PERFORMANCE ENHANCEMENT IN PROTON EXCHANGE MEMBRANE FUEL CELL – NUMERICAL MODELING AND OPTIMISATION

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Presentation overview

- Introduction (Fuel cell technology & challenges)
- Objective of the research
- Research Methodology
- Trends and results
- Conclusion, recommendations & remarks

World Energy concerns:

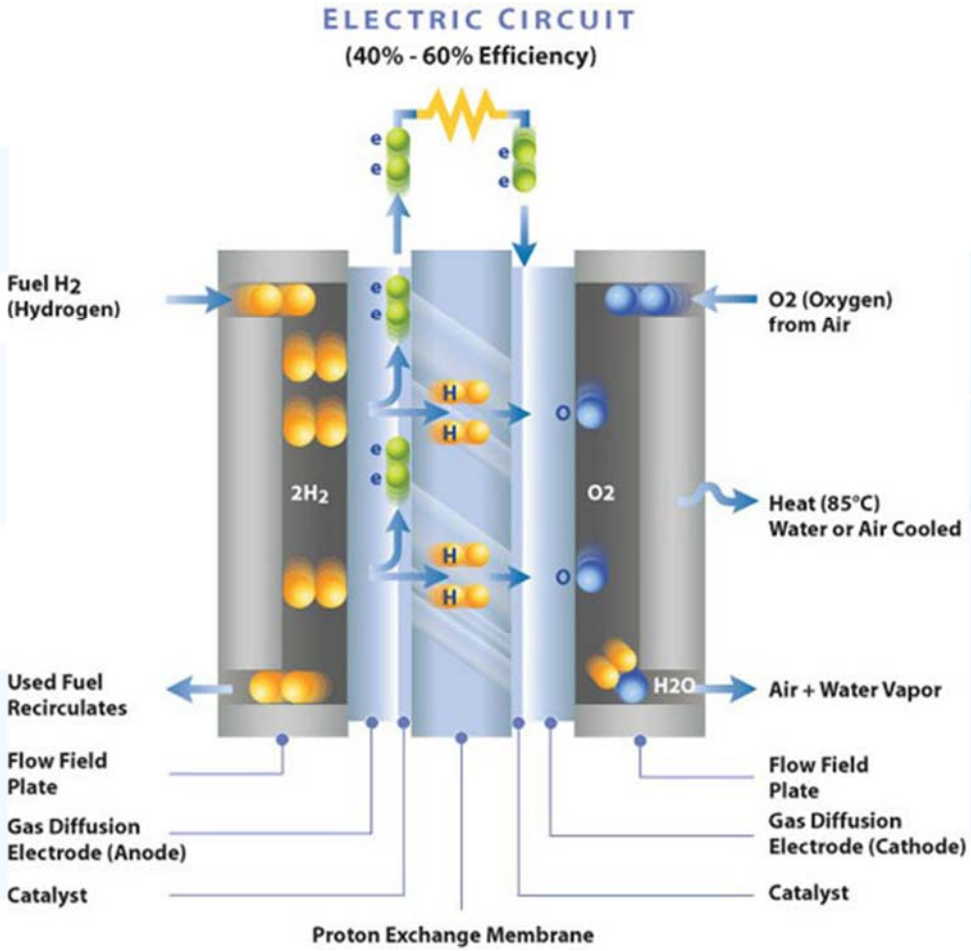
- **Increasing world population and production activity.**
- **Pollution increase through fossil fuels.**
- **Emergence of renewable energy sources (solar, Fuel cell, wind, etc.).**
- **Fuel cell potentials (PEMFC, SOFC, AFC, DMFC):**

  - *Low pollution potentials*
  - *Highly efficient power devices*
  - *Portability & remote application*
  - *South Africa platinum exploration (80% of world production)*

A case for PEM fuel cell:

- High power density
- High efficiency
- Fast start-up (low temperature of operation)
- Remote applications
- Dynamic response capability in automobile application

Basics of fuel cell reactions: generates electricity by chemical reaction taking place at two electrodes (anode & cathode)



- **Electrochemical Reaction**:

- At the anode: $2H_2 \rightarrow 4H^+ + 4e^-$

- At the cathode: $O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$

- Total cell reaction: $2H_2 + O_2 \rightarrow 2H_2O$ + Heat + Electricity

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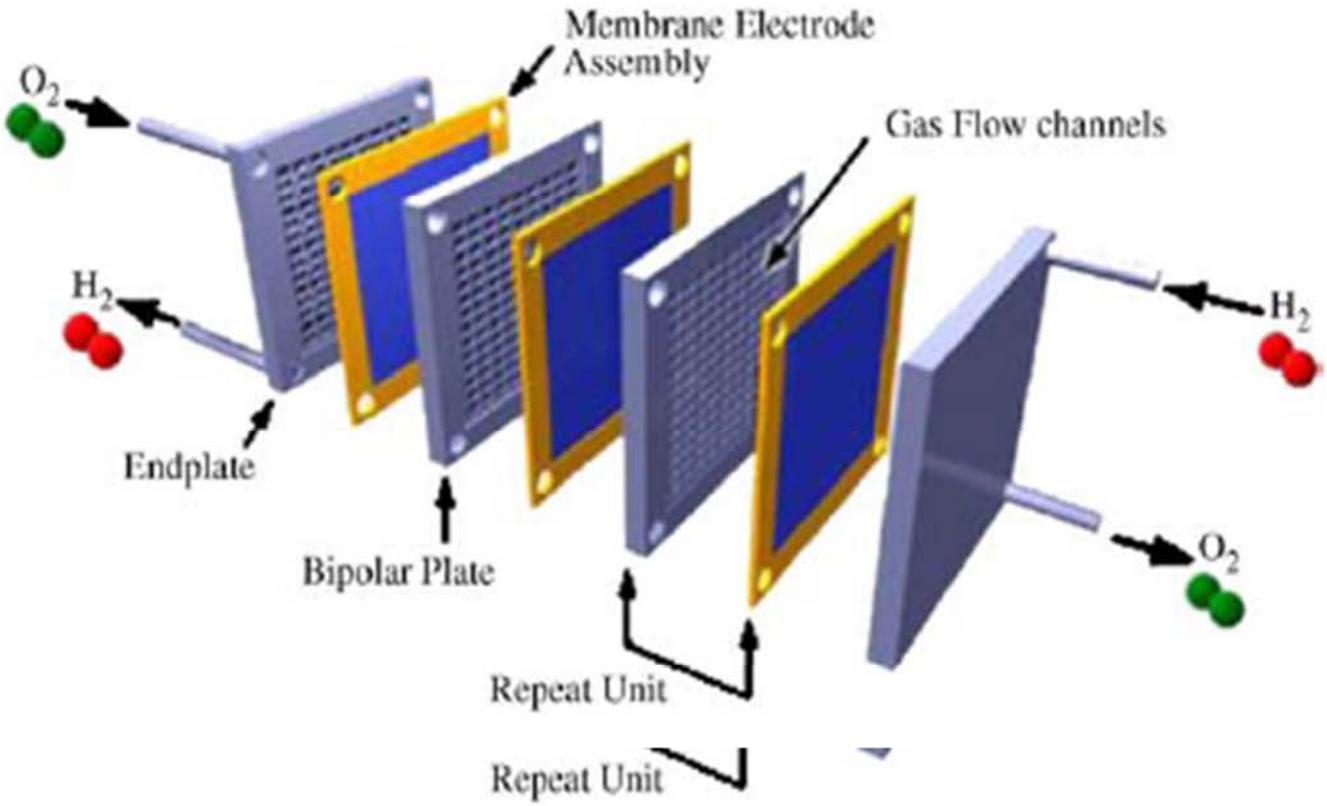
Source: http://auto.howstuffworks.com/fuel-efficiency /alternative-fuels/fuel-cell5.htm.

Fuel cell stack system



Multifaceted research field & Niche area for thermoflow research

- Flow reactant topology (Mech. Engrs.)
- Reactant species transport (Mech. Engrs)
- Material development (Material Sci & Engrs.)
- Electrochemistry (Chemistry & Chemical Engrs.)
- Thermal & water Management (Heat transfer & polymer scientist)
- Durability & life-span of auxiliary components (Metallurgist & Materi. Sci)
- Catalyst issues (Chemistry & polymer)

Thermoflow research niches:

- Flow field enhancement
- Species reactant transport enhancement
- Thermal cooling in structures

<u>The main research objective is</u>: ***to investigate on new methodologies towards performance enhancement in PEM fuel cell system.***

- To realise this main objective, the study focus on the following research activities:

- To numerically predict the performance of PEM fuel cell under different operating conditions

- To optimise the performance of PEM fuel cells through gas channel modification considering species flow rate and GDL porosity

- to develop a novel design approach towards maximised reactant species diffusion on the GDL

- To investigate cooling channel geometric scheme in conjunction with operating parameters (that are temperature related) to enhance PEM operation beyond the critical temperatures (80 ^{0}C)

Numerical Modeling & optimisation

- CFD code – ANSYS FLUENT (Fuel cell add-on)
- Dynamic-Q algorithm (Prof. J.A. Snyman)
- ***Basic assumptions***:

➢ Cell operates under steady-state conditions,

➢ Flow in the cell is considered to be laminar,

➢ Reactant and products are assumed to be ideal gas mixtures,

➢ Electrode is assumed to be an isotropic and homogeneous porous medium.

Fuel cell model basic equations

Continuity equation:

$$\nabla \cdot (\varepsilon \rho U) = S_m$$

Momentum conservation:

$$\nabla \cdot (\varepsilon \rho \mathbf{U}\mathbf{U}) = -\varepsilon \nabla p + \nabla \cdot (\varepsilon \mu_{eff} \nabla \mathbf{U}) + S_u$$

Species conservation:

$$\nabla \cdot (\varepsilon \mathbf{U} Y_i) = \nabla \cdot (D_{i,eff} \nabla Y_i) + S_i$$

Energy conservation:

$$\nabla \cdot (\lambda_{eff} \nabla T) = \nabla \cdot (\varepsilon \rho C_p \mathbf{U}\mathbf{T}) + S_T$$

Mathematical optimisation:

❖ Standard optimization problem

$$\underset{\text{with respect to x}}{\text{minimize}}\ f(\boldsymbol{x}),\quad \boldsymbol{x}=[x_1,x_2,..x_l..,x_n]^T, x_l \in \square^n$$

subject to the constraints:

$$g_i(\boldsymbol{x}) \le 0,\quad i=1,2,...,m$$

$$h_j(\boldsymbol{x}) = 0,\quad j=1,2,...,r$$

❖ DYNAMIC-Q Algorithm

- Spherical approximations are developed at each design point to approximate the objective function and constraints.

$$\tilde{f}(x) = f(x^k) + \nabla^T f(x^k)(x-x^k) + \frac{1}{2}(x-x^k)A(x-x^k)$$

$$\tilde{g}_i(x) = g_i(x^k) + \nabla^T g_i(x^k)(x-x^k) + \frac{1}{2}(x-x^k)\boldsymbol{B}_i(x-x^k)$$

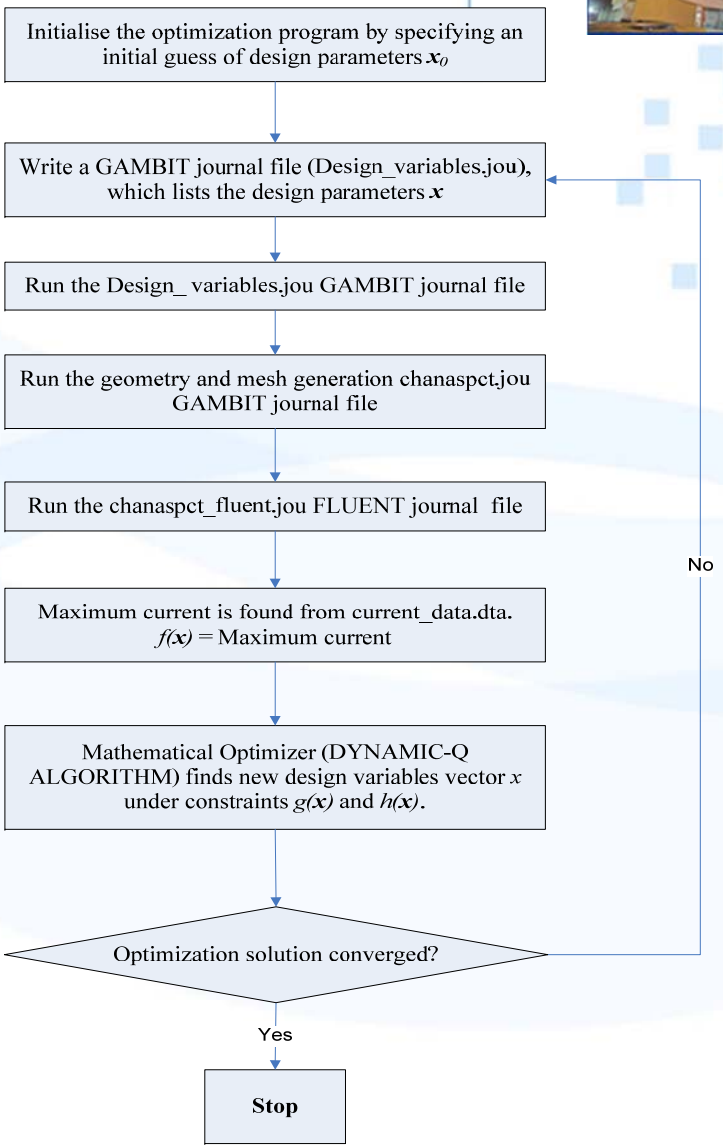
$$\tilde{h}_j(x) = h_j(x^k) + \nabla^T h_j(x^k)(x-x^k) + \frac{1}{2}(x-x^k)C_j(x-x^k)$$

- A robust multidimensional gradient based optimization algorithm.

- Three phase penalty function implementation scheme.

Optimization code (Dynamic-Q):

- Ideally robust for cases where the function evaluation are expensive.
- Applied to successive quadratic approximations of the actual optimization problem.
- Offers a competitive advantage compared to other algorithm in term of computational and storage requirement, especially when number of variables are large.
- Automation of process.



Previous studies in area of research (Operating conditions & flow field performance)

- Liu X. *et al* (2007). Studied experimentally the effect of flow field type, cell temperature, cathode flow rate and operation time on water build-up and cell performance.

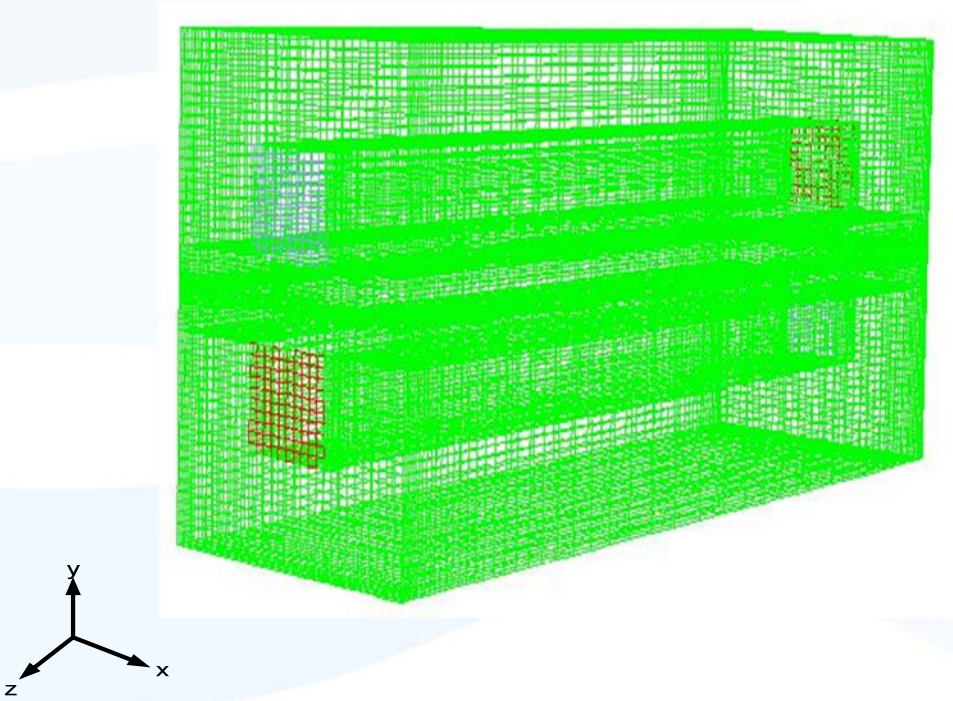
- Ahmed *et al* (2006). Performed numerical model to investigate PEMFC performance at high operating current densities for various configuration while maintaining the same reactant flow rates.

