Parametric Optimization for PEM Fuel Cells based on Numerical Simulation

利用數值模擬進行燃料電池參數最佳化

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Outline

- Introduction
- Inverse Theory
- PEM Fuel Cell Modeling & Experiments
- PEM Fuel Cell Optimization
- Concluding Remarks

Power and Light












民國96年台灣地區能源分配:
(經濟能源局統計資料)

單位:公秉油當量

能源類別	總計		自產能源		進口能源	
	數量	分配比(%)	數量	分配比(%)	數量	分配比(%)
總計	146,237,480	100.00%	2,495,296	1.71%	143,742,184	98.29%
煤炭及煤產品	47,004,652	32.14%	0	0.00%	47,004,652	32.14%
原料煤	3,698,034	2.53%	0	0.00%	3,698,034	2.53%
燃料煤	42,876,055	29.32%	0	0.00%	42,876,055	29.32%
煤產品	430,563	0.29%	0	0.00%	430,563	0.29%
石油	74,749,980	51.12%	17,778	0.01%	74,732,202	51.10%
原油	57,491,122	39.31%	17,778	0.01%	57,473,344	39.30%
石油產品	17,258,858	11.80%	0	0.00%	17,258,858	11.80%
液化天然氣	11,935,402	8.16%	0	0.00%	11,935,402	8.16%
天然氣	412,204	0.28%	412,204	0.28%	0	0.00%
水力發電	2,065,314	1.41%	2,065,314	1.41%	0	0.00%
核能發電	10,069,928	6.89%	0	0.00%	10,069,928	6.89%

CH_3OH in

Evaporator

Phase Conversion

converts liquid methanol to gaseous methanol

Heat in

Reformer

Catalytic Conversion

converts methanol to hydrogen

Air in

Fuel Cell

Electro-chemical Conversion

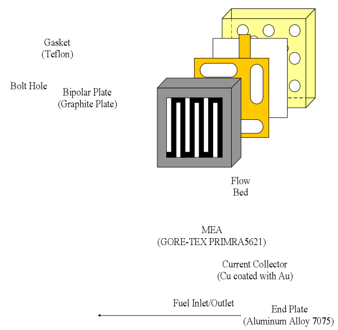
converts hydrogen to water and electricity

Electricity + Water out

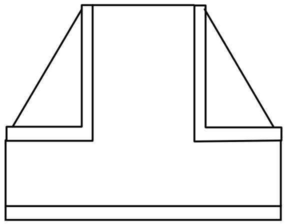
Electro-chemistry (Bulter-Volmer Kinetics)
Electromigration/convection/diffusion
Heat and mass transfer in porous media
Vaporization/condensation
Water and thermal management
Electron/proton conduction

