CFD SIMULATION OF PEMWE FLOW-FIELD DESIGN BASED ON A BIO-INSPIRED

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ABSTRACT

For the generation of green hydrogen, electrolysis in conjunction with renewable energy sources is the most viable approach. The capacity of the Polymer Electrolyte Membrane Water Electrolyzer (PEMWE) to generate compressed hydrogen with high purity at comparatively moderate working temperatures (70–90 C) has drawn attention. The bipolar plates (BPPs) are the PEMWE stack's major cost contributors. Flow distributor impact has a major effect on Polymer Electrolyte Membrane Water Electrolyzer (PEMWE) performance and durability. Several leaves were used as a very similar example inspired by the plant to study how to get the most out of bio-inspired design as a great convergence accelerator track for creating new bipolar plates (BPPs) geometries. The hydraulic pathway through a leaf can be thought of as analogous to an electrical circuit, which represents the channel geometry of BPPs. In order to assess the flow field performance of the proton exchange membrane water electrolysis (PEMWE) under the same operating conditions (operating temperature, anode pressure, current density) and design parameter (anode channel (ACH), porous gas diffusion layer (AGDL), and catalyst layer (ACL) thickness), a 3D numerical model based on COMSOL Multiphysics Software (version 6.1 COMSOL) is integrated with the Electrochemistry and Flow field distribution analysis. The primary design criteria in this study are centered on more even and consistent fluid pressure/velocity distributions, homogeneous water distribution, homogeneous species molar spreading along the flow channels, and efficient gas removal throughout the active area. which consequently enables the stack to operate at high pressure and high current density. Nature-inspired designs show their prominent characteristics such as low-pressure drops and effective fluid distribution. In turn homogeneous sufficient water sufficient removal.

Keywords: Flow field, PEMWE, bio-inspired, CFD, bipolar plates

INTRODUCTION

The world's need for energy is quickly rising these days, and access to energy resources is becoming more and more important to maintaining human well-being. The majority of the world's energy needs are met by fossil fuels, which will eventually cause the finite supply of fossil energy resources to gradually run out. [1]. In this situation, switching to hydrogen energy is typically an effective way to streamline the shift to a low-carbon community. PEMWE definition: A PEMWE consists of a membrane (PEM) positioned between two electrodes. The PEMWE is separated into the cathode and anode by the membrane; each section is made up of a catalyst layer, a gas diffusion layer, and a gas channel. Figure 1 displays a schematic diagram of a typical PEMWE. Equation (1) illustrates how water enters the anode channel (ACH) on the anode side and travels via the porous gas diffusion layer (AGDL) and anode catalyst layer (ACL), where it undergoes semi-reactions of oxidation that split the water into protons, oxygen, and electrons. Protons of hydrogen travel through the membrane to reach the cathode catalyst layer (CCL), while electrons move there through an external circuit. Equation (2) describes how hydrogen protons and electrons combine on the cathode side to form hydrogen gas through semi-reactions of a reduction. Equation (3) presents the overall response [4-6].

$$H_2O_{(liq)} \rightarrow \frac{1}{2}O_{2(g)} + 2H^+ + 2e^- \quad (1)$$

$$2H^+ + 2e^- \rightarrow H_{2(g)} \quad (2)$$

$$H_2O_{(liq)} + \text{electricity} + \text{heat} \rightarrow \frac{1}{2}O_{2(g)} + H_2 \quad (3)$$

Name	Side	Material	Value	Unit	Source
PTL thickness	Anode	Ti mesh	2E−4	m	[7]
	Cathode	Ti mesh			[7]
CL thickness	Anode	Iridium dioxide (IrO2)	1E−5	m	[2]
	Cathode	platinum with carbon (Pt/C)			[2]
Membrane thickness		Nafion® 117	1.78E−4	m	[7]
Channel thickness			0.001	m	[7] [3]

