Advanced Numerical Modeling of Cavity Growth Under Extreme Solicitations

Context

This project addresses significant societal challenges, particularly in the fields of energy and the environment. Research on the mechanical properties of polymer materials under pressure is crucial for improving the durability and reliability of batteries, which power a wide range of electrical devices, from mobile appliances to electric vehicles.

High-pressure gaseous hydrogen, reaching up to 90 MPa, is stored in fuel cell vehicles and hydrogen refueling stations. Similarly, rubber materials are used as seals for high-pressure gaseous hydrogen, subjected to cyclic pressurization and depressurization. This cyclic exposure leads to the formation of gas cavities within the rubber materials. A previous study demonstrated that the pre-existing pore model explains the growth of a single cavity inside the rubber [J. Jaravel, et al., Int J Solids Struct, 2013]. In other words, a cavity is already nucleated within the rubber as a "pre-existing pore filled with gaseous hydrogen," which expands when the external pressure is released.

The cavity growth is primarily governed by the competition between the mechanical properties of the cavity's internal walls and the concentration of H_2 within the cavity, which generates internal pressure. An initial attempt to study these phenomena provided an estimation of the evolution of local mechanical fields during the decompression of an elastomer under mechanical loading (Figure 1). However, this study did not take the interface into account.

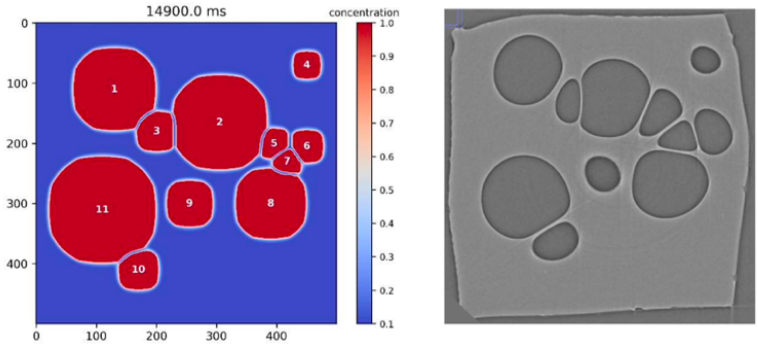

Figure 1: *Comparison of Interactions Between Simulated Cavities (Mesh 500x500, 150 Iterations) (Left) and Observed Interactions (Right) at the SOLEIL Synchrotron.*

The main focus of this doctoral work is to develop efficient numerical tools to model the evolution of cavities embedded in a polymer matrix. The phase-field method appears to be particularly well-suited for studying interfaces in 2D. More specifically, previous studies on EPDM exposed to pressures of up to 30 MPa [Kane Diallo 2016] have revealed that a Morphological Representative Volume Element, representative of the spatial distribution of cavities, includes a significant number of them.

In the literature, mechanical calculations that account for cavitation and its effects are generally performed at the cavity scale rather than at the level of a field of cavities. One obvious reason for this limitation is the complexity of handling large data volumes and the high computational cost associated with mesh generation, particularly in finite element cases. Moreover, the effects of the matrix/cavity interface are not considered, whether in terms of diffusion or mechanics, such as surface tension, for example.

To model the evolution of cavities through the resolution of a gas diffusion problem, simulations will be performed using a phase-field method. This numerical regularization method will allow for a better consideration of gas exchanges across the cavity wall. This method is particularly appropriate for interface problems by smoothing strong gradients.

The objective of this thesis is to model the evolution of cavities by solving a gas diffusion problem using simulations based on a phase-field method. This numerical regularization approach will enhance our ability to effectively consider gas exchanges across the cavity wall.

The PhD candidate will enroll at the University of Poitiers in the 2025 academic year Short research stays at Onera Châtillon are planned. The supervisory team will consist of Jérôme Colin (University of Poitiers/Pprime); Azdine Naït-Ali (ISAE-ENSMA/Pprime) and Aurélien Vattre (Onera Châtillon)

Applicants should have strong knowledge in material mechanics, continuum mechanics, and finite element methods. Applications should be sent to: jerome.colin@univ-poitiers.fr ; azdine.nait-ali@ensma.fr; aurelien.vattre@onera.fr