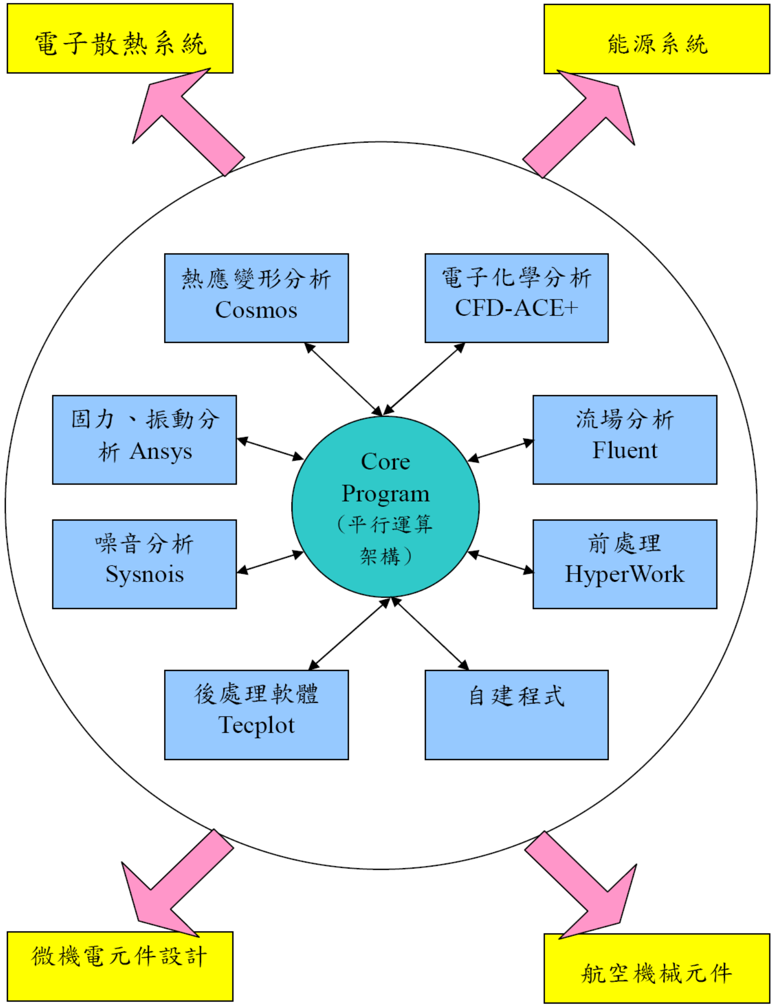
Influential Parameters

- **Operation:**
  Cell Temperature, Packing Pressure, Contamination, ….
- **Bipolar Plates-Fuel Channels:**
  Channel Pattern, Channel Width Ratio, Cross-Sectional Shape, Electric Conductivity, Thermal Conductiviy, ….
- **Fuels Fed at Anode & Cathode:**
  Fuel Inlet Temperature, Inlet and Outlet Pressures, Composition, Humidity, ….
- **Gas Diffusion Layers:**
  Characteristics of Porous Material, Thickness, Electric Conductivity, ….
- **Catalyst Layers:**
  Characteristics of Porous Material, Pt Loading, Thickness, Electric Conductivity, Electro-Chemical Characteristics, ….
- **Membrane:**
  Characteristics of Porous Material, Thickness, Proton Conductivity, Water Content, ….



Optimal Design





Direct Problem (Forward Problem)

Causes		**Effects**
history boundary conditions properties & coefficients geometry	→	performance thermal behavior flow pattern stress & strain

Inverse Problem (Backward Problem)

Causes		Effects
history	⇐	performance
boundary conditions		thermal behavior
properties & coefficients		flow pattern
geometry		stress & strain

Inverse Heat Transfer Problems (IHTPs)