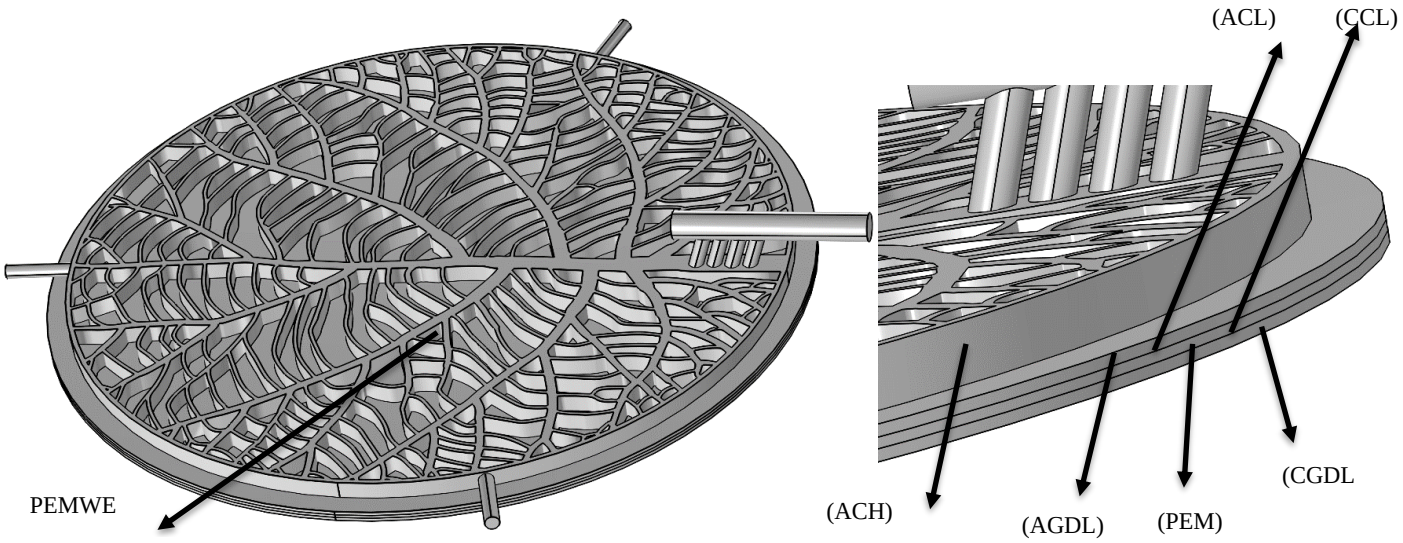


Figure 1 PEMWE

MODELING DEFINITION

This work employs a single-phase-domain approach to implement the nonlinear differential equations for a three-dimensional single-half-cell PEMWE. The finite element method is used to model the conservation equations for electrochemical reactions that must be solved simultaneously across seven regions of the cell, including the anode and cathode catalyst layer, GDLs, anode channel, and membrane. Utilizing COMSOL Multiphysics 6.1, the numerical model is constructed. To solve the set of equations, an iterative procedure is used until the residual approaches 10-6. Because there are seven distinct geometries, the mesh count required to ensure the independence of the results is roughly between 1E6 and 2E6 cells. The mesh independence of the results is verified in order to certify that the results are independent of the mesh. The geometry parameters, physical parameters, and operating conditions for the PEMWE are shown in Table 1.

Assumption: The modeling studies focus on optimizing the anode channel patterns using the leaf-biomass-flow-field of five leaf vein patterns in order to improve PEMWE performance. A few presumptions are made in this model in order to avoid confusion and maintain consistency in a fruitful compromise. It is assumed that the model is operating in a steady state. Laminar flow has one or more inlets and one or more outlets, and it is incompressible. Isothermal Newtonian fluid that disregards gravity Potential and kinetic energy changes are ignored, One bar of anode pressure is present. The gas mixture is subjected to ideal gas behavior. There has been a disregard for the contact resistance between different layers. It is assumed that the GDL, catalyst layer, and membrane are homogeneous and isotropic.

