

Electrochemists going with the flow: CFD-guided optimization of flow-engineered 3D electrodes and cells for alkaline water electrolysis

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Abstract

Introduction: The role of green hydrogen in the energy transition has been widely recognized by the scientific community and the International Energy Agency (IEA) [1], as it provides a pathway to store and deliver clean and usable energy. Currently, the two most mature technologies for green hydrogen production are alkaline and proton exchange membrane (PEM) water electrolysis. Recent experimental studies conducted in our group have demonstrated that the performance of alkaline water electrolyzers (AWE) can be significantly enhanced by incorporating three-dimensional (3D) porous electrodes in a zero-gap cell configuration with forced electrolyte flow [2]. Attempts were made to apply the same methodology (i.e. zero-gap cell with knitted mesh-type spacer and forced flow) to a 6 kW industrial-scale prototype electrolyser installed in our facilities. However, similar performance improvements to those observed at lab scale could not be achieved, mainly due to non-uniform electrolyte distribution in the anodic and cathodic half-cells [3].

Objectives: This work aims to demonstrate how Computational Fluid Dynamics (CFD) simulations, combined with experimental characterization, can be used to optimize both lab- and industrial-scale AWE cells. At lab scale, accurate 3D reconstructions of porous electrodes (i.e. foams or triply periodic minimal surfaces – TPMS – structures) enable the investigation of electrolyte transport from the catalytic layer, where gas is generated, to the porous transport layer (PTL), where gas bubbles are evacuated. Furthermore, numerical simulations provide insights into the performance limitations observed at industrial scale and support the design of improved cell configurations with enhanced flow distribution and electrochemical performance.

Material and methods: Single phase and multiphase flow simulations are performed considering a 30 wt% KOH solution at 80°C as the liquid phase and hydrogen as the gas phase. The discretized continuity and momentum equations are solved using pressure-based solvers implemented in OpenFOAM and ANSYS Fluent. The corresponding meshing utilities are employed to generate volume meshes of the complex 3D electrode geometries. At larger scale, these porous structures are represented implicitly using the Darcy-Forchheimer approximation. The electrolyte flow rate is imposed at the domain inlet to match experimental operating conditions. In multiphase simulations, a gas flux derived from Faraday's law is imposed at the electrode surface.

Results: As shown in Figure 1, single-phase simulations allow the extraction of lateral velocity profiles within explicit bi-layer structures at lab scale, highlighting electrolyte transport from the catalytic layer towards the PTL. The results indicate that 3D-printed bi-layer TPMS electrodes not only offer greater design flexibility but also promote improved lateral transport, consistent with the enhanced electrochemical performance observed experimentally.

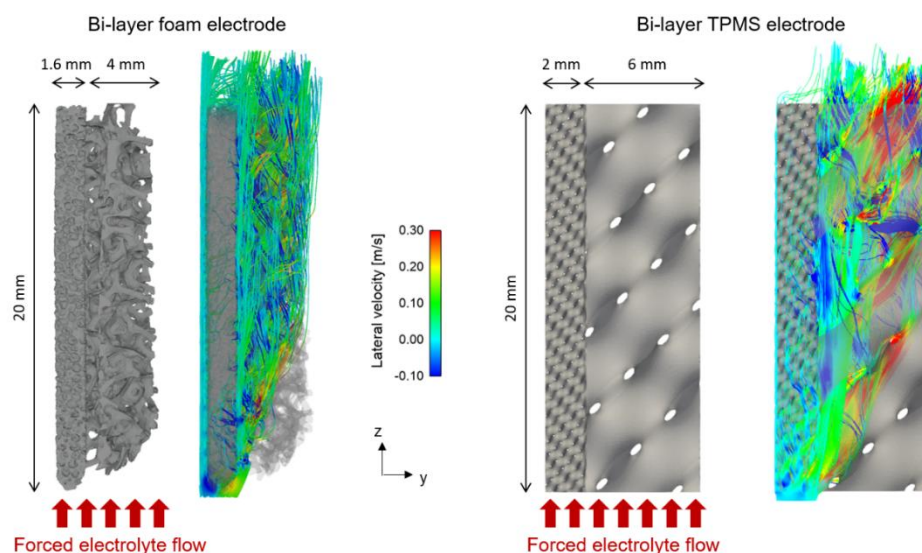


Figure 1: Lateral y-velocity streamlines emitted from the catalytic layer comparing a bi-layer foam (left) and a bi-layer TPMS (right).

These single-phase simulations can be extended to the industrial scale. Figure 2 shows that the use of a 3000 μm foam as PTL results in a more uniform flow distribution within the cell compared to a knitted mesh-type spacer. However, implementing such 3D structures may lead to gas accumulation at the top of the cell. This suggests that current industrial cell designs, characterized by small inlets and outlets, are not optimized for the use of a foam-based PTL, as gas evacuation is hindered.

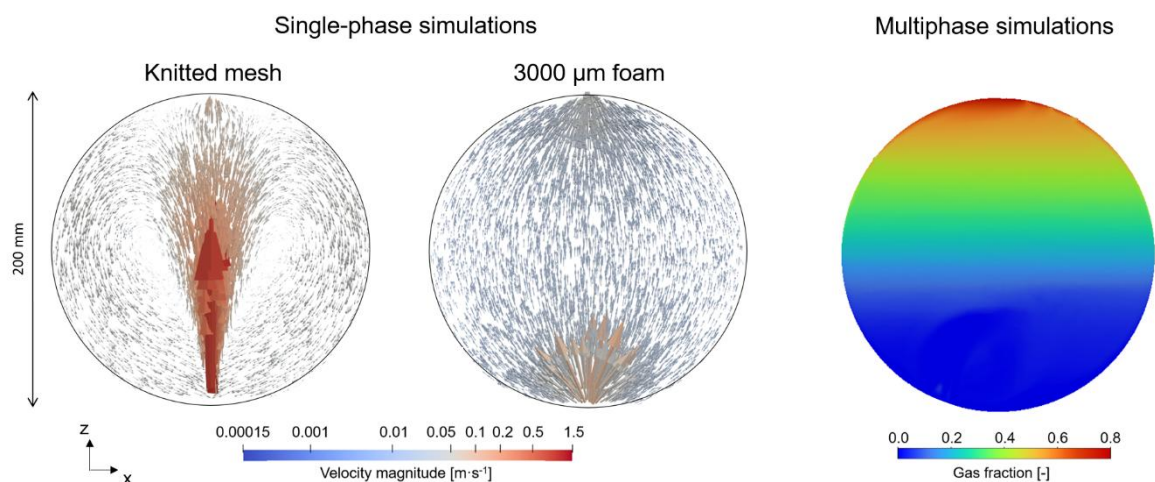


Figure 2: Velocity vectors colored by magnitude comparing a knitted mesh and a 3000 μm foam as PTL (left) and gas fraction profile (right) within industrial cells.

Conclusions: As electrochemists increasingly implement forced electrolyte flow in AWE cells incorporating complex 3D electrodes to enhance bubble removal, CFD simulations become a valuable tool for cell optimization. This approach is applicable at both lab- and industrial-scale, while also revealing the limitations of current cell designs. A paradigm shift in electrolyzer development is therefore required, in which flow fields, gas evacuation pathways, and overall cell architecture are co-designed. In this context single- and multiphase CFD emerge as powerful tools to support a more integrated and performance-driven design strategy.

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