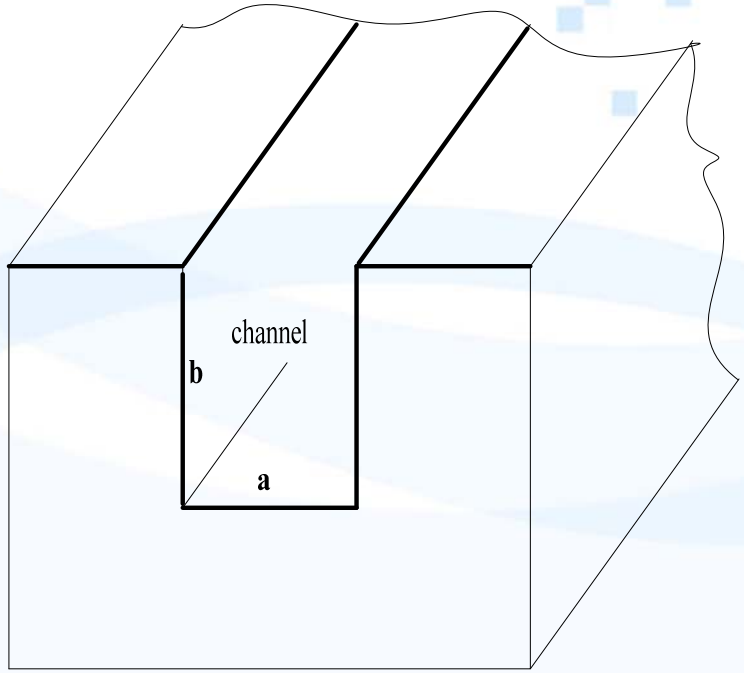
Issues of interest:

- *What effect does the GDL porous media has on species distribution?*

- *What effect does varying reactant flow rates has on performance at changing channel configuration?*

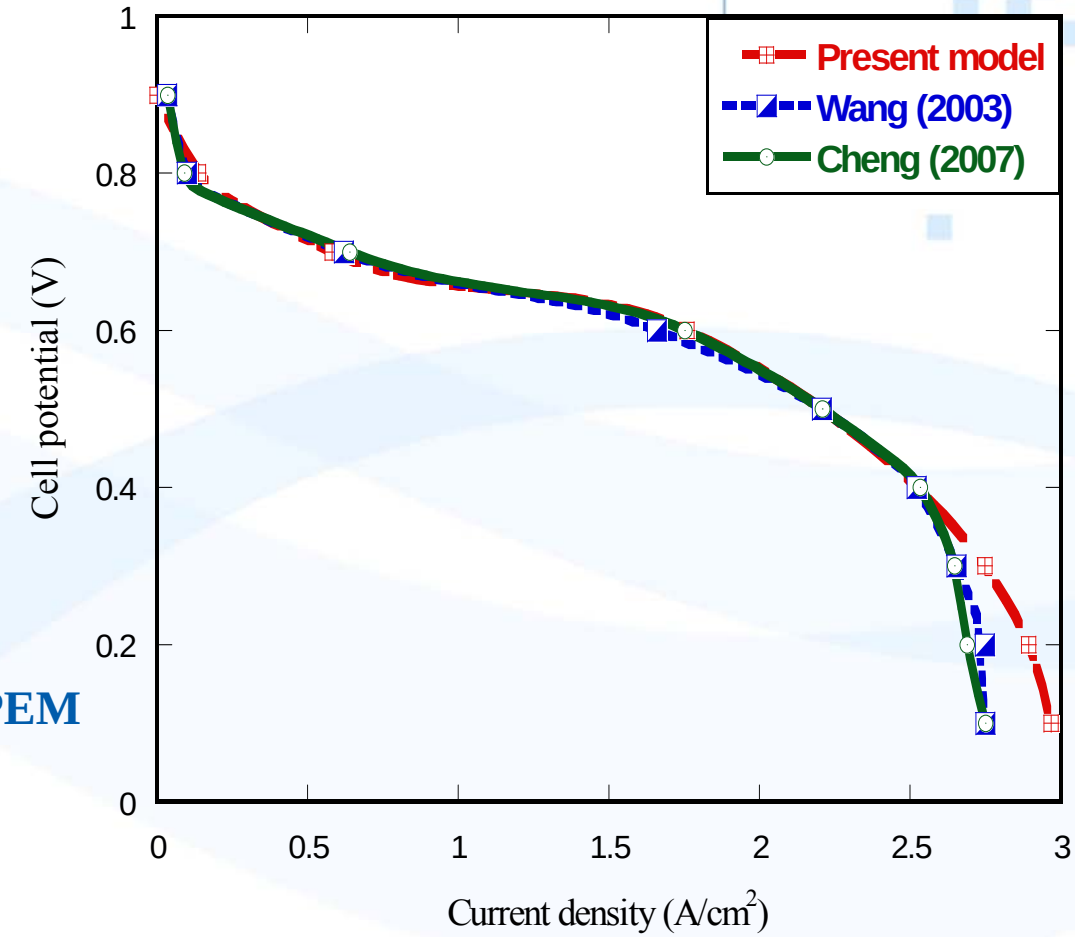
Model 1 description: *Discretised 3-D computational domain & channel cross-section.*





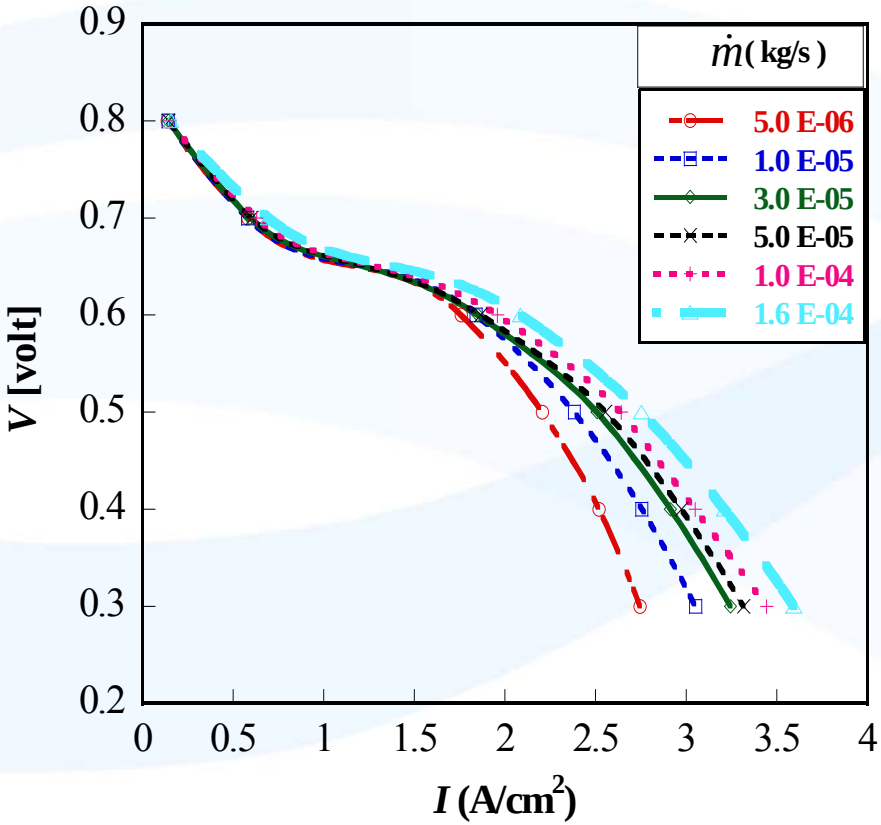
Results highlight & Model validation:

- ✓ **Comparison of numerical and experimental results**
  - *Polarization curve*
- ✓ **Effect of physical parameters on performance**
  - *Oxygen gas flow rate effect*
  - *GDL porosity effect*
- ✓ **Effect of design parameters on performance**
  - *Channel depth*
  - *Channel width*
- ✓ **Optimal channel geometries for PEM performance**
  - *varying GDL porosities*
  - *varying oxygen mass flow rates*

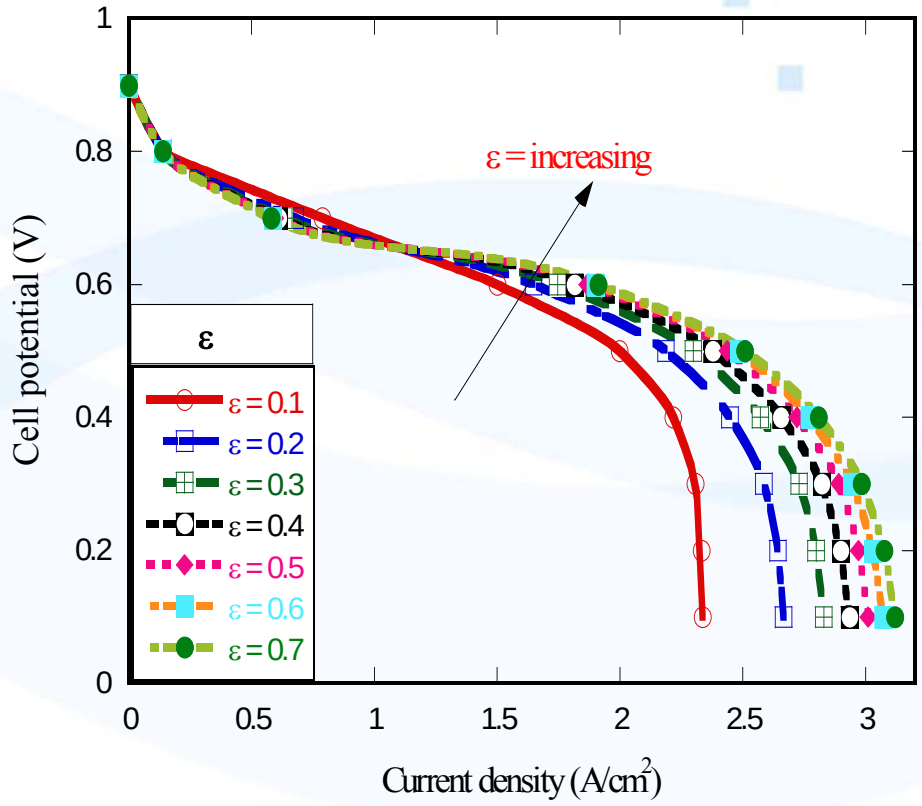


Parametric results:

Effect of cathode gas flow rate on cell performance

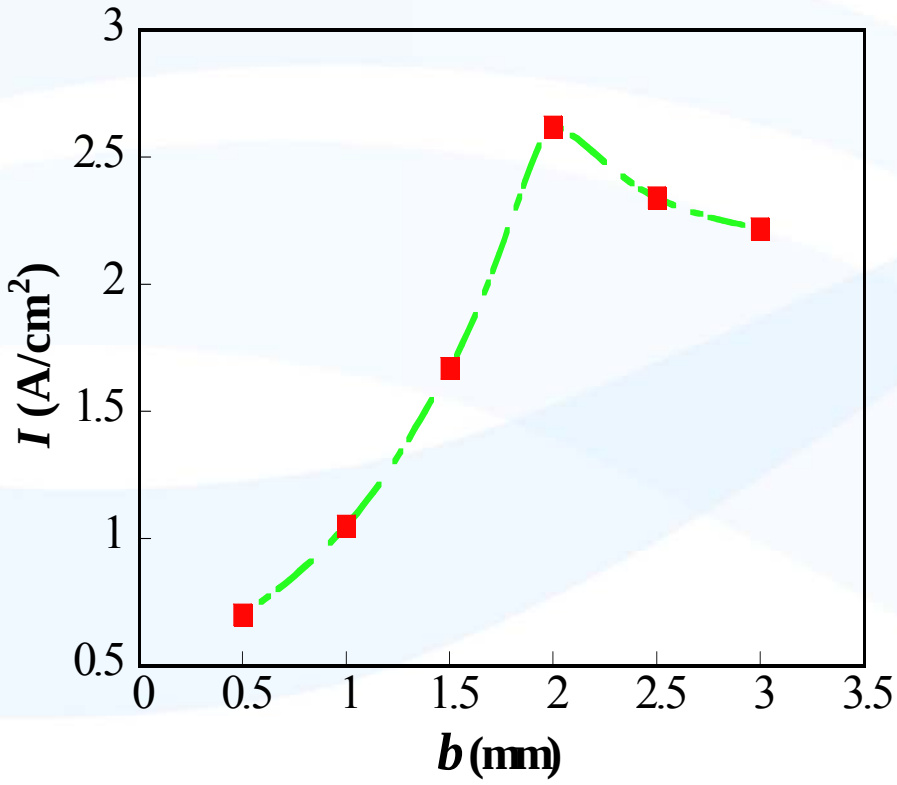


Effect of GDL porosity on cell performance

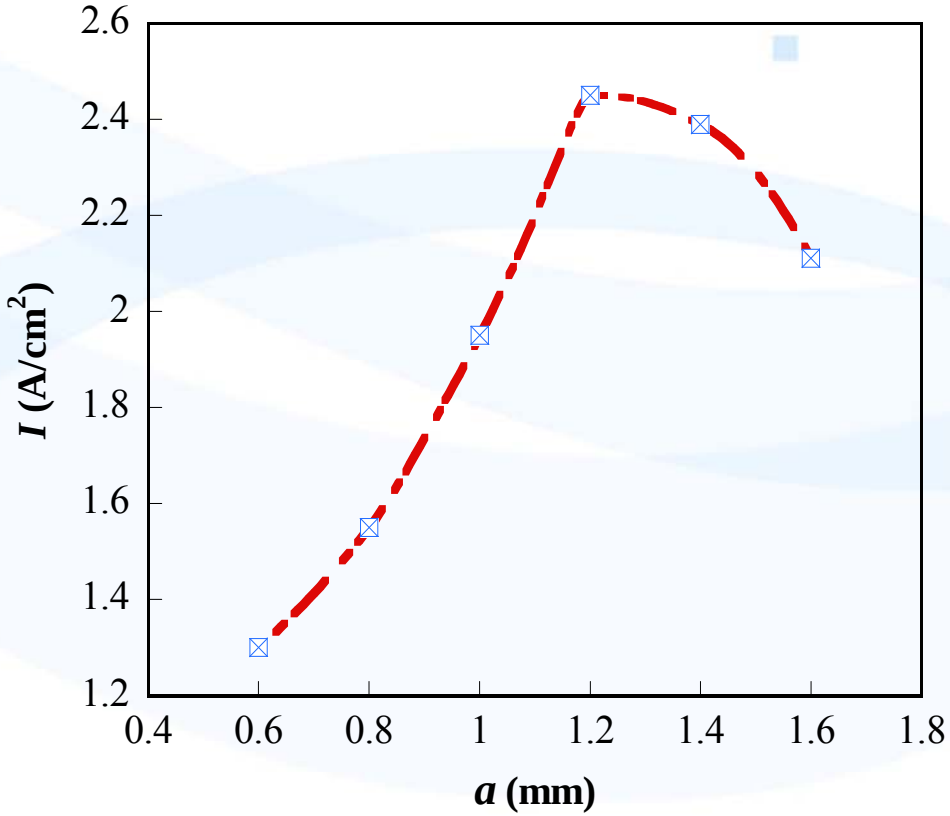


Effect of channel depth and width:

Optimal channel depth: 2.0mm (*I* = 2.62 A/cm^2) @ 5E-06 kg/s mass flow rate and fixed channel width