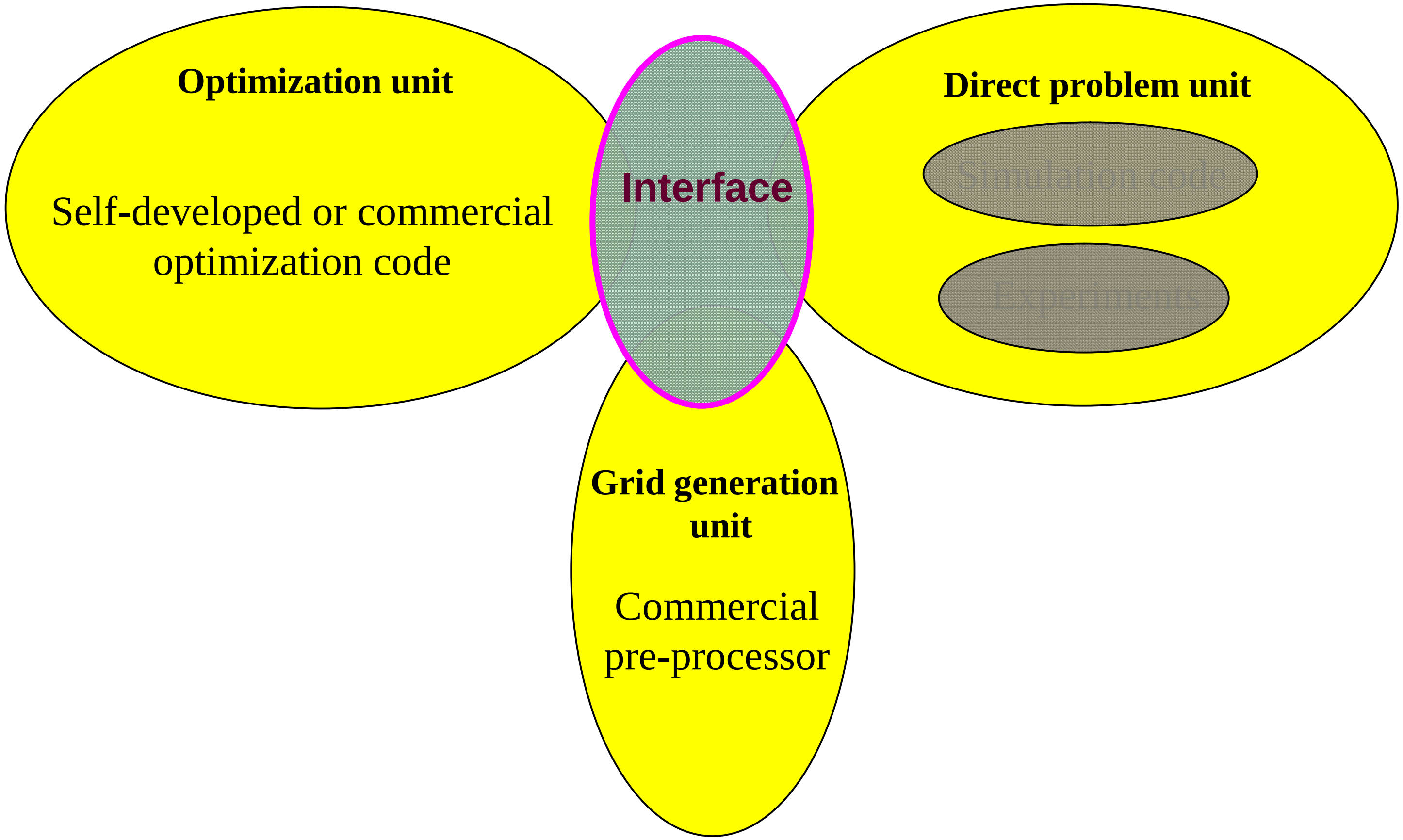
Retrospective inverse problem – history

Boundary inverse problem – boundary conditions

Coefficient inverse problem – properties & coefficients

Geometric inverse problem – geometry

Structure of Optimizer



SCGM Method

Variables updated $A_k^{n+1} = A_k^n - \beta \cdot \xi_k^n$

Search direction $\xi_k^n = \dfrac{\partial J^n}{\partial A_k} + \gamma_k^n \cdot \xi_k^{n-1}$

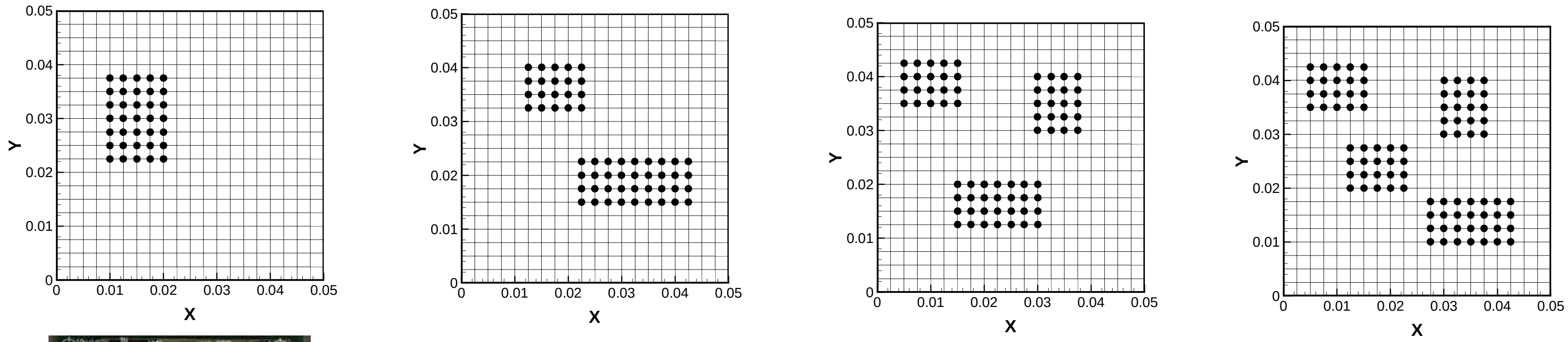
Conjugate-gradient coefficient $\gamma_k^n = \left[\left(\dfrac{\partial J}{\partial A_k} \right)^n \Big/ \left(\dfrac{\partial J}{\partial A_k} \right)^{n-1} \right]^2$

