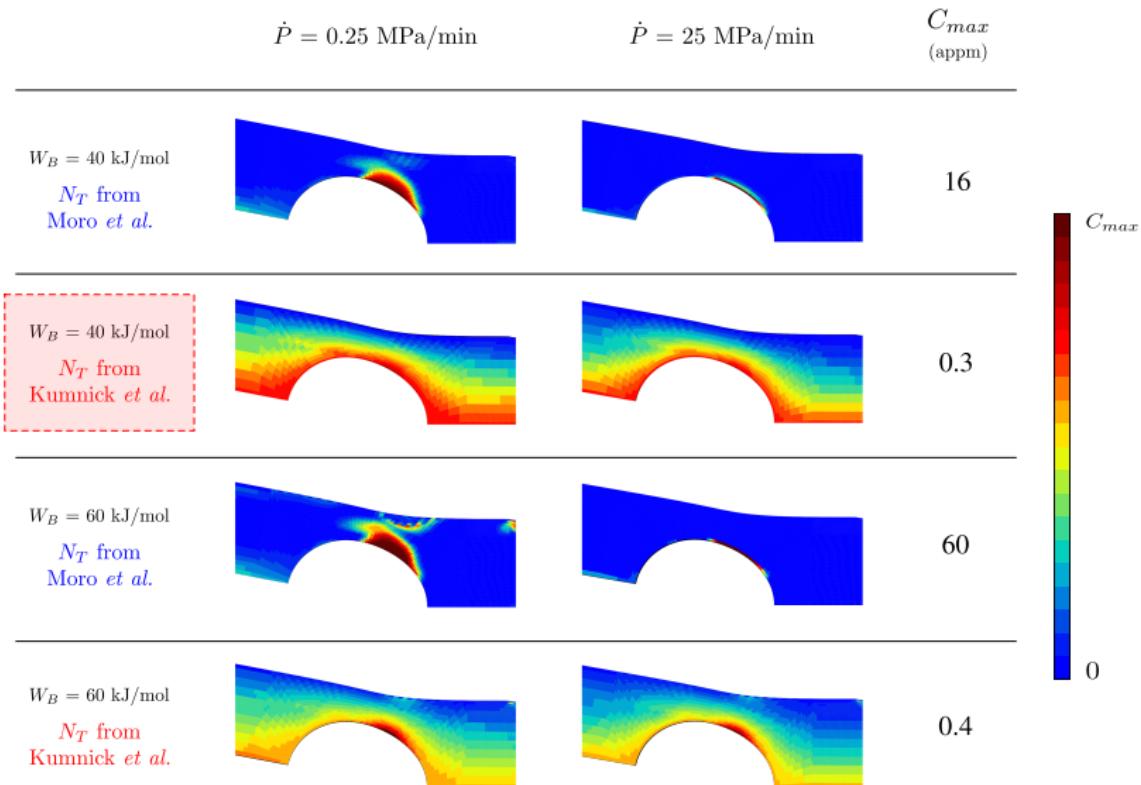
- ▶ Considers only one kind of trap: dislocations
- ▶ Trap binding energies (W_B) and trap densities (N_T) were taken from the literature and analyzed based on the experimental observations
- ▶ Based on the models proposed by Moro *et al.* (2010) and Kumnick *et al.* (1980), four cases emerge

$$W_B = \begin{cases} 40 \text{ kJ/mol} \\ 60 \text{ kJ/mol} \end{cases}$$

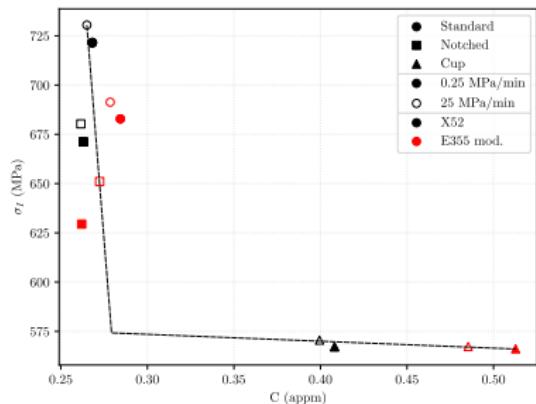
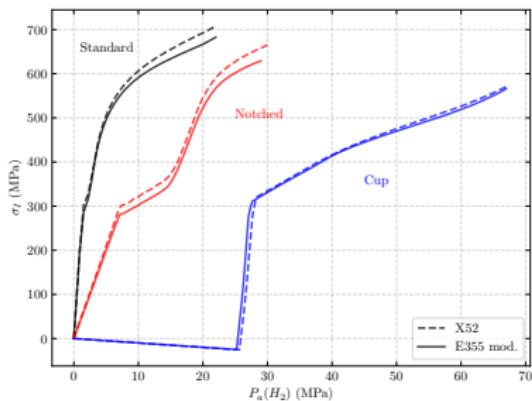
$$N_T = \begin{cases} \log_{10} N_T = 24.73 - 3.74 \exp(-60.17\kappa) \\ \log_{10} N_T = 23.26 - 2.33 \exp(-5.5\kappa) \end{cases}$$



