3D, Two Phase Multispecies Transport Model of PEM Fuel Cells

COMSOL Conference
November 30-December 01, Bengaluru

Image courtesy: TechCrunch

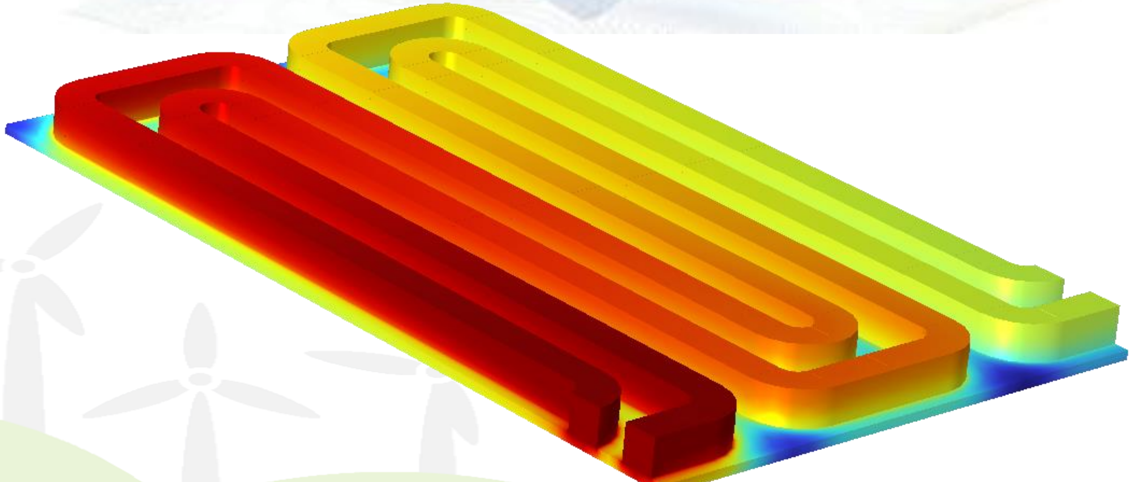

Image courtesy: COMSOL Multiphysics

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- System configuration

2. Research

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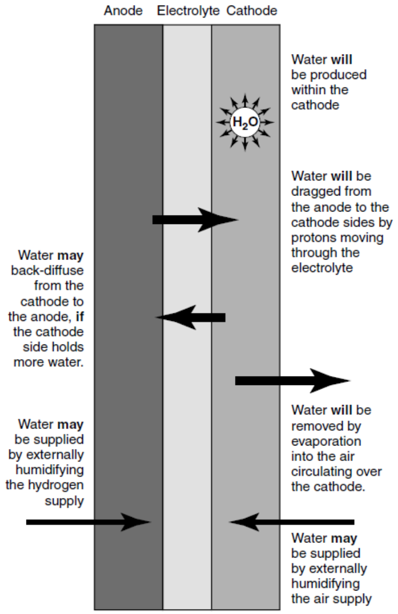
Introduction: Research In Hydrogen Fuel Cell

Water Management

Water, Where is it coming from? Formed water at cathode keep the **electrolyte** at the correct **level of hydration**. Supplied air over the cathode would also dry out any excess water.

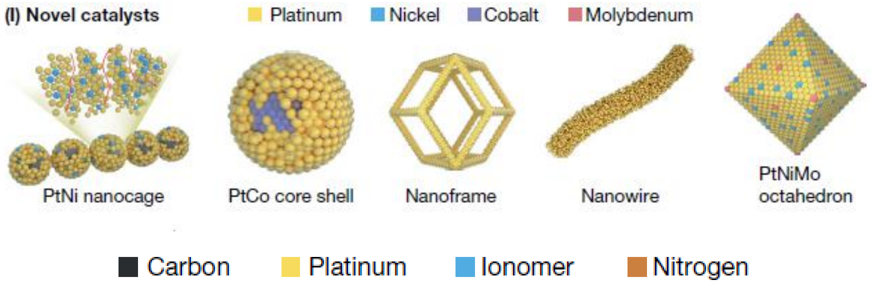
Solution-

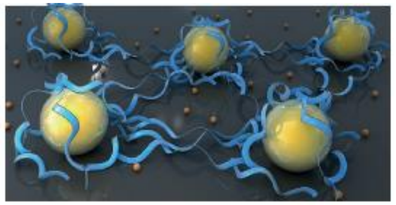
- **Humidifying** the air/hydrogen or both
- **Designing of Flow field** for the PEMFC.
- Proper **optimization of parameters** like- Air flow rate, humidity level (Relative humidity), Temperature, Stoichiometry (λ), pressure.
- Different methods like- **wick** with GDL, directly injecting water, utilizing the o/l water to humidify I/L air, and **self humidification**.



Catalyst & Membrane Design

- **Slow reaction** rate leads to low current and voltage.
- **Novel catalyst architectures** (such as nanocages, core–shell, nanoframes, nanowires, nanocrystals) can increase the activity of the catalyst.
- Nowadays, **nitrogen-doped carbon supports** ensure uniform coverage of the ionomer, owing to the Coulombic attraction between the ionomer and N groups on the carbon support.
- Catalyst designing can **increase the performance** of fuel cells by **40%**.