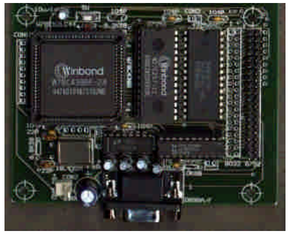
Step size $\beta_k^n = 0.01 \sim 0.001$

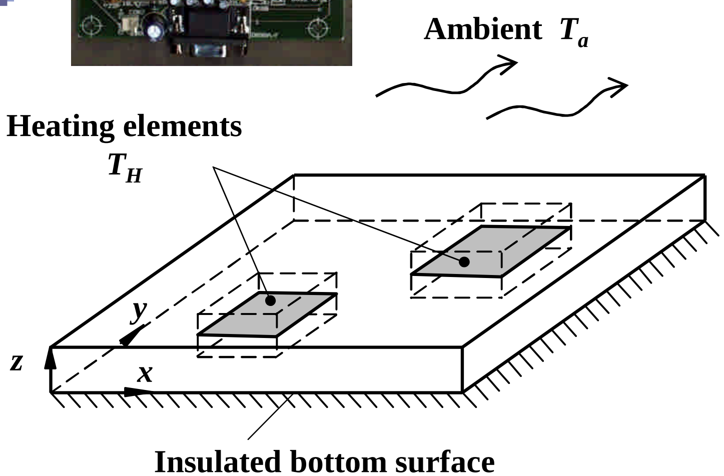
Source: Chang, M.H. and Cheng, C.H., "A Simplified Conjugate-Gradient Method for Shape Identification Based on Thermal Data", *Numerical Heat Transfer* B, **43**, 489-507, 2003.

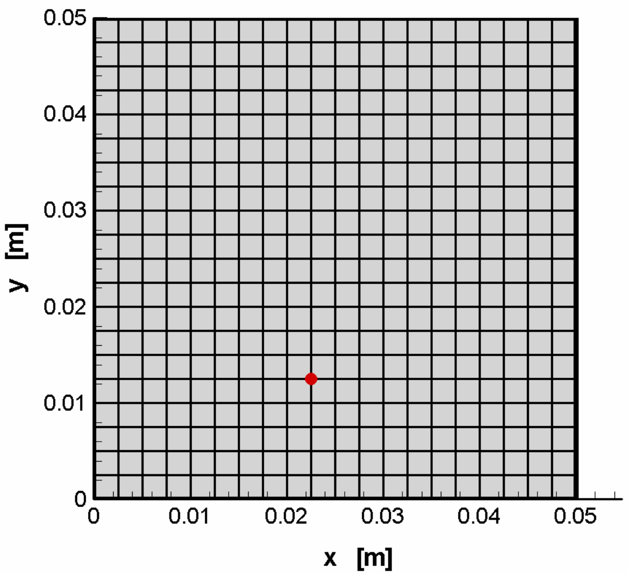
Optimizer with SCGM

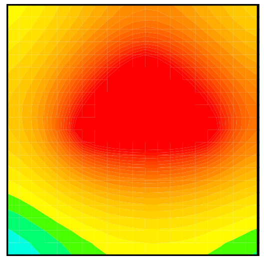
Identification of Heating Chips in MCM Packages

