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Design of Gas Channels for an Electrochemical Compressor

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ABSTRACT

The fundamental mechanisms behind electrochemical compression have long been understood. However, only now is this technology coming to fruition. The electrochemical compressor offers several key advantages over traditional mechanical compressors. Its lack of moving parts eliminates energy losses due to friction and reduces noise. Electrochemical compression of hydrogen has already been realized at scale, but its usefulness is generally limited to fuel cell applications. A major obstacle to useful electrochemical compression lies in the design of the gas distribution and collection channels, which supply to and collect gases from an ion exchange membrane. Here, we present a method for improving the gas channels using computational fluid dynamics to analyze the distribution of gas for different channel geometries. Several designs, including conventional fuel cell as well as nature-inspired geometries, were evaluated to determine which design is most effective for the electrochemical compressor. We conducted these analyses using performance data determined empirically from previous ammonia compression experiments and the known material properties of the ion exchange membrane. The results indicate a nature-inspired distribution network is likely to improve the compressor performance.

1. INTRODUCTION

Electrochemical compression is a relatively new technology with potentially far-reaching applications, from air conditioning to hydrogen infrastructure to carbon capture. The electrochemical compressor (EC) is a solid-state compression device that uses an electrochemical reaction to incite mass transport of a given working fluid across a solid membrane. Thus far, research groups around the world have verified the electrochemical compression process for several different working fluids, including hydrogen, ammonia, and carbon dioxide (Rohland *et al.*, 1998; Strobel *et al.*, 2002; Onda *et al.*, 2007; Grigoriev *et al.*, 2011; Tao *et al.*, 2017; Tao, 2017). The majority of these research efforts into electrochemical compression dealt with characterization of the electrochemical processes occurring in the compression cell. As consequence, there are several aspects of the compressor that have not yet been analyzed. One such aspect is the handling of the working fluid as it is supplied to and received from the membrane electrode assembly.

1.1. Working Principle

The EC device consists of three main components, the gas distribution channels, the electrodes, and the membrane. The gas distribution channels, shown in Figure 1(a), supply the working fluid to the electrodes, which are made of a porous, electrically conductive material. Within the electrodes, two separate half-reactions occur. In the first half-reaction, the working fluid reacts to form an ionic species that is permeable through the membrane. The ion then passes through the membrane, after which the second half-reaction occurs in the opposite electrode. In the second half-reaction, the ionic species reacts to reform the working fluid at a higher pressure. A second gas distribution channel receives the high pressure fluid from the electrode. Figure 1(b) illustrates the process.

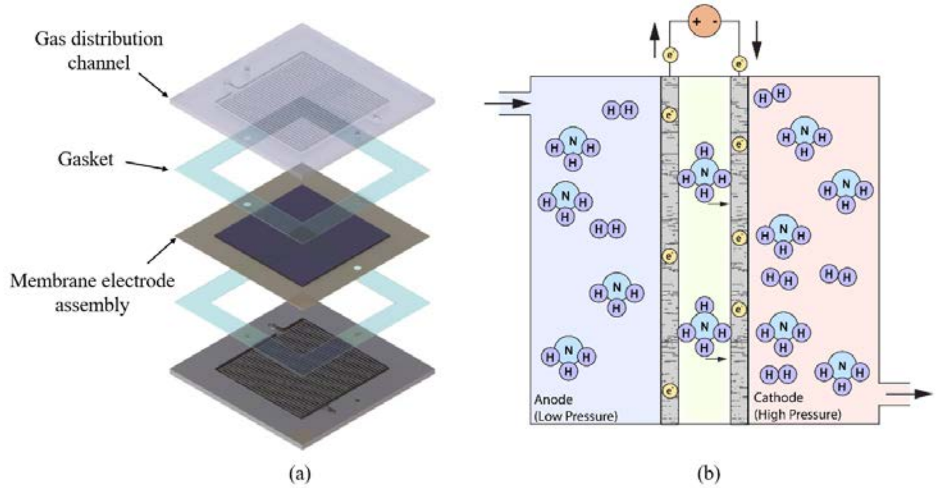

Figure 1: (a) Exploded view of EC cell, (b) Illustration of EC working principle

The following analysis considers an ammonia compression process. Equation (1) governs the oxidation reaction on the anode side, while equation (2) governs the reduction reaction on the cathode side.