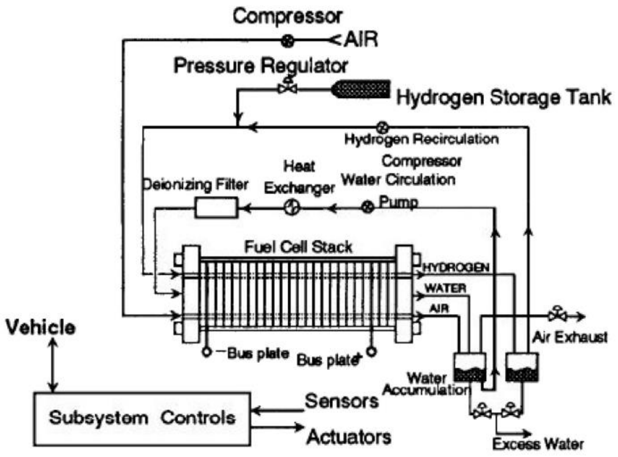




Pt/N-doped carbon supports

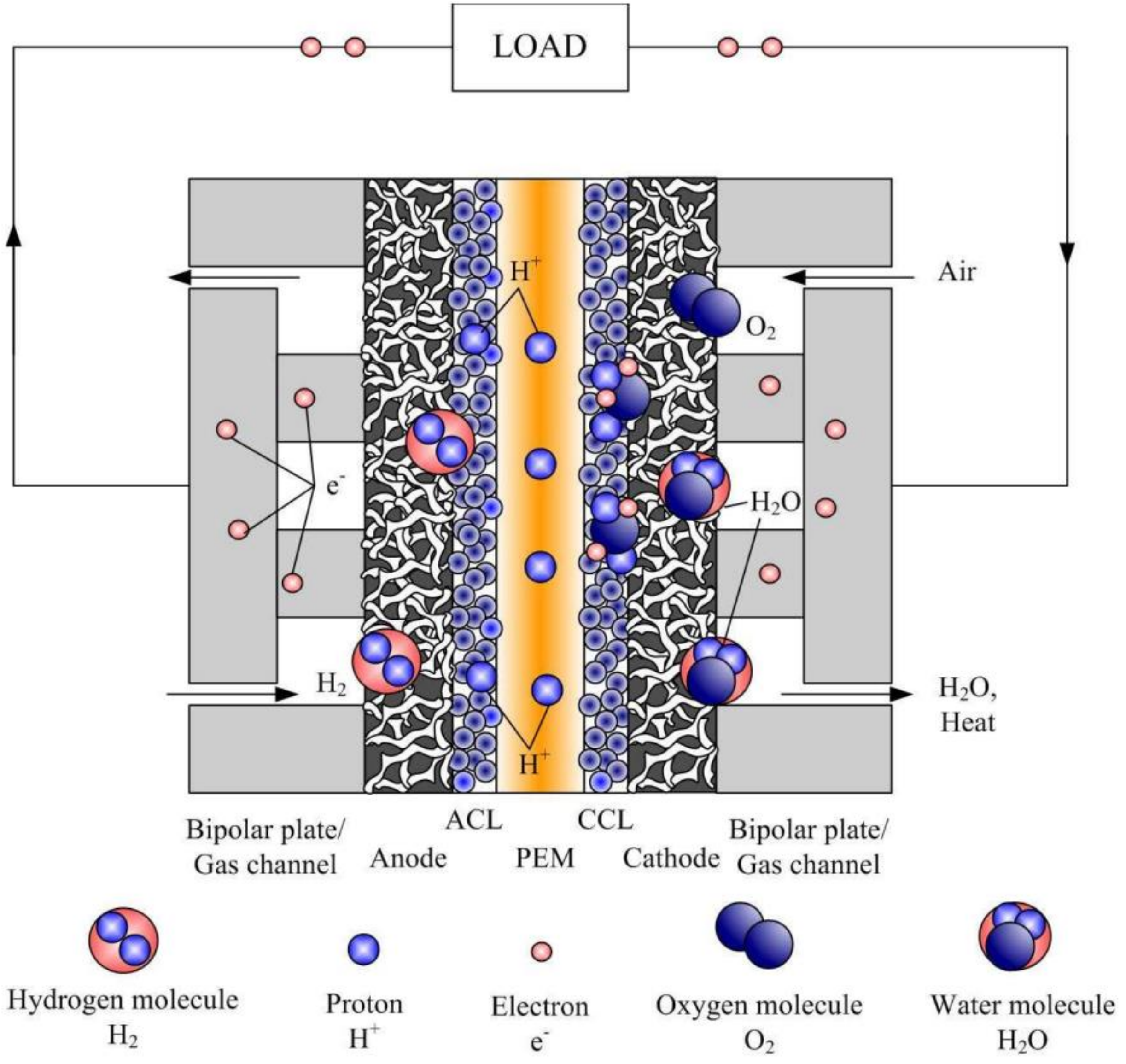
BOP & System Configuration

- **Design** related to **Gas Flow**- for hydrogen and oxygen.
- **Humidification** system designing- Bubbling, Direct water or steam injection method, Enthalpy wheel method, Membrane humidification method.
- **Air Compressor**-for improving the air pressure of the fuel cell.
- **Air recycle/bypass design**- the outlet air having heat can be used to warm up fuel cell system during cold-startup process.
- **Fuel Cell cooling system**



Reference: *K. Jiao et al. "Designing the next generation of proton-exchange membrane fuel cells." Nature 595 (2021), 361-369.*

Fundamental of PEM Fuel Cell



Reactions:

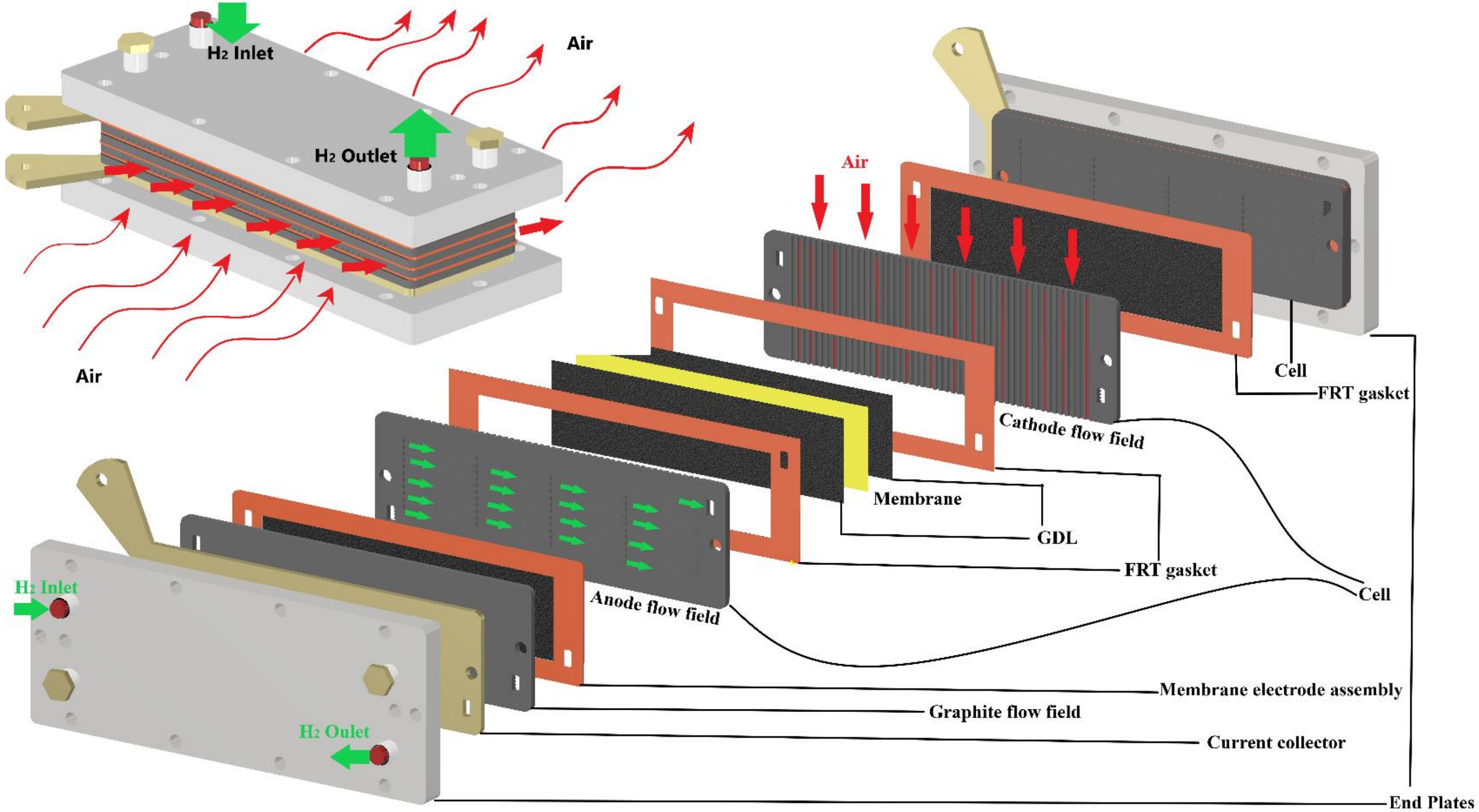
HOR at Anode: $H_2 \rightarrow 2H^+ + 2e^-$

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

Overall: $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$ + Heat + Electrical energy

***Reference**: H. Wu, Mathematical Modeling of Transient Transport Phenomena in PEM Fuel Cells, (Ph.D. thesis), University of Waterloo, 2009.*

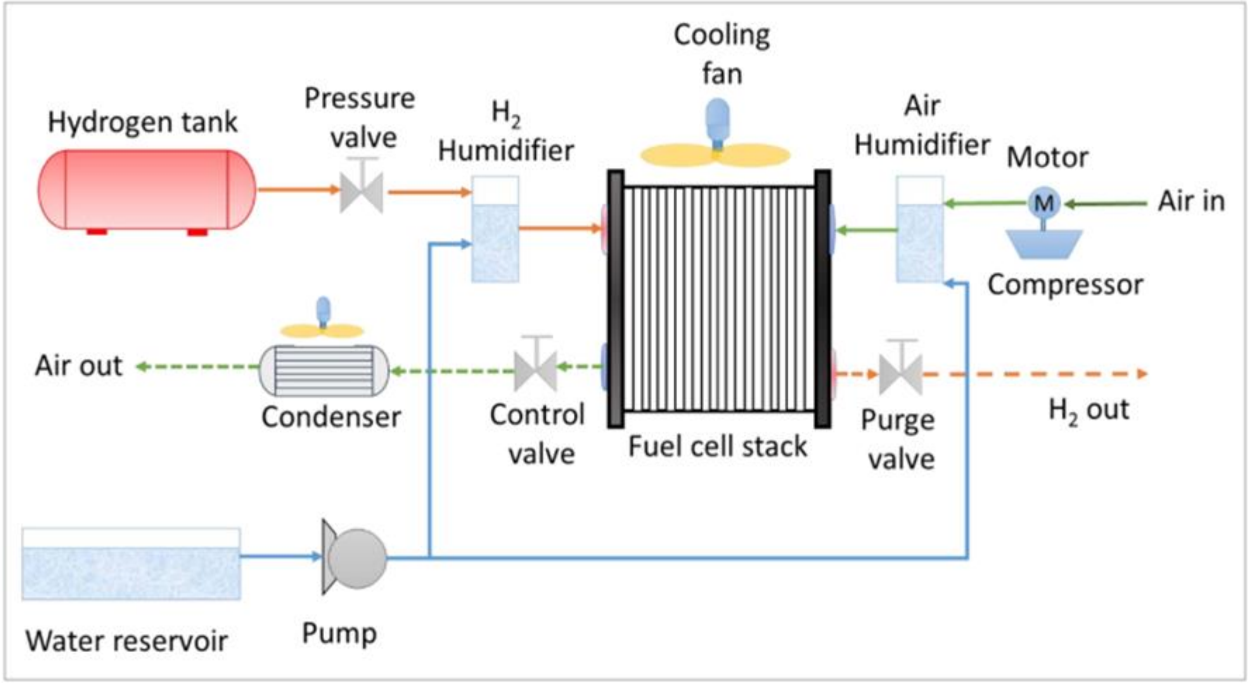
Schematics Representation of four cells PEMFC stack