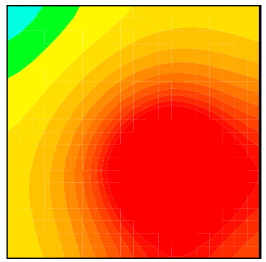






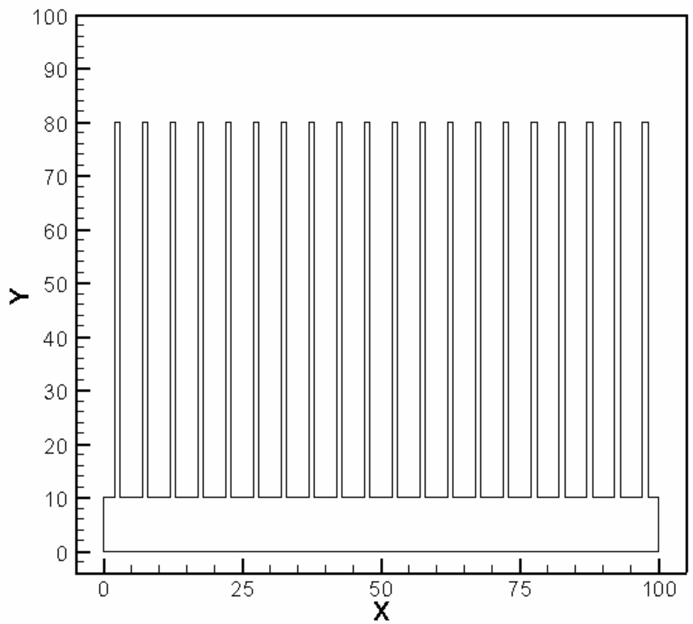


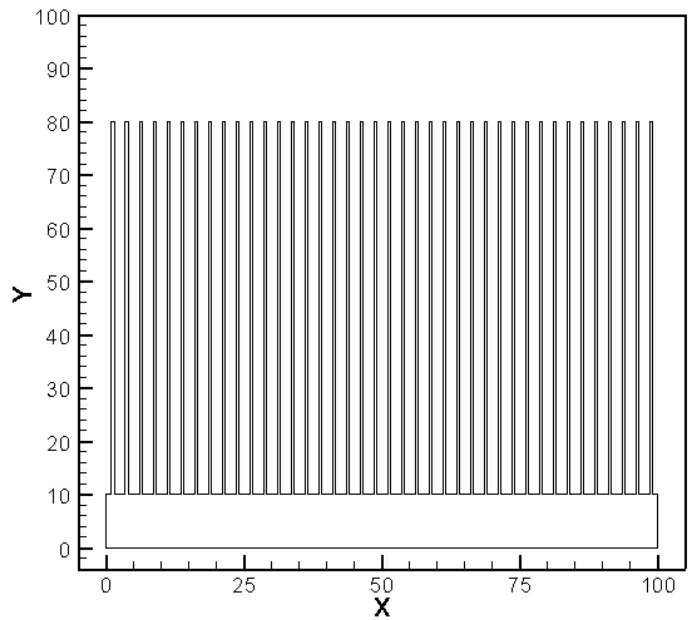


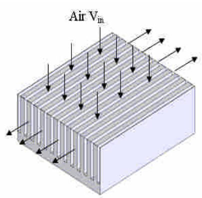


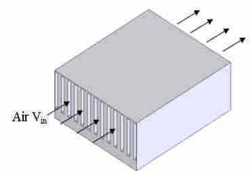
Optimizer with SCGM

