Gas Release in Porous Electrodes for Water Electrolysis: Numerical Simulation of Two-Phase Flow

I. Scientific Context and Challenges

Hydrogen is a versatile energy carrier with applications ranging from steelmaking to fertilizer production, and its demand has surged in recent years. However, approximately 99% of global hydrogen production still relies on fossil fuel-based methods. As a key enabler for decarbonization, water electrolysis—powered by low-carbon electricity—offers a sustainable alternative. Among electrolysis technologies, proton exchange membrane water electrolyzers (PEMWEs) and anion exchange membrane water electrolyzers (AEMWEs) stand out for their adaptability to intermittent renewable energy sources. Yet, both face critical challenges. Among the factors limiting electrolyzer efficiency, bubble dynamics emerge as a major bottleneck—particularly at high current densities. This phenomenon triggers a cascade of performance losses:

- Active site blocking (increased activation overpotentials),
- Mass transport limitations (ion pathway obstruction, gas accumulation),
- Mechanical degradation (*eg.* catalyst delamination),
- Microstructural alterations (non-uniform current distributions).

These challenges are exacerbated in AEMWEs, where thicker PGM-free electrodes amplify transport constraints and bubble accumulation. Moreover, the complex interplay between gas-liquid-solid interactions—governing bubble nucleation, growth, coalescence, and detachment with potential bubble issues—remains poorly understood, particularly in AEMWEs, due to limited experimental access to dynamic processes.

II. Objectives and Methodology

This 6-month internship aims to develop a 3D model to simulate two-phase flow in porous electrodes and investigate mass transport limitations during gas release. The work will be structured as follows:

1. Microstructural Reconstruction: The intern will leverage tomographic images obtained from prior collaborations with the SIMaP laboratory, literature data, or in-house generated images to faithfully reconstruct the microstructure of porous media.
2. Geometry Implementation and Meshing: The reconstructed geometry will be implemented in simulation software (COMSOL Multiphysics® or OpenFOAM) to generate a computational mesh. This step is critical to strike the right balance between computational cost and result resolution, particularly at reactive interfaces.
3. Two-Phase Flow Modeling: A two-phase flow modeling framework integrating advanced Computational Fluid Dynamics (CFD) will be developed. The intern will explore different two-phase flow descriptions, such as: Volume of Fluid (VOF), Level Set, and Phase Field methods.
4. Parametric Studies: The impact of the following parameters will be evaluated: (1) geometric properties: porosity, tortuosity, and permeability, (2) material properties: hydrophobicity (contact angle, capillary pressure), specific surface area, and conductivity and (3) operating conditions: current density, temperature.

The models will guide the development of design guidelines for bubble-tolerant electrodes, optimizing parameters such as pore size distributions, hydrophobicity patterns, and identifying efficient gas evacuation scenarios. This work could also find applications in other fields.

III. SIMaP and LEPMI Collaboration

The SIMaP and LEPMI laboratories share strong collaborative ties and complementary expertise in materials science, creating an ideal environment for this project.

- SIMaP contributes mechanical and materials engineering expertise, with a focus on materials processing, design, and microstructural characterization. Their know-how includes: the effects of micro/nanostructures on physical and mechanical properties, and multi-scale and multi-physics modeling and simulations. Their expertise in the mechanical behavior of structured materials will be invaluable for accurately reconstructing and analyzing electrode microstructures and modeling.
- LEPMI provides electrochemical expertise, both experimental and computational, with a strong background in electrochemical engineering, microstructure characterization, and interfacial electrochemistry. Their research spans from fundamental to applied studies, ensuring that the developed models are physically sound and relevant to real-world applications.

Together, the two laboratories offer a synergistic framework, combining mechanical, materials, and electrochemical perspectives to address the challenges of this project.

IV. Integration of the Intern Within the Laboratories

The intern will be fully integrated into the research teams of both SIMaP and LEPMI, benefiting from a rich, collaborative, and interdisciplinary experience.

- Resources and Workspace: The intern will have access to a dedicated high-performance workstation at LEPMI, equipped with COMSOL Multiphysics® (with CFD licenses) and/or OpenFOAM, as well as computational resources from both laboratories. While the intern will not perform image acquisition themselves, expert support from both labs will be available if needed for tomography or microscopy.
- Mentorship and Training: The intern will be co-supervised by experts from both laboratories, ensuring guidance in materials science, electrochemistry, and numerical modeling. He/she will also participate in lab meetings, seminars, and workshops, engaging with ongoing research and expanding their technical skills.
- Collaborative Environment: The intern will work alongside PhD students, post-docs, and researchers, fostering a dynamic and supportive atmosphere for learning and innovation. Regular joint meetings with experts from both labs will ensure progress alignment and knowledge exchange.

An existing 2D model (see **Figure 1**) will serve as a foundation for the intern to build upon. This internship is ambitious, but if successful—even if not all objectives are fully completed—the student will have the opportunity to pursue a PhD.

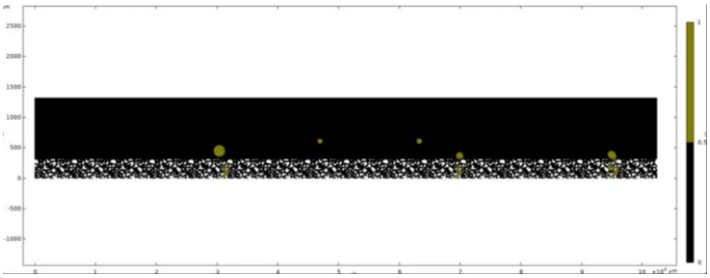

Figure 1. Gas release from porous media into a channel during water electrolysis: 2D simulation using the phase-field method.