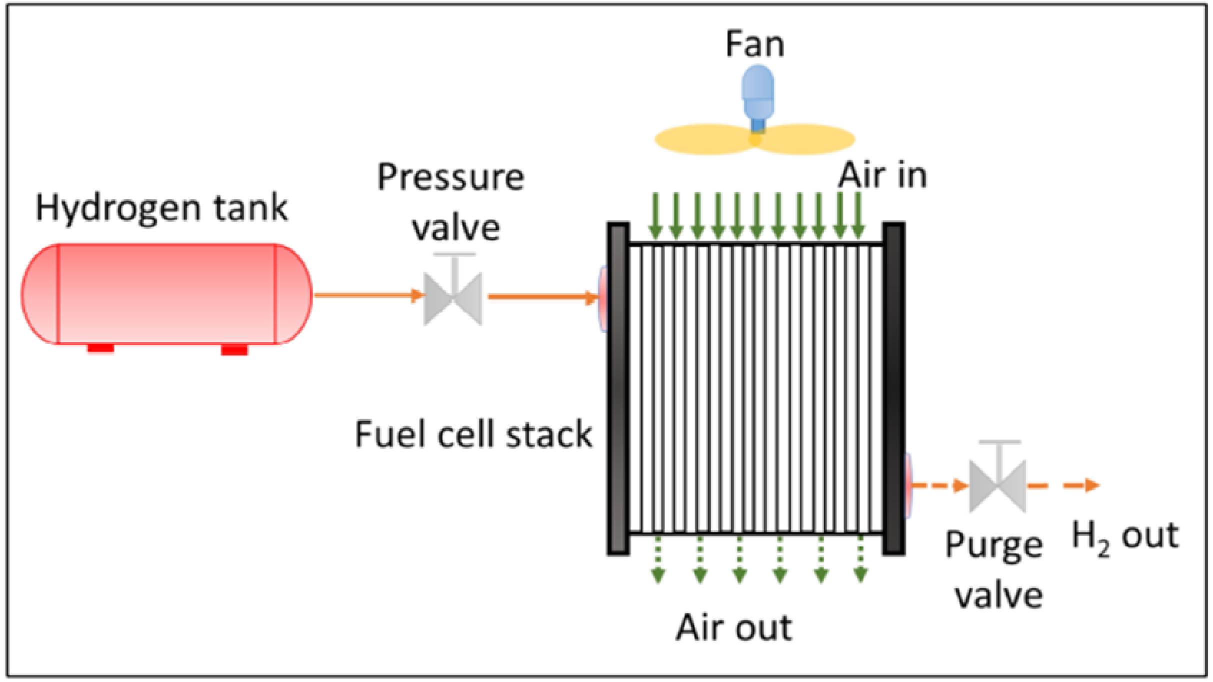
Function & Transport Phenomena
Bipolar Plate ➢ Guiding gas reactant flow ➢ Provide structural support for stack assembling ➢ Electron transport ➢ Liquid water transport ➢ Heat transfer
Gas diffusion layer (GDL) ➢ Gas reactant porous media flow ➢ Water evaporation and condensation ➢ Liquid water porous media flow ➢ Electron transport ➢ Heat transfer
Catalyst layer ➢ Electrochemical reactions ➢ Gas reactant porous media flow ➢ Water evaporation and condensation ➢ Liquid water porous media flow ➢ Membrane (dissolved) water transport ➢ Membrane water sorption/desorption ➢ Electron/proton transport ➢ Heat transfer
Membrane ➢ Repelling electrons ➢ Impermeable barrier to gas reactants ➢ Membrane (dissolved) water transport ➢ Proton transport ➢ Heat transfer

System Configuration for PEMFC and OC-PEMFC

Polymer electrolyte membrane fuel cell

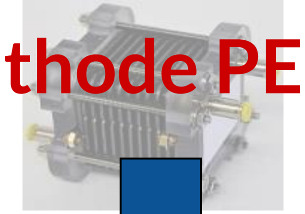


Open cathode polymer electrolyte membrane fuel cell



PEM Fuel Cell Stack to System level development

Open Cathode PEMFC Stack

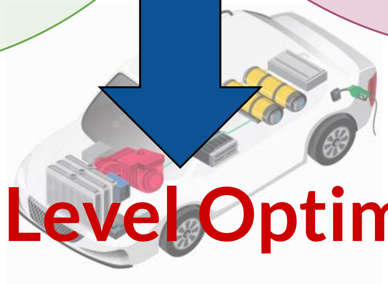


Parametric optimization

- *Pressure*
- *Gas flow rate*
- *Temperature*
- *Cooling rate*

Power optimization

- *Stack power*
- *Net power output*
- *Overall system output*



System Level Optimization

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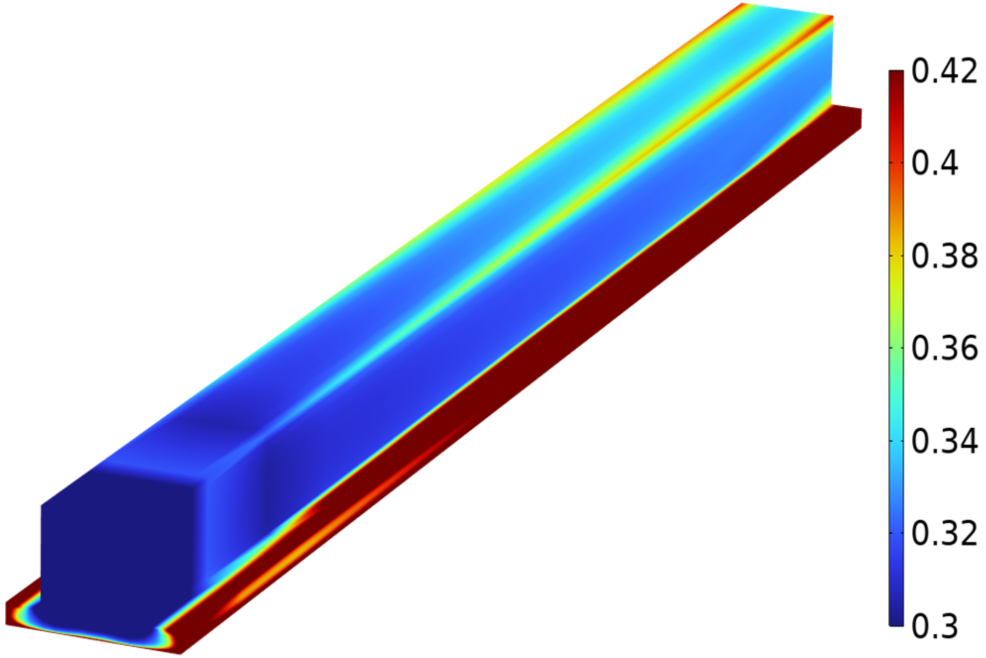
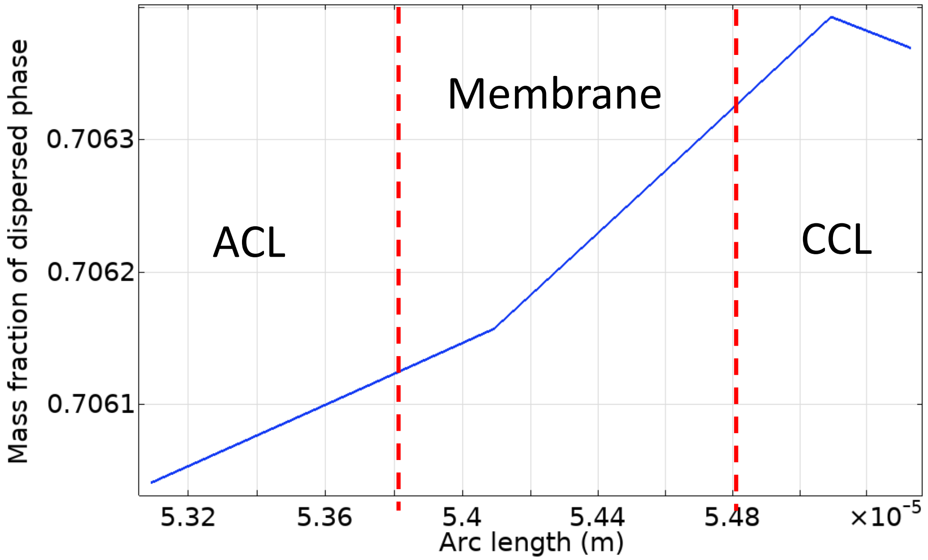
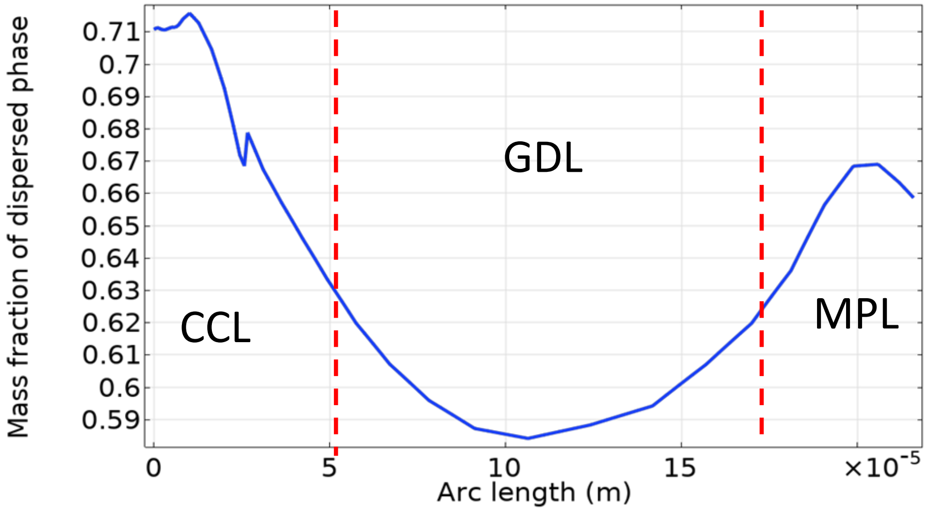
Visualization of liquid water content in PEMFC





