Thermal and Electrochemical Energy Laboratory (TEEL)

A Computational Study on Flowrate Sensitivity of a PEM Fuel Cell with Multi-Parallel Flow Channels

M. A. Rahman, J. M. Mora*, P. A. Chuang
Thermal and Electrochemical Energy Laboratory (TEEL)
Department of Mechanical Engineering, University of California, Merced

*Department of Chemical Engineering, College of Engineering
University of the Philippines, Diliman

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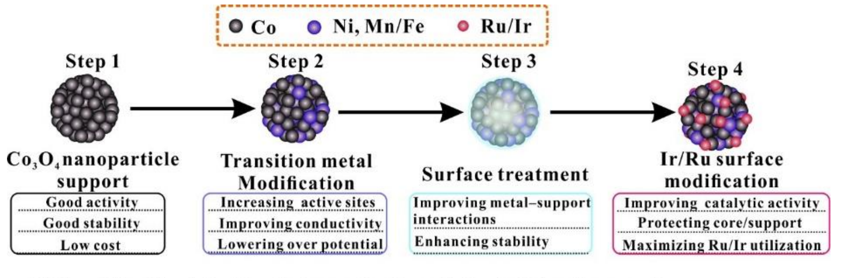
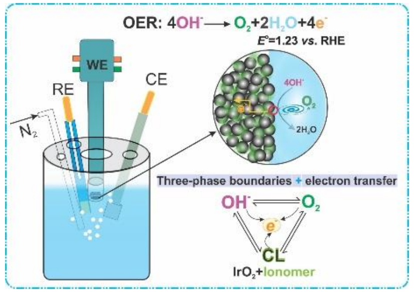
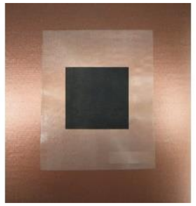
Material Synthesis and Evaluation



**Steps 2-4: without significantly increasing the cost of materials and preparation

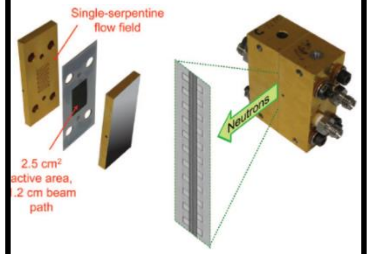


MEA Integration

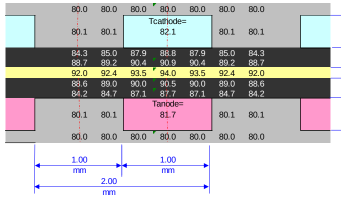


Fuel Cell Experiment

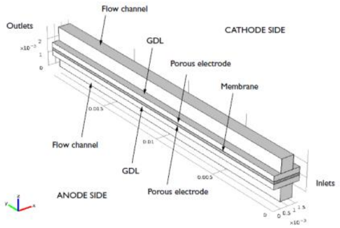
Fuel Cell Diagnostic



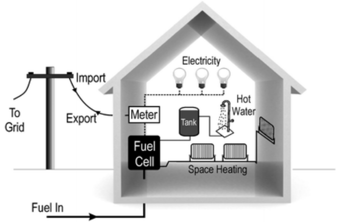
Fuel Cell Modeling

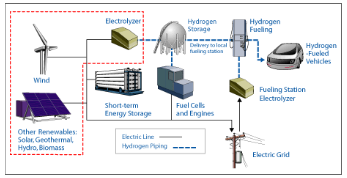


80.0	80.0	80.0	80.0	80.0	80.0	80.0
80.1	80.1		Tcathode= 82.1		80.1	80.1
84.3	85.0	87.9	88.8	87.9	85.0	84.3
88.7	89.2	90.4	90.9	90.4	89.2	88.7
92.0	92.4	93.5	94.0	93.5	92.4	92.0
88.6	89.0	90.0	90.5	90.0	89.0	88.6
84.2	84.7	87.1	87.7	87.1	84.7	84.2
80.1	80.1		Tanode= 81.7		80.1	80.1
80.0	80.0	80.0	80.0	80.0	80.0	80.0



