

Multiphase Modeling of Enhanced Bubble Evacuation in Alkaline Water Electrolysis Cells based on Laterally-Graded 3-D Electrodes

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To mitigate the challenges posed by anthropogenic climate interference, substantial efforts are imperative in order to limit the rise in global average temperature. One major declaration made by the international community through various climate agreements [1,2] calls for an elimination of greenhouse gas emissions, necessitating a shift from fossil fuels to sustainable renewable energy sources. Hydrogen and hydrogen-based fuels emerge as promising candidates to decarbonize a wide range of sectors – including transport, industry and chemical manufacture – due to hydrogen's remarkable flexibility and storage capacity. At present, water electrolysis conducted by renewable electricity is considered as the most sustainable technology to produce green hydrogen.

Among the various approaches for water electrolysis, two commercially available methods stand out: alkaline and proton exchange membrane (PEM) [3]. Alkaline water electrolysis (AWE) has the advantage of presenting the lowest cost per kilowatt of electricity but yields lower hydrogen production rates. In contrast, PEM electrolysis achieves superior performance, thanks to the use of costly and scarce electrocatalytic materials like Ir and Pt. Considering the unique strengths of each system, it is appealing to try to integrate the best of these two technologies, yielding high production rates per electrode area while benefiting from more cost-effective electrode materials.

To this end, recent experimental work in our group has focused on the conception and analysis of flow-engineered 3-D electrodes into a novel laterally-graded cell configuration to allow alkaline water electrolysis to become PEM-like [4,5]. More specifically, 3-D electrodes such as foams were integrated into a zero-gap cell using a bi-layer configuration in which a fine foam (450 μm pore size) working as a catalytic electrode is put in contact with a coarser foam (3000 μm pore size) acting as a porous transport layer (PTL). Because of the high production rate in the 450 μm foam, a high forced upstream electrolyte flow is used to favour bubble removal and hence decrease the Ohmic resistance of the system. Thanks to the use of a bi-layer configuration in flow-through upstream flow mode, the many bubbles generated near the diaphragm were believed to be evacuated laterally towards the coarser foam, keeping the catalytic surface of the finer foam active throughout the process. The enhanced performance of this PEM-like system was confirmed experimentally and current densities of 2 A/cm² were observed at cell voltages lower than 2 V (for 2 x 2 x 0.56 cm³ electrodes).

The aim of this work is to use Computational Fluid Dynamics (CFD) simulations in order to assess flow behaviour into the bi-layer and validate the assumptions that were made based on the experimental results. First of all, a single-phase model (i.e. considering only the electrolyte) was used to solve the incompressible Navier-Stokes equations in OpenFOAM. The objective is to shift towards multiphase simulations by considering a simple mixture model to account for the presence of gas bubbles. The driftFluxFoam solver will be used to solve the general mixture model equations, in which velocity, density and viscosity are weight-averaged based on gas fraction and on the properties of both phases. This work also highlights two ways of incorporating porous media in the numerical simulations. The first way, called explicit, is based on the exact geometry of the foams, obtained thanks to high-resolution micro-CT (computed tomography) scanned data, but is extremely costly from a numerical point of view. The other method, called implicit, uses the Darcy-Forchheimer approximation to

spatially average porosity over a given domain, which is less representative of the exact foam structure but generally allows to get first useful insights of the flow behaviour in porous media.

An example of a laterally graded bi-layer configuration and some initial multiphase results are shown in Figure 1. The velocity vectors and the lateral velocity profile confirm that hydrogen bubbles can indeed be expected to be evacuated from the fine catalytic 450 μm into the coarser 3000 μm PTL foam. The main objective of our modeling approach is to demonstrate the relation between the observed electrochemical performance enhancement with multiphase mass transport phenomena occurring inside the 3-D electrodes in order to show the intrinsic interest of using such laterally graded bi-layer approach in all future alkaline water electrolyzers.

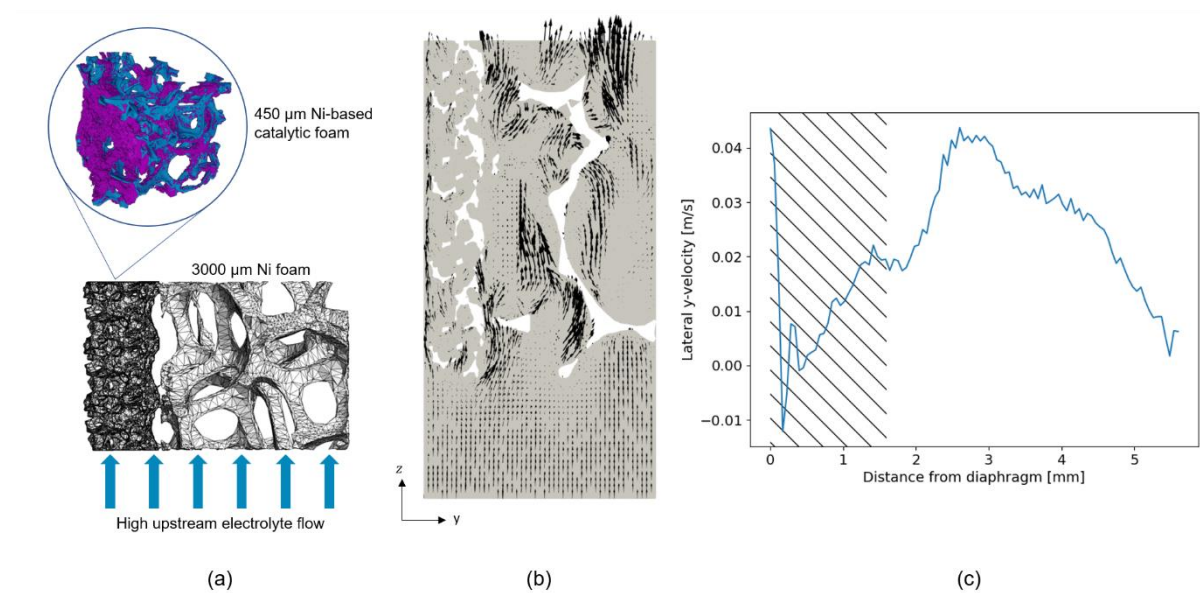


Figure 1 – (a) Bi-layer foam configuration with a 450 μm Ni-based catalytic foam in contact with a 3000 μm Ni foam used as Porous Transport Layer. (b) Velocity vectors inside the bi-layer considering a gas fraction of 40% on the diaphragm side. (c) Averaged lateral y-velocity component as a function of diaphragm distance for an electrolyte inlet velocity of 0.22 m/s.

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