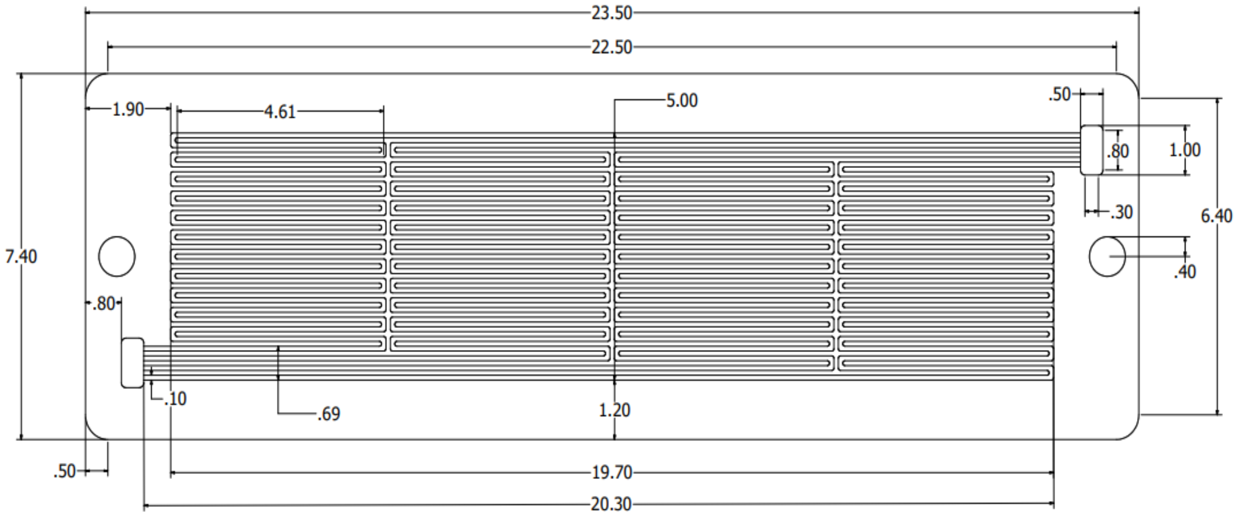


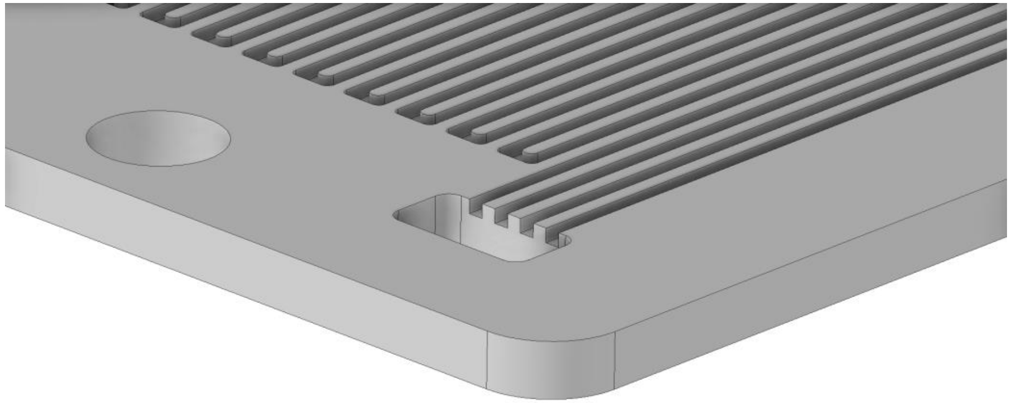
- Transport of water, condensation and evaporation phenomenon in anode and cathode domains are solved using temperature dependent vapor pressure.
- The reactant gases enters the flow channels in laminar flow and liquid in dispersed phase, with additional mass transport source from porous gas diffusion layer, governed by eqn. 1.

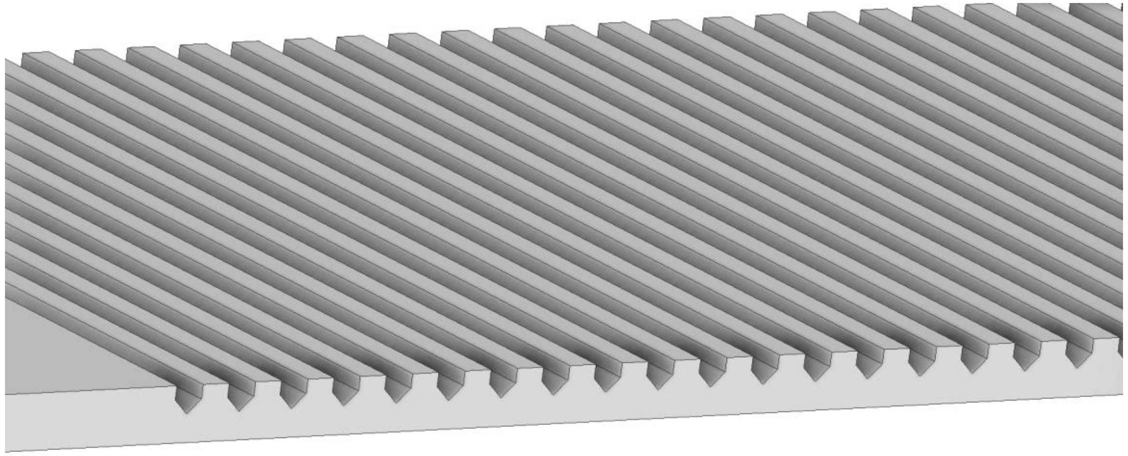
$$m = k\left(c_{channel} - c_{porous\ media}\right)M \qquad (1)$$

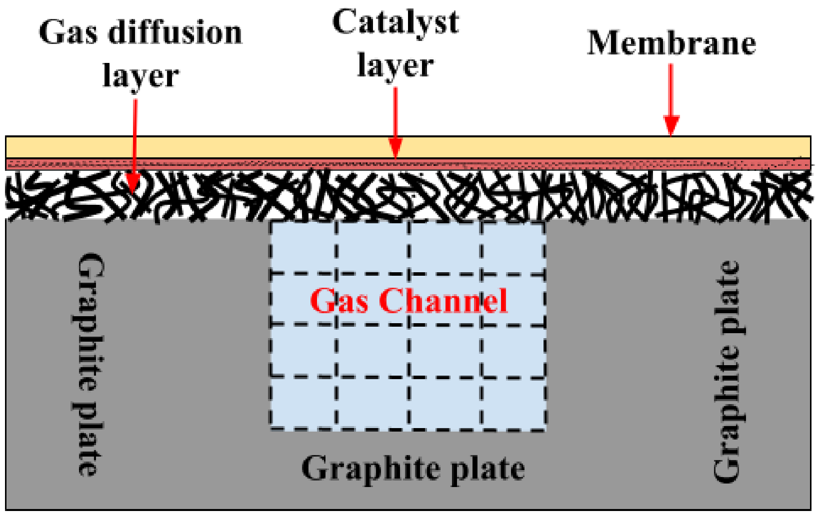
k- mass transfer rate; c-concentration; and M- molecular wt.