$$2NH_3 + H_2 \rightarrow 2NH_4^+ + 2e^- \quad (1)$$

$$2NH_4^+ + 2e^- \rightarrow 2NH_3 + H_2 \quad (2)$$

The EC is a modular device, meaning that we may "stack" several individual cells on top of one another to increase the compressor output. Grigoriev *et al.* (2011) created a stack of three hydrogen compression cells, demonstrating that the EC technology may be scaled up relatively easily. Naturally, if one desires to scale up the EC for practical applications, it is important to derive the best performance possible from a single cell. It is apparent that one of many areas for improvement lies in the delivery of gas to the membrane. To achieve a uniform chemical reaction across the membrane and to avoid internal pressure gradients within the compressor cell, we must design the gas distribution system for an EC operating in a closed loop. In previous EC research endeavors, the gas channel geometry was taken from conventional proton exchange membrane fuel cell designs. These channel geometries, while effective in fuel cell applications, are not necessarily practical for a closed-system EC. This paper compares conventional gas channel designs to several new designs with the objective of minimizing pressure drop within the gas channel.

2. GAS CHANNEL GEOMETRY

Fuel cell researchers have conducted extensive research on different gas channel geometries. However, there is little to no research investigating the effectiveness of gas channel geometry under EC conditions. Fortunately, EC design is very closely related to fuel cell design, so many of the same parameters that affect fuel cell performance also affect EC performance. When designing flow channel layouts for fuel cells, researchers examine the distribution of pressure on the membrane, pressure drop through the gas channels, distribution of temperature across the membrane, and uniformity of reactant concentration over the whole active membrane area (Wilberforce *et al.*, 2017). As such, considerations must be made for fluid flow and heat transfer in the system in addition to the obvious electrochemical considerations.

2.1. Common Fuel Cell Channels

Each channel geometry has its own unique set of advantages and disadvantages. While fuel cell researchers around the world have analyzed these geometries both numerically and empirically, there is no clear consensus as to which is best. Two of the most common geometries are parallel and serpentine channels. Parallel channels, shown in Figure 2, are advantageous due to their intrinsically low resistance to flow, but offer poor distribution, as individual gaseous species may pool in one area, leaving parts of the membrane unsupplied with reactants. Contrarily, serpentine channels create an even distribution of reactants at the cost of higher pressure drop (Larminie and Dicks, 2003). When applying fuel cell flow channels to an electrochemical compressor, it is imperative that the internal pressure drop is minimized and that the membrane receives an even mixture of reactants everywhere across its surface.

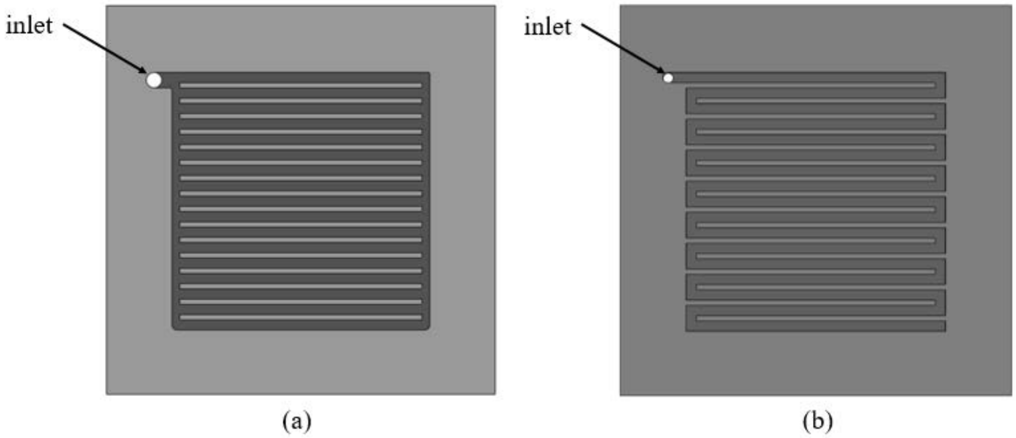

Figure 2: (a) Parallel gas distribution channel, (b) Serpentine gas distribution channel.