GOVERNING EQUATION AND NUMERICAL METHODS :

Conservation of mass - In the Flow fluid model part a free and porous media is applied to enable porous media domains and neglect the gravity effect. for zero velocity condition at the wall, mass exchange occurs at Porous Medium calculated by equation (4) :

$$\rho \nabla \cdot \mathbf{ua} = Q_{\mathrm{m}} \tag{4}$$

where *u* is the mixture velocity vector (m/s), ρ is the mixture density (kg/m^3), *Q* is the source term or mass source [kg/(m^3 s)].

conservation of momentum - the momentum conservation applied for the channel fluid and Porous Medium GDL as shown in equations (5-8) respectively :

$$\rho(\mathbf{ua} \cdot \nabla)\mathbf{ua} = \nabla \cdot [-p\mathbf{I} + \mathbf{K}] + \mathbf{F} \tag{5}$$

$$\mathbf{K} = \mu\left(\nabla \mathbf{ua} + (\nabla \mathbf{ua})^{\mathsf{T}}\right) \tag{6}$$

$$\frac{1}{\epsilon_{\mathrm{p}}}\rho(\mathbf{ua} \cdot \nabla)\mathbf{ua}\frac{1}{\epsilon_{\mathrm{p}}} = \nabla \cdot [-p\mathbf{I} + \mathbf{K}] - \left(\mu\kappa^{-1} + \beta\rho|\mathbf{ua}| + \frac{Q_{\mathrm{m}}}{\epsilon_{\mathrm{p}}^2}\right)\mathbf{ua} + \mathbf{F} \tag{7}$$

$$\mathbf{K} = \mu\frac{1}{\epsilon_{\mathrm{p}}}\left(\nabla \mathbf{ua} + (\nabla \mathbf{ua})^{\mathsf{T}}\right) - \frac{2}{3}\mu\frac{1}{\epsilon_{\mathrm{p}}}(\nabla \cdot \mathbf{ua})\mathbf{I} \tag{8}$$

Where p is the pressure (N/m2), μ is the dynamic viscosity of the mixture [kg/(m s)], K is the viscous stress tensor (Pa), F is the volume force vector (N/m3) and, T is the absolute temperature (K) , ε_P is the GDL porosity, κ the permeability of the GDL (m^2), and β drag force coefficient which is assumed to be zero

Mass Diffusion (Maxwell–Stefan) - In the electrochemical model part PEMWE selected including H2O species, gas phase diffusion, and H2O(L) in reaction stoichiometry. In order to solve for the fluxes of each species in terms of mass fraction, The whole computational domain multispecies mass transports are described by the Maxwell–Stefan equation (diffusion equation) (9-13) respectively:

$$\nabla \cdot \mathbf{j}_i + \rho(\mathbf{u} \cdot \nabla)\omega_i = R_{i,\text{total}} \tag{9}$$

$$\mathbf{j}_i = -\rho\omega_i \sum_k \tilde{D}_{ik,\text{eff}} \mathbf{d}_k \tag{10}$$

$$\mathbf{d}_k = \nabla x_k + \frac{1}{p_A}\left[(x_k - \omega_k)\nabla p_A\right], \quad x_k = \frac{\omega_k}{M_k} M_n \tag{11}$$

$$p_i = x_i p_A \tag{12}$$

$$M_n = \left(\sum_i \frac{\omega_i}{M_i}\right)^{-1} \tag{13}$$

Where **u** is the mass averaged velocity of the mixture (m/s), $\mathbf{j}_i$ is the mass flux relative to the mass-averaged velocity (kg/(m^2·s)) , $\boldsymbol{\omega}_i$ is the mass fraction (1), R_i is the rate expression describing its production or Consumption (kg/ (m^3·s)).where, $\mathbf{d}_k$ is the diffusional driving force (1/m) acting on species k, x_k mole fraction (1), p_A is the total anode pressure (Pa) Mn mean molar mass (kg/mol), and p_i partial pressures (Pa)