Flow Fields for OC-PEMFC









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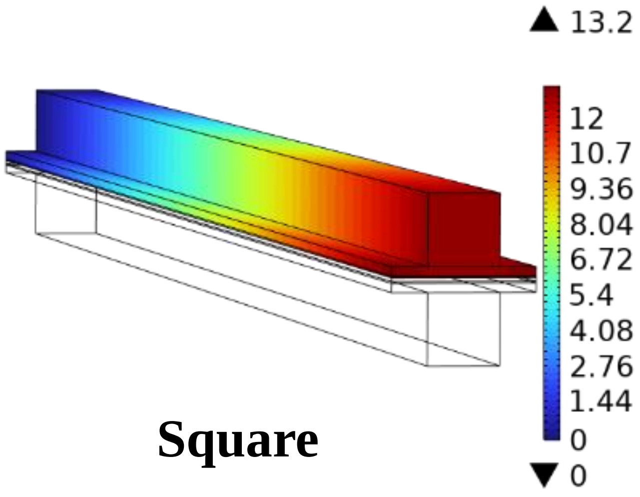
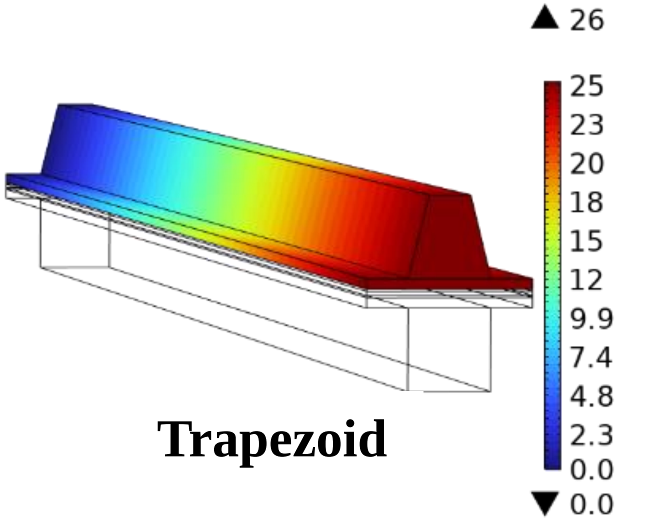
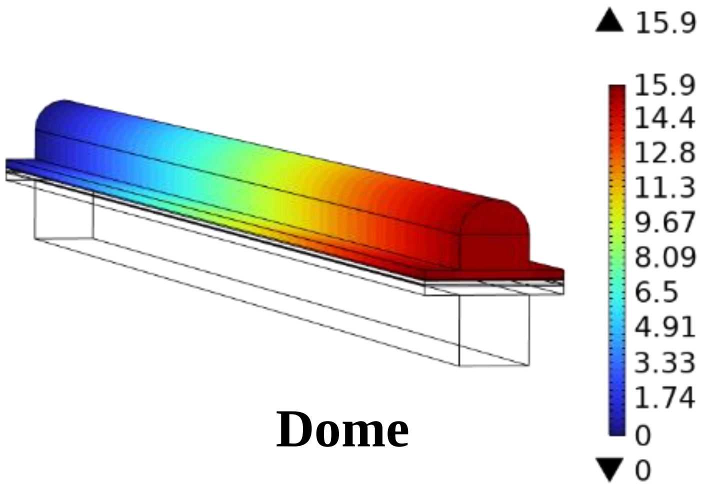
Pressure Drop



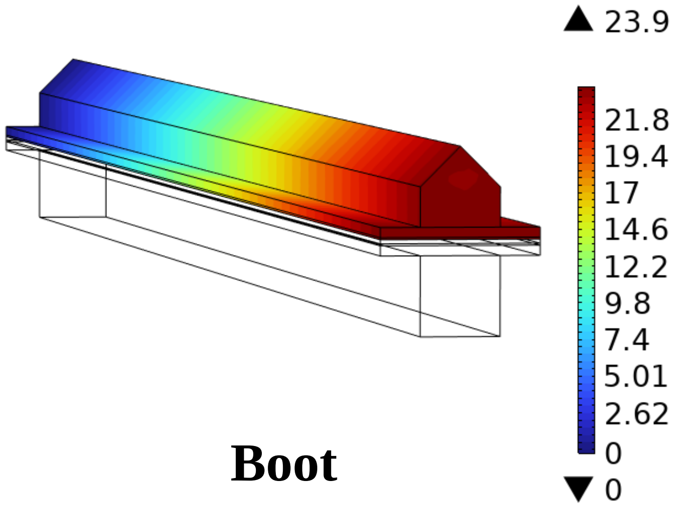
Square



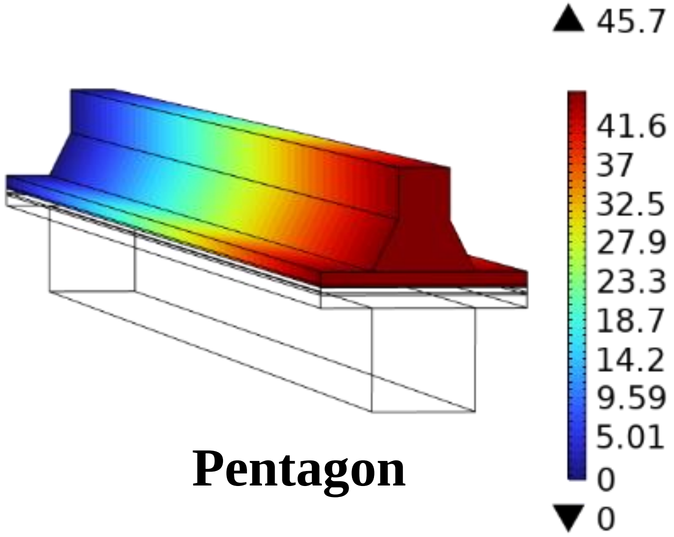
Trapezoid



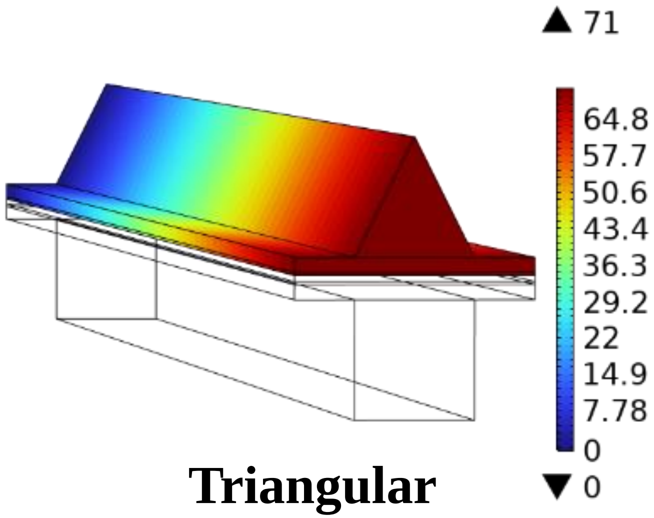
Dome



Boot



Pentagon



Triangular

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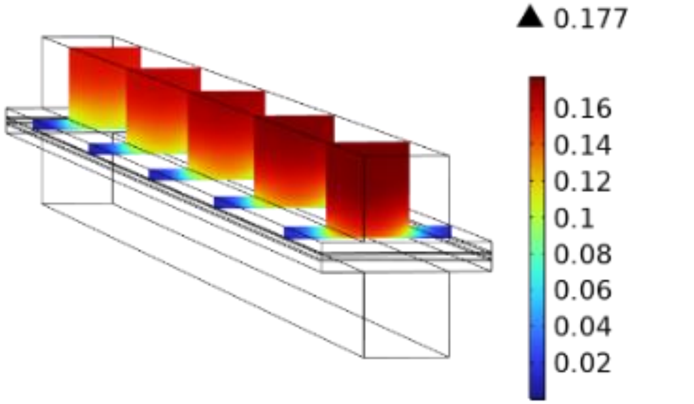
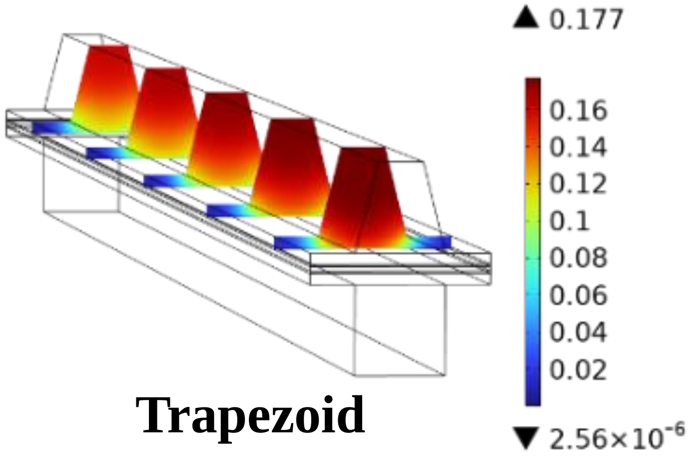
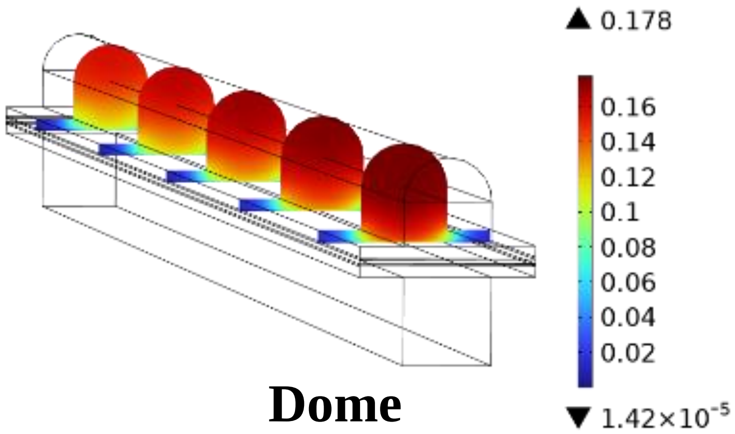
Oxygen Concentration



