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INVESTIGATION OF ELECTROLYTE FORCED FLOW FOR ALKALINE WATER ELECTROLYSIS USING COMPUTATION FLUID DYNAMICS

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ABSTRACT

Green hydrogen production by water electrolysis constitutes a fundamental process for the transition to the hydrogen economy. While alkaline water electrolysis is considered a mature technology to this end, recent work has shown that we can achieve further process intensification with forced electrolyte flow through macro-porous 3D electrodes. The objective of this work is to simulate and analyze electrolyte flow through an industrial-scale pilot and through lab-scale 3D printed electrodes using Computational Fluid Dynamics (CFD). Initial results show that our current pilot cell design is inadequate for forced flow and offer insights in order to design a cell structure that is more suited for gas removal.

Keywords: Computational Fluid Dynamics, Alkaline water electrolysis, Forced Flow

INTRODUCTION

Recent experimental results show that forced electrolyte flow through foams or 3D printed electrodes can offer a significant increase in performance [1,2]. Increased surface area offered by these structures leads to a higher hydrogen production rate while forced flow permits efficient bubble removal. The aim of this work is to complement experimental work with CFD simulations in order to obtain a better understanding of the full field flow characteristics inside the electrode. Reviewing the relevant literature we observe this kind of analysis has rarely been addressed [3].

Our lab-scale experiments on 3D printed structures show the benefits in terms of performance. Unfortunately, we do not observe the same behaviour in an industrial-scale pilot that is modified for electrolyte flow. We perform here simulations of single-phase flow of electrolyte to assess the hydrodynamic behaviour of the cell for both cases: the industrial-scale pilot and the lab-scale 3D printed electrodes. Our objective is to associate electrochemical performance with flow characteristics in order to design an appropriate geometry for industrial-scale electrolyzers.

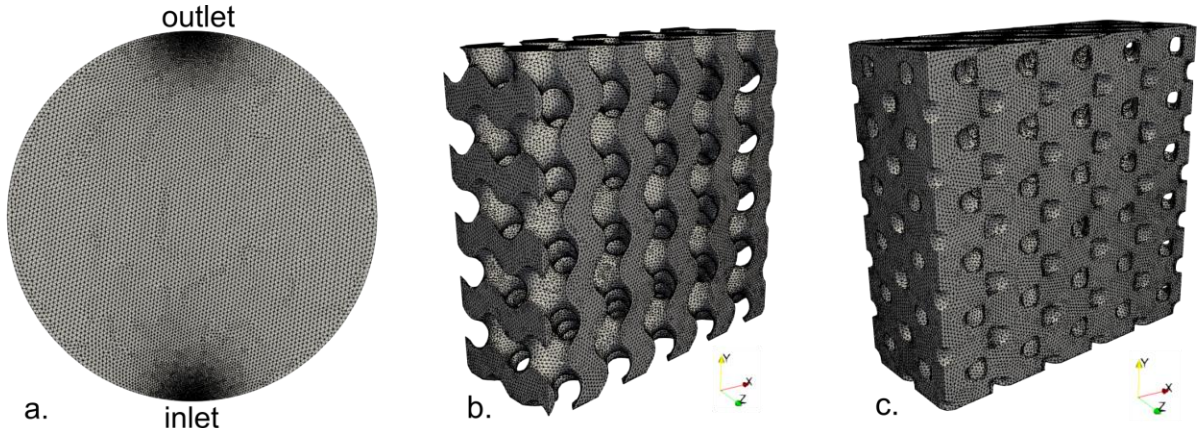

Fig. 1. Computational meshes. a) 2D pilot. b) Gyroid structure. c) Schwarz structure.

MODELING

The geometry of the pilot-scale electrolyzer is circular with a radius of 195 mm and a width between the front and the back plate of 6mm. The inlet at the bottom has a diameter of 2mm and the extractor outlet has a diameter of 4mm. The model geometry of the cell was created and meshed using Gmsh [4] with an interior mesh size of 0.025 m and reduced mesh size of 0.0125 m near the inlet and the outlet (Fig. 1.a.). For the 3D printed electrodes, we use the equations of [5] and create models for a Gyroid and a Schwarz structure. We generate the geometry on a 20x20x8 mm rectangular region and we mesh with an element size of 0.005 m (Gyroid on Fig. 1.b. and Schwarz on Fig. 1.c.). Mesh element sizes were chosen to resolve the flow scales of interest, for which the explicitly described geometries of the 3D printed electrodes require a smaller mesh size.