System Integration

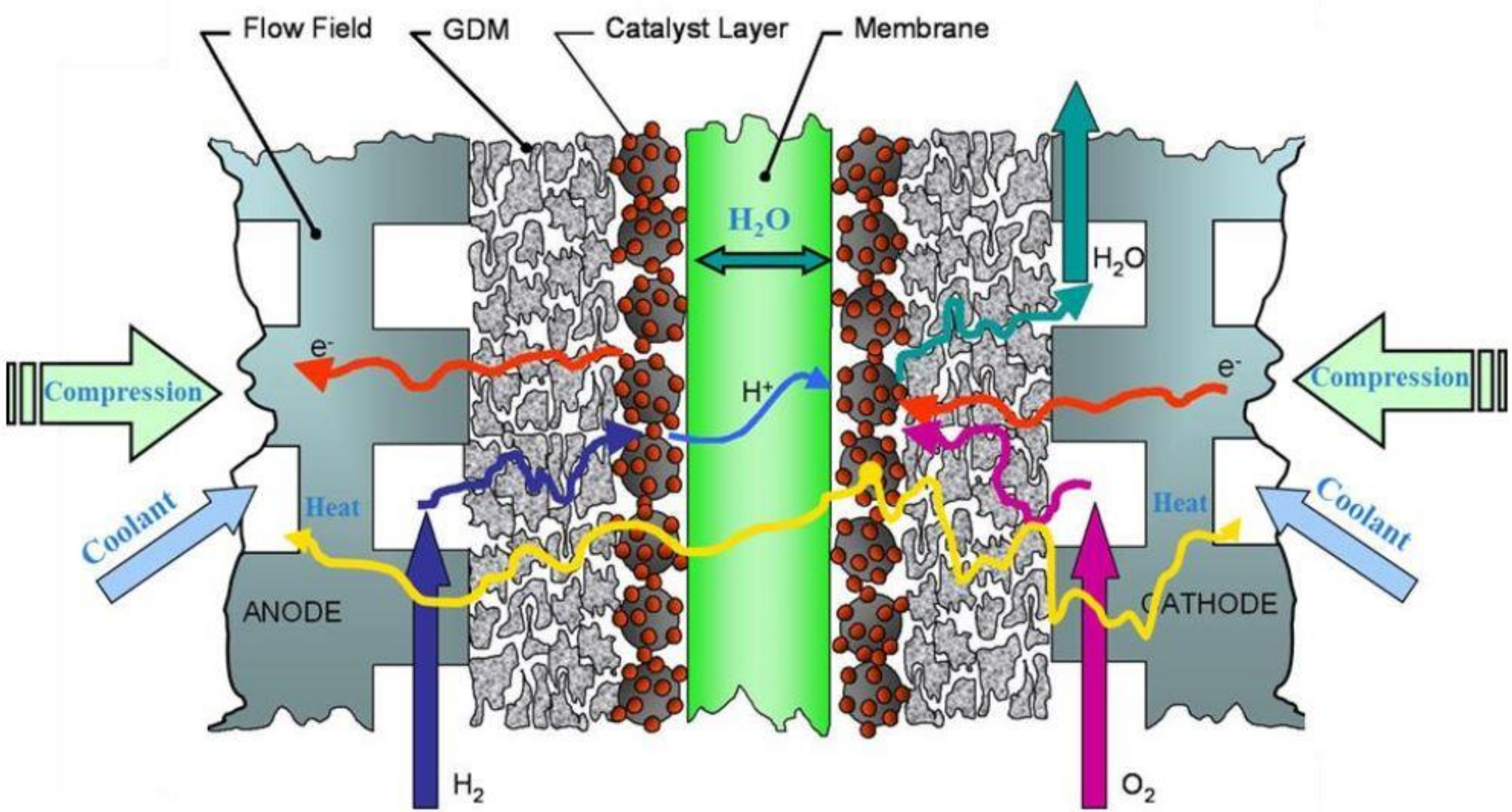




Objectives

- Simulate electrochemistry, reactant flow and porous media transport in a Proton Exchange Membrane (PEM) Fuel cell with parallel flow fields under three constant flowrate operating conditions.
- Obtain the reactant and relative humidity distributions in the flow channels and membrane electrode assembly (MEA).
- Study the effect of flowrate on fuel cell performance.

PEM Fuel Cell Schematic Diagram



Anode: $H_2 \rightarrow 2H^+ + 2e^-$

Cathode: $\frac{1}{2}O_2 + 2H^+ + 2e^- \rightarrow H_2O$

COMSOL Model Description

- In this model the steady-state transport of hydrogen, nitrogen, oxygen, and water in a parallel channel PEM fuel cell is simulated.
- This model includes both anode and cathode mass and momentum transports in flow channel, gas diffusion layers (GDLs) and porous electrode.
- **Kinetics**: The electrochemical reactions are modeled using “Secondary Current Distribution” interface to solve for the electronic and ionic potential.
- **Mass Transport**: The mass fraction of Hydrogen, Oxygen and water are solved by “Transport of concentrated species” interface.
- **Convective Flow**: : The “Brinkman Equation” interface is used to solve for the velocity field vectors and pressure in Anode and Cathode compartment .

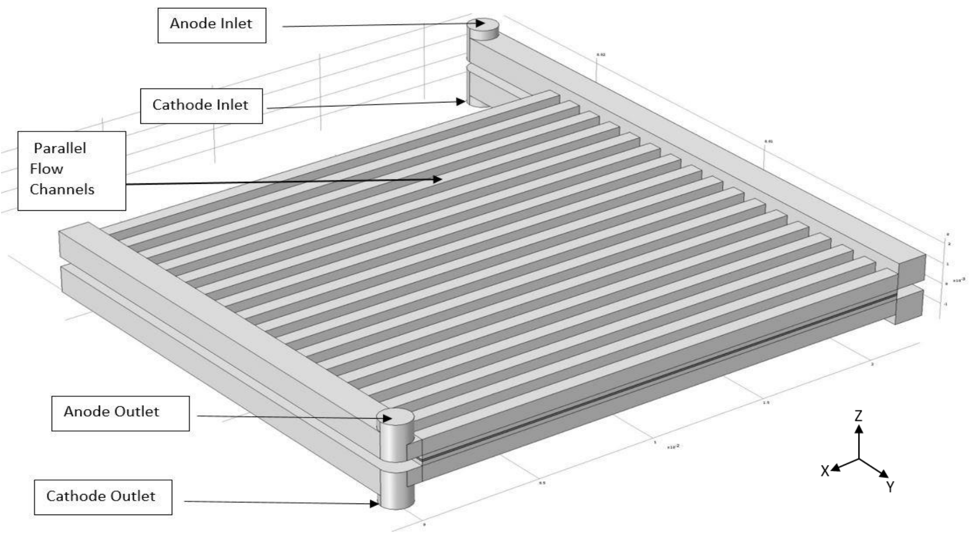


Figure 2a: Geometry of the cell

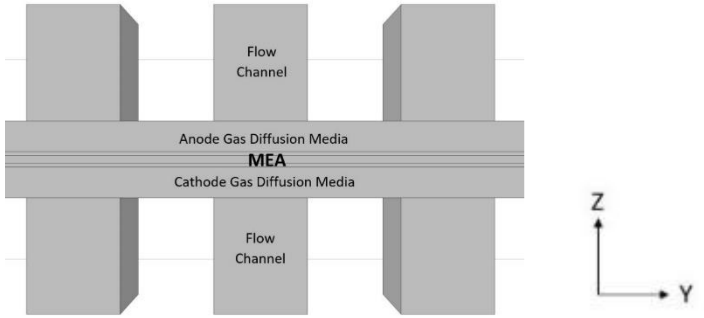


Figure 2b: Through plane cross sectional view

Modeling Equations - Kinetics

Kinetics:

