Towards multi-physics and multi-scale modelling of pilot-scale photo-electrochemical cells for hydrogen production

The production of chemical molecules and synthetic fuel, from non-fossil resources and renewable energy, is one of the solution envisaged to face climate issues. In this context, the use of photo-electrochemical cells (PEC) solar-driven water splitting is seen as promising route for hydrogen production. The hydrogen thus produced could be used for the conversion of carbon dioxide into other chemical vectors (such as methane or methanol). Today, proofs of concept generally concern small objects (of the order of 1cm² of active surface) and operating-times limited to a few minutes or a few hours. It is therefore essential, in order to consider the rapid deployment of PECs, to be able to predict the influence of the architecture of the cell and scale-up on their performance, in terms of energy efficiency, kinetic efficiencies (volume and surface), stability of operation and aging of materials.

The thesis is part of the development of a generic simulation tool for PECs, with the main objective to develop optimised technologies by inverse design. From a critical analysis of the state of the art, in order to identify the locks specific to the simulation of these intrinsically multiphysical and multiscale devices controlled by radiative transfer, **it aims to develop original knowledge models, capable of robustly representing the effect of couplings and of the different scales on the final kinetic and energy performances of the PEC**. First, the 1D modelling of the rate-limiting steps regarding kinetic and energy performance (optical properties, radiation transfer, charge separation and transport, interfacial reaction rates, etc.) together with gas separation will be undertaken. **A major effort will be focused on the representation of the semiconductor-electrolyte junction which has a strong impact in the knowledge model**. These model bricks can be developed in different languages, integrating the state of the art existing in the laboratories. The models will be tested and validated using analytical solutions, when they exist, and experimental data obtained independently on small-scale PEC devices, implementing a model of photocatalyst, $BiVO_4$, considering progressively a complex nanostructuration. **Finally, the transposition to 3D devices will be considered via the reformulation of the solutions in the form of path integrals, allowing a statistical resolution, using the Monte Carlo method**. This method, under development via the EDStar platform, have the advantage of being insensitive in terms of computation time to the space and time dimensions and to the geometric complexity of the cell at each scale.

The proposed research project will be carried out in collaboration between **Institut Pascal**, for its expertise in the modelling of photo-reactive processes; **CEA**, for its expertise in the modelling of multiphase processes, and the ENGIE R&D center dedicated to new energy resources **ENGIE Lab GRIGEN**, which is funding the thesis. ENGIE Lab CRIGEN and CEA are also partners in the PROSPER-H2 Industrial Chair project, aimed at developing a PEC producing hydrogen. The results of the integrated tests carried out within PROSPER-H2 will valuably supplement the database used for the validation of the models to be developed in the thesis.

You have a solid background in Physics, Energy, Thermodynamic or Chemical Engineering, with particular attraction for modelling and computer science; you have also a strong capacity for collaborative work, and you want to contribute actively the energy transition? By choosing this thesis, you will join a multidisciplinary consortium and contribute to an active field of research, at the interface between fundamental research and industry.

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