2.2. Fractal-Like Channels

We turn to nature for a new gas channel geometry that will provide us with both low pressure drop and high uniformity of distribution. Nature-inspired fractal channels are increasingly common in heat exchanger design due to their intrinsic advantages for high heat transfer and low resistance to flow (Huang *et al.*, 2017). Therefore, it seems reasonable that such a geometry will be advantageous to an EC cell's performance. A handful of research groups have analyzed the feasibility of nature-inspired flow channel designs in a fuel cell environment, noting distinct improvements in pressure drop and power density (Kloess *et al.*, 2009; Damian-Ascencio *et al.*, 2017). Damian-Ascenco *et al.* (2017) studied a tree-like branching channel design using numerical methods, finding that a branching design improved current density in a fuel cell environment. Moreover, nature-inspired designs have shown promise in heat exchanger design. Pence (2002) designed a fractal-like microchannel heat sink following constructal theory, showing that pumping power was significantly reduced in a fractal-like branching network compared to a straight channel array. In light of these findings, we hypothesize that a bifurcating, fractal-like network will improve both pressure drop and distribution of gas in the EC. We propose a constructal channel network, such as the one depicted in Figure 3.

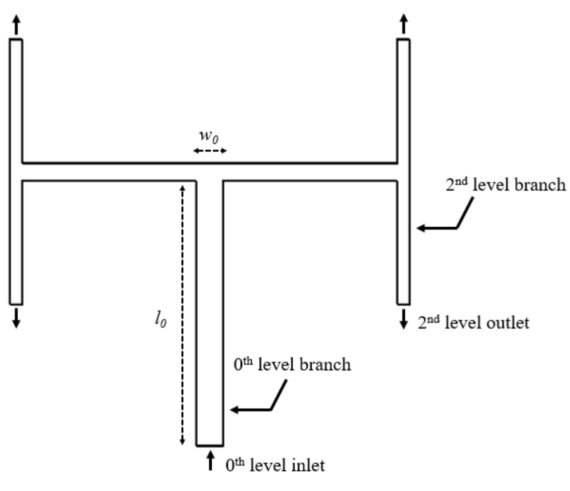

Figure 3: Bifurcating, fractal-like gas channel segment.

We used a parametric CFD analysis to evaluate the internal pressure drop of the experimental geometry under experimentally observed operating conditions. To keep the model relatively simple, the analysis only considered bifurcating channels with a constant channel length (*l*) and a rectangular cross section. The channels follow Pence's construcatal method for fractal-like flow networks, where the width of the kth channel varies as:

$$w_k = \frac{\beta H w_{k-1}}{w_{k-1} + H - \beta w_{k-1}} \tag{3}$$

where β is the branching diameter ratio and H is the channel height (Pence, 2002). The expression relates the hydraulic diameter of consecutive branches using Constructal Law, which governs the way that finite-sized systems must evolve to provide easier access to the imposed currents that flow through it (Reis, 2006). Similarly, the relationship between consecutive channel lengths is:

$$l_k = \gamma l_{k-1} \tag{4}$$

where γ is the length ratio. The values of β and γ considered in the analysis were 0.7937 and 0.7071, respectively (Pence, 2002). Using this methodology, we investigated the effect of the bifurcation angle and hydraulic diameter on the total pressure acting on the membrane surface, which comprises the top surface of the flow channel.

3. MODELING AND SIMULATION

In the analysis, we simulated several different channel geometries to determine which configuration is most suitable for use in a closed-loop electrochemical compression device. The present study compares the fractal-like channels to a chosen baseline system. In this case, the serpentine flow channel was selected as the baseline system. Despite the possibility for low pressure drop in the parallel channel, the issue of misdistribution of species inside the flow field makes this geometry a poor reference. The serpentine channel, however ensures that the reactants appear on the membrane in even concentrations. Because the branching fluid network has the same advantages as the serpentine for misdistribution, we wish to observe the difference in pressure drop between these two types of flow channels.

