Numerical Modeling of Hydrogen Induced Cracking in Hydrogen Transportation Systems

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Abstract

Hydrogen offers vast potential as a clean energy source, pivotal for reducing reliance on fossil fuels. It can power heavy industry, transportation, buildings, and homes sustainably [1]. Existing gas pipelines could potentially transport hydrogen, but thorough investigations are needed to assess safety risks, especially with hydrogen/natural gas mixtures [2]. Hydrogen embrittlement (HE) weakens metals by promoting crack growth and leading to sudden failure. It occurs due to hydrogen exposure, either through electrochemical processes or high-pressure environments, and reduces crucial properties like ductility, toughness, and strength [3].
The goal of the present study is to track the growth hydrogen assisted cracking for the prediction and prevention of catastrophic failures in hydrogen rich environments. To this purpose, numerical simulations are performed on a phase field modelling framework that incorporates a coupled mechanical and hydrogen diffusion response, driven by chemical potential gradients, and a hydrogen-dependent fracture energy degradation law derived from first-principles calculations [4].The analyses enable the characterization of crack growth under hydrogen influence, susceptibility of the material to hydrogen embrittlement, cracking thresholds under sustained loading, and crack paths stemming from local defect.

1.Introduction

Hydrogen holds immense promise as a clean, sustainable energy source that can play a pivotal role in mitigating climate change. However, realizing this potential requires addressing key challenges such as storage, manufacturing, distribution, infrastructure, and safety [5]. The establishment of a robust transportation infrastructure is essential to realize the full potential of hydrogen energy while ensuring safety, reliability, and economic viability. Leveraging the extensive natural gas pipeline network offers a cost-effective solution for transporting hydrogen-blended natural gas. However, the inherent disparities in the physical and chemical properties of hydrogen and natural gas present significant safety challenges to pipeline operations [6]. Exposure to hydrogen can significantly compromise steel's mechanical properties, leading to unexpected failures. Hydrogen Embrittlement involves three stages: hydrogen absorption, diffusion, and induced cracking. Hydrogen penetrates

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[6] Tian, X., & Pei, J. (2023). Study progress on the pipeline transportation safety of hydrogen-blended natural gas. Heliyon, 9(11), e21454. https://doi.org/10.1016/j.heliyon.2023.e21454

steel's surface, diffuses through its lattice, and accumulates at stress points like grain boundaries and dislocation clouds and defects. In some case weakens atomic bonds, reducing ductility and toughness. Eventually, cracks form due to localized stress, even under low external pressure [2]. The anticipation and mitigation of material failures necessitate the utilization of sophisticated numerical methodologies aimed at scrutinizing material behaviour across diverse environmental and operational scenarios. Exciting advancements in computational modelling to understand the initiation and propagation of complex fractures include utilizing phase field methods [7]. Martinez et al. (2018) investigate hydrogen transport towards the fracture process zone and subsequent cracking utilizing a coupled mechanical-diffusion-phase field finite element framework. This approach integrates various components, including a phase field description of fracture, an extension of Fick's law for mass diffusion, and a quantum-based relationship between hydrogen content and fracture surface energy [8]. The computational approach the presented builds upon the code framework illustrated in [9,10]. By employing this code, our primary aim is to conduct an extensive inquiry into the implications of fluctuating hydrogen concentrations and temperatures on the occurrence of hydrogen-assisted cracking. This capability unveils pivotal factors that influence the durability and resilience of natural gas pipelines blended with hydrogen. Such insights serve as invaluable resources for risk assessment and design optimization strategies, crucial for safeguarding the integrity of natural gas infrastructure amid the transition towards a hydrogen-based economy.

2.Phase-field damage models for hydrogen assisted cracking

Industrial equipment in high-pressure hydrogen environments faces varied loads. HE impacts mechanics in two ways: quasi-static and dynamic. Quasi-static loads, relevant for high-pressure parts, are assessed for HE susceptibility. Tests quantify tensile properties, fracture resistance, and fatigue crack growth rate, this evaluation is vital for ensuring the integrity of components in the hydrogen value chain [11]. The constitutive theory, rooted in the free energy function, represents a comprehensive framework that seamlessly incorporates mechanical deformation, phase field modeling for fracture, and the transport of diluted species, notably emphasizing the intricate phenomena associated with hydrogen diffusion [8]. It is crucial to underscore that the formulation of this model involves the intricate coupling of three fundamental equations, which collectively govern the complex interactions between these interconnected processes.