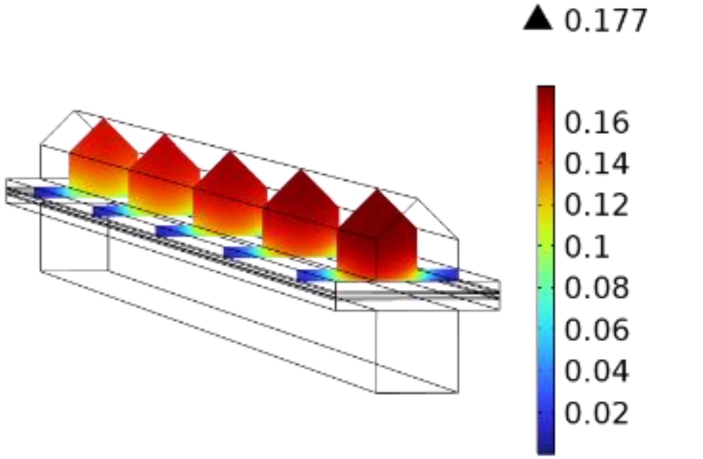
Square



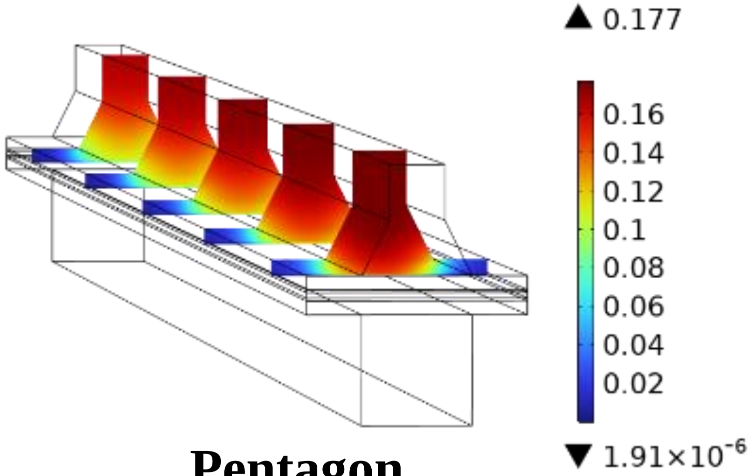
Trapezoid



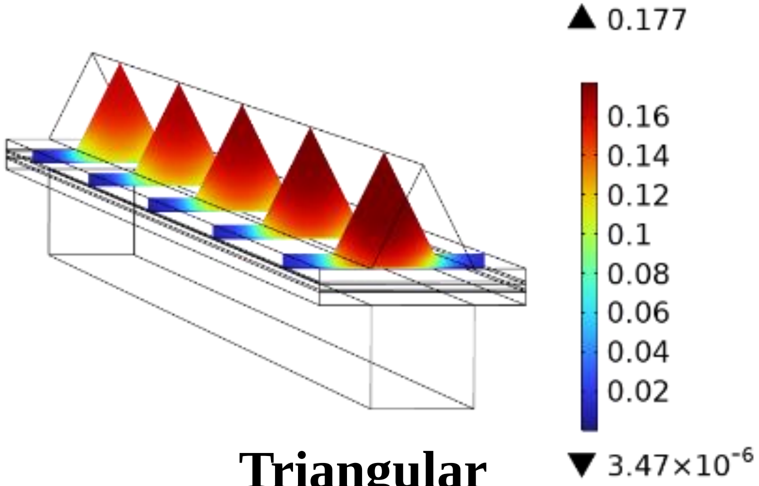
Dome



Boot



Pentagon



Triangular

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I-V Polarization Curve

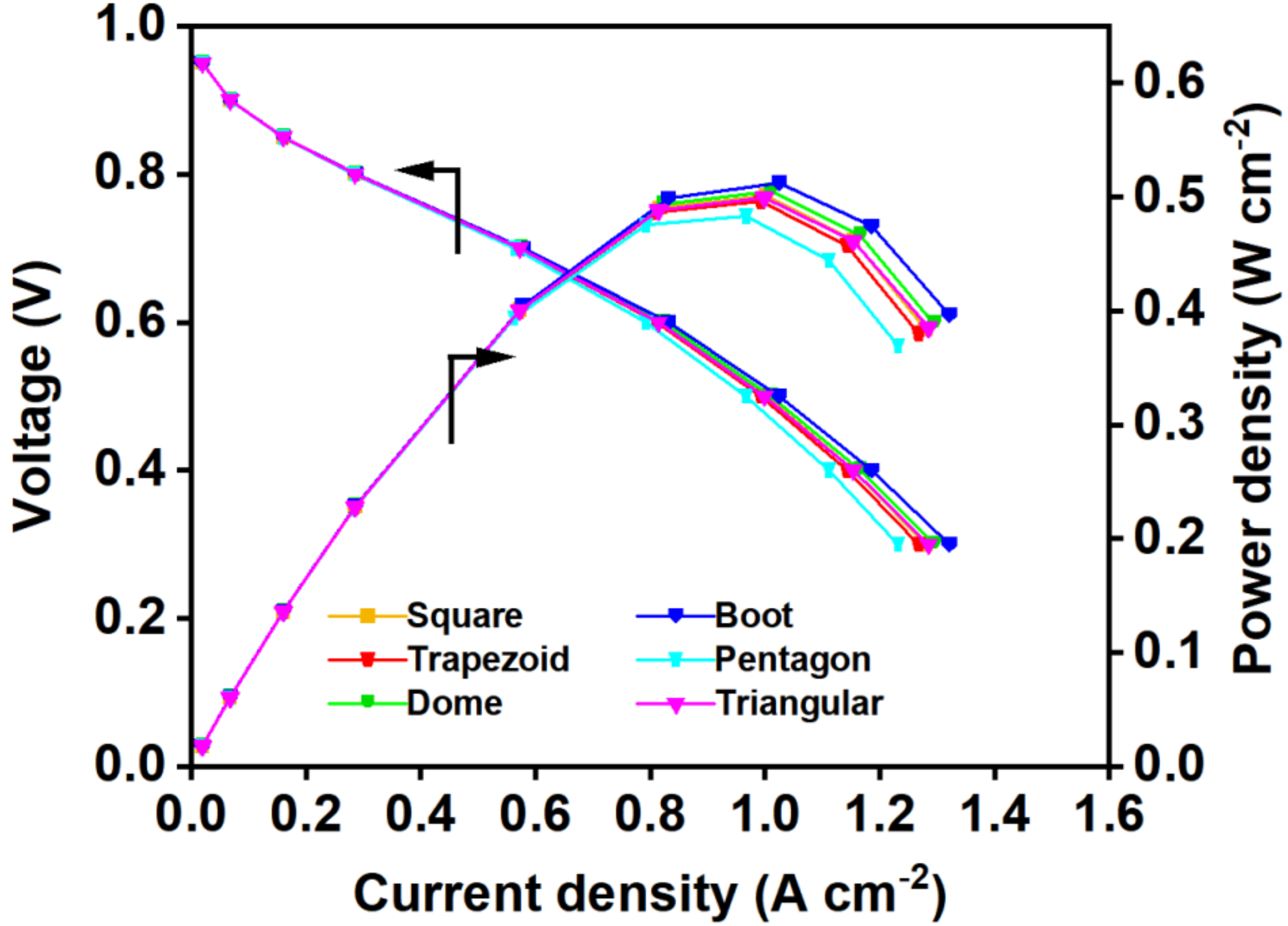

Figure: I-V polarization curve for varying cross-sectional designs obtained via simulation.

