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10.02.2025	Daniella LOPES PINTO

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Report on the PhD thesis
"Finite element models for the study of hydrogen embrittlement of steel structures"

by Daniella LOPES PINTO

submitted to Mines Paris-PSL

Hydrogen embrittlement (HE) is a critical issue in materials science, particularly for metallic structures exposed to hydrogen. When hydrogen molecules diffuse into metals, they can lead to embrittlement, making the material more susceptible to cracking and failure under stress. HE is especially significant for steels, which are widely used in critical infrastructure such as pipelines, pressure vessels, and other high-strength components. As hydrogen becomes a key player in the global energy transition, especially in hydrogen storage and transport systems, understanding and mitigating the effects of HE is crucial for ensuring the safety and reliability of steel structures. HE can compromise the integrity of materials, leading to catastrophic failures in systems that are essential for industries such as energy, aerospace, and transportation. The PhD thesis of Daniella LOPES PINTO is highly relevant to the ongoing research and practical challenges related to HE. The thesis work develops a finite element modeling (FEM) framework to simulate and predict the impacts of hydrogen diffusion and embrittlement on steel materials. The research connects experimental observations with advanced numerical methods to provide insights into the HE mechanisms, including ductile failure, damage evolution, and hydrogen transport. This integrated approach enhances our ability to model and understand HE in steel, contributing to safer designs in industries where hydrogen occurs.

The thesis is organized into 7 well-structured chapters that provide a detailed description of the research and major findings. The overall organization of the thesis follows a logical progression, with each chapter building on the previous one to develop a comprehensive understanding of HE in steel structures and the methods used to study it. The thesis begins with an introduction to the research, followed by a bibliographic review that lays the theoretical groundwork. Subsequent chapters delve into specific experimental and numerical studies, including pressurized disk tests, hydrogen uptake during tensile test, comprehensive modeling framework, and fracture toughness testing. The main content of each chapter is briefly summarized below.

- The Chapter 1 Introduction provides a brief overview of the research objectives and motivation. It introduces the challenges associated with HE and outlines the importance of developing reliable testing and simulation methods.

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- The Chapter 2 Bibliography presents a comprehensive review of the literature, covering key topics such as ductile failure mechanisms, regularized damage models, locking-free finite element methods, and hydrogen transport equations. The chapter sets the theoretical foundation for the rest of the thesis, offering insights into the state-of-the-art knowledge in the field and serves as a reference for the methodologies employed later.

- The Chapter 3 combines experimental testing and numerical analysis of HE using pressurized disk tests in two types of steel (X52 and E355 mod. steel). It introduces new disk geometries and discusses the effects of hydrogen and pressurization rate on the embrittlement process. The work provides a detailed analysis of fracture surfaces and compares experimental results with simulations. The results support the hydrogen enhanced decohesion (HEDE) theory and establish a quantitative relationship between hydrogen concentration and critical stress for fracture, contributing to a complete understanding of HE. This part of the work has been published as *Study of hydrogen embrittlement in steels using modified pressurized disks, International Journal of Hydrogen Energy, 2024, 88: 498-514*, in which the PhD candidate is the second author.

- The Chapter 4 investigates the hydrogen uptake during tensile tests under different loading condition. The effect of absorbed hydrogen content at various strain levels, strain rates, and dwell times is examined. The developed numerical model, validated through Thermal Desorption Spectroscopy (TDS), accurately predicts hydrogen concentrations in steel, improving the understanding of how hydrogen uptake evolves during mechanical loading.

- A comprehensive modeling framework that integrates plasticity, damage mechanics, and hydrogen diffusion is developed in the Chapter 5. To mitigate volumetric locking, a mixed formulation in displacement, pressure, and volume variation is employed. The coupled model is validated against experimental data from various mechanical tests, including tensile tests, pressurized disk tests, and fracture toughness tests. It highlights the importance of combining these phenomena to better predict the effects of hydrogen on material properties and structural integrity. The model's ability to predict hydrogen distribution and its impact on material properties is an essential step forward in simulating real-world conditions and reducing the need for costly experimental tests. This work has contributed to a publication *Simulation of hydrogen embrittlement of steel using mixed nonlocal finite elements, European Journal of Mechanics – A/Solids, 2024, 104: 105116*.

- The Chapter 6 reports on experimental and numerical results from fracture toughness tests. The study investigates the impact of specimen size and thickness on fracture toughness, using both standard and sub-size specimens. A parametric study on specimen geometry is conducted to examine how different testing conditions influence fracture behavior in hydrogen-exposed steel, offering critical insights into how to accurately assess fracture toughness in the presence of HE.

- The last Chapter 7 summarizes the main findings of the thesis and discusses potential future research directions, paving the way for continued advancements in this critical area of HE.

The thesis work makes significant contributions to the field of HE. First, it provides a comprehensive computational framework for simulating hydrogen effects on steel structures, integrating plasticity, damage mechanics, and hydrogen diffusion into a unified model. This framework allows for more accurate predictions of material failure under hydrogen exposure, a significant advancement over traditional methods that may only address one aspect of the problem at a time. Additionally, the thesis has contributed to the development of new testing methodologies that can better replicate the conditions under which HE occurs. It also optimizes specimen geometries, which are crucial for obtaining reliable experimental data and improving the precision of simulations. These contributions enable more effective material testing and provide a stronger basis for designing steel components, with direct implications for industries involved in hydrogen production, storage, and transportation.

In conclusion, the PhD thesis by Daniella LOPES PINTO noticeably advances the study of HE in steel structures by developing new testing methods, creating an advanced numerical framework, and providing in-depth experimental analysis. The work contributes not only to a better understanding of HE mechanisms but also offers practical tools for improving the safety and performance of materials exposed to hydrogen, with clear implications for industries involved in hydrogen transport and storage. **I agree to grant the candidate a "Thèse de Doctorat de l'université Paris Science Lettre préparée à MinesParis"**.

Sincerely,

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Suggested questions for discussion

The thesis should have a sub-section to summarize the main contribution to the field.

What are the main challenges you faced when developing the modeling framework? Are there any unexpected results during the validation of the numerical model?

All experimental specimens are extracted from intact pipe. How about weldments that have distinct properties from base material?

Is it possible to incorporate microstructure of materials into the modeling framework, such as phases, different boundaries, precipitates, and secondary particles?

What are the limitations of the current model when applied to real-world scenarios? How transferrable is the model from small specimen to field applications? Are there additional experimental datasets that could be used to further validate the numerical framework?

How can the findings from the thesis be used to inform industry standards, especially for design of hydrogen-resistant materials?

While the hydrogen diffusion model based on the work of Sofronis and McMeeking is widely accepted, it would be interesting to discuss how it compares to more recent models.

It is concluded that the hydrogen concentration is nearly independent of pressurization rate. This is somewhat unexpected. Could this be due to the specific materials or geometries used in this study?

Given the significance of accurate hydrogen concentration predictions, how do you ensure the models remain adaptable to different steel alloys and industrial applications?

How can the thermal desorption spectroscopy (TDS) tests be expanded to better identify trap sites and their associated parameters that affect hydrogen embrittlement?

Are there any emerging experimental techniques that could help further refine your model?

How does carbon monoxide oxidize pipeline surface? What is the mechanism of carbon monoxide inhibiting hydrogen embrittlement?

How does the inclusion of mobile dislocations affect the overall hydrogen diffusion process?

If you were to continue the research in HE, what specific research direction or focus would you pursue next?