Displacement(u): $$\nabla.\left[(1-\phi)^2\sigma\right]=0$$

Damage(ϕ): $$G_c(C)\left(\frac{\phi}{L}-L\nabla^2\phi\right)-2(1-\phi)\psi(\mathcal{E})=0$$

Hydrogen Diffusion(C): $$\frac{\partial C}{\partial t}-D\nabla^2 C+\nabla.\left(\frac{DC}{RT}\overline{V_H}\nabla\sigma_H\right)=0$$

The finite element (FE) method serves as the cornerstone of the computational framework for tackling the intricate interplay between mechanical deformation, diffusion, and phase field evolution, often referred to as the coupled mechanical-diffusion-phase field problem. Employing Voigt notation, the FE method interpolates nodal values, establishing a robust

[7] Diehl, P., Lipton, R., Wick, T., & Tyagi, M. (2022). A comparative review of peridynamics and phase-field models for engineering fracture mechanics. Computational Mechanics 2022 69:6, 69(6), 1259–1293. https://doi.org/10.1007/S00466-022-02147-0

[8] Martínez-Pañeda, E., Golahmar, A., & Niordson, C. F. (2018). ScienceDirect A phase field formulation for hydrogen assisted cracking. https://doi.org/10.1016/j.cma.2018.07.021

[9] https://www.empaneda.com/codes/

[10] https://www.imperial.ac.uk/mechanics-materials/codes/

[11] Campari, A., Ustolin, F., Alvaro, A., & Paltrinieri, N. (2023). A review on hydrogen embrittlement and risk-based inspection of hydrogen technologies. International Journal of Hydrogen Energy, 48(90), 35316–35346. https://doi.org/10.1016/J.IJHYDENE.2023.05.293

numerical framework capable of capturing the complex interactions between these phenomena with high accuracy [8, 12]. This framework is particularly adept at elucidating the role of hydrogen diffusion within this intricate interplay:

$$u = \sum_{i=1}^{m} N_i u_i \quad ; \quad \phi = \sum_{i=1}^{m} N_i \phi_i \quad ; \quad C = \sum_{i=1}^{m} N_i C_i$$

Where m is the number of nodes and N_i, utilized for interpolation, are diagonal matrices with the nodal shape functions N_i serving as their constituent elements.
A square plate featuring a horizontal crack serves as a pivotal benchmark for investigating the model's response under tensile loading conditions Figure1. (a). Initially, the plate contains a uniform hydrogen concentration $C(t = 0) = C_0$, a configuration maintained at the boundaries throughout the simulation $C_b = C_0$. This setup closely mimics pre-charged materials commonly encountered in real-world applications. To expedite the simulation, a coarse mesh is employed, supplemented by a finer mesh concentrated along the crack propagation trajectory to ensure precise resolution of the fracture process zone. Notably, the characteristic element length along the crack path measures 0.005 mm, with a corresponding length scale of 0.05 mm, ten times greater than the characteristic element length Figure1. (b).