Hydrogen embrittled depth



- ▶ Specimens that develop higher principal stress (σ_I) in the fracture zone fail at a lower hydrogen pressure ($P_a(H_2)$)
- ▶ The total hydrogen concentration reduces the maximum principal stress that triggers fracture



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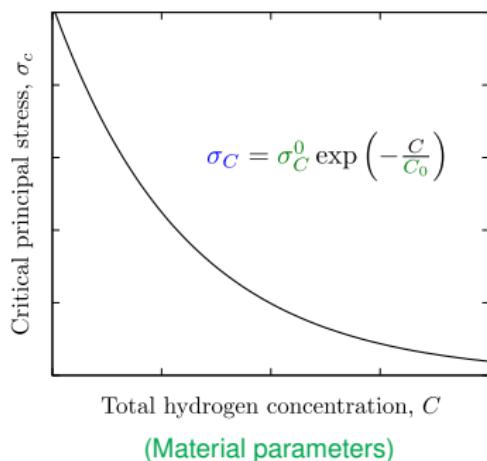
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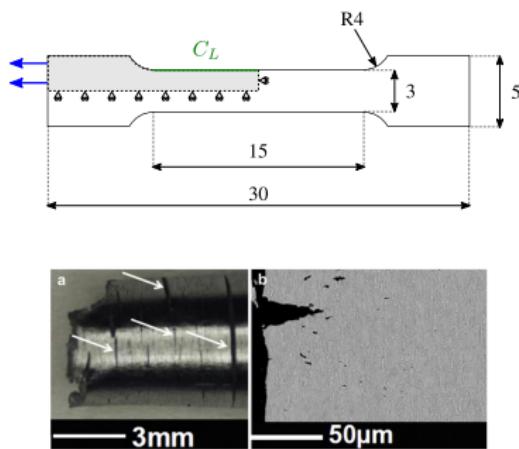
- ▶ **Database:** Briottet *et al.*, 2012 and Moro *et al.*, 2010: *Effect of gaseous hydrogen on the mechanical properties of steel*
- ▶ **Material:** high-strength steel (API X80 grade) in an environment of hydrogen and neutral gas
- ▶ As HE corresponds to **quasi-cleavage**, a **stress dependance** is introduced to the nucleation law
- ▶ The function expressing the nucleation rate due to quasi-cleavage is:

$$B_n(C) = \frac{B_0}{\sigma_C^0} (\sigma_I - (1 - q_1 f_*) \sigma_C)$$

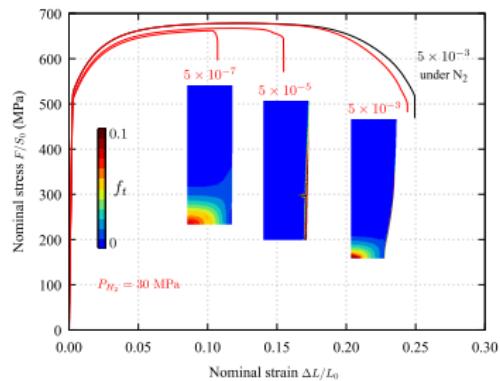
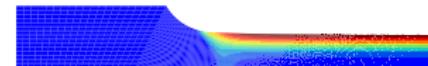
- ▶ Hydrogen decreases the critical stress to trigger void nucleation