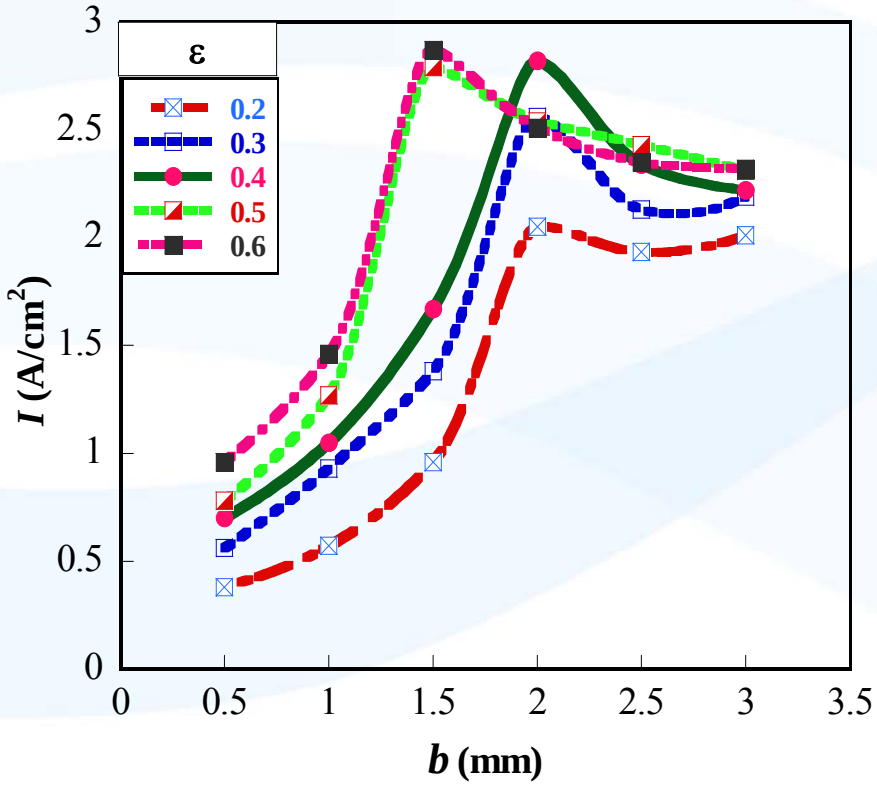


Optimal channel width: 1.2 mm (*I* = 2.45 A/cm^2) @ 5E-06 kg/s mass flow rate and fixed channel depth

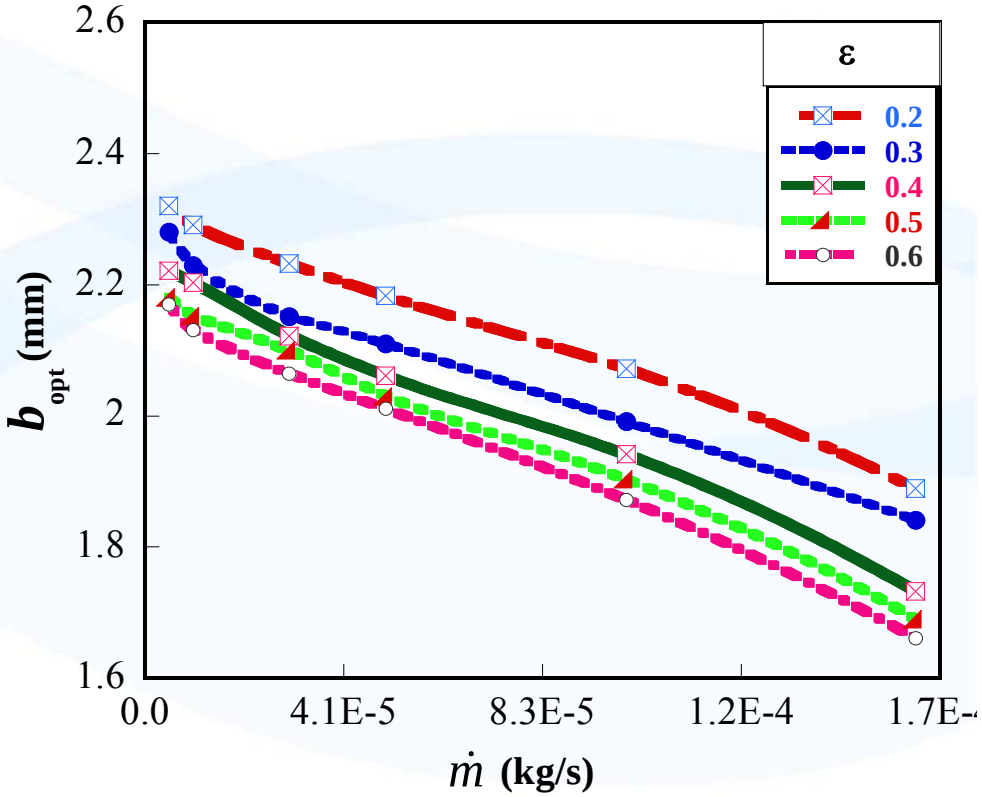


Channel depth, GDL porosity & mass flow rate

Effect of GDL porosity and channel depth on performance @ 5E-06 kg/s mass flow rate and width of 1.2mm

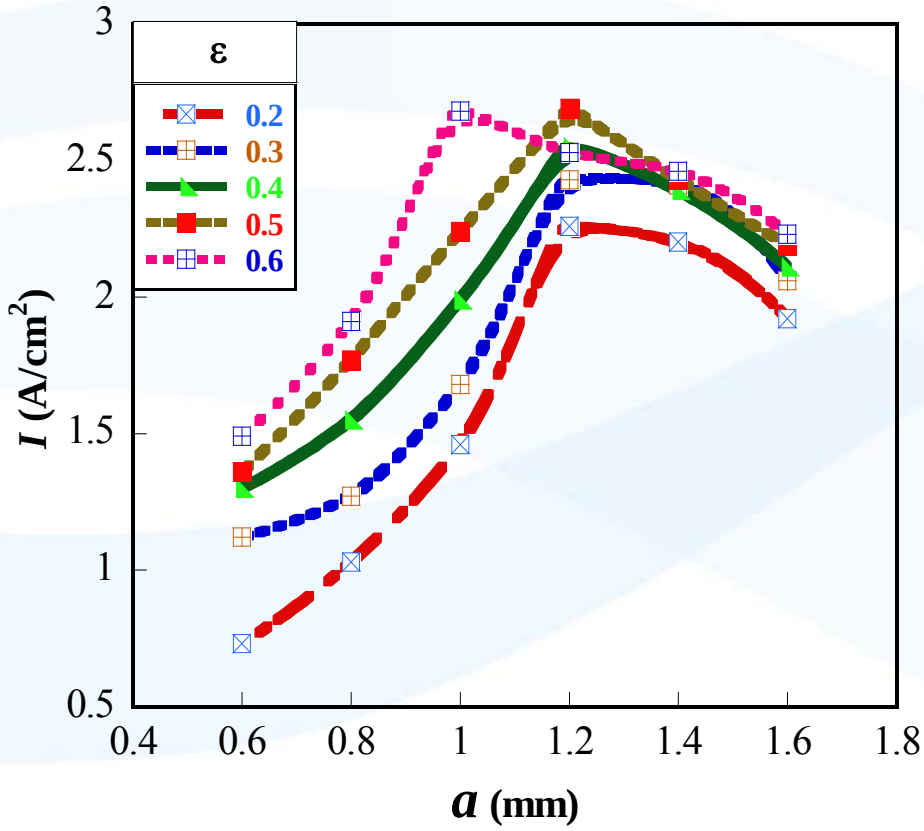


Optimal depths as a function of mass flow rate and gas diffusion layer porosity

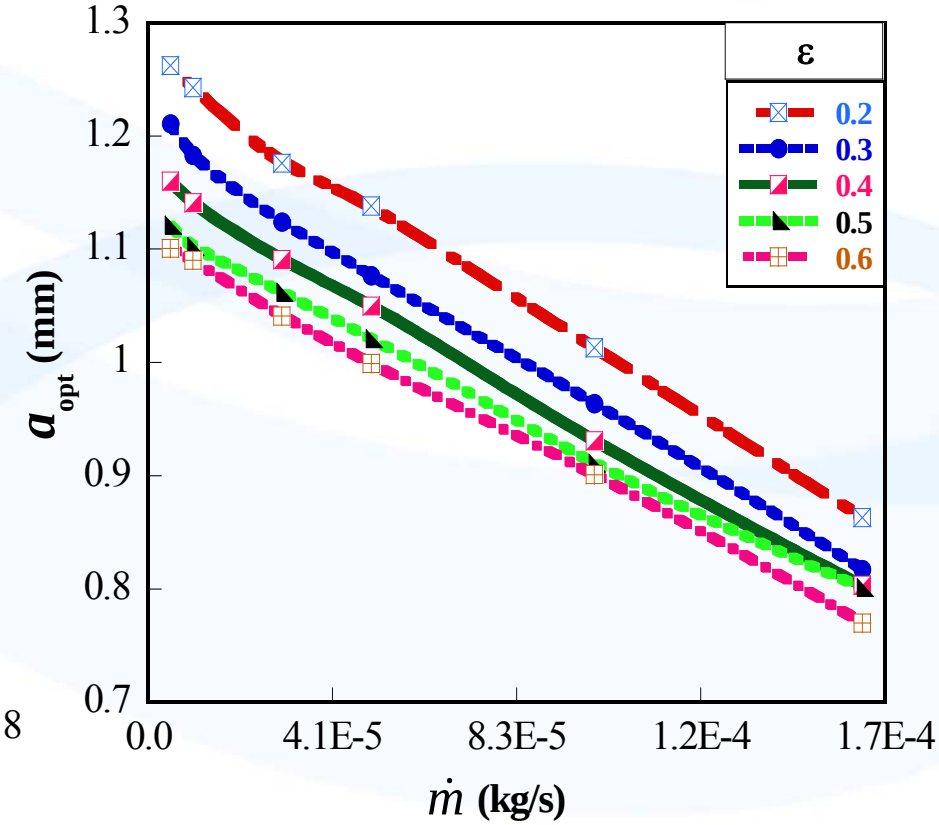


Channel width, GDL porosity & mass flow rate

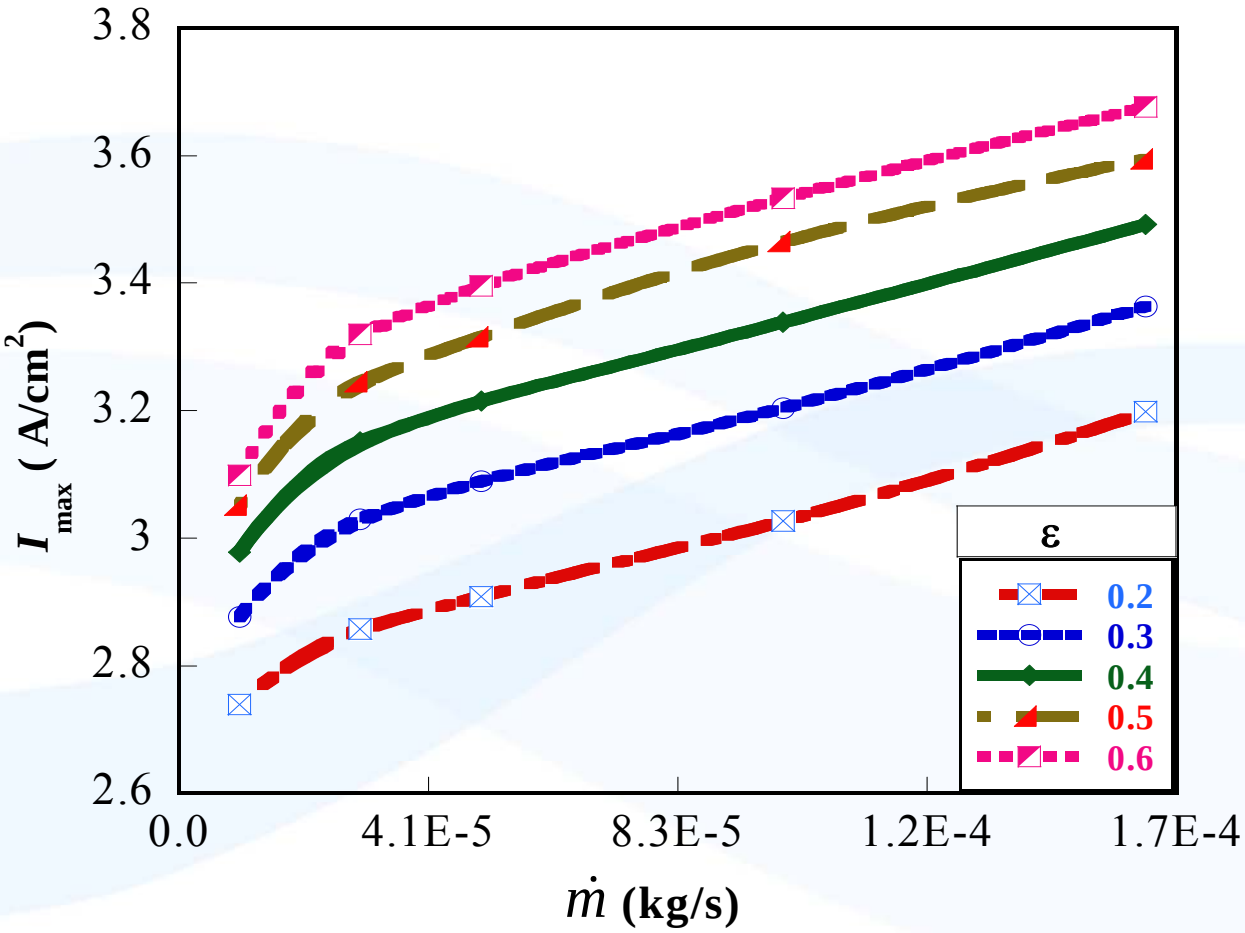
Effect of GDL porosity and channel width on performance @ 5E-06 kg/s mass flow rate and depth of 2.0mm



Optimum widths as a function of mass flow rate and gas diffusion layer porosity



Effect of mass flow rate and GDL porosity on the cell performance (*maximised current density*)



Research objective 2:
Previous studies in area of research (Species diffusion optimisation in flow field)

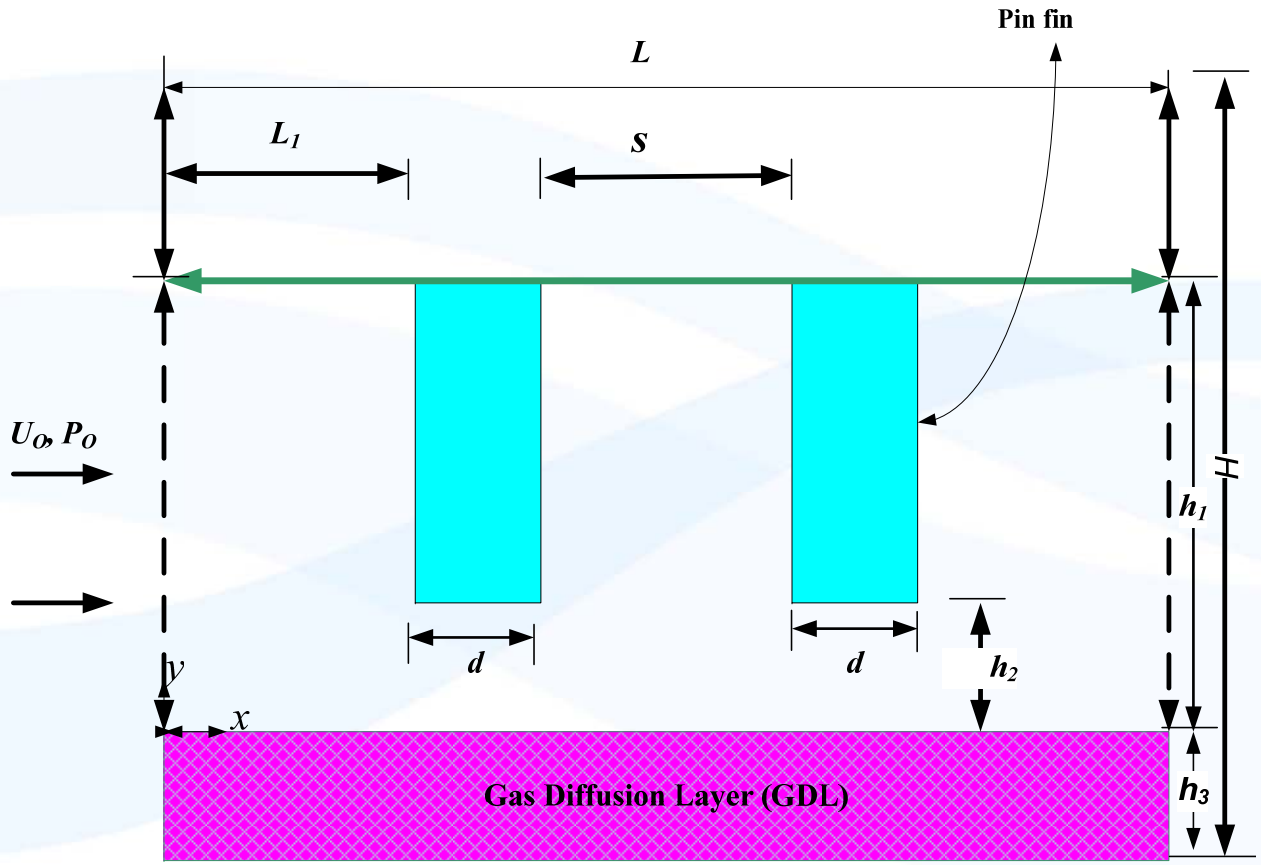
- Soong. *et al.* (2005). Developed a flow channel configuration by inserting baffles in the conventional flow field channels. Performance was enhanced though with penalty of higher pressure loss.