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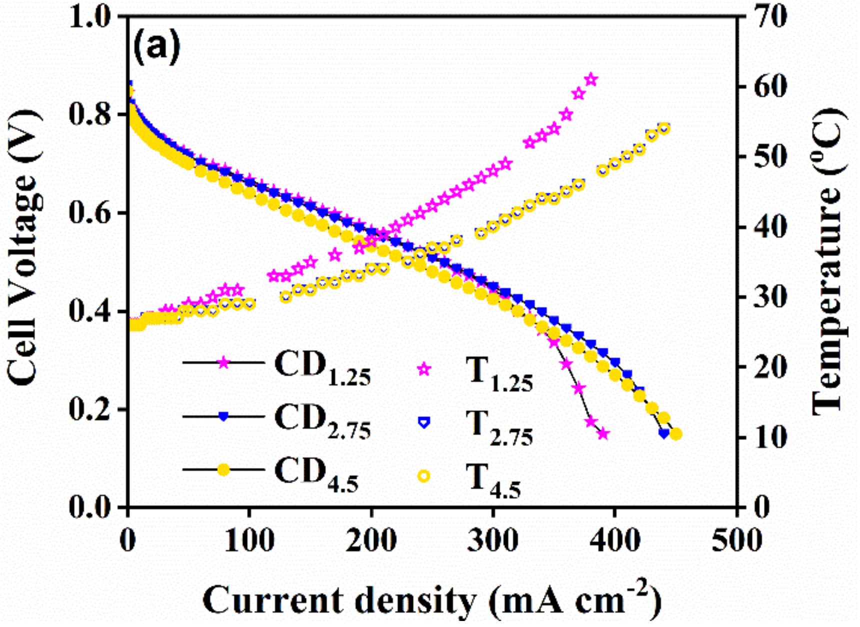
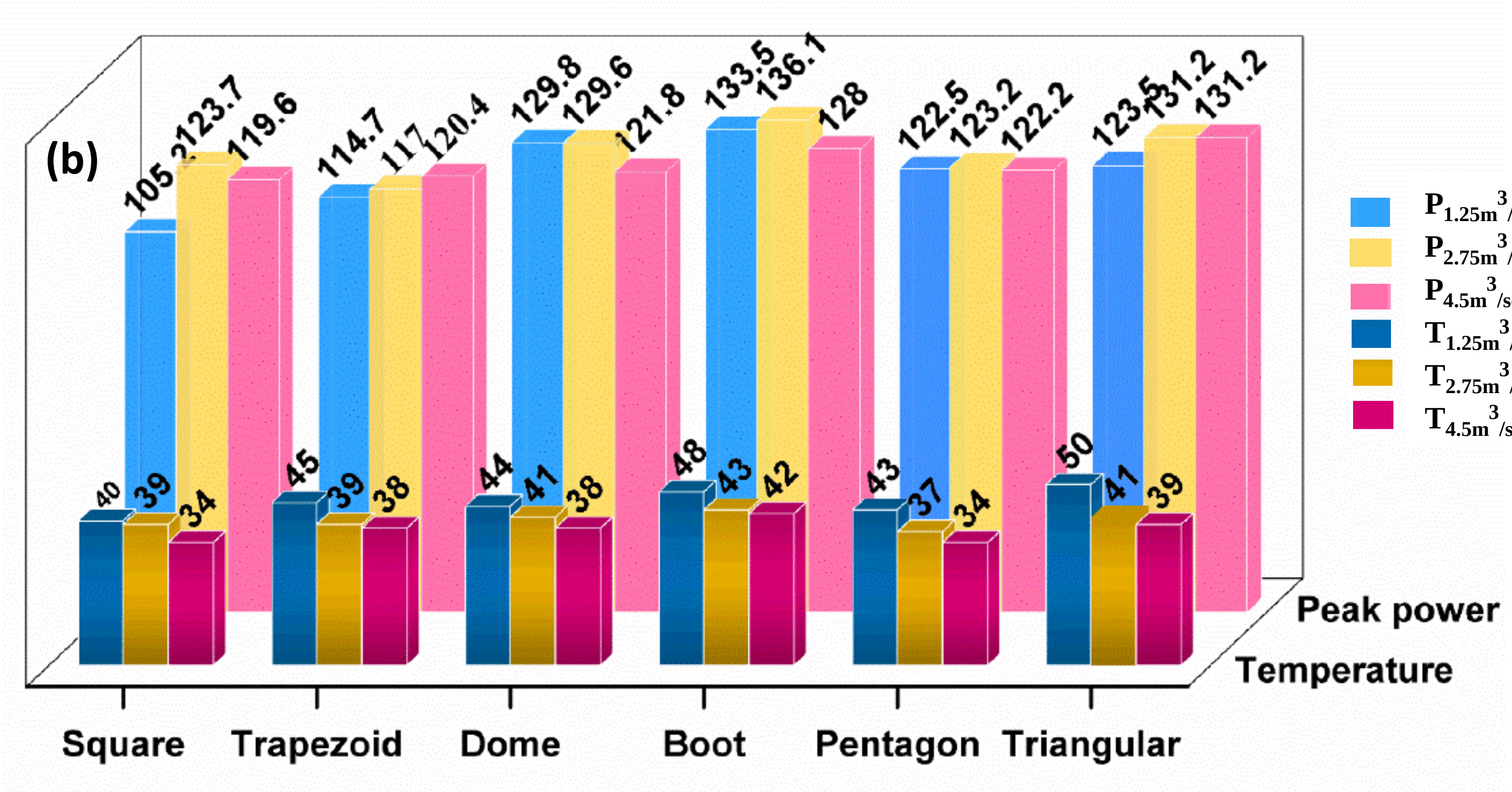
Experimental Results at different Airflow Rate





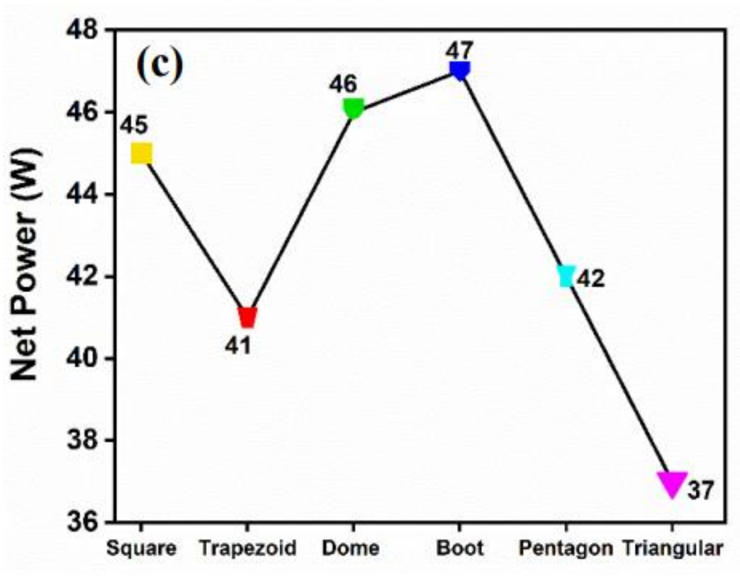


Figure: **(a)** I-V curve and temperature plot for boot CSD at different AFR $1.25 m^3/sec$, $2.75 m^3/sec$, and $4.5 m^3/sec$; **(b)** Histogram plot for peak PD in mW/cm^2 and corresponding stack temperature in °C for various CSDs at different AFR; and **(c)** The net system power plot at corresponding OC-PEMFC stack peak power density for different CSDs at AFR $2.75 m^3/sec$. CD-Current density, T-temperature, and P-Peak power density.

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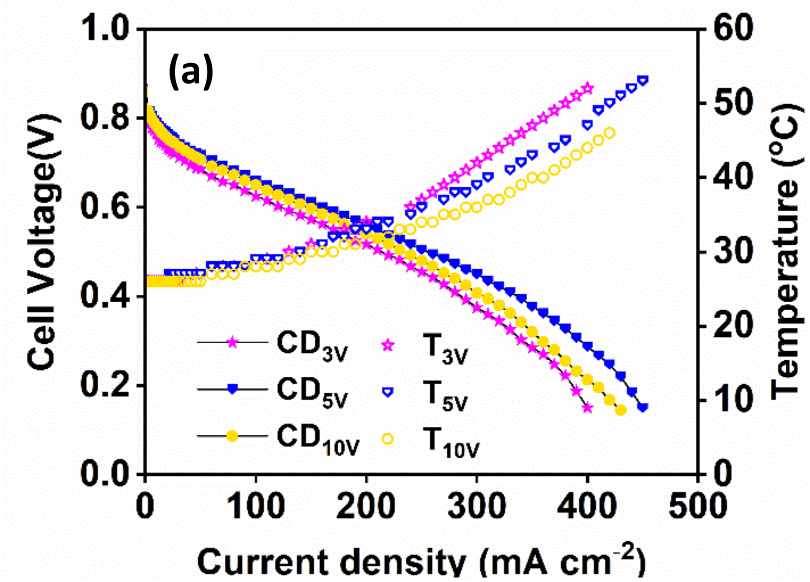
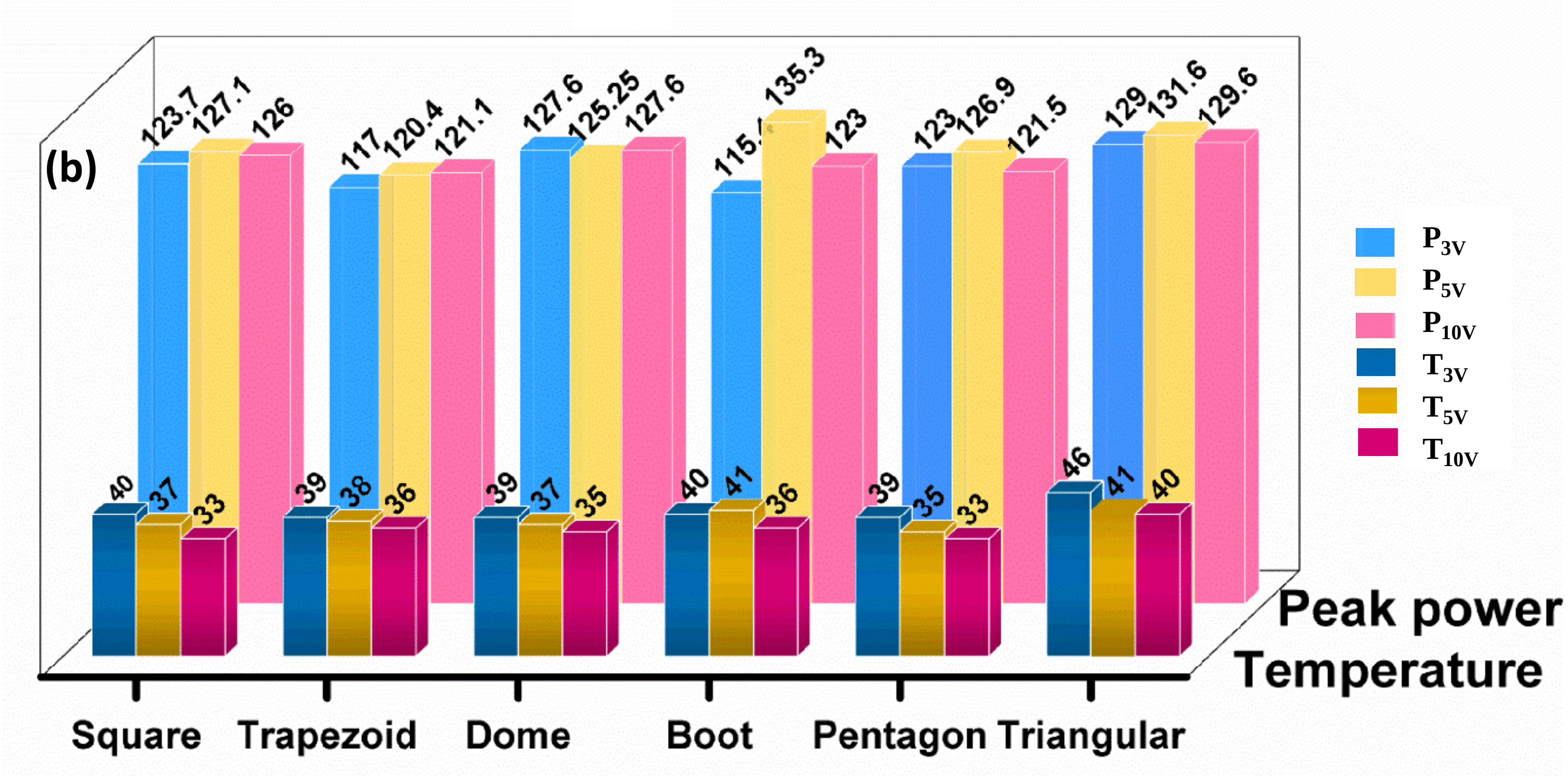
Experimental Results at different Blower Power