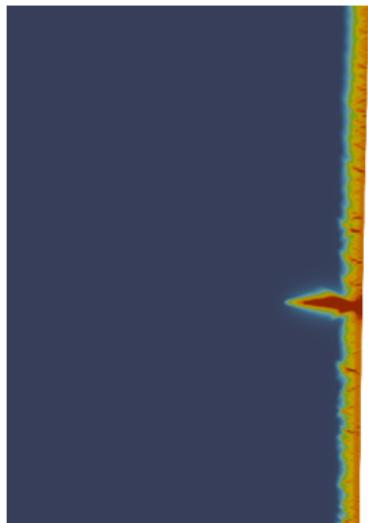
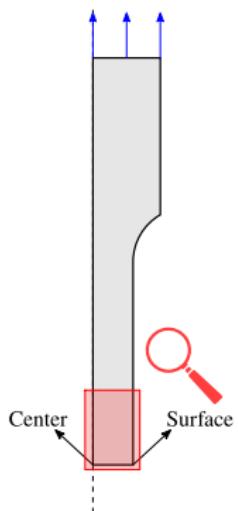
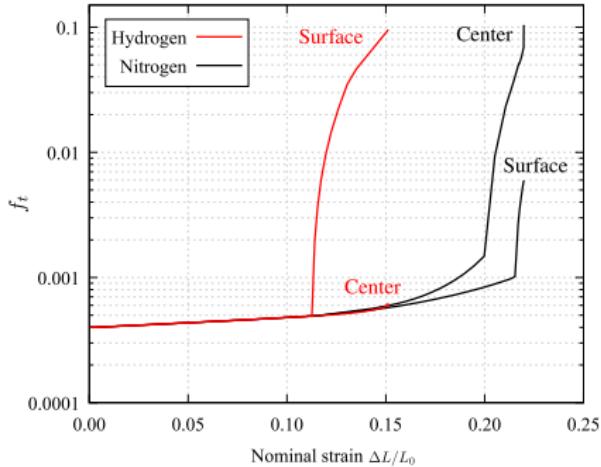
- ▶ Tensile tests under different strain rates under hydrogen gas
- ▶ Slower rates lead to important ductility losses



(Experimental data: Briottet *et al.*, 2012)

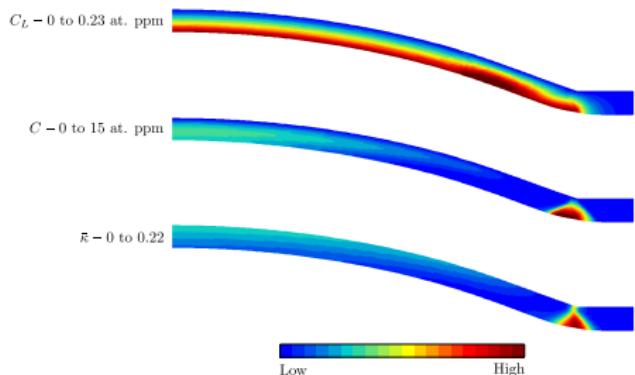
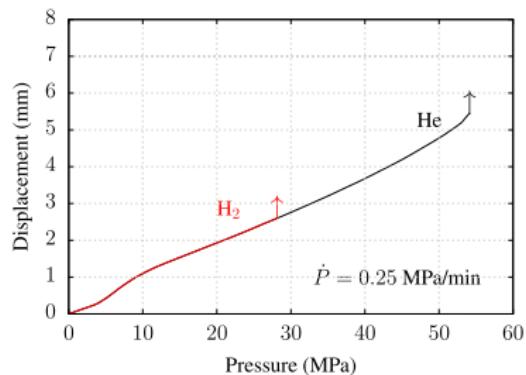


- ▶ Different damage evolution under hydrogen environment
- ▶ Multicrack initiation on the surface



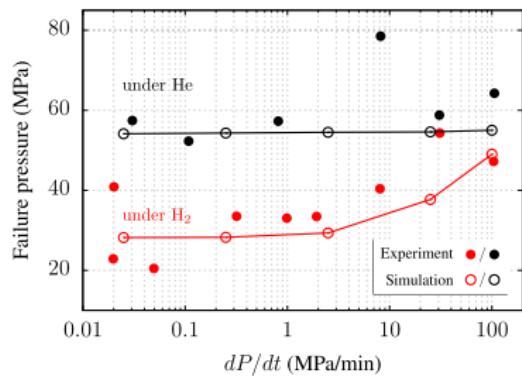
Hydrogen effect:

- ▶ Lower pressure at rupture with decreased ductility
- ▶ Higher hydrogen concentration in the rupture zone