- Wang *et al.* (2007). Studied the use of baffles in a serpentine flow field to improve performance in PEM fuel cell. The baffles helps gas diffusion leading to enhanced current density though at higher pressure difference between adjacent flow channels.

Issues of interest:

- *Investigate on pin fins geometry on reactant gas distribution in PEM fuel cell*
- *Investigate of a trade-off between the performance enhancement & pumping power requirement due to pressure drop.*

Model 2 description: *2-D computational domain of cathode channel & GDL section.*



Optimization problem formulation:

Objective function : optimised pin fin geometry giving optimal performance

Total pin fin area constraint:

$$\therefore \sum A^c{}_j = \text{Constant}$$

$$\sum \pi D_j H_j = C$$

$$\sum D_j H_j = \frac{C}{\pi}$$

for $j = 1, 2$

Other geometric constraints:

$$0.2 \le \left[\lambda = \frac{h_2}{h_1} \right] \le 0.6$$

$$5 \le \left[\zeta = s/d \right] \le 10$$

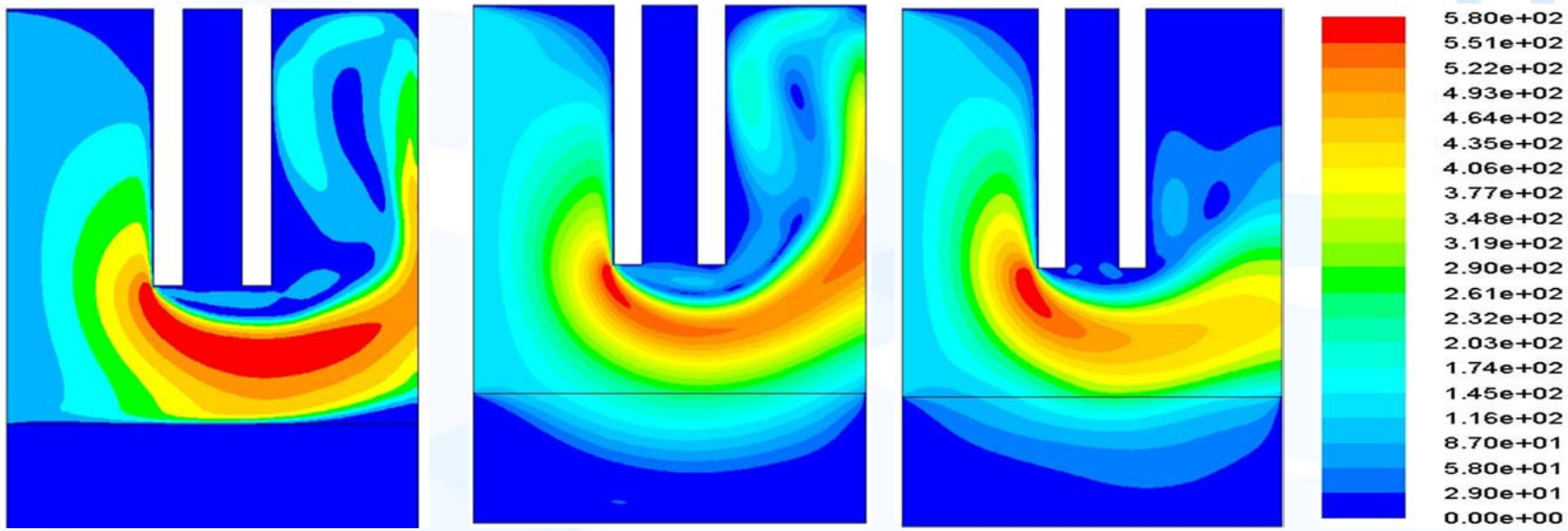
$$0.5 \le \left[\varphi = \frac{h_1 - h_2}{d} \right] \le 4$$

$$s \ge 50 \ \mu m$$

Results highlights:

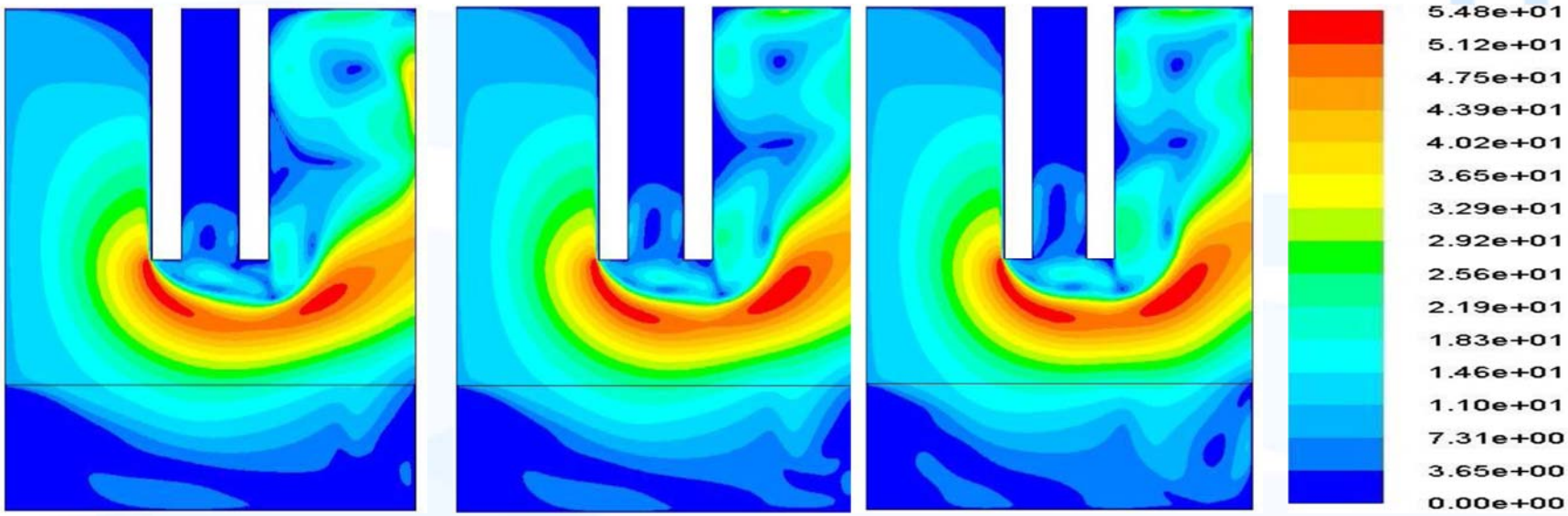
- ✓ **Results of flow field:**
- ✓ **Results of pin fin geometry:**
- ✓ **Optimization results:**
- ✓ **Performance evaluation:**

Effect of Reynolds number on the flow field: (a) Re = 50, (b) Re = 150, © Re = 250. (s/d = 5 & λ= 0.2)



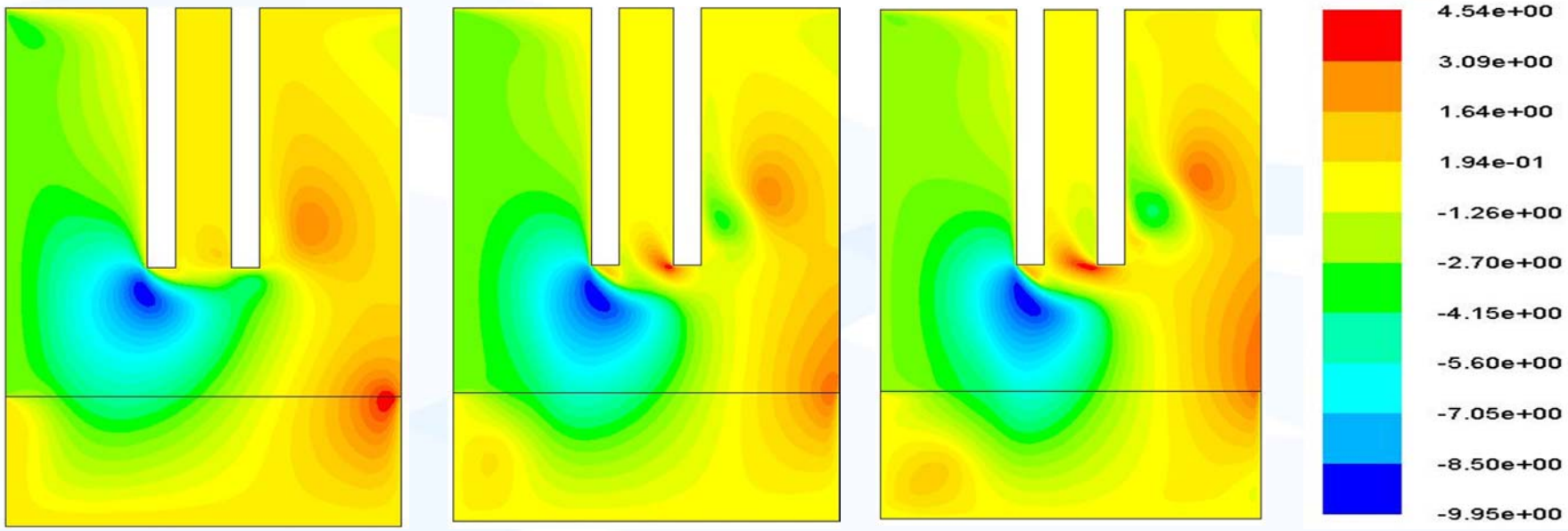
(a) **(b)** **(c)**

Effect of Reynolds number on the flow field: (a) Re = 50, (b) Re = 150, © Re = 250. (s/d = 5 & λ= 0.6)



(a) **(b)** **(c)**

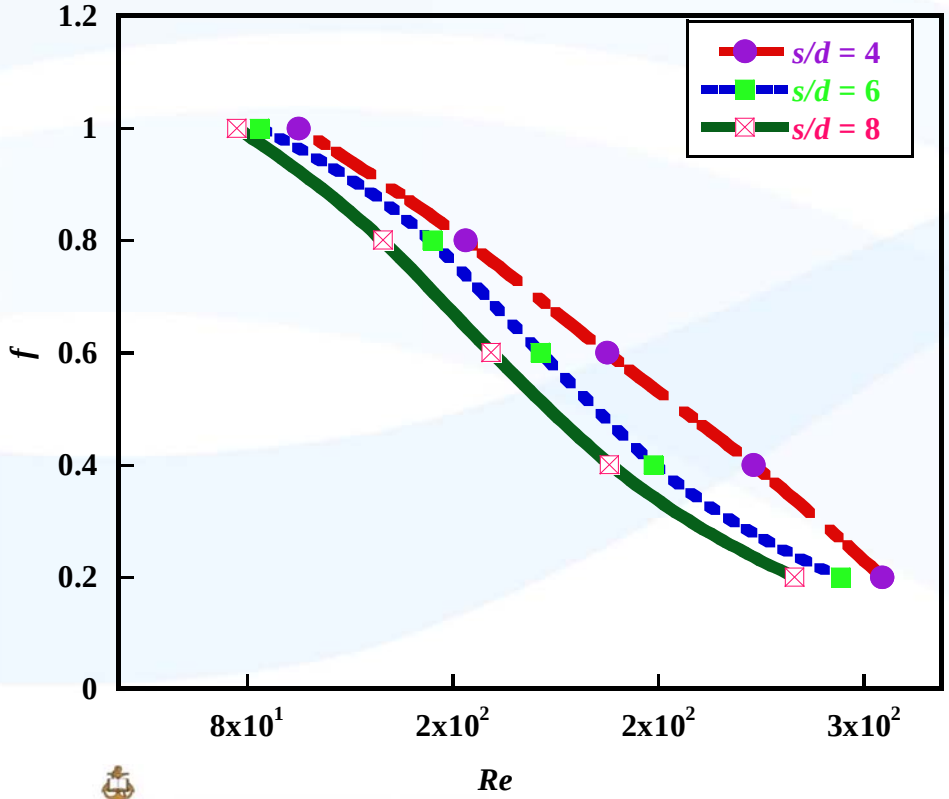
Contours of tangential velocity at different Reynolds number : (a) Re = 50, (b) Re = 150, © Re = 250. (*s/d* = 5 & λ= 0.6)



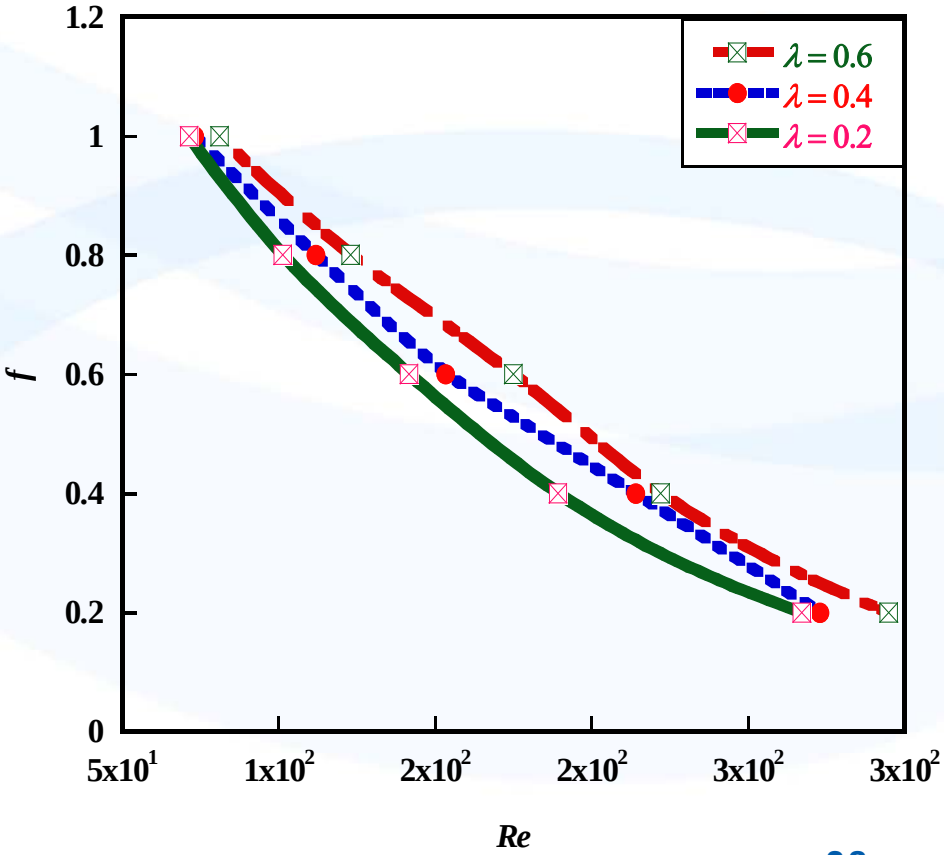
(a) **(b)** **(c)**

Friction factor, pitch & clearance ratio (Need for trade-off between performance and pumping power)