Optimal Design for Heat Sink Modules





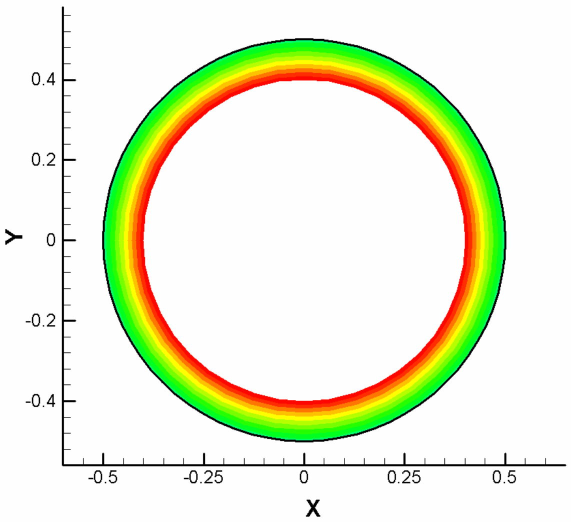


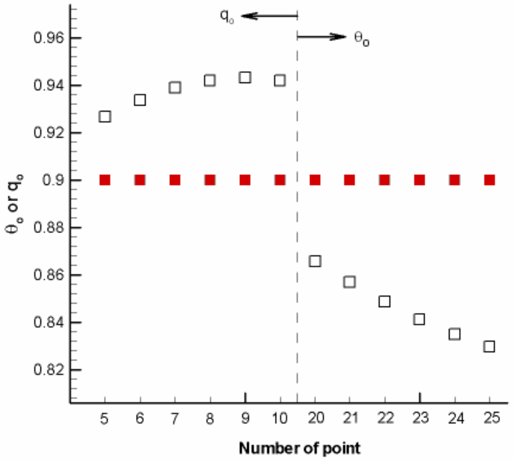


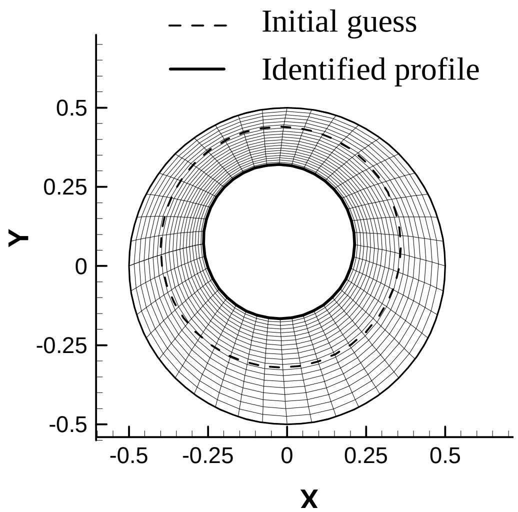
Source: http://www.cooljag.com (courtesy of COOLJAG, Inc.)