3.1. Finite Element Analysis of Membrane Material

One challenge in designing gas channels for both fuel cells and the EC unit is that the channel width must not be so wide that the membrane deforms under the differential pressure developed during regular operation. Therefore, we need to determine the threshold for a safe channel width. To do so, a mechanical finite element analysis (FEA) study was conducted. A section of the membrane was analyzed assuming fixed supports on either end of the test specimen and a uniform pressure load on the top surface. The maximum Von Mises stress was measured in the test section and compared to the yield strength of the membrane material, which is fumasep® FAB-PK-130. The membrane has an average yield strength of 25 MPa, modulus of elasticity of 1,400 MPa, and density of 920 kg/m^3 (Fuel Cell Store). The Poisson ratio was assumed to be 0.47, which is equal that of PTFE. After applying these engineering parameters to the structural model, a parametric FEA simulation was conducted to evaluate the maximum equivalent stress for a variety of channel widths and pressure loads. Figure 4 shows a contour plot of the equivalent stress developed in the test section for a given set of input parameters.

The results are shown in Figure 5. From the FEA results, it is apparent that the channel width must be kept relatively short, around 1 mm. Thus, it was determined that the flow simulation should test channel widths of 0.25 mm, 0.5 mm, and 1.0 mm. To control the hydraulic diameter, the channel heights were similarly set to 0.25 mm, 0.5 mm, and 1.0 mm. Each channel geometry was analyzed for all combinations of channel width and height.

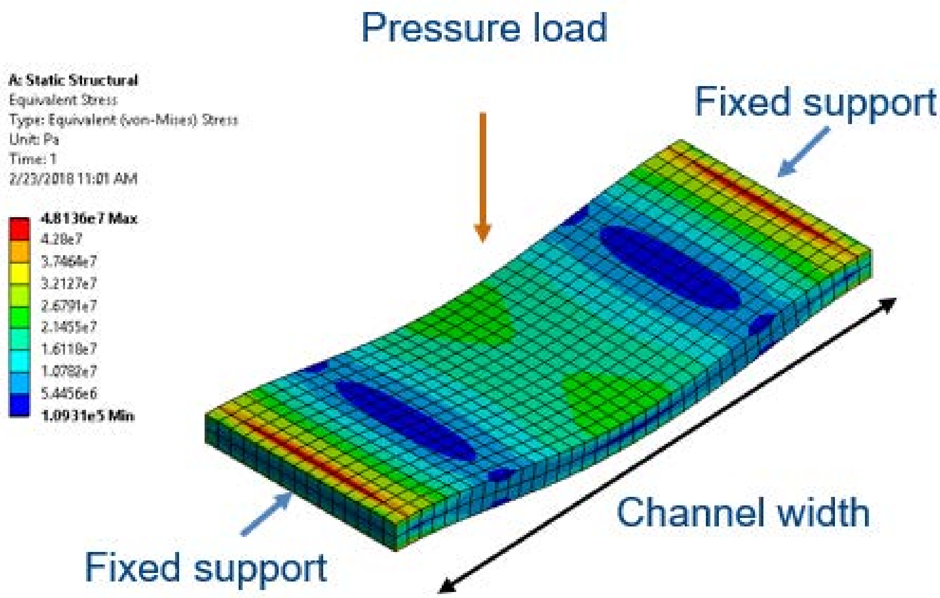

Figure 4: Contour plot of membrane equivalent stress.