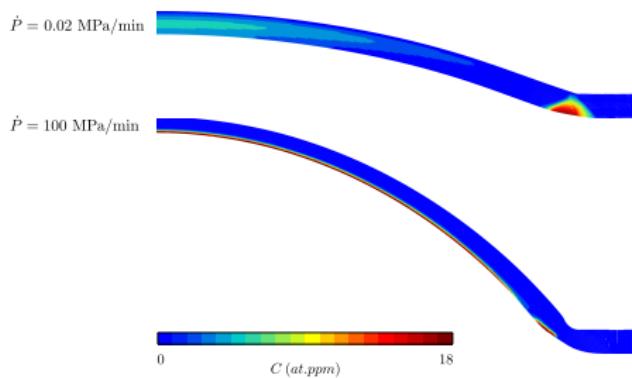


Effect of the pressurization rate:

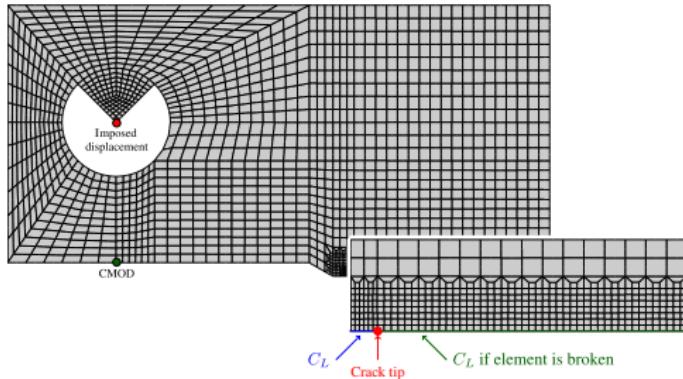
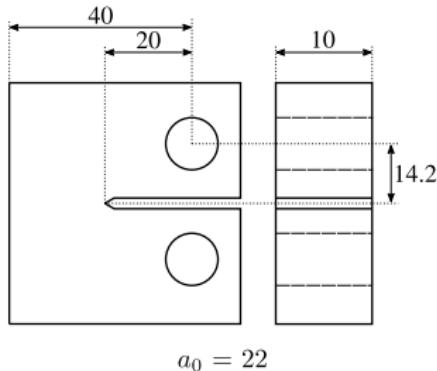
- ▶ Tests under different pressurization rates on H_e and H₂ gases
- ▶ **Lower pressurization rate → Higher embrittlement** since has a longer time to diffuse



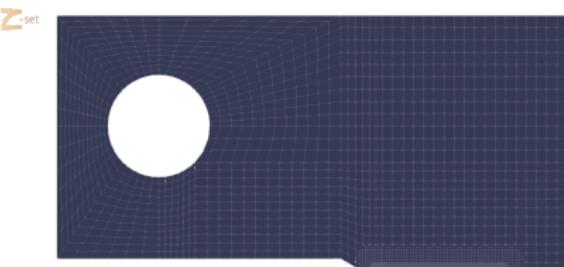
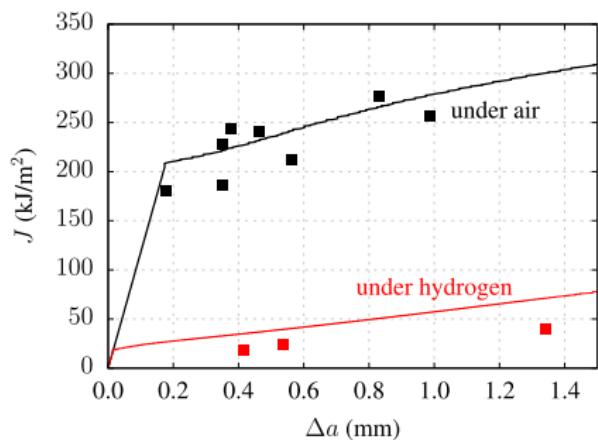
(Experimental data: Briottet *et al.*, 2012)



- ▶ 2D Compact Tension (CT) specimen - *plane strain*
- ▶ Uniaxial imposed displacement
- ▶ Environment: air and hydrogen (30 MPa)
- ▶ Lattice concentration (C_L) derived from Sieverts' law imposed on the newly formed crack



- ▶ Crack length: post-processing considering broken elements $f_* = 0.99 \times 1/q_1$
- ▶ J computation: ASTM E1820 standard considering the simulated Load-CMOD curve



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Thank you

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