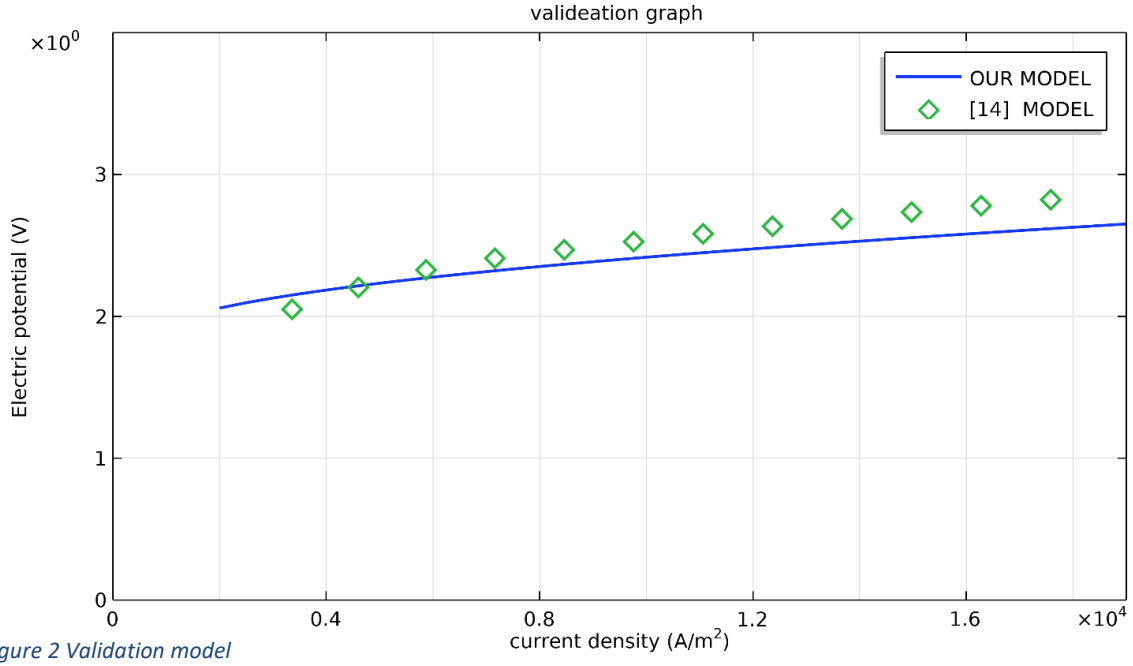


Figure 2 Validation model

Validation: To verify the simulation model's findings, Upadhyay [2] presents the data from an experimental investigation, which is compared with the numerical results. As shown in Figure 2, the polarization curve of the experimental study created from [2] is compared to the polarization curve predicted by the current model at operating conditions of pressure at 1 bar and temperatures of 328.15. The experimental findings and the model predictions agree fairly well [2].

RESULT AND DISCUSSION

POLARIZATION CURVES - The operating conditions are the basis for the simulation curves displayed in Figure 3, and the constants listed in Tables 2 demonstrate how significantly bio-inspired designs can enhance PEMWE performance. The L4k bipolar plates (BPPs) geometry outperformed the other bioleaf designs, most likely because of the design's abundance of redundant channels, which raise the interface active area. and because of the longer channels than the multi-serpentine, record better performance. Water accumulation in bends reduces point flow and local current density.