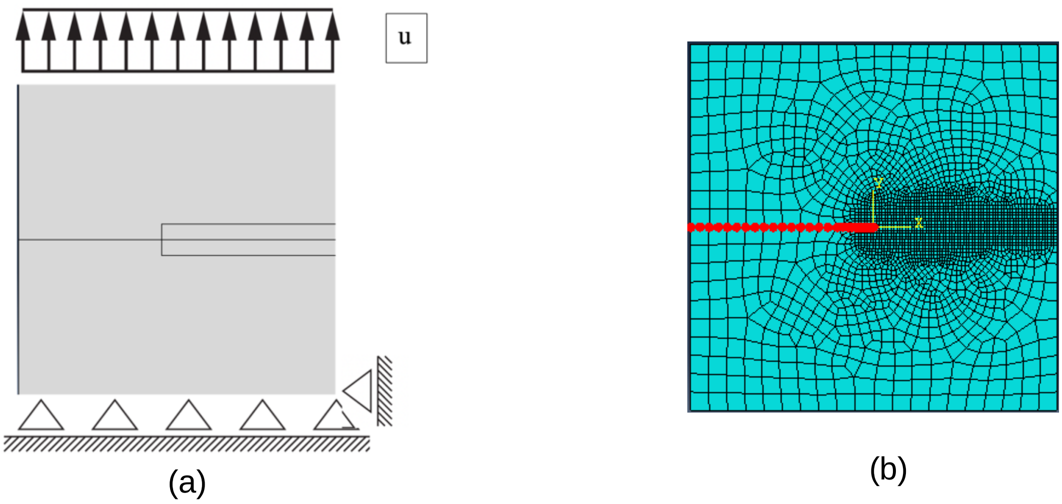

Figure 1. Schematic description of the square plate: (a) geometry and (b) mesh.

3.Results

The finite element analysis results, depicted in Figure 2, illustrate the evolution of the parabolic degradation function within the notched square plate, with $C_b = C_0 = 0.5$ wt ppm. The hydrogen concentration in the fracture process zone is typically around 0.5 wt ppm for a high strength steel [13]. Phase field contours show intact material in blue $(\phi \approx 0)$ and cracks in red $(\phi \approx 1)$. Remarkably, the consistent crack path observed across all environments suggests a universal trend in crack propagation. Temperature plays a crucial role in the interaction between hydrogen and metal, influencing surface reaction kinetics, hydrogen solubility, diffusion, and trapping. These properties are intricately linked to the specific material system [11]. Due to the complexity involved in studying temperature effects, we aim to observe temperature changes using the current model. While understanding the impact of temperature is crucial for engineering applications, there is a lack of studies that adequately explain or predict its influence on the mechanical properties of structural materials.

[12] Cui, C., Ma, R., & Martínez-Pañeda, E. (2021). A phase field formulation for dissolution-driven stress corrosion cracking. Journal of the Mechanics and Physics of Solids, 147, 104254. https://doi.org/10.1016/J.JMPS.2020.104254
[13] Kristensen, P. K., Niordson, C. F., & Martínez-Pañeda, E. (2020). Applications of phase field fracture in modelling hydrogen assisted failures. Theoretical and Applied Fracture Mechanics, 110, 102837. https://doi.org/10.1016/j.tafmec.2020.102837

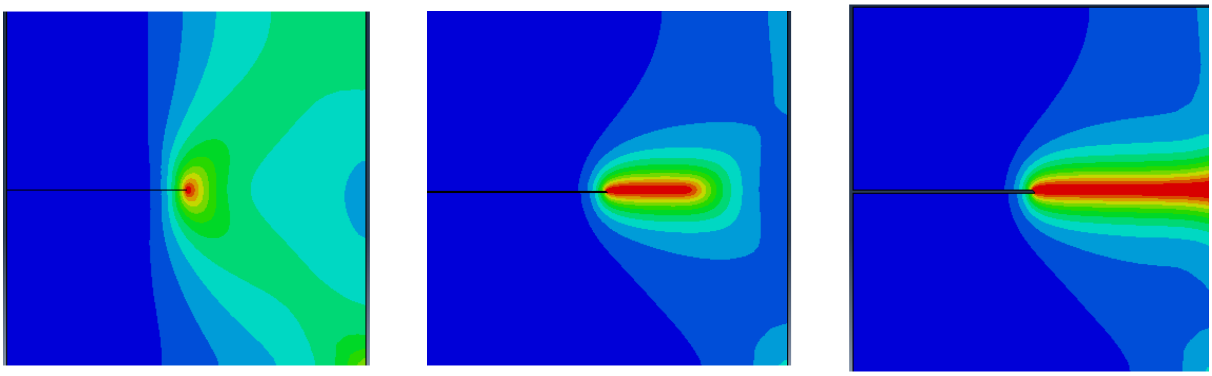

Figure 2. Notched square plate subjected to tension test. $C_0 = 0.5$

Figure 3 illustrates the impact of temperature variations within the range of 273 K to 333 K as modeled in this study with $C_0 = 0.5$ wt ppm.