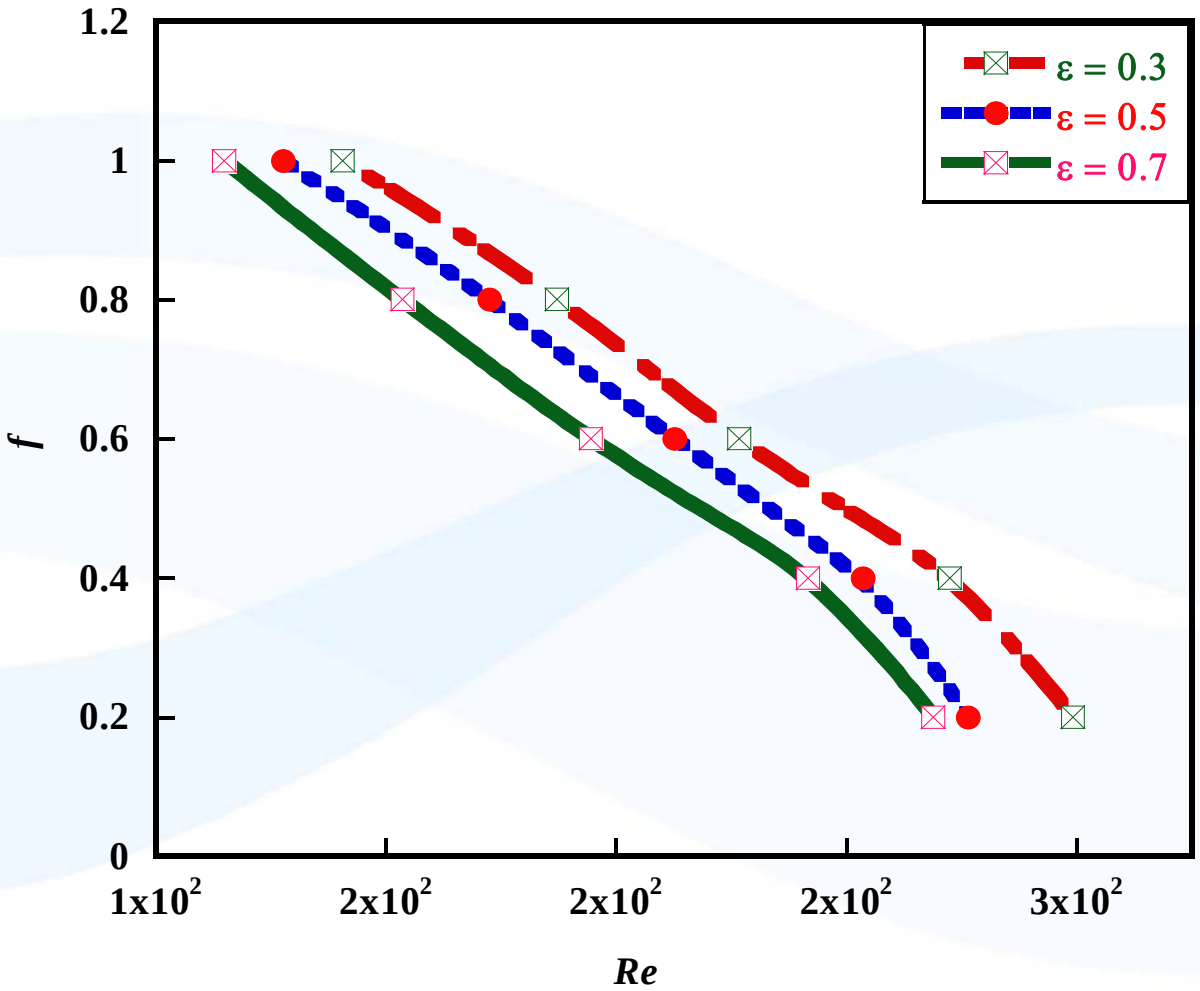
Cathode gas channel friction factor as a function of the Reynolds number and pitch, (λ = 0.3).



Cathode gas channel friction factor as a function of the Reynolds number and clearance ratio, (s/d = 5).

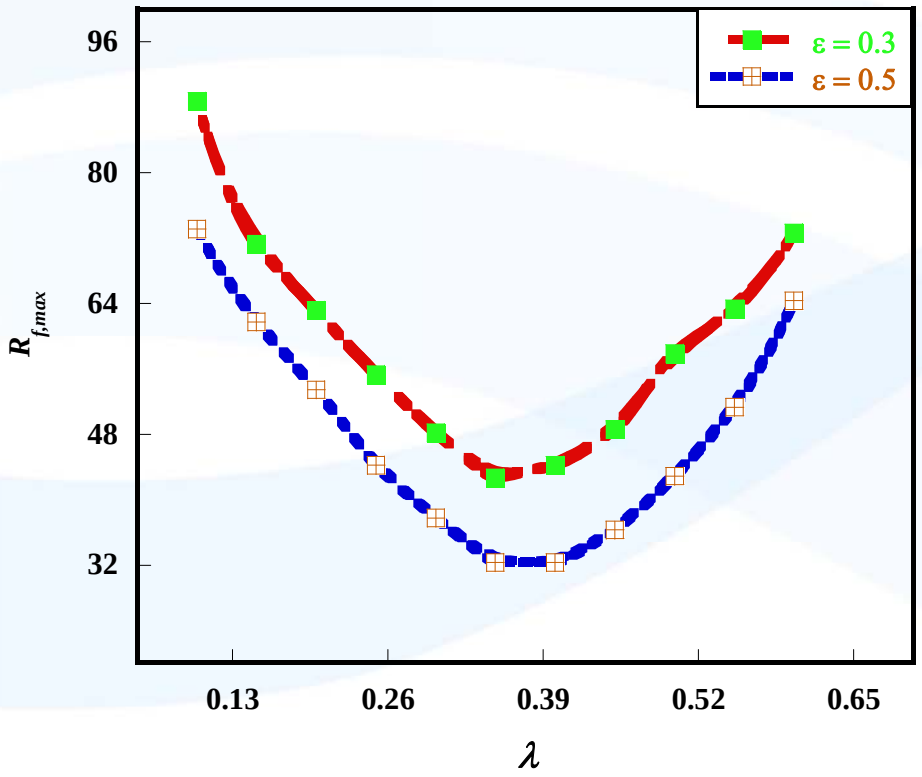


Cathode gas channel friction factor as a function of the Reynolds number and GDL porosity, (λ = 0.3 & *s/d* = 5).

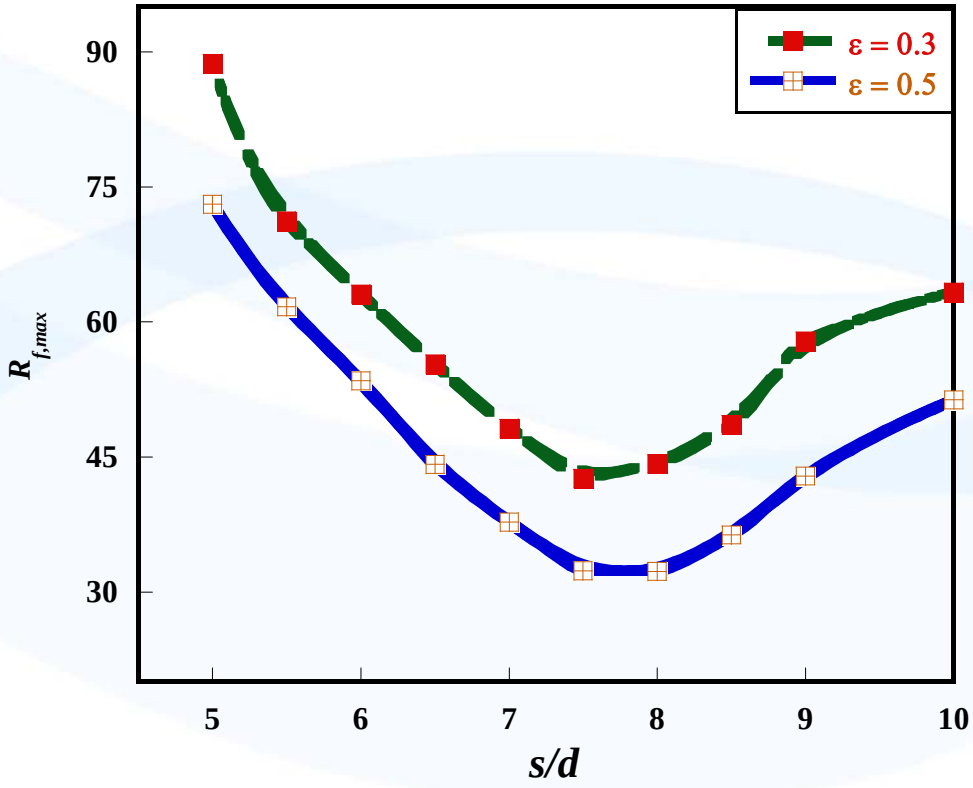


Results of optimised clearance ratio & pitch

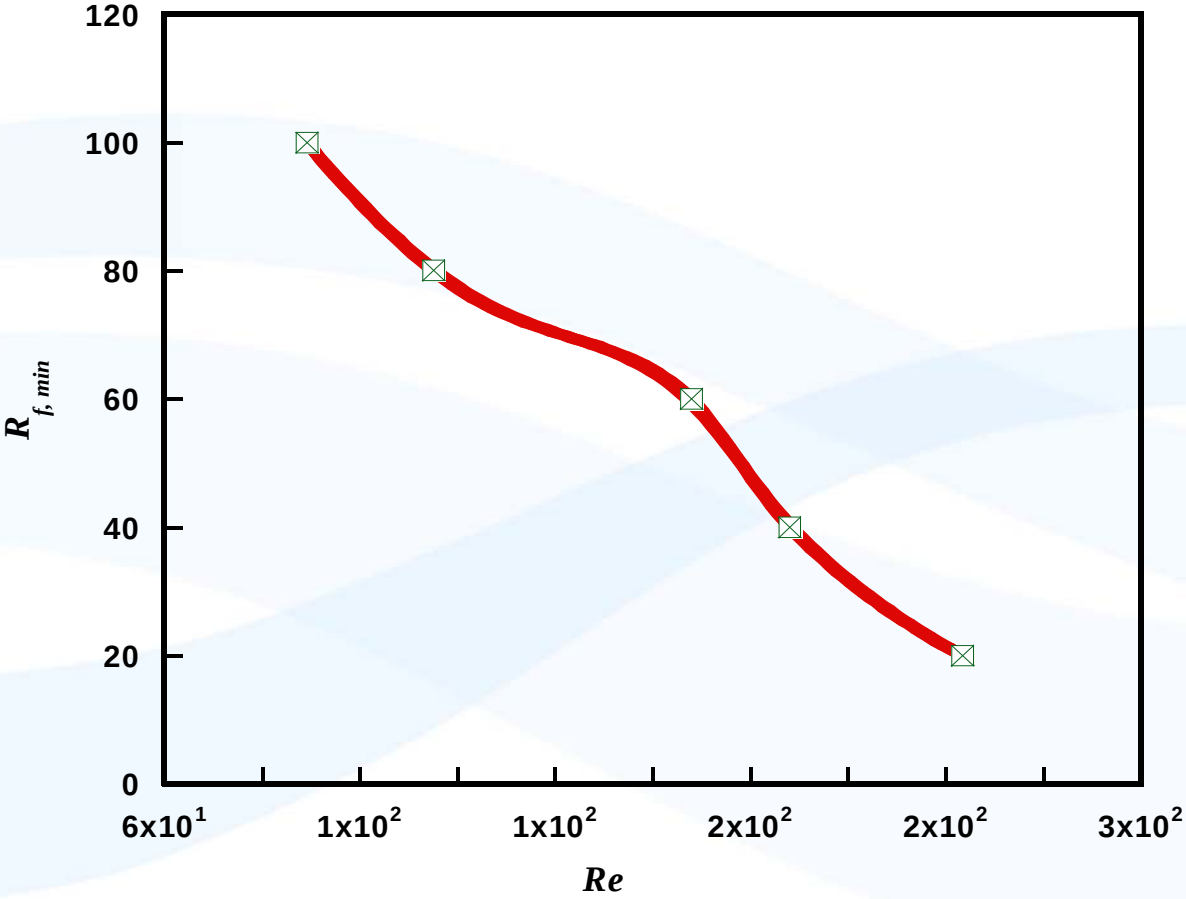
Effect of optimised clearance ratio on the peak cathode channel flow resistance



Effect of optimised pitch on the peak cathode gas channel flow resistance

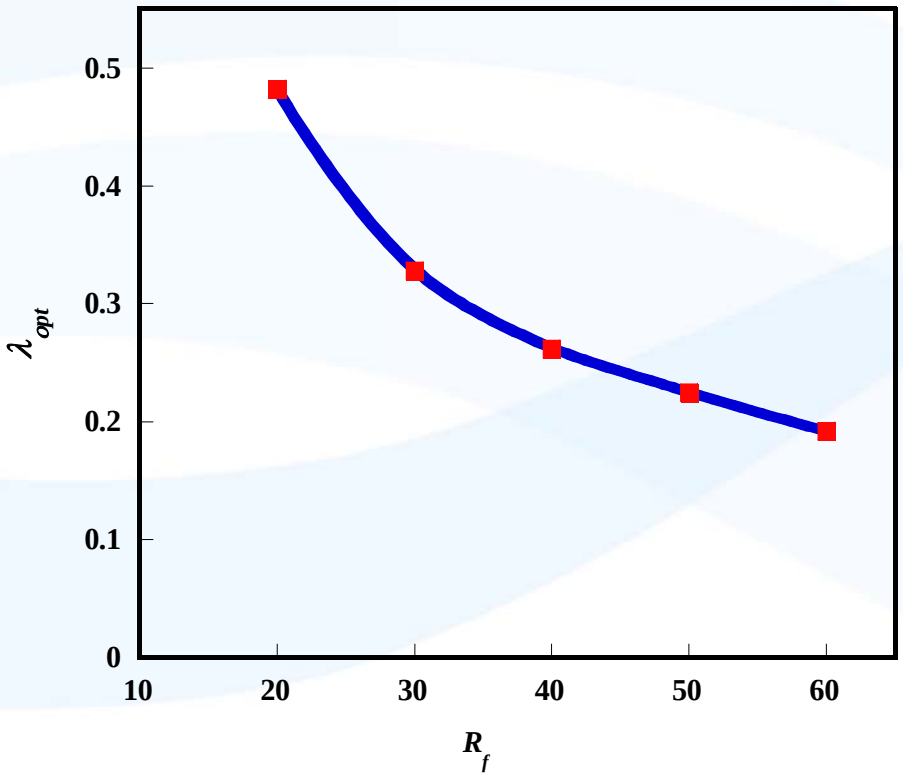


Minimised cathode gas channel flow resistance as function of Reynolds number, (ε = 0.5 & λ = 0.3).

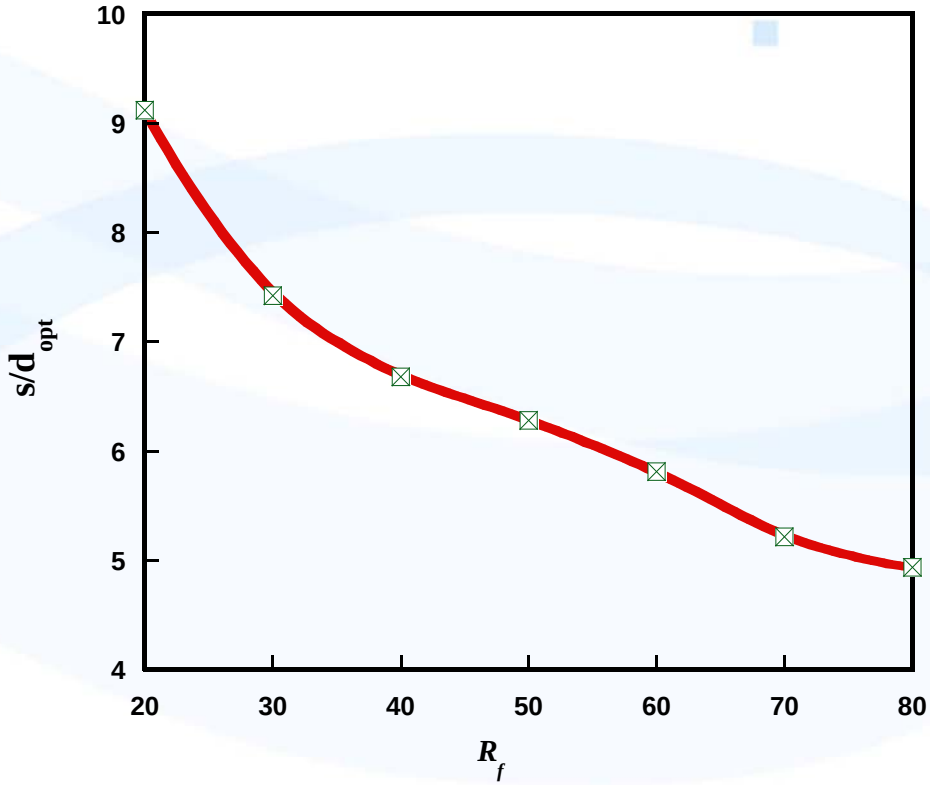


Channel flow resistance, optimised clearance ratio & optimised pitch

Effect of channel flow resistance on the optimised clearance ratio (s/d = 5, ε = 0.5 & Re = 250)