- This model solves for electrochemical reactions in the porous electrodes, and ohmic current flux in the GDLs and the polymer membrane.
- Linearized Butler-Volmer equation in anode electrode and Cathodic Tafel equation has been solved to find the local current density.

$$i_a = i_{o,a}\left(\frac{c_{H_2}}{c_{h_2}^{ref}}\right)^{0.5}\left(\frac{(\alpha_a+\alpha_c)F\eta_a}{RT}\right) \qquad i_c = -i_{0,a}\left(\frac{c_{O_2}}{c_{O_2}^{ref}}\right)\exp\left(-\frac{\alpha_c F\eta_c}{RT}\right)$$

Kinetic parameters	
Exchange current density HOR ($i_{0,a}$)	1×10^5 A/m^2
Exchange current density ORR ($i_{0,c}$)	1 A/m^2
Anodic and cathodic Transfer coefficient	0.5

Modeling Equations – Mass Transport

Mass Transport:

- $w_{\mathrm{H_2}}$, $w_{\mathrm{H_2O}a}$, w_{O_2}, and $w_{\mathrm{H_2O}c}$ are solved for in the flow channels, GDLs and porous electrode using the Maxwell-Stefan equations.

$$\nabla \cdot \mathbf{j}_i + \nabla \cdot (\rho \omega_i \mathbf{u}) = R_i$$

$$\mathbf{j}_i = -\rho \omega_i \sum_{k=1}^{Q} \tilde{D}_{ik} \mathbf{d}_k - D_i^T \nabla \ln T$$

$$\mathbf{d}_k = \nabla x_k + \frac{1}{p}\left[(x_k - \omega_k)\nabla p - \rho \omega_k \mathbf{g}_k + \omega_k \sum_{l=1}^{Q} \rho \omega_l \mathbf{g}_l\right]$$

$\tilde{D}_{ik}$ = multicomponent Fick diffusivities (m^2/s)

D_i^T = Thermal diffusion coefficients $(\mathrm{Kg/m \cdot s})$

$\mathbf{d}_k$ = Diffusional driving force acting on species k

ω = mass fraction

x_k = mole fraction = $\dfrac{\omega_k}{M_k} M$

M = mean molar mass = $\left(\sum_{i=1}^{Q} \dfrac{\omega_i}{M_i}\right)^{-1}$

Modeling Equations – Convective flow

- **Convective flow:** The flow in porous media governed by a combination of the continuity equation and momentum equation which together form the Brinkman Equations. The dependent variables are Darcy velocity and the pressure.

$$\frac{\rho}{\varepsilon_p}\left((u.\nabla)\frac{u}{\varepsilon_p}\right)=\nabla\left(p+\frac{\mu}{\varepsilon_p}(\nabla u+\nabla u^T)-\frac{2\mu}{3\varepsilon_p}(\nabla u)\right)-\left(\mu\kappa^{-1}+\beta_F u+\frac{Q_{br}}{\varepsilon_p^2}\right)u+F$$

$$\nabla\cdot(\rho u)=Q_{br}$$

In these equations

$\mu =$ Dynamic viscosity of the fluid (Kg/m-s)

$\mathbf{u} =$ velocity vector (m/s)

$\rho =$ density of fluid (kg / m^3)

$p =$ pressure

$\varepsilon_p =$ porosity

$\kappa =$ Permeability tensor of the porous medium

$Q_{br} =$ Mass source or sink

F = influence of gravity and other volume forces is accounted via F

$\beta_F =$ Forccheimer drag (kg / m^4), adds a viscous orce porportional to the square of fluid veloctiy

Boundary Conditions

The following boundary conditions have been applied to solve the modeling equations:

- **Current Distribution and Kinetics**
  - Anode side – Grounded
  - Cathode side – Cell potential
- **Mass transport**
  - Inlet mass fraction
- **Convective flow**
  - Inlet – Inlet velocity
  - Outlet – Atmospheric pressure
- **Multiphysics Coupling**
  - Chemical reactions in electrode were coupled with mass fractions in electrode

Mesh

- The cross-section geometry and mesh are shown in figure 3.
- User controlled mesh has been created to solve the modeling equation.
- In the flow channels unstructured triangular mesh was created on the YZ plane and structured rectangular mesh was created in the gas diffusion media and MEA.
- Then the 2D mesh was swept in X direction.
- In cathode and anode intake and outlet manifold, tetrahedral mesh has been used.