The incompressible Navier-Stokes equations for a single-phase flow were solved using the Finite Element Method (FEM) implemented in MigFlow software [6]. The electrolyte is water with density ρ = 1000 kg/m^3 and kinematic viscosity v = 0.003 Pa s. For the case of the pilot cell we make the assumption of a 2D flow since the width is small compared to the diameter. To account for the drag of the front and the back walls of the cell we make the hypothesis of a Poiseuille flow in the direction of the flow. For the electrode structures we run 3D simulations since we want to observe the associated flow phenomena such as the vorticity intensity. The boundary conditions for the simulation are the inlet velocity of the electrolyte and zero pressure at the outlet.

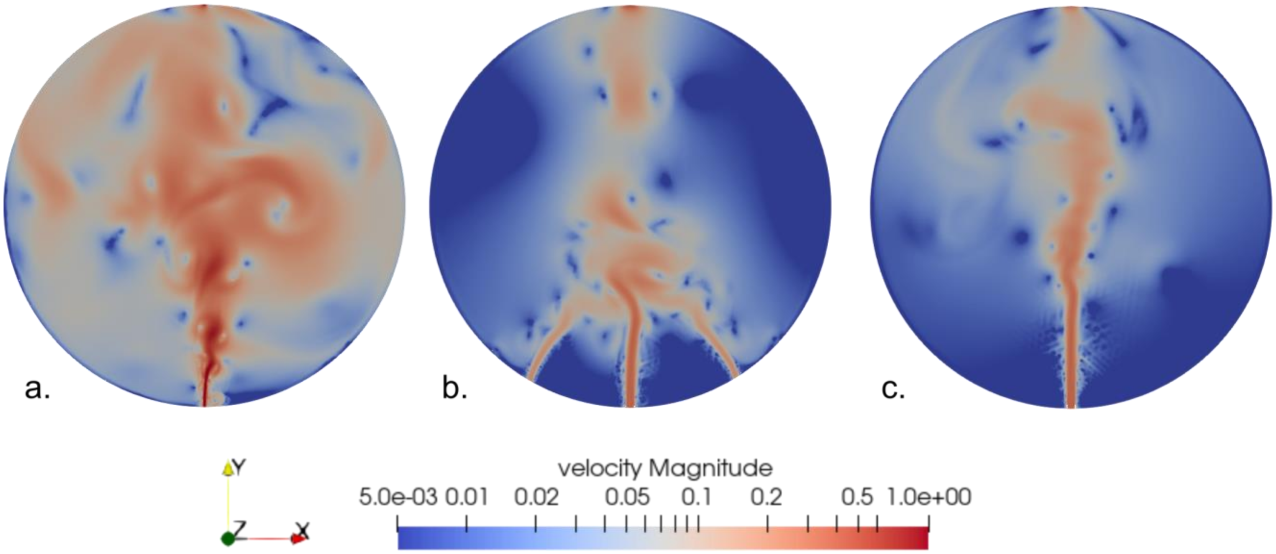

Fig. 2. Velocity profiles for three pilot inlet configurations. a) Current experimental setup. b) Three inlets. c) Inlet of bigger size.

RESULTS AND DISCUSSION

The flow rate chosen for the pilot simulations is 62.5 L/h. This value is a bit higher than the experimentally measured flow rate for the operation of the pilot cell with natural convection. It is therefore the lower limit for which we should consider forced flow. The inlet velocity of the fluid is then calculated at 1.45 m/s for an inlet area of 0.002m x 0.006m = 0.000012 m^2. High inlet velocity through the small opening produces a jet stream flow, which quickly evolves to a shear layer and leads to flow instabilities. Vortical structures are generated and convected throughout the domain, as visualized in Figure 2.a. This kind of flow would lead to concentration of gases that circulate or even remain stagnant in certain regions of the cell.