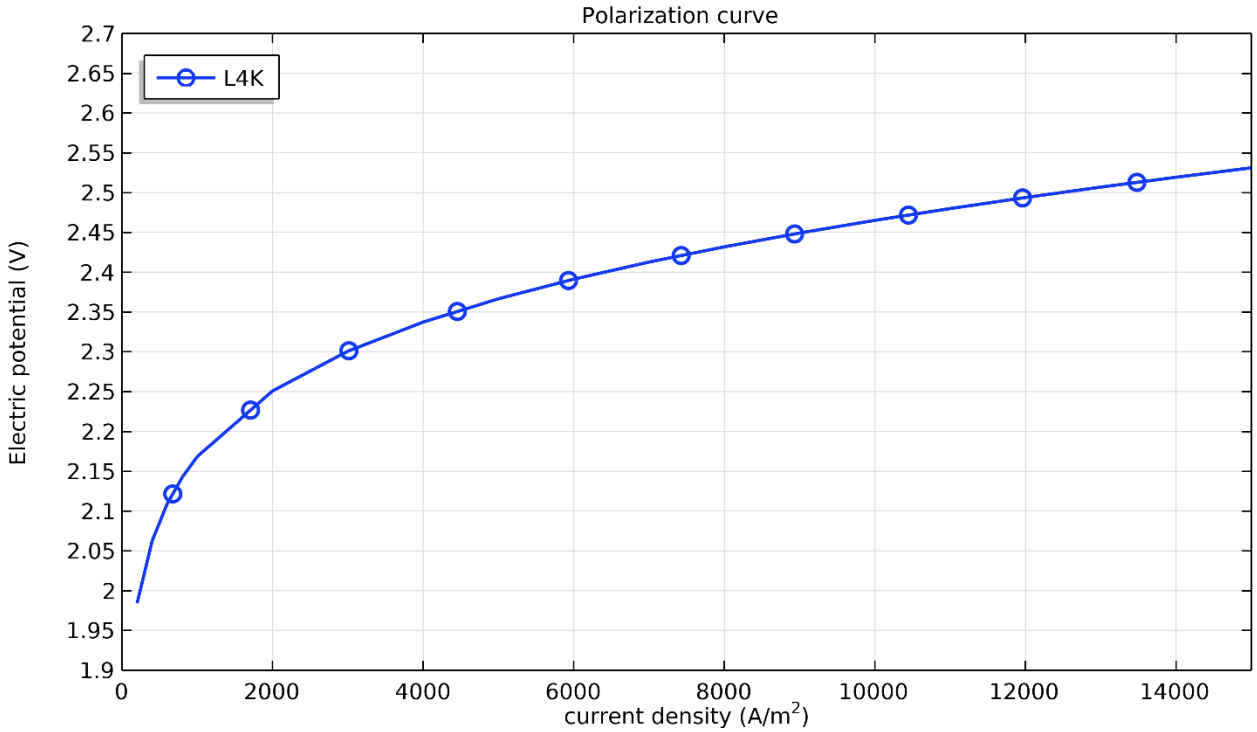


Figure 3 Polarization curve of the BPPs Kiwi leaf

PRESSURE CONTOURS

The performance of PEMWE is significantly influenced by the pressure distribution. Reactant problems are brought on by the high-pressure drop across the electrolyzer. Thus, the ideal pressure distribution is the one that genuinely prevents water buildup in the cell. The static pressure of L4K flow field designs in the GDL is displayed in Figure 4. The designs with the largest pressure drop are the multi-serpentine. But by a wide margin, the bio-leaf design has the lowest pressure drop. Longer average path lengths increase pressure drop, which is shows Figure 5.