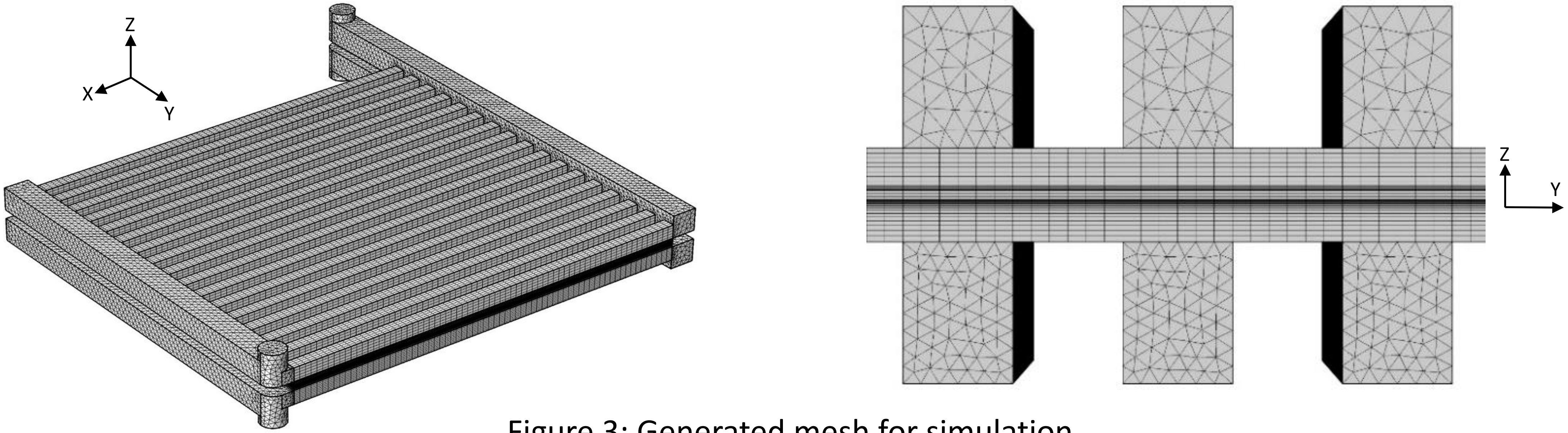


Figure 3: Generated mesh for simulation

Parameters Used

Geometry Parameters	
Parameter	Value
Membrane/CL/ GDM width	2.108 cm
Membrane/CL/ GDM Length	2.013 cm
GDM Thickness	0.020 cm
Catalyst layer thickness	0.0025 cm
Membrane thickness	0.005 cm
Channel width	0.061 cm
Rib width	0.061 cm
Channel height	0.076 cm
Inlet/Outlet manifold width	0.127 cm
Inlet/Outlet manifold height	0.127 cm
Inlet manifold length	2.584 cm
Outlet manifold length	2.013 cm
Inlet diameter	0.127 cm
Outlet diameter	0.127 cm

Reactant gas properties	
$D_{O_2\text{-}N_2}$ (calculated)	2.47×10^{-5} (m^2/s)
$D_{O_2\text{-}H_2O}$ (calculated)	2.9×10^{-5}(m^2/s)
$D_{H_2\text{-}H_2O}$ (calculated)	9.47×10^{-5} (m^2/s)
$D_{N_2\text{-}H_2O}$ (calculated)	2.65×10^{-5}(m^2/s)
Mass fraction of H_20 (cathode)	0.023
Mass fraction O_2 (Cathode)	0.228
Mass fraction H_2 (Anode)	0.743
Reversible cell voltage	1.229
Dynamic viscosity (Anode gas mixture)	1.19×10^{-5} (Pa-s)
Dynamic viscosity (Cathode gas mixture)	2.46×10^{-5} (Pa-s)

Material Properties	
Electrolyte conductivity	9.825 S/m
Catalyst layer conductivity	222 S/m
GDM Porosity	0.4
GDM Permeability	1.18×10^{-11} (m^2)
Catalyst layer Porosity	0.3
Catalyst layer Permeability	2.36×10^{-12} (m^2)

Parameters Used - Flowrate

- In “Brinkman equation” interface, inlet velocity is provided as an input.
- The velocity is calculated based on the stoichiometric flow rate required to generate 1 A/cm^2 current density.
- Flowrate A, B and C corresponds to stoichiometric flow of 1, 5 and 15, respectively, at 1 A/cm^2 output current density.
- The following table shows the flowrate values used for the three constant flow simulation cases.

	Flowrate A (SLPM)	Flowrate B (SLPM)	Flowrate C (SLPM)
Anode inlet	0.0416	0.208	0.527
Cathode inlet	0.0736	0.368	0.932

Results – Polarization and Power Density

- Operating condition: T = 40°C, P = 101.325 kPa, RH = 50%
- Overall performance of the fuel cell is shown in the polarization and power density curves.
- The results indicate that fuel cell performance improves with increasing flow rate for the studied channel design.

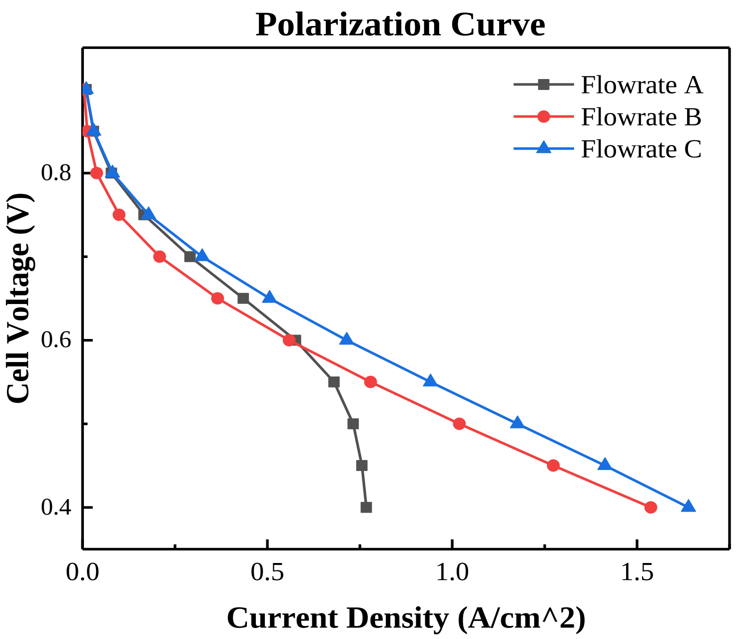


Figure 4a: Polarization curve

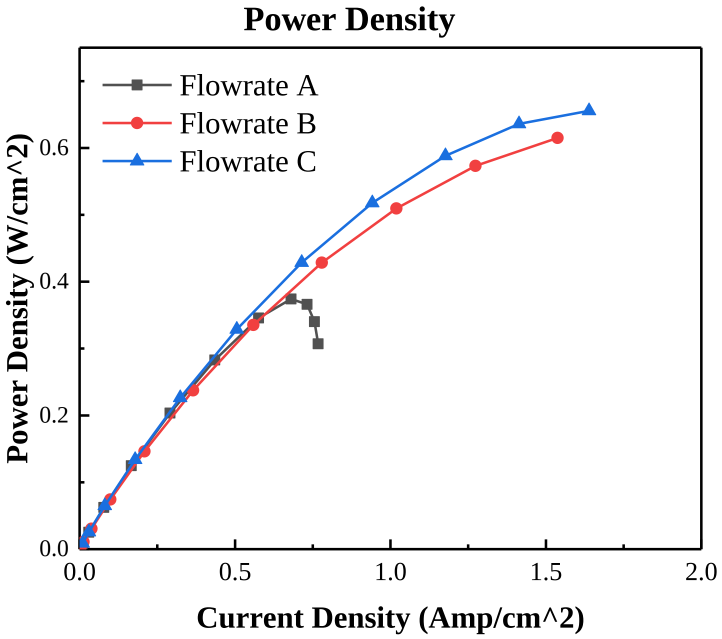


Figure 4b: Power density

Current Density distribution

- Current density along flow channel direction is more uniform compared to the transverse direction.
- In transverse flow direction for all flow rates the current density curve shows a similar oscillating pattern. The peak of each oscillation occurs at the center of each flow channel where reactant supply is highest.
- But the current density distribution along the flow channel direction becomes more uniform as flow rate is increased.