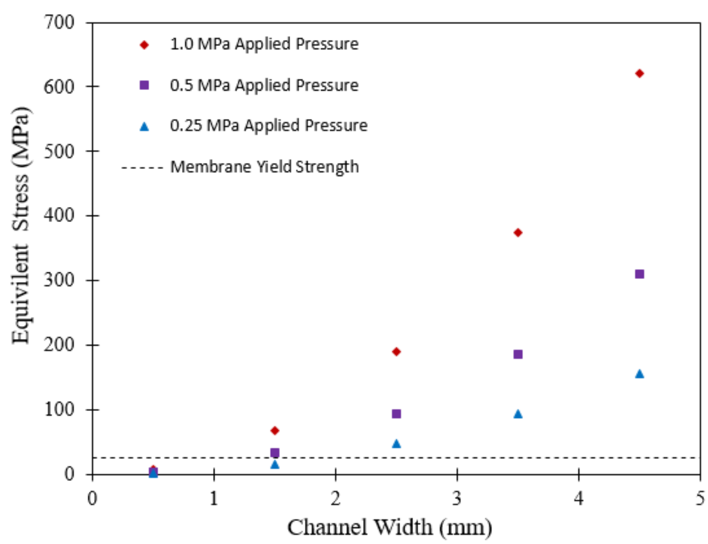

Figure 5: Results of membrane parametric FEA.

3.2. Real EC Operating Conditions

We applied operational data from Tao's ammonia compression experiments (2017) to evaluate the system boundary conditions. In his experiment, Tao (2017) used acid/base titration to measure the total flow rate of ammonia and hydrogen molecules leaving a single EC cell in moles per second. Knowing the rate of ammonia molecules leaving the system, we were able to determine the total mass flow rate of the working fluid through the membrane. Additionally, knowing the active membrane area, we determined the average mass flux through the membrane. However, the present study is focused on the fluid leaving the top of the gas channels rather than the diffusive flow through the membrane, so the mass flux leaving the flow channel was calculated as the total flow through the membrane divided by the open channel area. These mass flow input parameters are summarized in Table 1**.** Because the present study only examines a representative sample of the entire flow channel, an additional flow outlet, besides the mass flux condition on the top fluid boundary, was included to satisfy conservation of mass. This outlet flow rate was calculated as the total inlet mass flow rate minus the product of the average open channel mass flux and the area of the top surface of the fluid body. The working fluid was defined in the simulation as a mixture of ammonia and hydrogen at standard conditions according to the stoichiometric coefficients from the overall cell reaction. The viscosity of the fluid mixture was determined by summing the products of the viscosities and mole fractions of the individual components (Davidson, 1993).

Table 1: CFD simulation input parameters

Simulation Input	Value
Total Flow NH_4^+ (mol s^{-1})	1.94E-06
Total Mass Flow Rate (µg s^{-1})	34.9
Membrane Area (mm^2)	575
Open Channel Area (mm^2)	413
Diffusive Flux (µg s^{-1} mm^{-2})	0.0607
Open Channel Flux (µg s^{-1} mm^{-2})	0.0845
Mixture Density (kg m^{-3})	0.4933
Mixture Viscosity (kg m^{-1} s^{-1})	9.81E-05

It is computationally expensive to simulate the entire gas distribution channel, so we limit the analysis to a small, representative segment. To enable a fair comparison, all sample channels with like design parameters have equal channel length. To achieve equal channel lengths in all channel designs, the serpentine channel's total length was set equal to the total length of the fractal channels. In total, we simulated four types of channel geometries, including a serpentine channel and three fractal-like channels of different bifurcation angles. Figure 6 shows the different geometries considered in the analysis. Additionally, because the flow in the bifurcating channels is symmetrical, we reduce computational time by evaluating the flow for half of the segment we wish to simulate. The simulation was carried out using ANSYS Fluent CFD software.