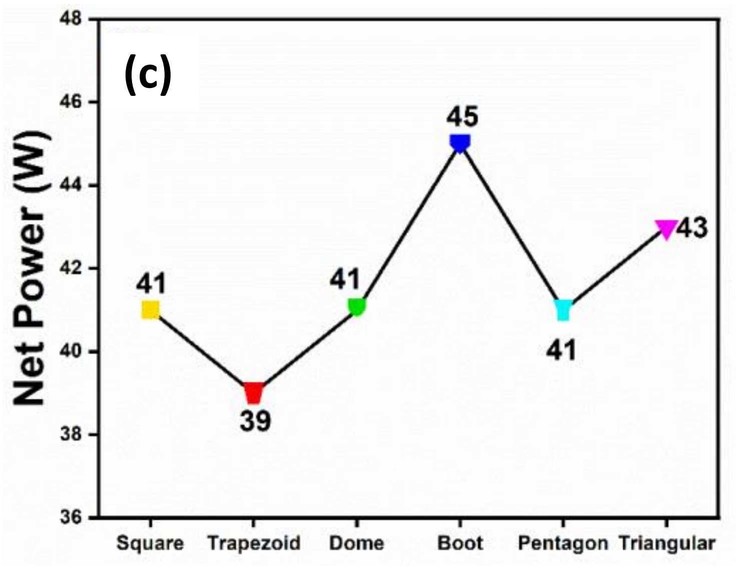


Figure: **(a)** I-V curve and temperature plot for boot CSD at different blower power of 3V, 5V, and 10V; **(b)** Histogram plot for peak PD in mW/cm^2 and corresponding stack temperature in ºC for various CSDs at different blower power; and **(c)** The net system power plot at corresponding OC-PEMFC stack peak power density for different CSDs at 5V BP rating. CD-Current density, T-temperature, and P- peak power density.

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Electrochemical Impedance Spectroscopy (EIS)

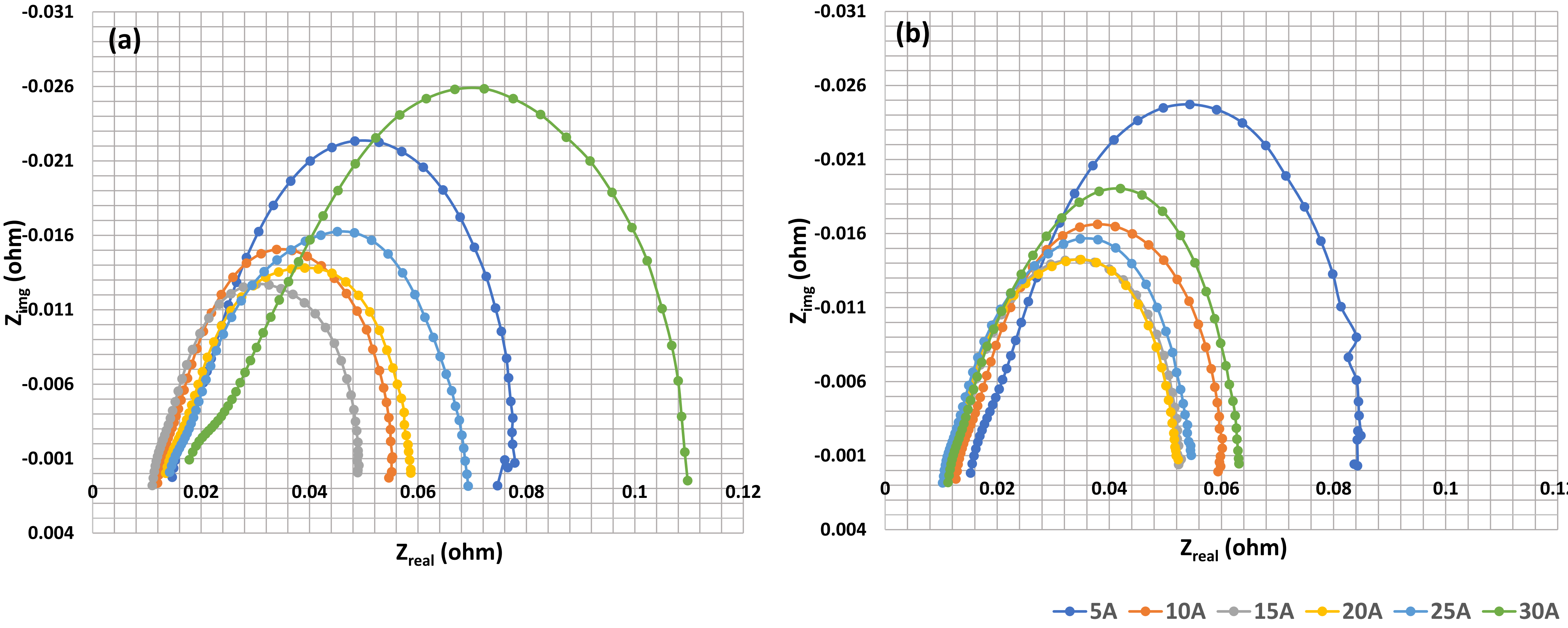

Figure: Nyquist diagram obtained from the EIS test for four cells OC-PEMFC stacks at different operating conditions **(a)** Airflow rate of 1 m^3/sec. **(b)** Blower power rating of 5V.

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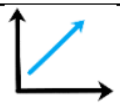
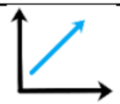
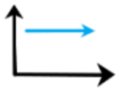
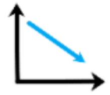
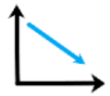
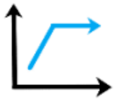
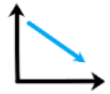
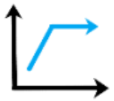
Table: Overall analysis of the Cross-Sectional Designs

CS Design	CSA (mm^2)	Pressure drop (Pa)	Airflow rate		Blower power		Stack temperature		Galvanostatic
Square	4	13.2		Excessive cooling		Excessive cooling			Effective cooling at 5, 7V
Trapezoid	3	26		Improved airflow rate		Improved airflow rate			Ineffective cooling
Dome	3.57	15.9		Excessive cooling; water removal		Complex balance of performance and temp			Effective cooling at 7, 10 V
Boot	3	23.9		Water removal		Water removal		Excessive drying	Ineffective cooling
Pentagon	2.5	45.7		Minimal effect		Excessive water removal		Excessive drying	Ineffective cooling
Triangular	2	71		No effect		Drying		Low dying; compensated by enhanced performance	Ineffective cooling

Unpublished work

Acknowledgement

- Director CSIR-CECRI, Dr. K. Ramesha.
- Supervisor- Dr. A.K. Sahu (Principal Scientist) and Mentor- Dr. Harshal Agarwal (Senior Scientist) for constant support and guidance.
- CSIR-HRDG and AcSIR for GATE-SRF (GATE31/0068(15842)/2022-EMR-I).
- Organizing committee and team members COMSOL Multiphysics.

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Thank you

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