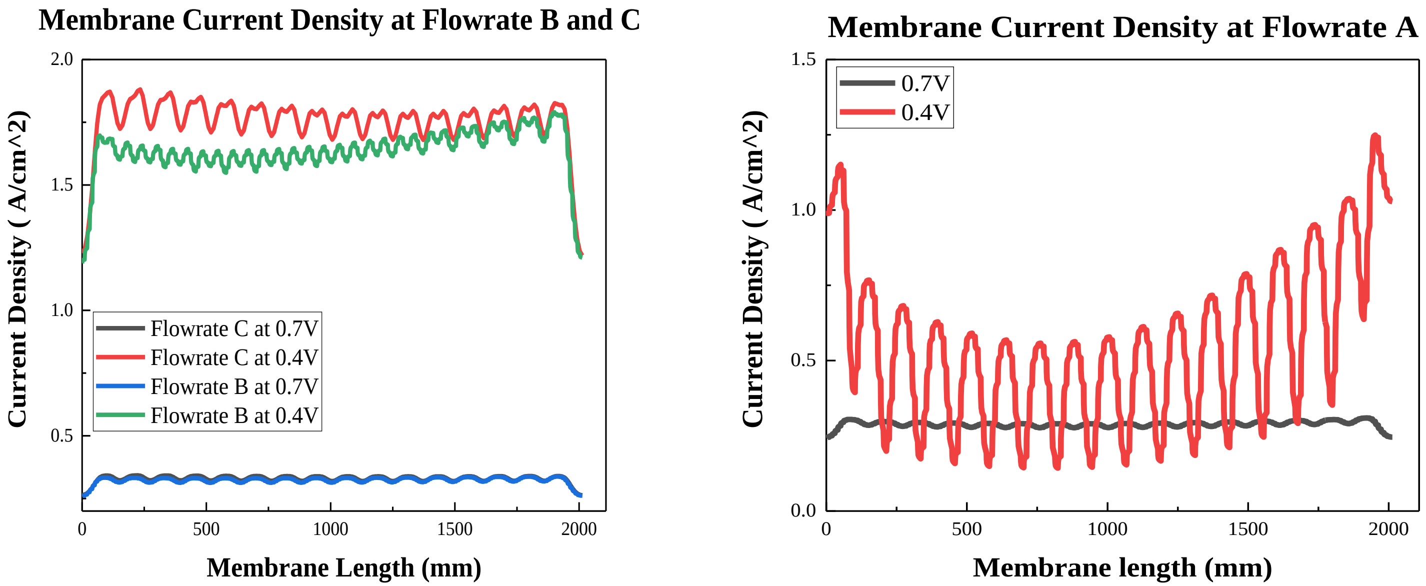


Fig 4c : Current Density in transverse to the parallel flow direction

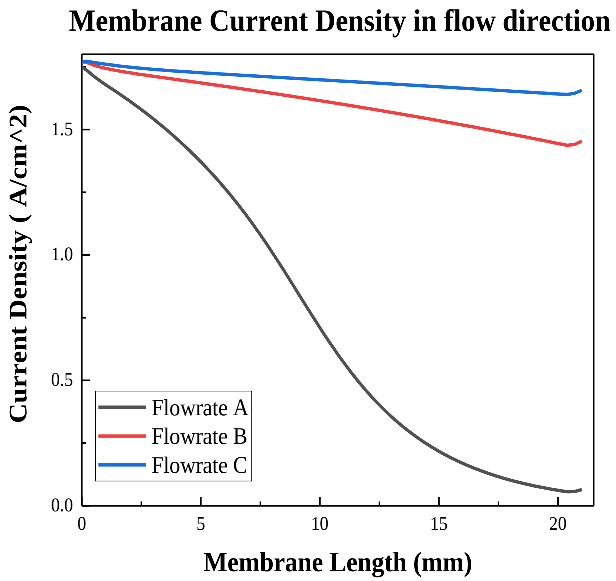


Fig 4b : Current Density in the parallel flow direction

Results - Reactant Distribution in Flow Channels

- Operating condition: T = 40°C, P = 101.325 kPa, RH = 50%, and **0.4 V**.
- Hydrogen and oxygen distribution in flow channel is shown in Fig 5a and 5b.
- Our results show that, at low flowrate of 0.416 slpm (flowrate A) the highest H_2 partial pressure drop occurs and as the flowrate is increased to 0.527 slpm (Flowrate C), the pressure drop reduces to 1 kPa.
- At flowrate A (0.073 slpm), O_2 partial pressure drop is 20kPa, which results in Oxygen depletion near channel outlet. This results in the limiting current behavior, which is observed in the polarization plot.
- As flowrate is increased, O_2 partial pressure drop in the channel reduces to 5kPa.