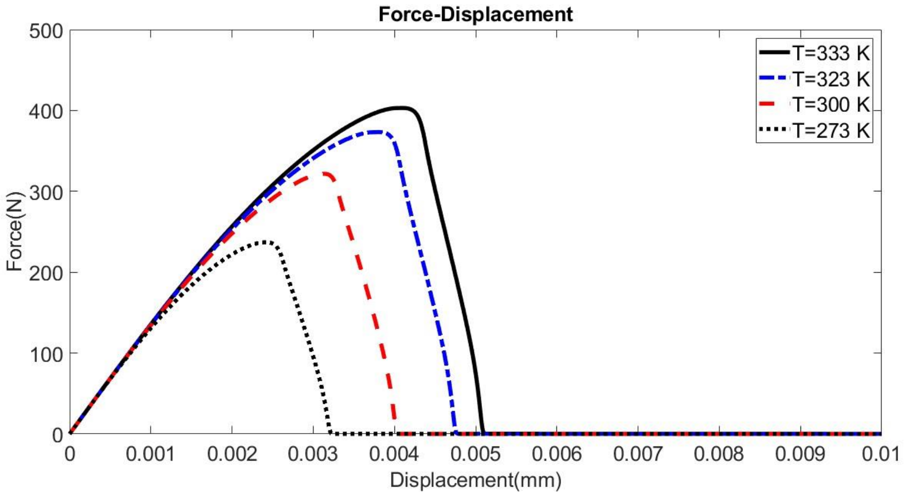

Figure 3. Force displacement response for a Hydrogen concentration of $C_0 = 0.5$ wt ppm in the temperature range of 273 K to 333 K.

The figure 4. depicts the load-displacement response as a function of hydrogen concentration. The specimen's load-bearing capacity diminishes as hydrogen concentration increases. As the figure shows, damage triggers a significant load drop, with the crack propagating unstably across the specimen.

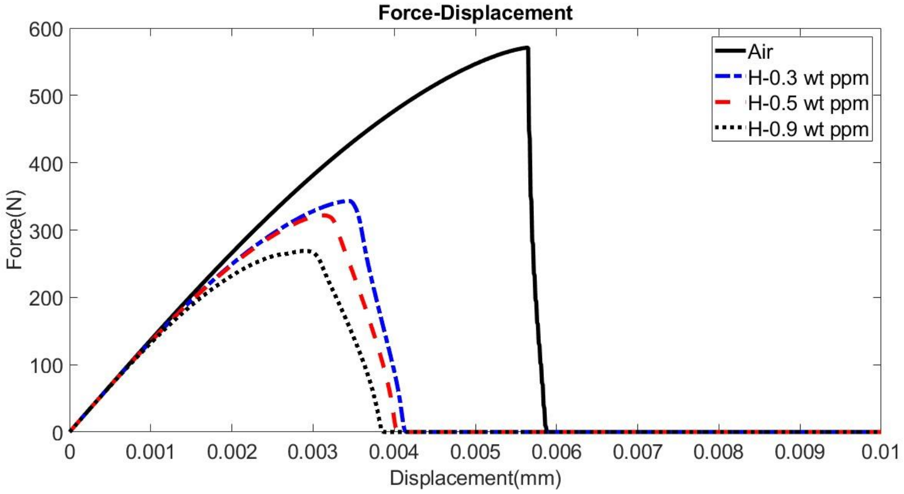

Figure 4.Graph depicting the load-displacement response in correlation with varying hydrogen concentrations.

4-Conclusion

This study starting from a well-established constitutive theory framework conducted an in-depth investigation of the interplay between mechanical deformation, fracture mechanics, and hydrogen diffusion, with a specific focus on parameters excluding high temperatures. By leveraging this framework, we successfully replicated the observed decrease in load capacity with increasing hydrogen concentration and the unstable crack propagation behavior. These findings highlight the model's effectiveness in capturing key aspects of hydrogen-related failure at moderate temperatures, which is particularly relevant for the emerging field of natural gas transmission lines blended with hydrogen.

Future endeavors will prioritize incorporating the effect of temperature into the model, with careful consideration to maintain safe testing conditions. As temperature plays a significant role in real-world applications like hydrogen-blended natural gas pipelines, its influence on crack growth remains under-explored. By extending the model's capabilities to encompass a wider range of temperatures while adhering to safety protocols, we aim to develop a more comprehensive framework for evaluating the integrity of these novel pipelines under varying environmental condition.