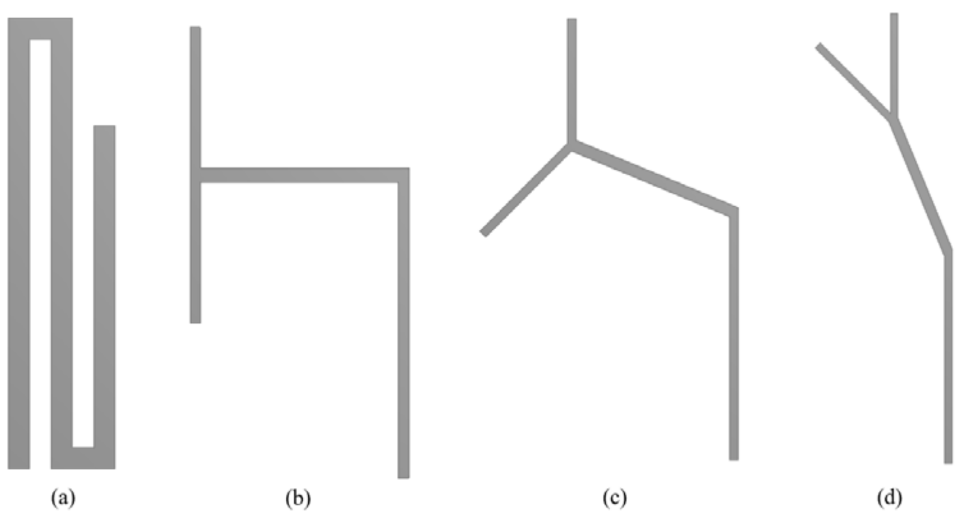

Figure 6: Experimental channel geometry: (a) Serpentine, (b) 180° bifurcation, (c) 135° bifurcation, (d) 45° bifurcation.

4. RESULTS

The results from the parametric study are summarized in Figures 7 and 8. As expected, the pressure drop observed in each simulation increases significantly as the hydraulic diameter decreases. As the hydraulic diameter approaches 1 mm, as is the case for the 1 mm by 1 mm channel, the pressure drop becomes negligible. Additionally, we see that the pressure drop increase more rapidly with decreasing channel height than it does with decreasing channel width.

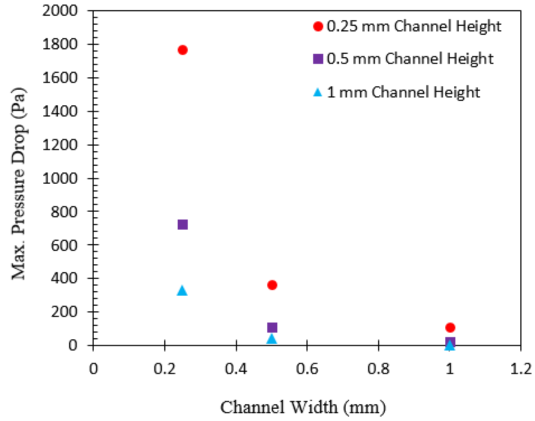

Figure 7: Minimum total pressure across membrane surface for serpentine channel geometry.