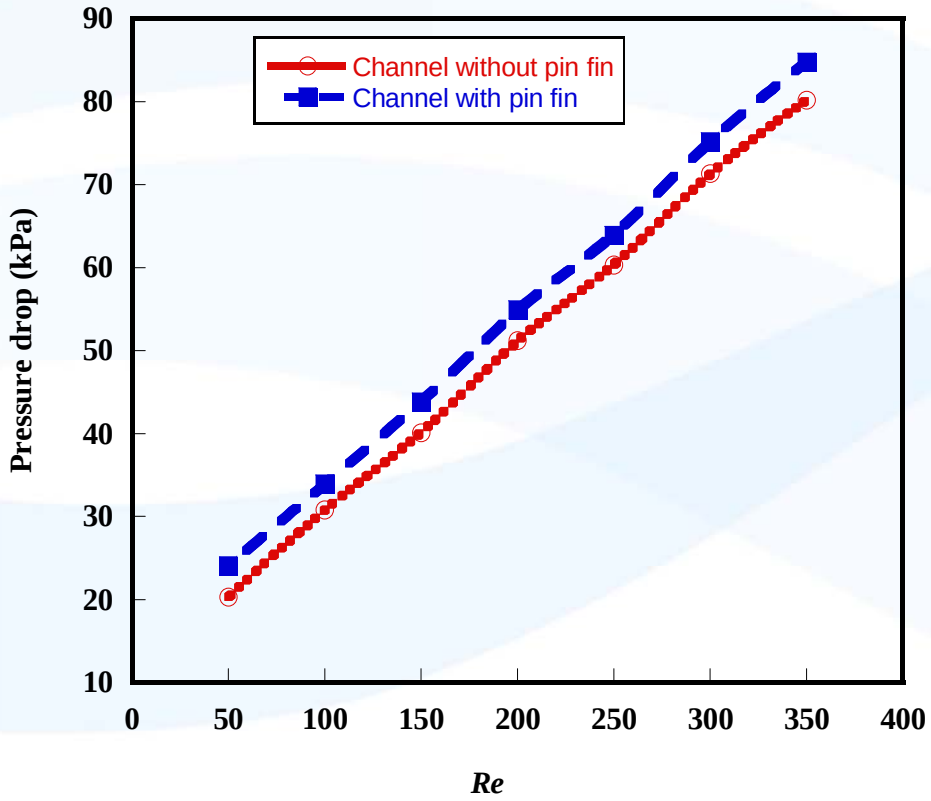


Effect of channel flow resistance on the optimised pitch (λ = 0.3, ε = 0.5 & Re = 250)

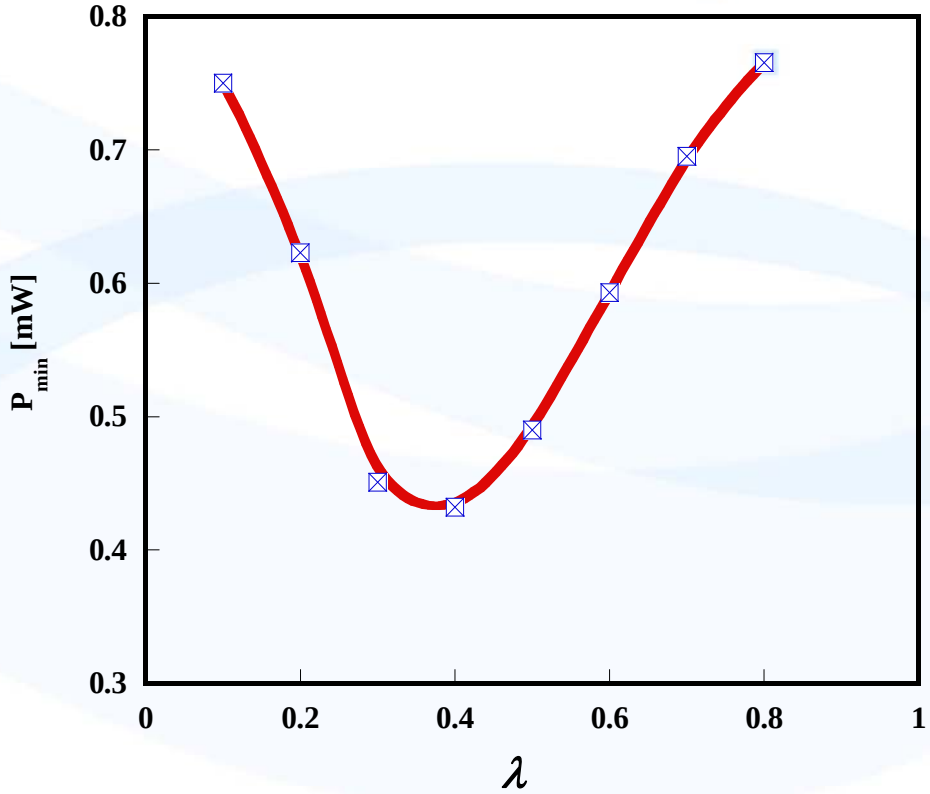


Performance evaluation:

Cathode channel pressure drop for a channel with pin fin (s/d = 5, λ = 0.3) and channel without pin fin.



Pumping power as a function of tip clearance ratio (s/d = 5, ε = 0.6 & Re = 250)



Research objective 3:
Previous studies in area of research (Thermal cooling for PEM fuel cell maximum performance)

- Coppo *et al.* (2006). Presented a 3D model to study the influence of temperature on PEM performance. Study confirms that water transport & removal from GDL surface by temperature variation affects the system performance.

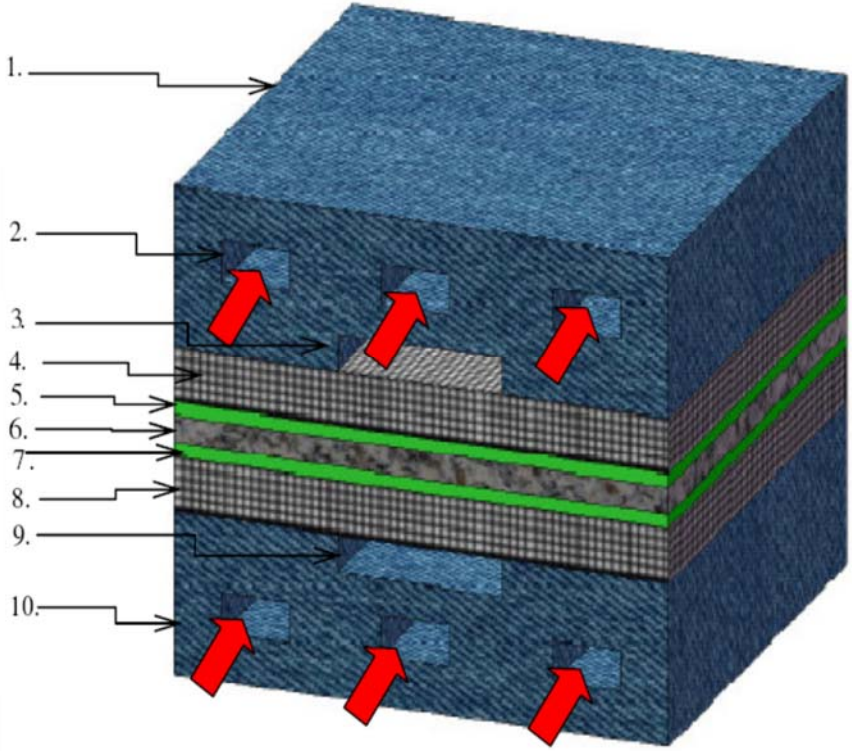
- Ramousse *et al.* (2005). Presented a numerical model accounting for heat and mass transfer. The study shows that thermal stresses are induced at higher current density of cell operation.

Issues of interest:

- *Investigate on operating PEM fuel cell beyond the critical temperature (~80 ^{0}C) without special high temperature materials.*

- *Develop a cooling channel geometry scheme for enhanced PEM fuel cell performance*

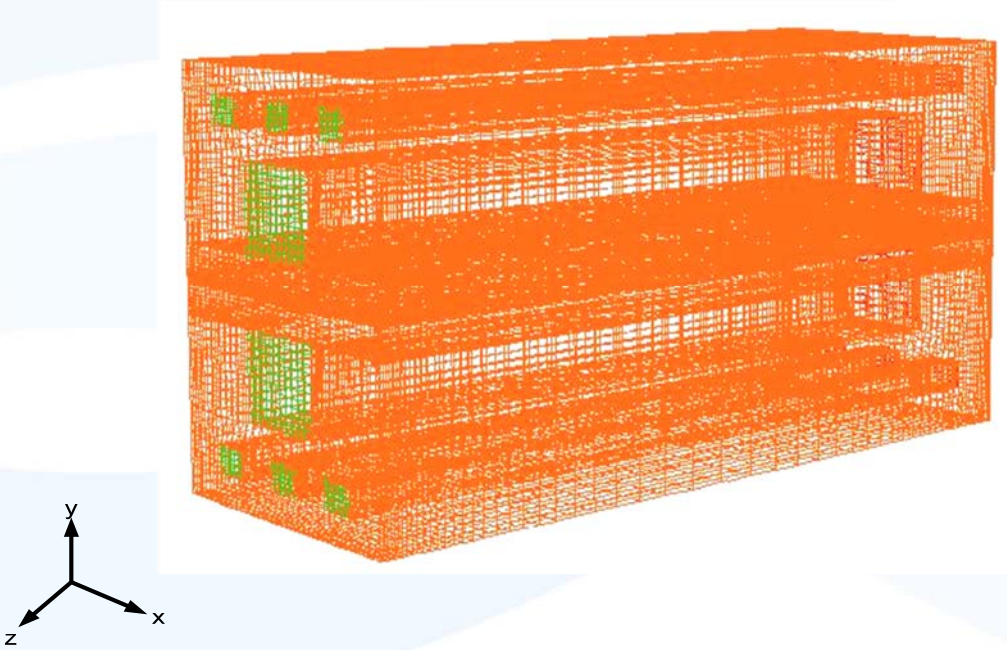
Model 3 description: *3-D computational domain of PEM fuel cell with cooling channels.*



1. Anode-side bipolar plate
2. Cooling channels
3. Hydrogen fuel channel
4. Anode GDL
5. Anode Catalyst layer
6. Membrane
7. Cathode catalyst layer
8. Cathode GDL
9. Air gas channel
10. Cathode-side bipolar plate

Discretised 3-D domain & temperature dependent parameters

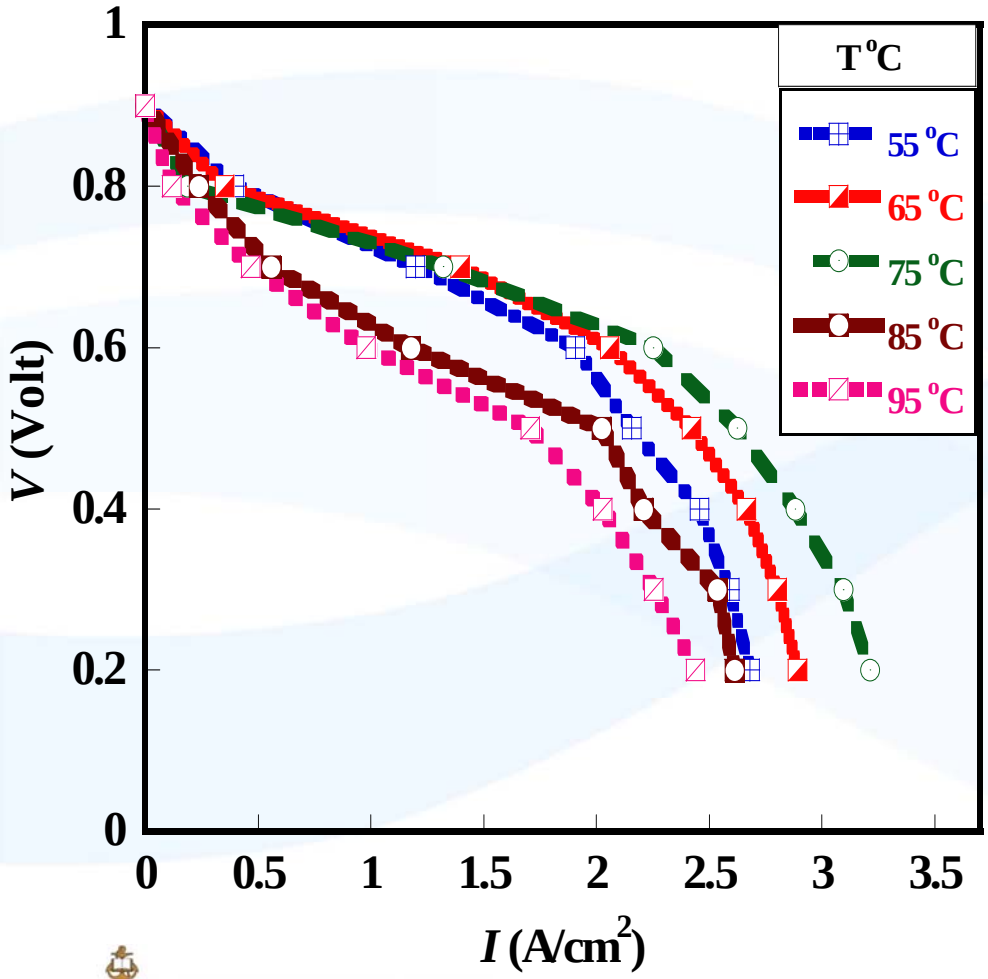
The discretised three-dimensional computational domain