Fig 5a

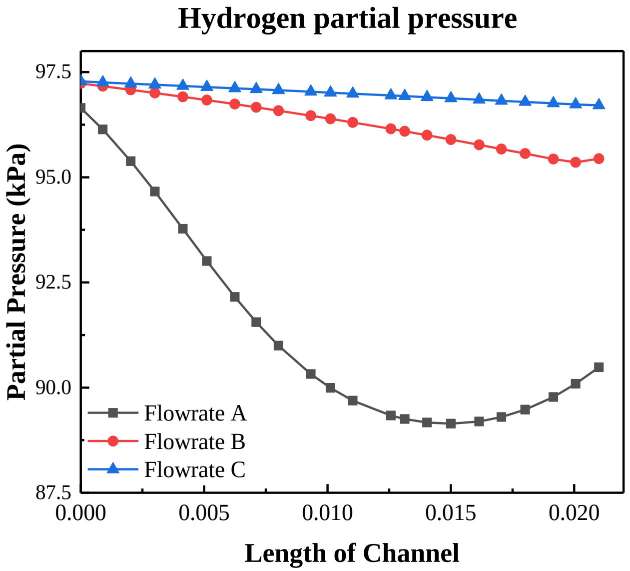
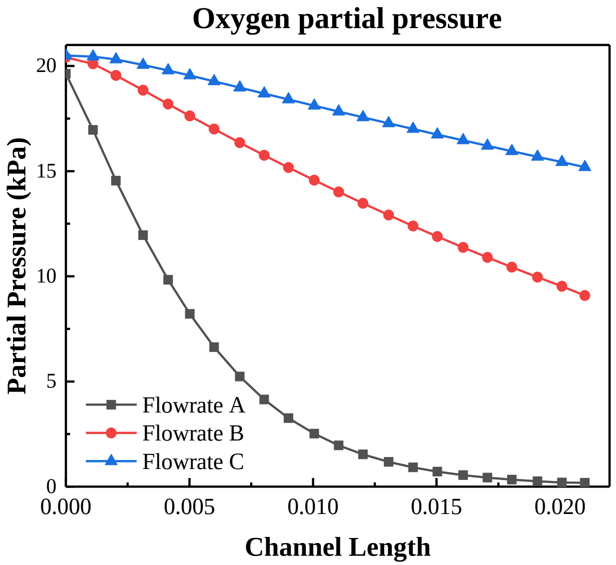
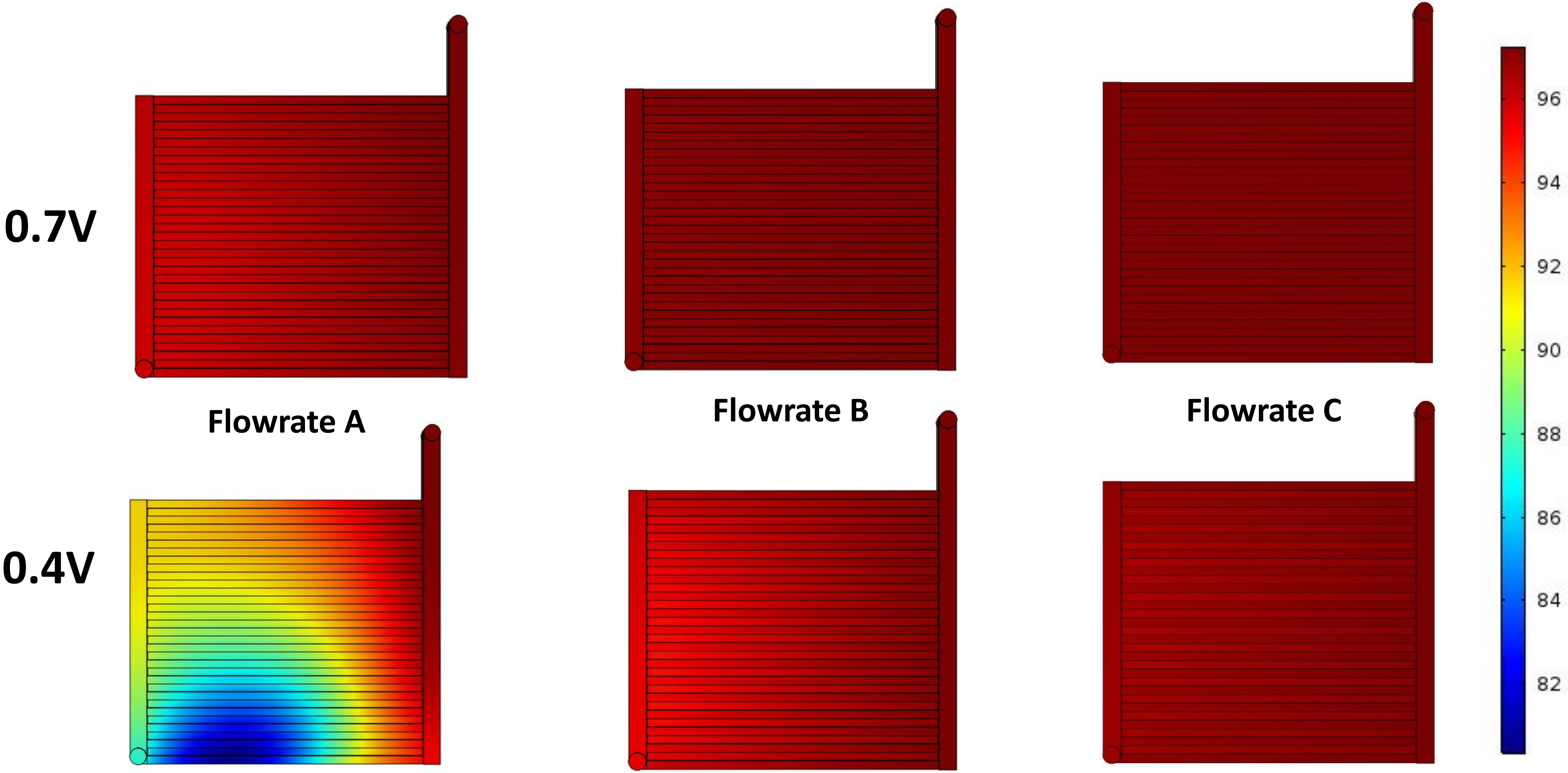