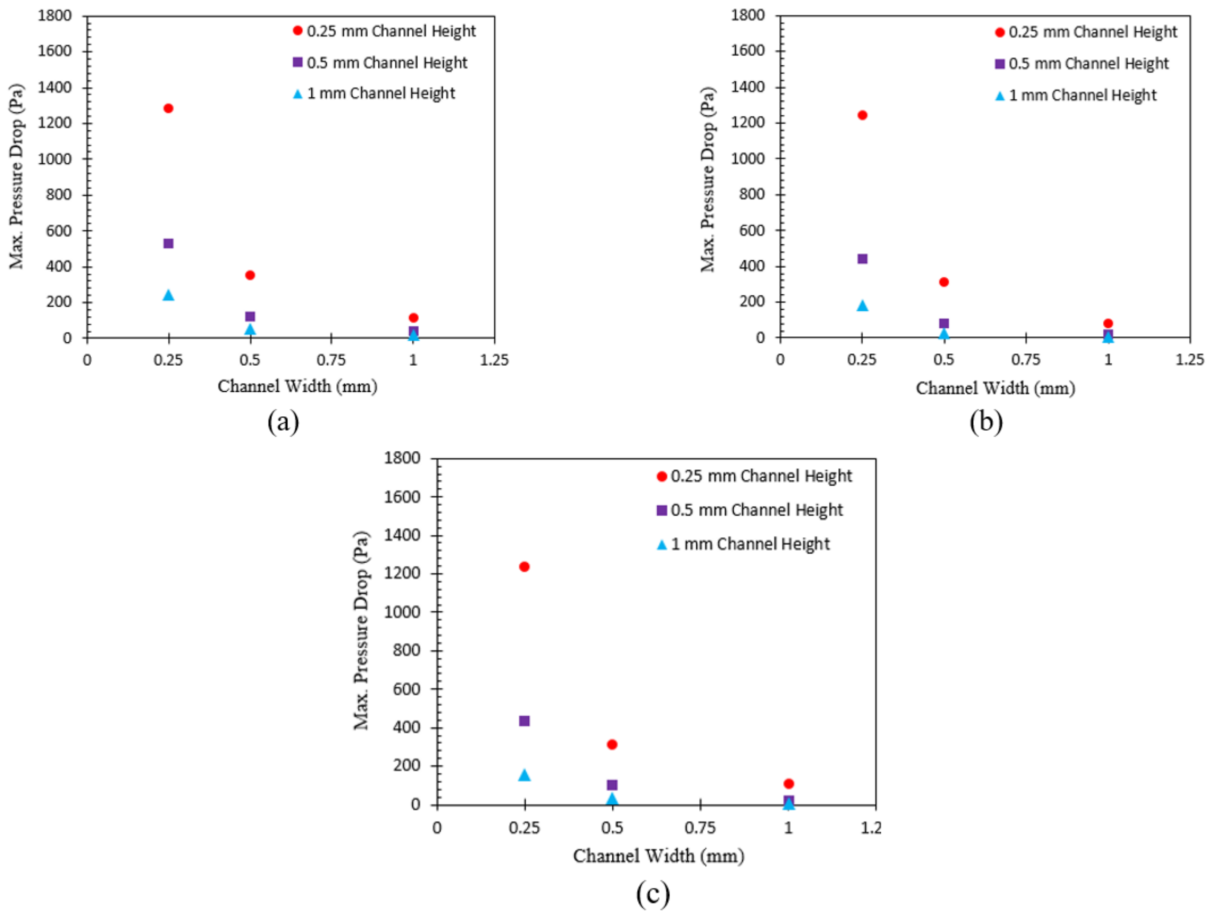

Figure 8: Minimum total pressure across membrane surface (a) 45° bifurcation, (b) 135° bifurcation (c) 180° bifurcation.

From the results shown in Figure 8, it is clear that the bifurcating channels exhibit lower pressure drop than the baseline in all instances. However, because there is no significant difference in the flow channel performance across different bifurcation angles, it is evident that the benefit seen in the bifurcating flow channels is the result of the decreased fluid velocity after the flow branches. In other words, the pressure drop in the flow field is dominated by major losses. Minor losses associated with bends in the channels are less significant.

The results indicate that there is a distinct benefit for pressure drop if the EC cell employs a fractal-like flow network. Furthermore, because there is no significant difference in performance of decreasing the bifurcation angle for the observed conditions, the 180° bifurcation angle may be used. The 180° geometry is advantageous because it can spread out over a larger area of the membrane surface, so one may implement this channel design without making major modifications to the existing membrane electrode assembly.

5. CONCLUSIONS

The present work is a general design study for a novel EC component technology. The minimum total pressure developed under real operating conditions in several samples of different EC flow channels was examined using CFD techniques. We found that a fractal-like bifurcating flow channel demonstrates a lower pressure drop than the conventional serpentine channel. The bifurcating and serpentine geometries are preferred of other geometries for their tendencies to avoid unequal distribution of reactants on the membrane surface. Therefore, the experimental geometry shows promise for improved EC performance with respect to the baseline. Because the pressure drop is not a significant function of bifurcation angle, the 180° fractal geometry is recommended for use in the EC due to its intrinsic advantages for space efficiency. While these results may be useful in designing an improved EC cell, the gas channels should be optimized for specific applications. Future research endeavors should seek to optimize the fractal flow network for specific applications and test their performance empirically.

NOMENCLATURE

EC	Electrochemical compressor	(–)
CFD	Computational fluid dynamics	(–)
FEA	Finite element analysis	(–)
H	Channel height	(mm)
l	Channel length	(mm)
w	Channel width	(mm)

Greek Letters

β	Channel width ratio	(–)
γ	Channel length ratio	(–)

Subscript

k	Channel branch number	(–)

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