PhD position in CNAM

Development of models to simulate the operation of an alkaline electrolyser

(CEA/TotalEnergies collaboration)

Context

TotalEnergies aims to become a pioneer in the production of green H2 and thus a key player in the new hydrogen ecosystem. Green hydrogen is produced using an electrolyser powered by a renewable energy source. The heart of the electrolyser is made up of electrochemical cells comprising a cathode and an anode separated by an ion-conducting membrane. Under polarisation, the water is dissociated into hydrogen at the cathode (HER reaction) and oxygen at the anode (OER), with the membrane ensuring that the gases do not mix. The cells are connected in series in the form of stacks with a power output of 1 to 10 MW for future industrial applications.

Two electrolyser technologies are considered mature, namely alkaline and PEM (proton exchange membrane) electrolysers. However, the development of a digital twin of the system is essential to gain a competitive advantage in terms of the design and operation of green H2 assets, as it will help us to predict the underlying behaviour.

To be effective, this numerical model of an electrolyser must cover two different aspects:

- A data-driven approach using artificial intelligence and data sets. This data will be generated as part of studies carried out outside this collaborative framework, typically via cell test benches and company assets to predict certain 'macro' behaviours (e.g. reduced performance).
- Physical models: The various physical aspects involved in such a problem are dominated by the chemical reactions producing hydrogen and its interaction with the surrounding fluid. In particular, the formation and propagation of bubbles, which have an impact on the overall performance of the cell itself, an aspect that is not yet well understood. Understanding this complex physical phenomenon requires a multiphysics and multi-scale approach, which we aim to develop and study in this project. The data generated by this effort can then be processed using artificial intelligence techniques for general prediction.

Such a tool will also enable us to carry out predictive maintenance and optimise operations. It will also enable the emergence of new R&D topics to improve the performance of alkaline electrolysers.

The DAWN project will be based on the use of two multiphase fluid simulation tools:

- canoP, a library for developing multiphase CFD applications with adaptive mesh refinement (Drui 2017, Chen 2019, Padioleau 2020).
- Flower.jl, a CFD code in Julia that enables bubbles and three-phase interfaces between gas, liquid and the wall to be studied locally (Quirós-Rodríguez 2022, Fullana 2023).

Mission

Initially, the mission will involve developing the Flower.jl CFD application, with the primary objective of studying the mechanism of bubble growth, their size and dynamics at the interface between the electrodes, the membranes and the electrolyte. Building an application with Flower.jl will require, in the first step, the following elements:

- Implementation of phase change models taking into account the effects of local concentrations and temperature on the rate of mass transfer.
- Implementation of slip models for the dynamics of the triple line (generalized Navier boundary condition) on rough walls.
- Addition of an electro-magnetic model compatible with the sharp representation of interfaces.

In a second phase, these developments will be used :

- a parametric study of thermochemical models and properties in preparation of performance optimisation, and
- a coupling with the CanoP application, in particular by proposing simple laws or reduced models compatible with the macroscopic models implemented in CanoP.

Finally, the assignment also includes writing deliverables (minutes, reports and documentation) as well as preparing and submitting articles to peer-reviewed scientific journals.

Skills

You have a thesis in physics/numerical chemistry and :

- You have a good command of one or more programming languages (C, Fortran, Python, Julia).
- You are familiar with the basic tools associated with collaborative development (git, github, etc.).
- You are interested in the challenges of the energy transition.

Timeline

The position is offered for the duration of 36 months, between October 1st, 2025 and September 30th, 2028. **Deadline for applications: 31/05/2024**

Information and contact

The applicant should include a CV, and a motivation letter.

Requests for information and applications should be sent by e-mail to Taraneh SAYADI (taraneh.sayadi@lecnam.net).