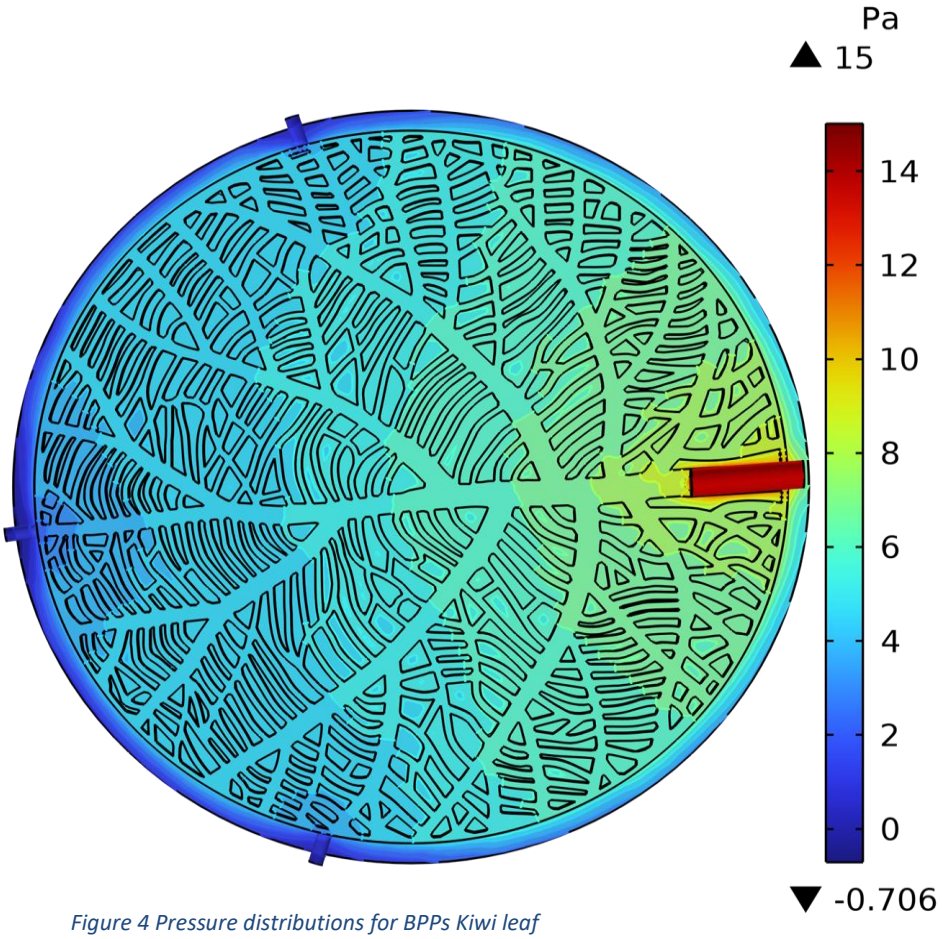


Figure 4 Pressure distributions for BPPs Kiwi leaf

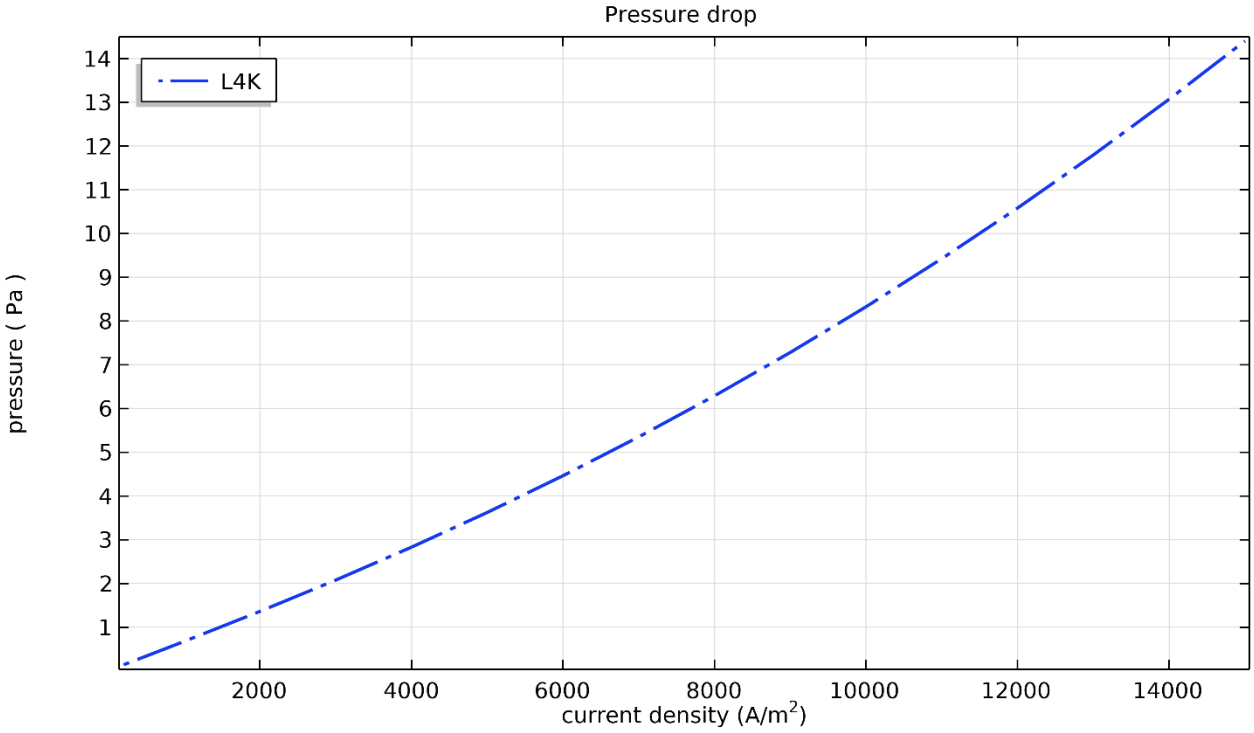


Figure 5 Pressure drop of BPPs Kiwi leaf

VELOCITY CONTOURS

PEMWE benefits greatly from even and high velocity profiles. A cell's capacity to expel liquid water and the time it takes to extract the generated gases from the cell are both greatly enhanced by higher velocities. Reactant residence times are similar and the reactant distribution is more even when the velocity profiles are uniform. This implies a more consistent distribution of hydrogen production. As a result, Figure 6 displays the L4K flow field design ' velocity distributions. the velocity profile of the bioleaf design is substantially more uniform.

