

Numerical assessment of electrolyte flow distribution through flow-engineered 3-D printed bi-layer electrodes for alkaline water electrolysis

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The use of porous electrodes within zero-gap cell configurations for alkaline water electrolysis has gained popularity over the past years. Even though these 3-D electrodes present an increased hydrogen production rate thanks to their high available surface area, bubble evacuation remains a challenge, as bubbles are trapped within the intricate porous structure of the electrodes. Recent studies in our group have shown that current densities of $2 \text{ A}\cdot\text{cm}^{-2}$ can be reached at cell voltages lower than 2 V when using flow-engineered laterally-graded bi-layer foam electrodes with forced electrolyte flow [1]. This performance improvement arises from the electrode design, which promotes efficient bubble removal and thereby reduces the Ohmic resistance. In this work, the bi-layer foams are compared to 3-D printed bi-layer geometries with so-called triply periodic minimal surfaces (TPMS) [2]. The latter are defined based on a mathematical expression involving void fraction and a lattice parameter. In a first approach, two so-called Schwarz CLP structures are combined with lattice parameters matching the pore sizes of the previously used $450 \mu\text{m}$ foam (catalytic layer) and $3000 \mu\text{m}$ foam (porous transport layer - PTL).

Computational fluid dynamics (CFD) simulations are combined with experimental data to correlate the electrolyte flow characteristics of various bi-layer structures with their electrochemical performance. In particular, single-phase electrolyte flow (30 wt% KOH solution at 80°C) through explicitly defined 3-D electrode geometries has been simulated using OpenFOAM. Postprocessing allows extraction of specific velocity components, in particular the lateral y-velocity, which describes electrolyte transfer away from the diaphragm, i.e. from the catalytic layer to the PTL.

As illustrated in Figure 1 below, the lateral velocity profiles differ markedly between the bi-layer foam and the bi-layer TPMS. The bi-layer foam exhibits a pronounced inlet effect, whereas the bi-layer TPMS provides a steadier and more uniform transfer towards the PTL as the electrolyte penetrates upwards through the electrode. This first 3-D printed bi-layer TPMS already achieves a performance comparable to that of the optimised bi-layer foam electrode. Importantly, TPMS structures offer far greater design flexibility. Indeed, by tuning parameters such as channel orientation, lattice size and porosity through 3-D printing, the velocity fields – and consequently bubble removal and overall cell efficiency – can be precisely tailored. We then believe that TPMS structures can overcome the current bi-layer foam in terms of performance.

[1] F. Rocha et al., “Proton exchange membrane-like alkaline water electrolysis using flow-engineered three-dimensional electrodes”, *Nat Commun*, vol. 15, no. 1, p. 7444, 2024.

[2] F. Rocha, R. Delmelle, C. Georgiadis and J. Proost, “Electrochemical Performance Enhancement of 3D Printed Electrodes Tailored for Enhanced Gas Evacuation during Alkaline Water Electrolysis”, *Advanced Energy Materials*, vol. 13, no. 1, p. 2203087, 2023.

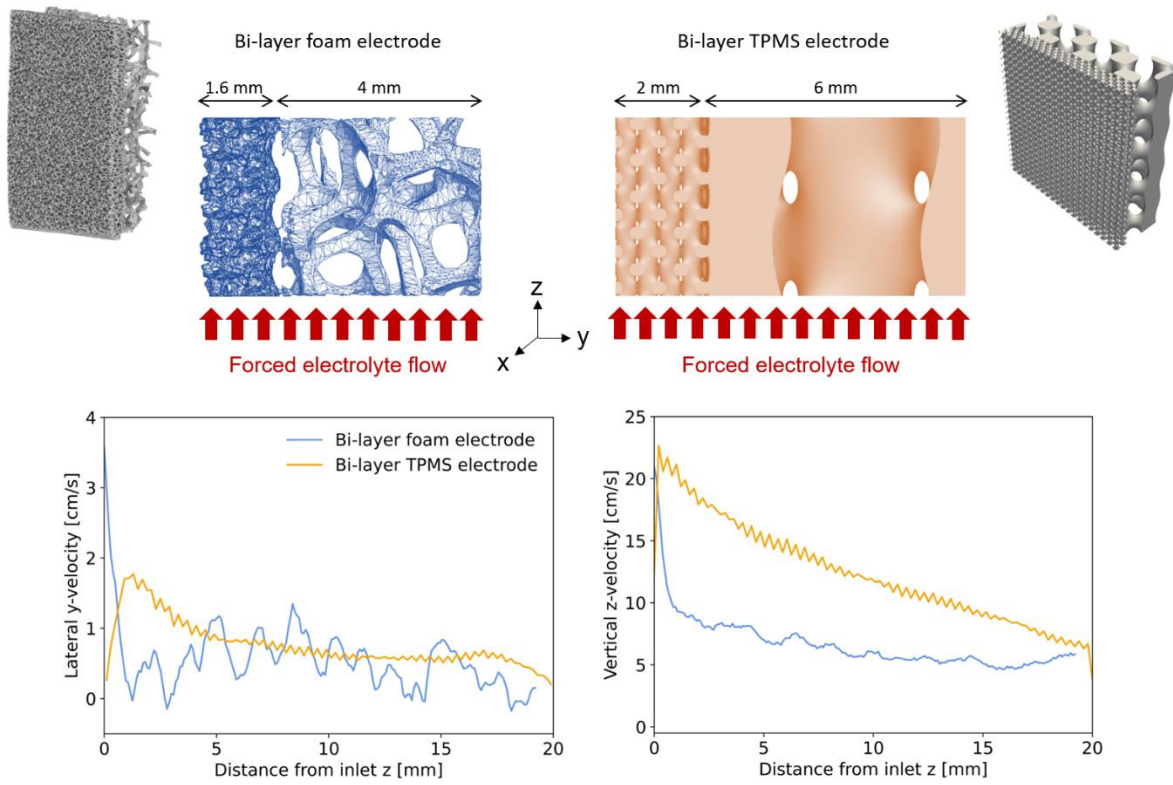


Figure 1: Lateral y-velocity profile (left) and vertical z-velocity profile (right) averaged over x-y planes within the catalytic layer.