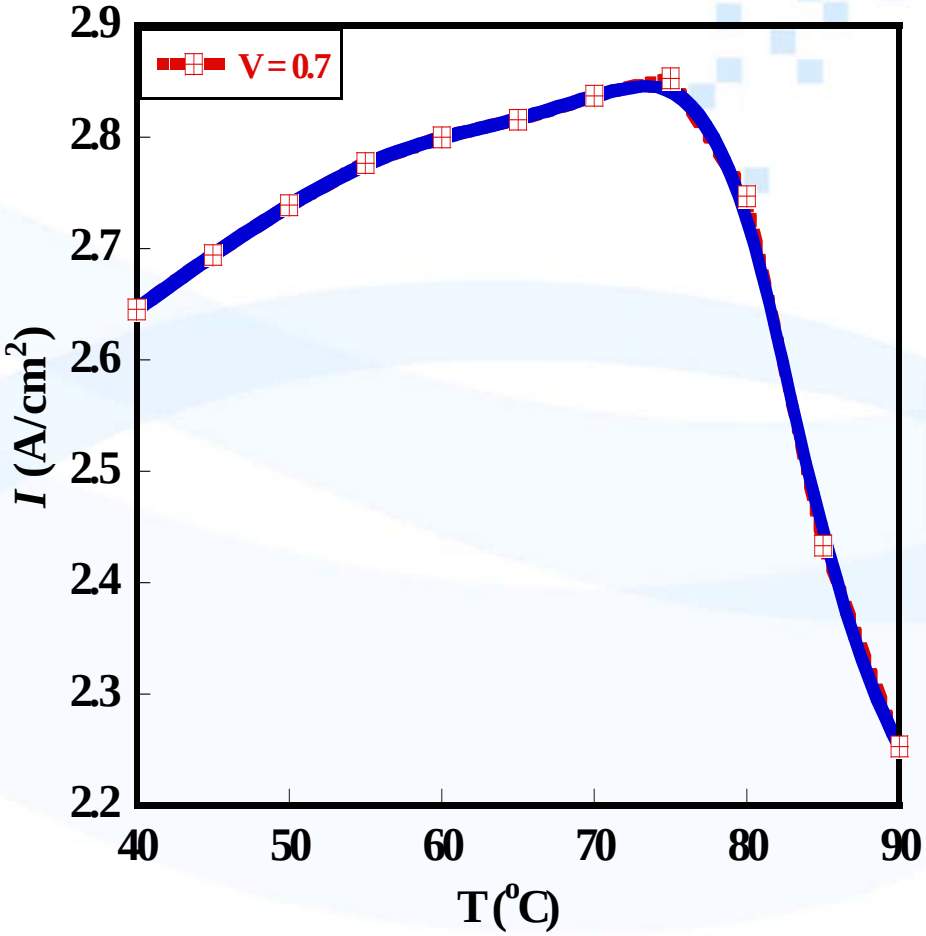


Temperature dependent parameters in PEM fuel cell

- Stoichiometry ratio
- Relative humidity (RH)
- Cooling channel aspect ratio

Effect of temperature on PEM fuel cell performance





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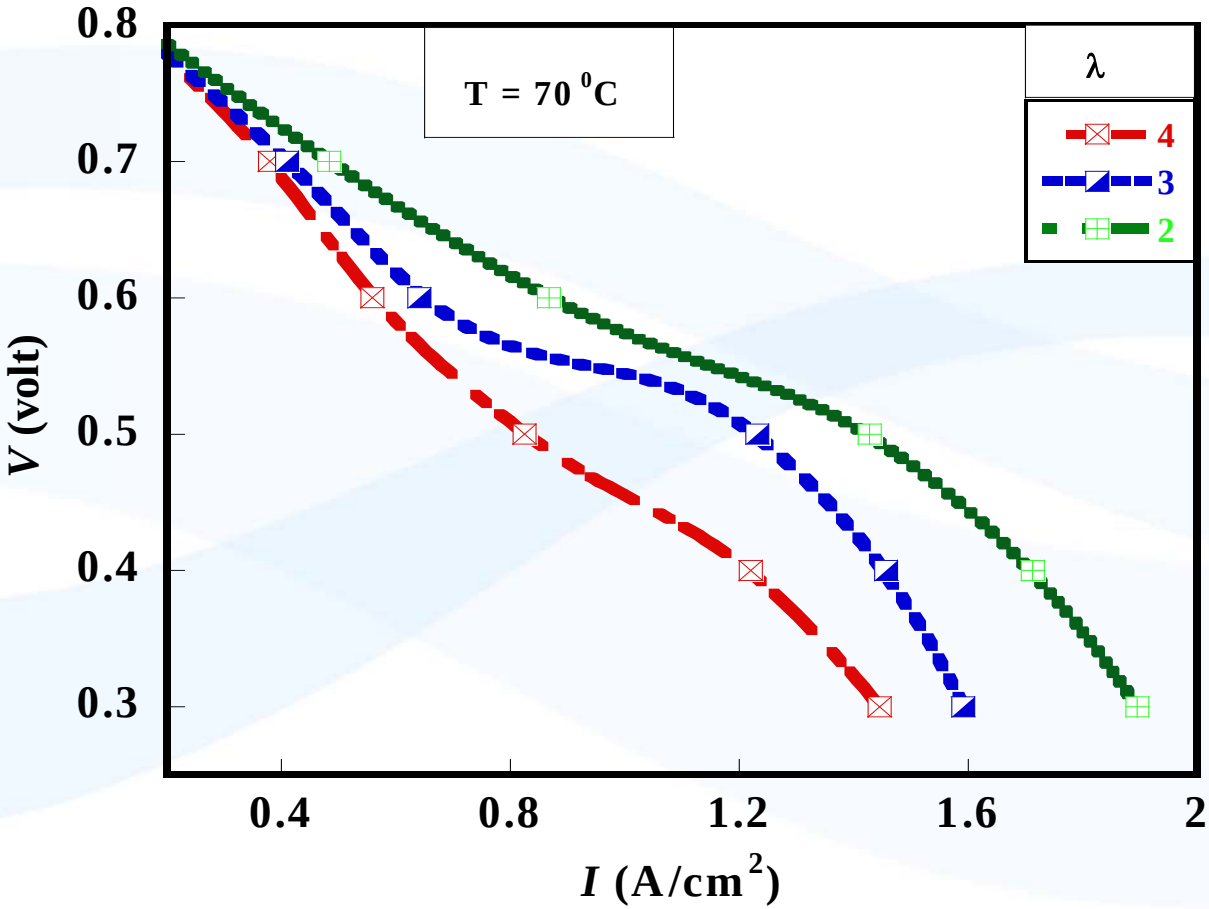
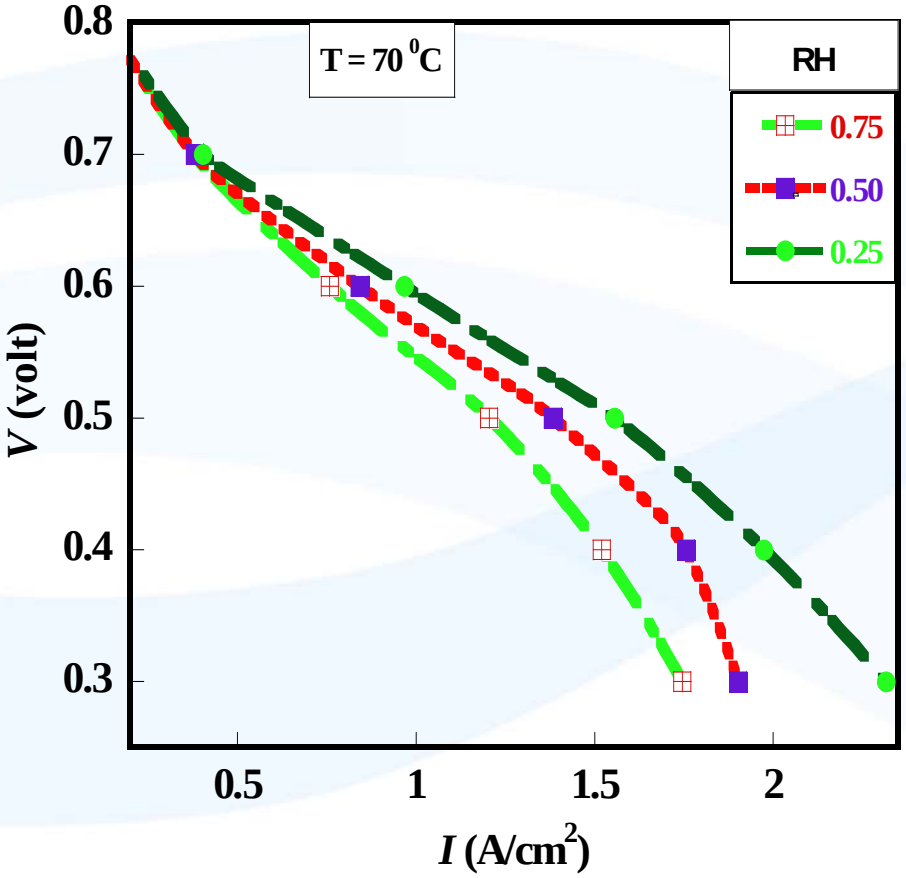
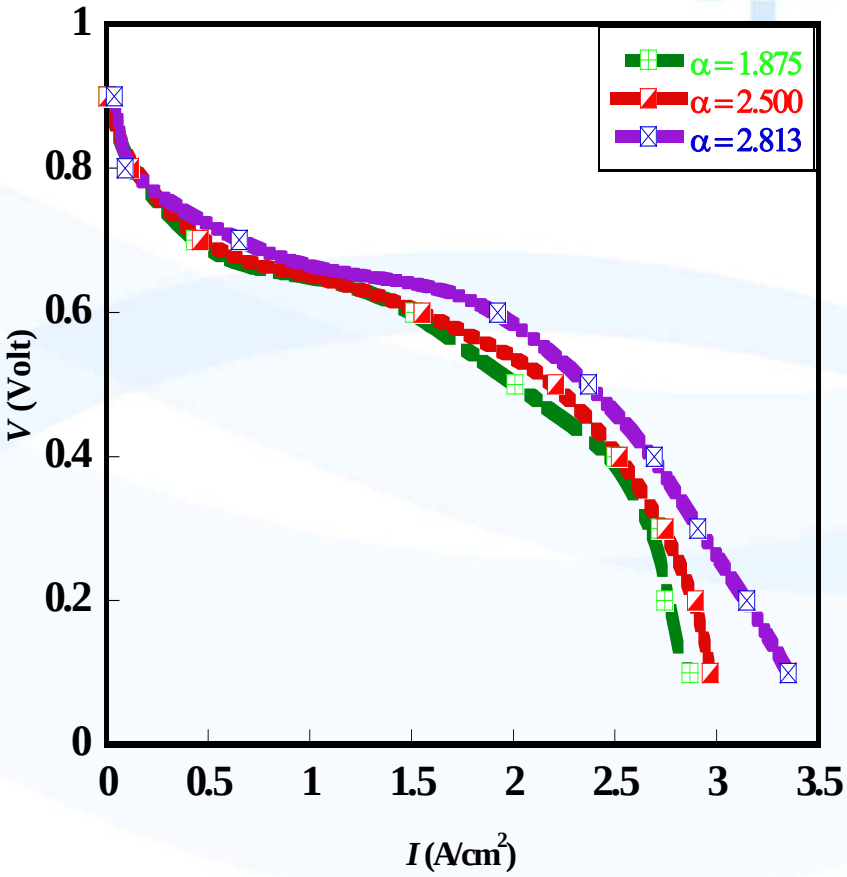
Effect of stoichiometry ratio on PEM fuel cell performance



Effect of relative humidity & cooling channel aspect ratio on PEM fuel cell performance





Optimization problem formulation:

To obtain maximised current density output for the optimised design variables.

- **The objective function for the study is:**

$$I_{max} = f(\lambda_{opt}, RH_{opt}, H/W_{opt})$$

- **Imposed constraints:**

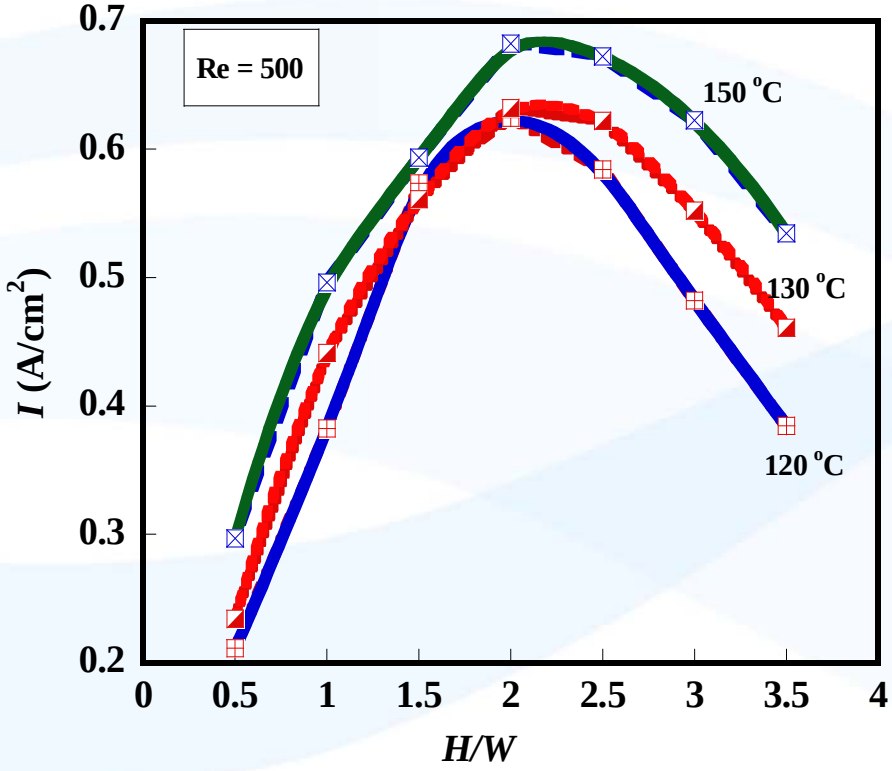
$$1 \leq \lambda \leq 5$$

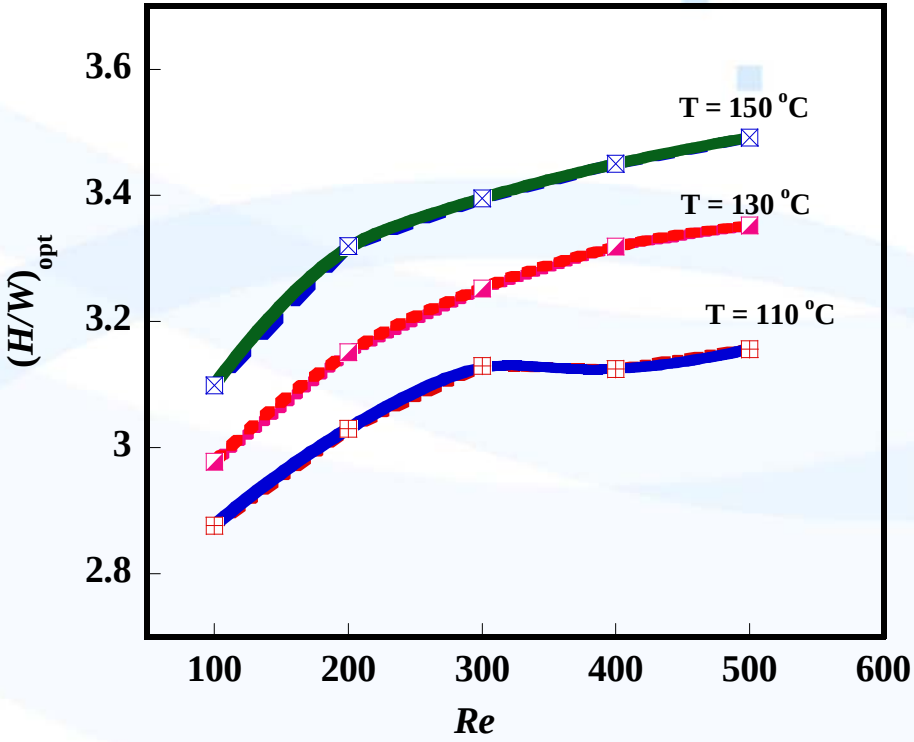
$$0.2 \leq RH \leq 1.0$$

$$1.5 \leq H/W \leq 3.5$$

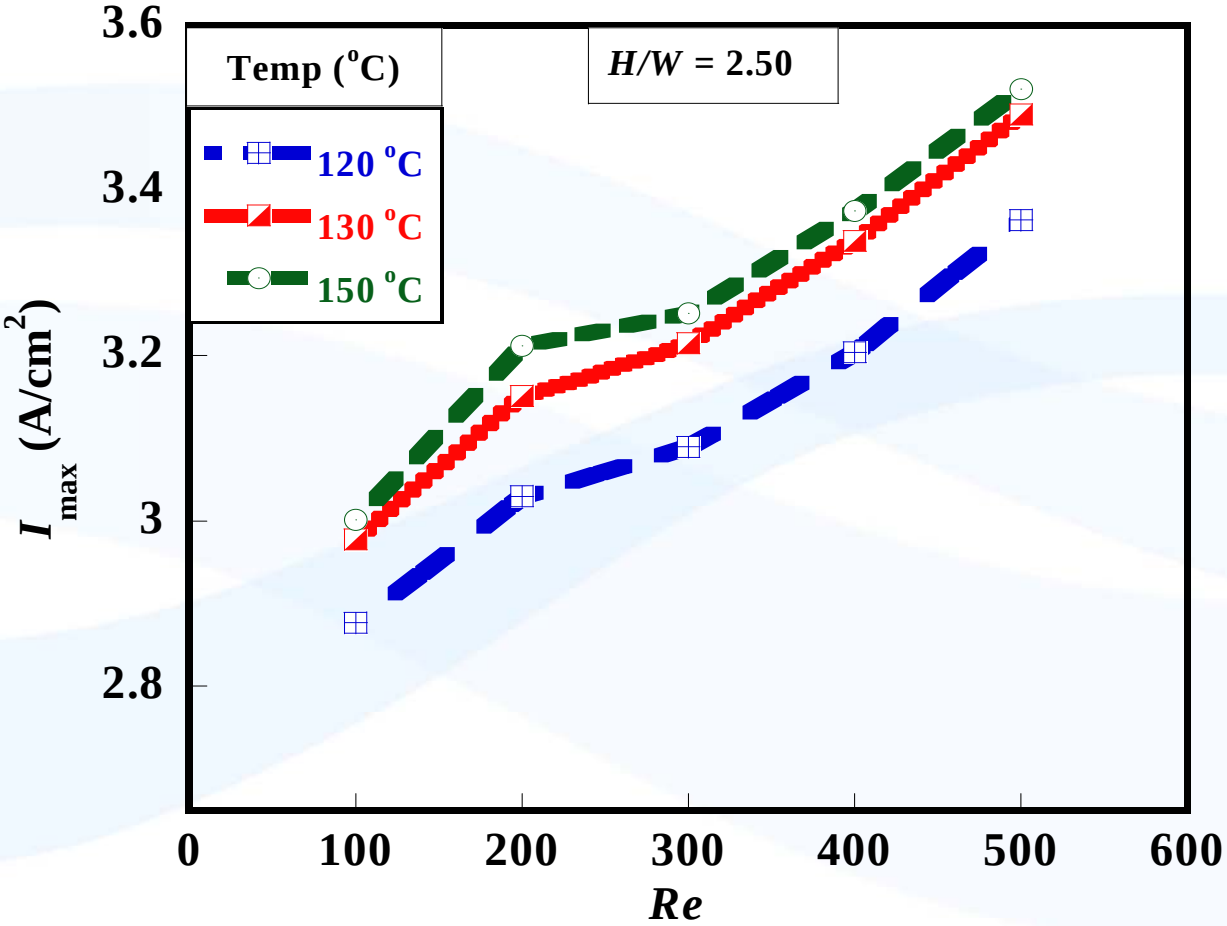
$$100 \leq \mathrm{Re} \leq 500$$

Effect of cooling channel aspect ratio on cell performance at different temperature