We investigated the possibility of modifying the inlet conditions in order to obtain smoother velocity profiles throughout the cell. At first, we use two supplementary inlets on symmetrical positions. The situation in this case gets more perplexed, as we would also have a mixing of the three jets in the middle of the cell (Fig. 2.b.). As another option, and since we identify as the cause of instability the high electrolyte velocity on the input, we also examined the possibility of a larger input area and thus lower velocity for the same flow rate. This choice only delays the onset of instabilities forming even though it leads to a less turbulent flow (Fig. 2.c.). In the general case though, we are aiming for flow rates up to 600 L/h where an enlarged inlet would not mitigate turbulent effects.

In the case of 3D printed structures the impact of forced flow is significant, and in particular we observe better performance on Schwarz structures compared to Gyroid ones. By performing 3D flow simulations on a Gyroid and a Schwarz structure of similar surface area, we can identify some qualitative characteristics that promote electrochemical efficiency. For average velocities of 1 m/s flow through the electrode, we can see that for Schwarz the flow is more laminar and thus could offer better gas removal (Fig. 3.b.). The structure of the Gyroid on the other hand leads to higher vorticity and mixing in the x-z directions, therefore there exist regions where gas evacuation may be hindered (Fig. 3.a.).

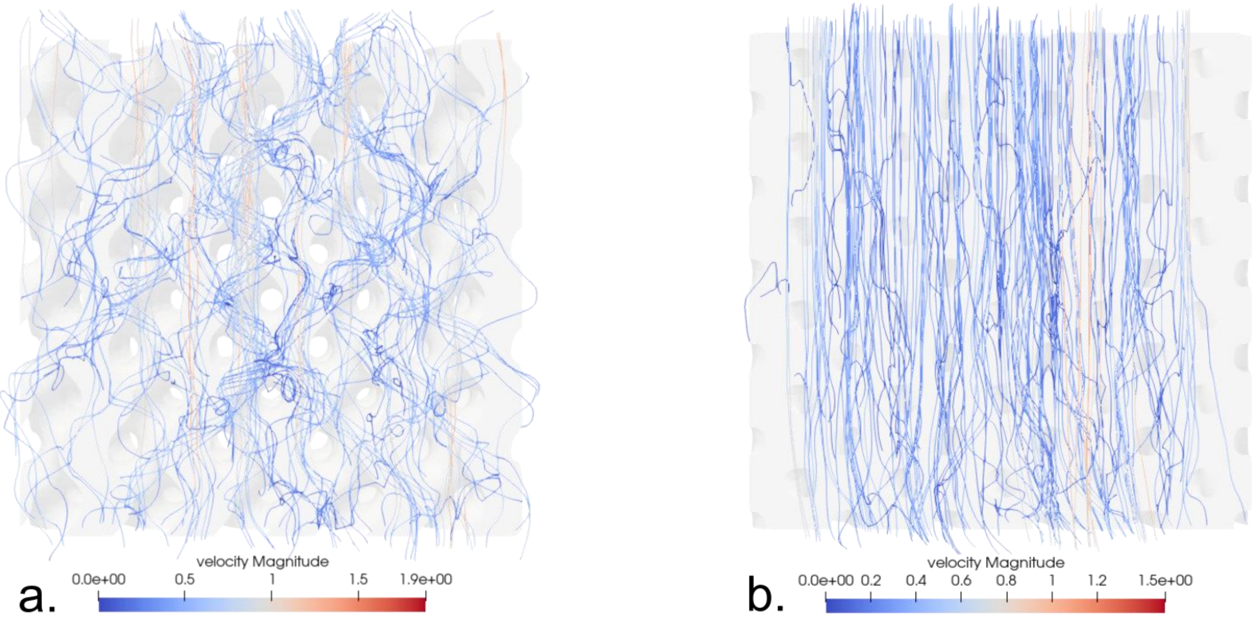

Fig. 3. Velocity streamlines on a) Gyroid and b) Schwarz 3D printed structures.

CONCLUSIONS

We performed computational fluid dynamics simulations to obtain insights about the performance of electrolysis with forced flow. Flow characteristics on the pilot show that the current setup is inadequate to enhance performance with forced flow. For 3D printed structures, we conclude that it is important to have geometries which on the one hand offer high surface area and on the other hand can accommodate a smooth flow evolution. The next step of our developments is to incorporate such a ‘flow-guiding’ structure in the pilot cell. This work is the initial step towards the modeling of the whole process that will simulate the two-phase flow of the electrolyte and the hydrogen gases.

ACKNOWLEDGEMENT

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