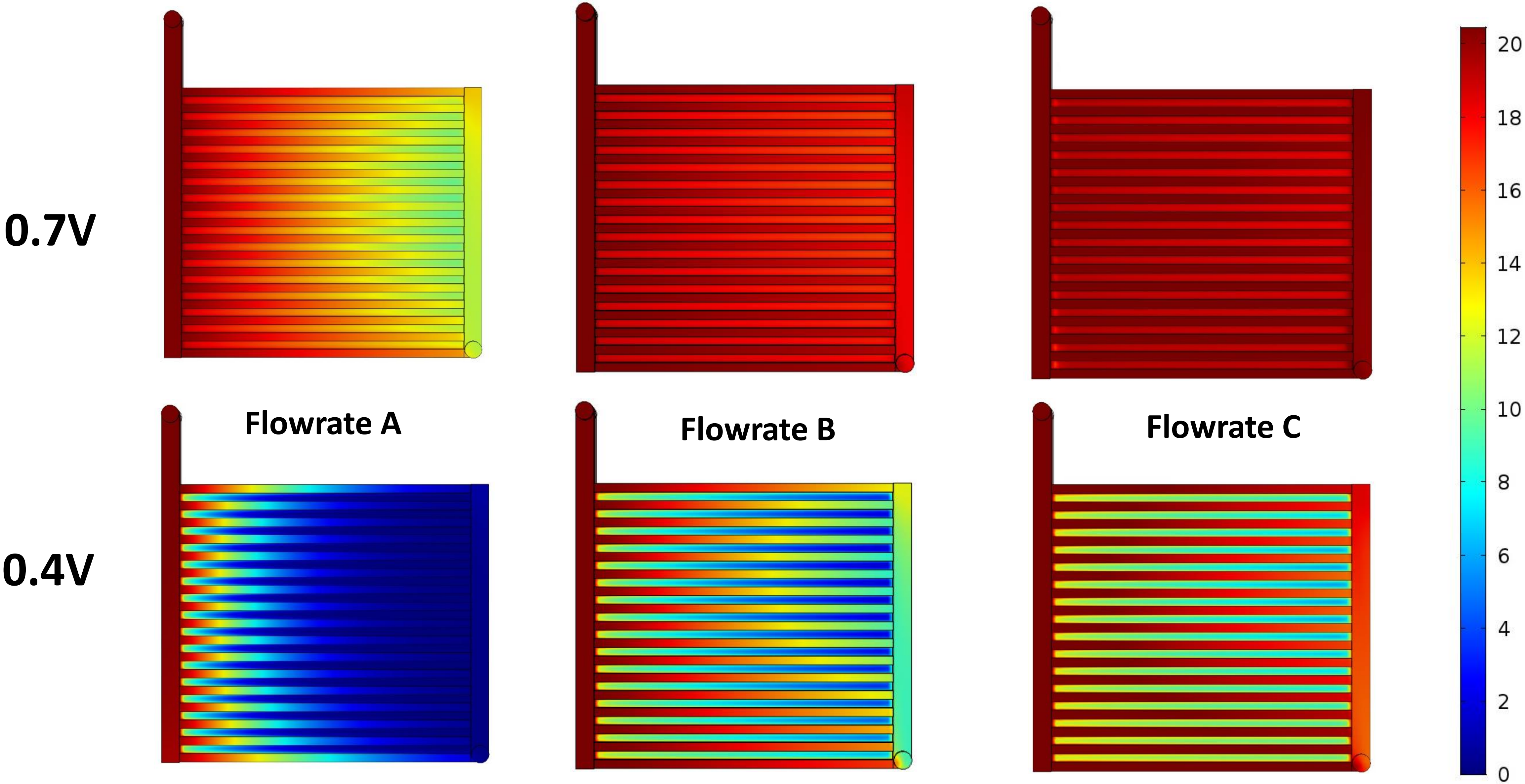
Fig. 5b



Results – Hydrogen Distribution in Anode Flow Channels



Results – Oxygen Distribution in Cathode Flow Channels



Results - RH in cathode flow channels

- The Relative humidity (RH) distribution in cathode flow channels at 0.7V and 0.4V are shown in figure 8a and 8b respectively.
- RH of 100% suggests saturated water.
- From Fig. 7a, it can be observed that at operating voltage of 0.7V and flowrate A, the reference channel is filled with saturated water and as flow rate is increased to flowrate C (0.932 slpm), saturated water is completely removed from the channel.
- Similar behavior is also observed at cell operating voltage of 0.4V.

Fig 7a

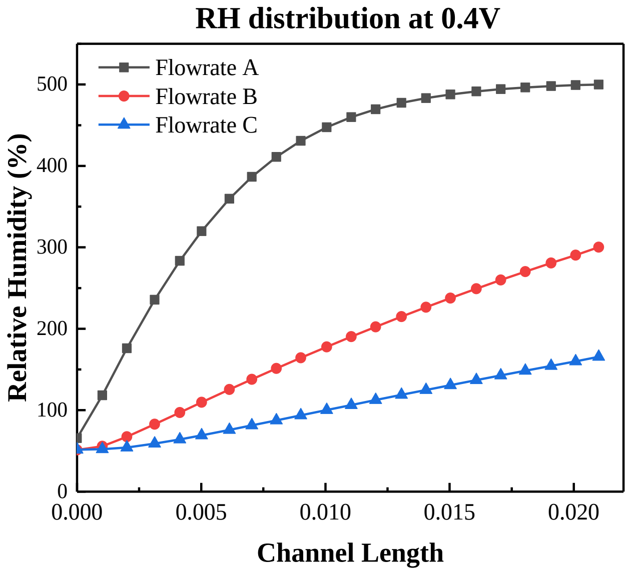
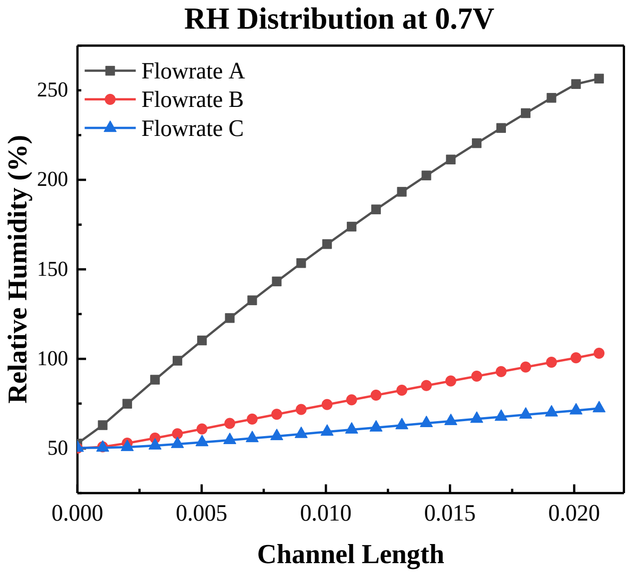