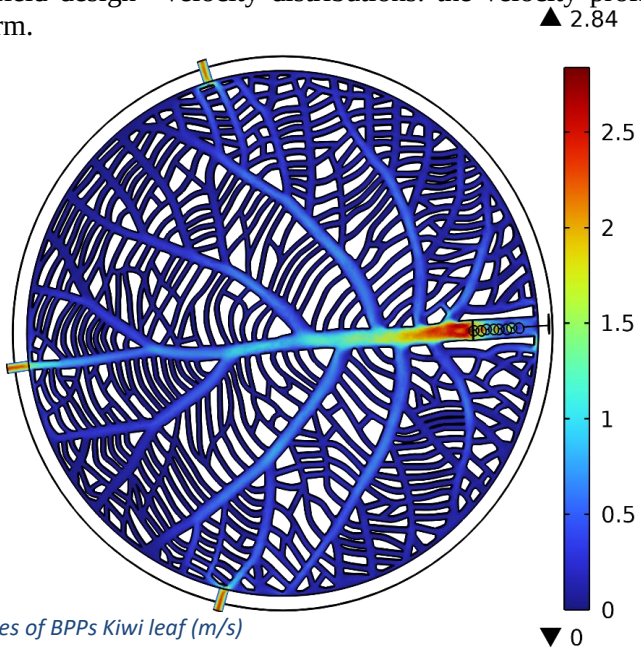


Figure 6 Velocity profiles of BPPs Kiwi leaf (m/s)

OXYGEN DISTRIBUTION

The water distribution for the various flow field designs is displayed in Figure 7. Comparing the bio-leaf design to the multi-serpentine, the bio-leaf design has a more uniform water distribution. More high-performance cells result from a more uniformly distributed design.

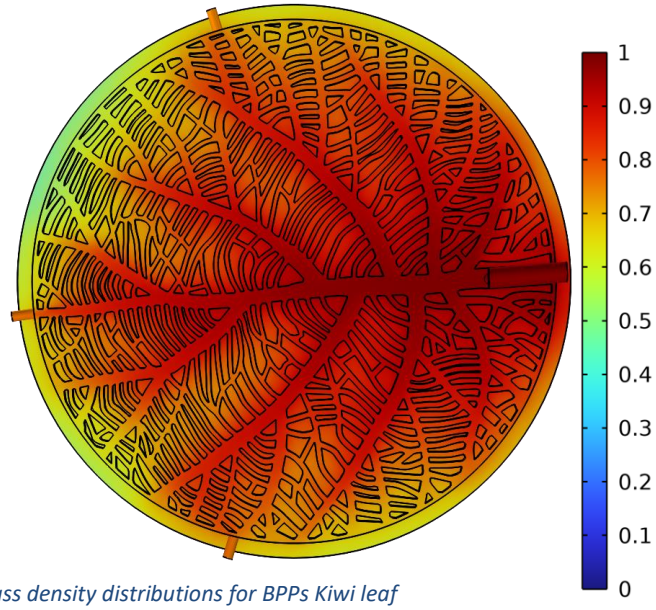


Figure 7 water mass density distributions for BPPs Kiwi leaf

CONCLUSION

To sum up, this study looked into how bipolar plates (BPPs) in polymer electrolyte membrane water electrolyzers (PEMWE) might perform better by using a bio-inspired design, more especially a leaf-like geometry. The outcomes showed that the bio-leaf design has a number of benefits with regard to pressure distribution, velocity profiles, and water distribution—all of which have a significant impact on PEMWE's effectiveness and performance. The bio-leaf design had the lowest pressure drop, according to the pressure distribution analysis. This was primarily because of its redundant and connected flow channels, which facilitated quick pressure equalization. The bio-leaf design's uniform velocity profile resulted in more uniform reactant distribution and quicker water removal, even though the latter designs recorded higher maximum velocities.

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