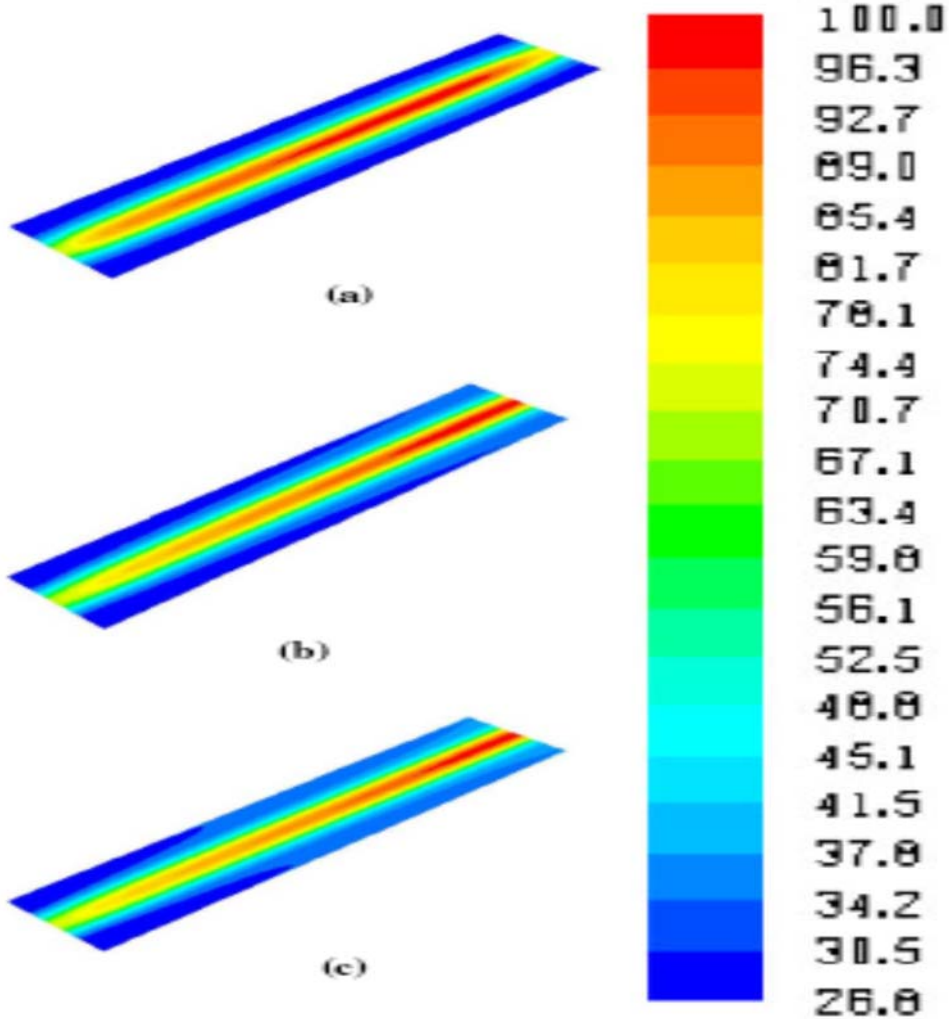
Maximised current density as a function of Reynolds number and cell temperature



PEM fuel cell performance at different operating cell voltages

Cell voltage (V)	*I* (A/cm^2) (T = 120 °C)	*I* (A/cm^2) (T = 130 °C)	*I* (A/cm^2) (T = 150 °C)
0.7	3.1421	3.6213	3.8228
0.6	4.0627	4.7341	5.1431
0.5	4.6814	5.4326	5.6314
0.4	5.3343	5.9531	6.3281

The local distribution of temperature along the membrane at different cooling channel aspect ratios and cell operating voltage of 0.7 V and Re = 500: (a) = 1.875, (b) = 2.50 and (c) = 2.813.



Conclusions: model case 1

- The model predictions are in good agreement with experimental data.
- Gas diffusion layer porosity and cathode gas mass flow rate affect the performance of the fuel cell.
- Porosity effect on cell performance are more significant at porosity levels of 0.1 to 0.4 than at 0.5 to 0.7.
- The study shows that appropriate match of PEM fuel cell parameters (i.e. porosity, species mass flow rates and channel geometry) can significantly improve fuel cell performance.

Conclusion: Model case 2

- **The flow Reynolds number had a significant effect on the reactant flow field, and the diffusion of the reactant gas through the GDL medium increased as the Reynolds number increased.**

- **The friction factor increased with an increasing clearance ratio of the pin fin in the channel.**

- **The optimal clearance ratio and pitch for the considered fuel cell channel decreased with an increase in the fuel channel friction.**

- **The friction factor decreased with an increase in the GDL porosity. Hence, the channel friction and pressure drop can be reduced significantly with increased GDL porosity.**

Conclusion model case 2 contd.

- **An optimal pin fin clearance ratio existed which offered minimum pumping power requirement.**

- **An enhanced fuel cell performance was achieved by using pin fins in a fuel cell gas channel, which ensured high performance and low fuel channel pressure drop of the fuel cell system.**

Conclusion: Model case 3

- **PEM fuel cell performance is considerably enhanced when PEM fuel cells operate at combined optimised design parameters.**

- **Performance is more outstanding at temperatures between 120°C and 130°C. However, the performance increment rate declines gradually from 130°C to 150°C.**

- **The study shows the possibility of operating a PEM fuel cell beyond the critical temperature range (80°C) by using the combined optimised stoichiometry ratio, relative humidity and cooling channel geometry.**

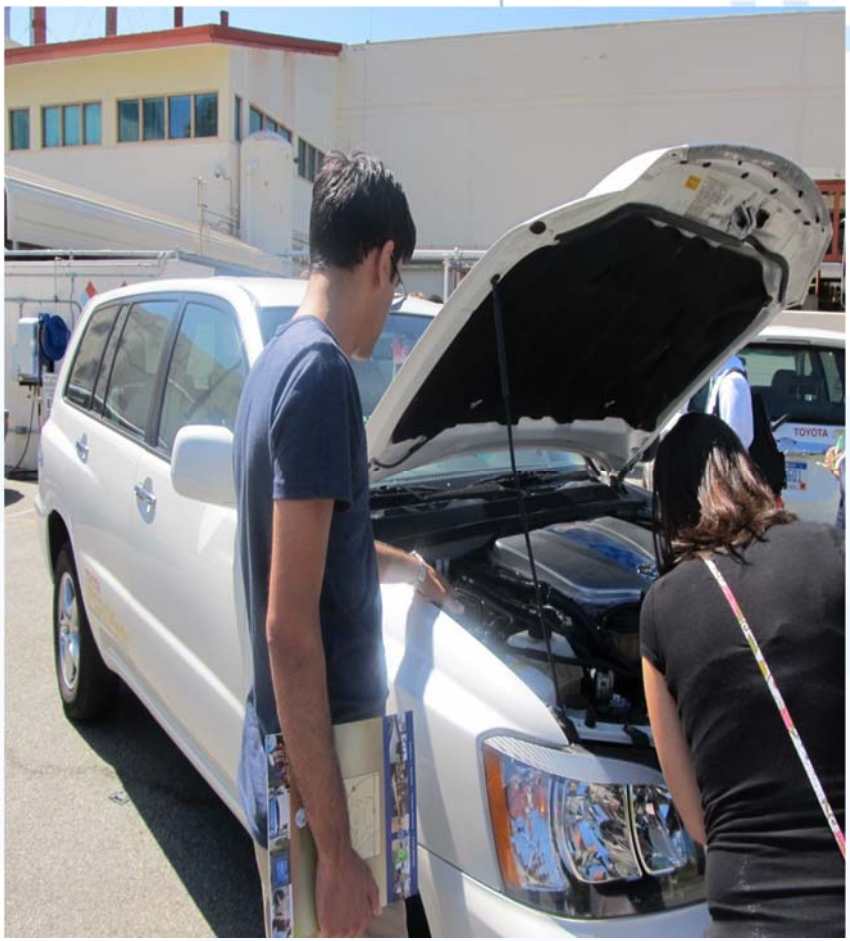
- **It should also be noted that this study can easily be extended to different cooling channels (apart from the rectangular channels used in this study) in order to enhance the performance of PEM fuel.**

Recommendation for future work

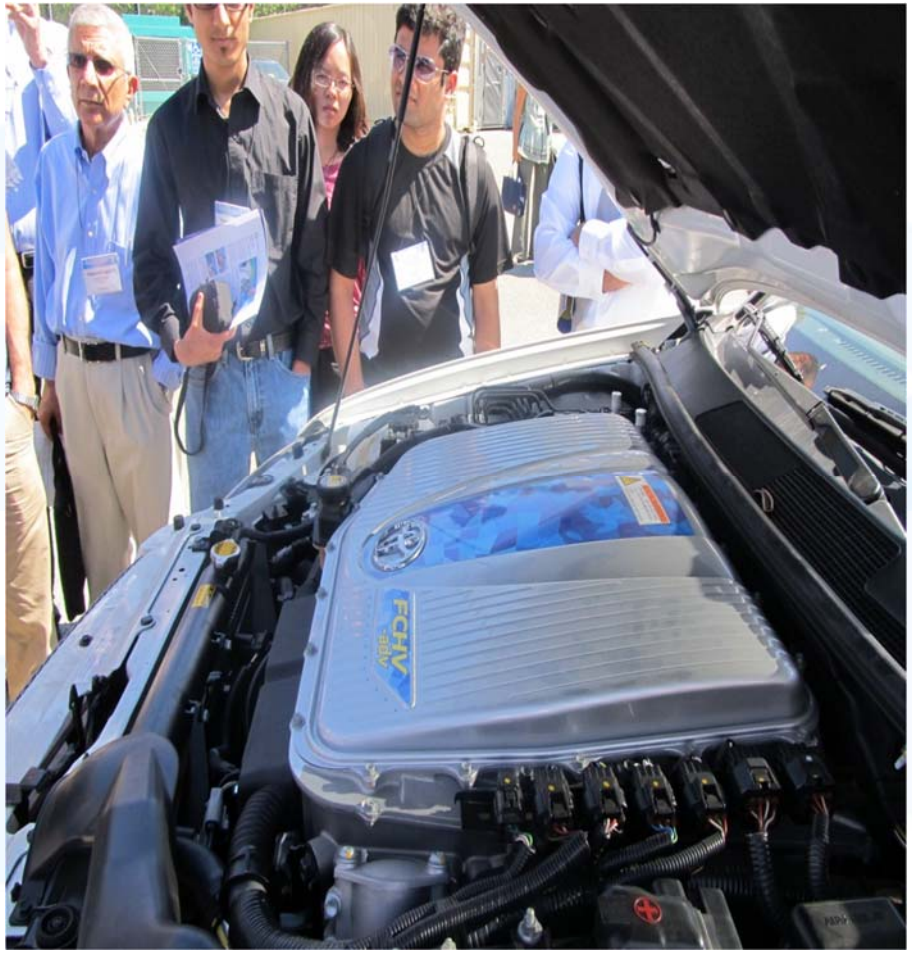
- **Evaluation of PEM fuel cell under different material properties rather than assuming isotropic & homogeneous**
- **Need for consideration for two-phase flow in the PEM fuel cell structures to enhance modeling results.**
- **Large scale simulations using parallel computing will reduce computational time especially in model with multi-parameter evaluation.**
- **Experimental validation of results in standard fuel cell test stations to enhance model result implementation.**

Fuel cells application: myth or reality

Fuel cell: *Energy of the future*:



Fuel cell: *Energy of the future*:



List of Publications from the study:

- **S.O Obayopo,** T.Bello-Ochende, J.P. Meyer (2011); **Three-dimensional optimization of a fuel gas channel of a PEM fuel cell for maximum current density**, *International Journal of Energy Research (Wiley Science)* paper no: DOI:10.1002/er.1935. ***Impact factor: 2.122***

- **S.O. Obayopo**, T. Bello-Ochende, J.P. Meyer (2012), **'Modelling and optimization of reactant gas transport in PEM fuel cell with transverse pin fin insert in channel flow',** *International Journal of Hydrogen Energy* 37 (13):10286-10298. ***Impact factor: 4.054***

- T. Bello-Ochende, **S.O. Obayopo**, J.P. Meyer, **'Conceptual design of high current density PEM fuel cell with optimized cooling channels' – *under review.***

- **S.O. Obayopo,** T. Bello-Ochende, J.P. Meyer, '**Impact of Cooling Channel Geometry on Thermal Management and Performance of a Proton Exchange Membrane Fuel Cell',** *Proceeding of the 9th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics*, HEFAT 2012, 16-18 July 2012,Malta

List of Publications contd:

- **S.O. Obayopo,** T. Bello-Ochende, J.P. Meyer, 'Numerical Study and Optimisation of Channel Geometry and Gas Diffusion Layer of a PEM Fuel Cell', *Proceedings of the ASME 2012 6th International Conference on Energy Sustainability & 10th Fuel Cell Science, Engineering and Technology Conference ESFuelCell2012*, July 23-26, San Diego, CA, USA.

- **S.O. Obayopo**, T. Bello-Ochende, J.P. Meyer, 'Optmising the Performance of a PEM Fuel Cell with Transverse Fins Insert in the Channel Flow using Mathematical Algorithm', *Proceedings of the ASME 2012 6th International Conference on Energy Sustainability & 10th Fuel Cell Science, Engineering and Technology Conference ESFuelCell2012*, July 23-26, San Diego, CA, USA.

- **S.O. Obayopo,** T. Bello-Ochende, J.P. Meyer, 'Numerical Study of effect of design and physical parameters on a PEM fuel cell performance', *Proceeding of the 8th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics,* HEFAT 2011, pp 567, Pointe Aux Piments, Mauritius, 11-13 July 2011.

- **S.O. Obayopo,** T. Bello-Ochende, J.P. Meyer, 'Thermodynamic Optimization of PEM Fuel Cell Stack Gas Channel for Optimal Thermal Performance', *Proceeding of the 14th "International Heat Transfer Conference (ASME),* IHTC-14, paper no. IHTC14-22233 Washington DC USA, 8-13 August 2010.

List of Publications contd:

- **S.O. Obayopo,** T. Bello-Ochende, J.P. Meyer, **'Numerical Optimization of a Single PEM Fuel Cell under Variable Operating Conditions**', *Proceeding of the 7th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics,* HEFAT 2010, pp 667-672, Antalya Turkey, 19-21 July 2010.

- **S.O. Obayopo**, T. Bello-Ochende, J.P. Meyer, **'Thermodynamic Optimization of Proton Exchange Membrane Fuel Cell System',** *Proceeding of the 1st National symposium on Renewable and Sustainable Energy Center for Renewable and Sustainable Energy Studies,* NCRS2010, Paper no. NCRS017. pp 1-15.Stellenbosh South Africa, 11-12 November 2010

- **S.O. Obayopo**, T. Bello-Ochende, J.P. Meyer, **'Performance enhancement of PEM fuel cell through reactant gas channel and gas diffusion layer optimization',** *Proceeding of the 2nd National symposium on Renewable and Sustainable Energy Center for Renewable and Sustainable Energy Studies,* NCRS2011, Paper no. NCRS010. pp 1-15.Stellenbosh South Africa, 17-18 November 2011.

Appreciation:

- My supervisors (Prof. T. Bello-Ochende & Prof. J.P. Meyer)
- Prof. J.A. Snyman.
- All academic & non-academic staff of Department of Mechanical Engineering University of Pretoria.
- My family: Rofiat , Abdul-Rahman, Mar'yam & Ibrahim.
- All research students and friends.
- Advanced Engineering Centre of Excellence at the University of Pretoria, NRF, TESP, NAC, the SOLAR Hub with the Stellenbosch University, EEDSM Hub and the CSIR.

THANK YOU FOR YOUR ATTENTION…..