Fig. 7b



RH Distribution in Cathode Flow Channels

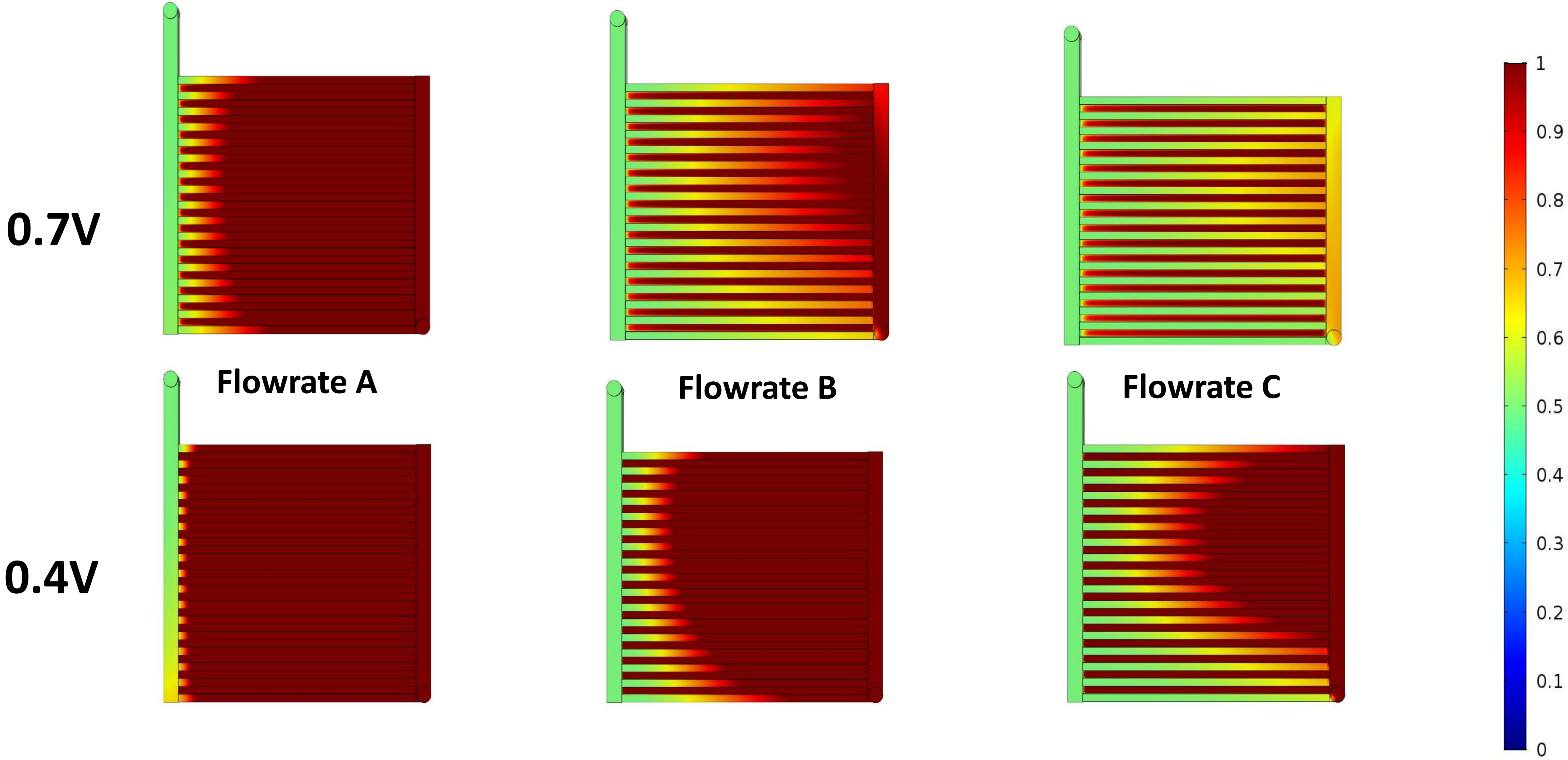


Fig 8: RH Distribution in cathode flow channels

Conclusion

- 3D isothermal steady state model has been developed to simulate reactant flow rate sensitivity of a PEM fuel cell with parallel channel flow field.
- Saturated water content in flow channel increases as higher current is drawn.
- The removal of liquid water from the channel is facilitated by increasing flow rate.
- Increasing flowrate shows better fuel cell performance.

References

- E. U. Ubong, Z. Shi,b, X. Wang, Three-Dimensional Modeling and Experimental Study of a High Temperature PBI-Based PEM Fuel Cell, *Journal of The Electrochemical Society,* **156** 10 B1276-B1282 (2009)
- “Batteries and Fuel cell user’s guide”, COMSOL Multiphysics 5.3

Acknowledgement

UC MERCED
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PHILIPPINE-CALIFORNIA
ADVANCED RESEARCH INSTITUTES

- GREEN Power Program (IIID 2015-09) from Commission on Higher Education – Philippine California Advanced Research Institutes (CHED-PCARI) of the Republic of the Philippines.

Questions?