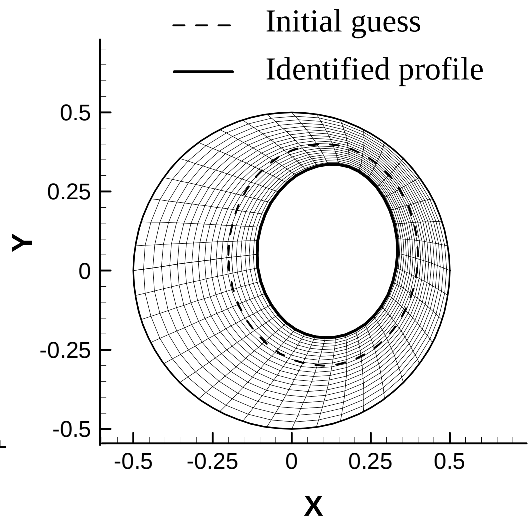
Optimizer with SCGM

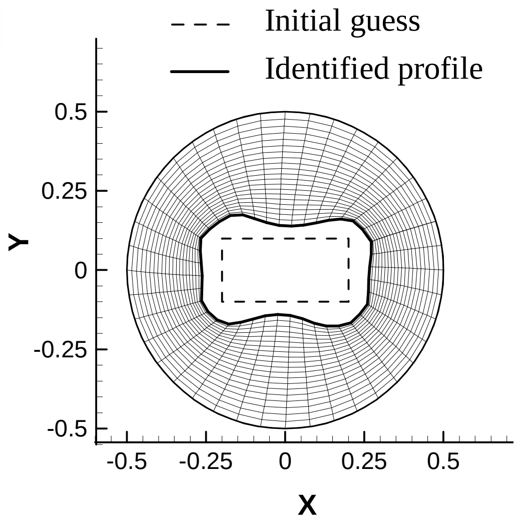
Identification of Fouling Layer in Pipes

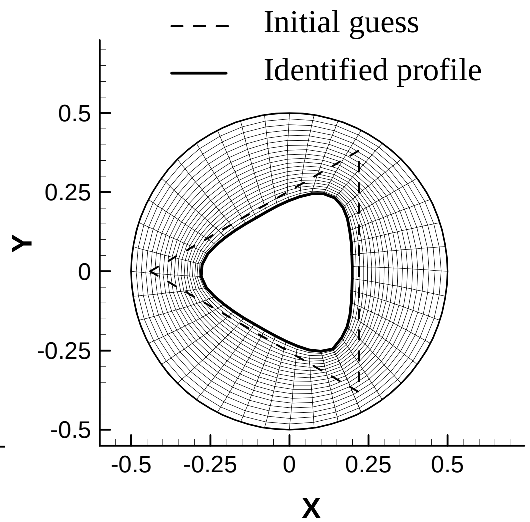








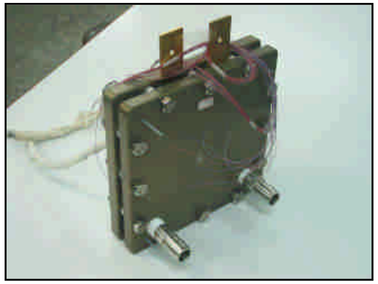


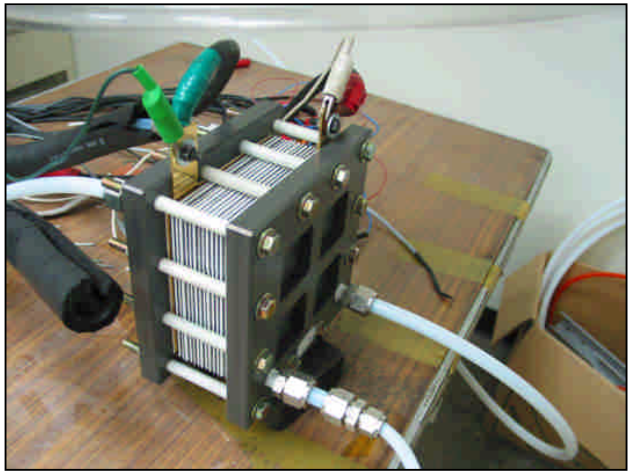


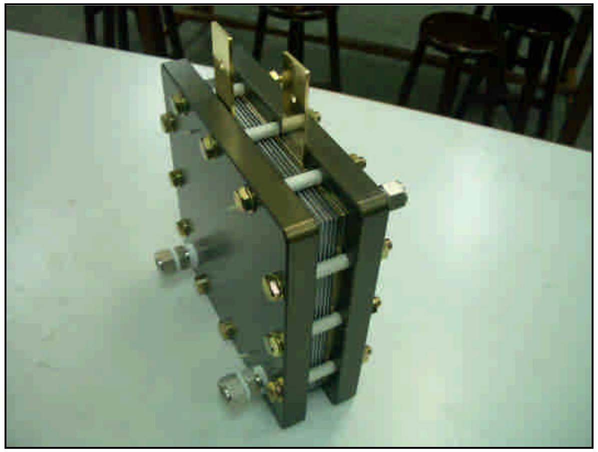
Why Numerical Simulation ?

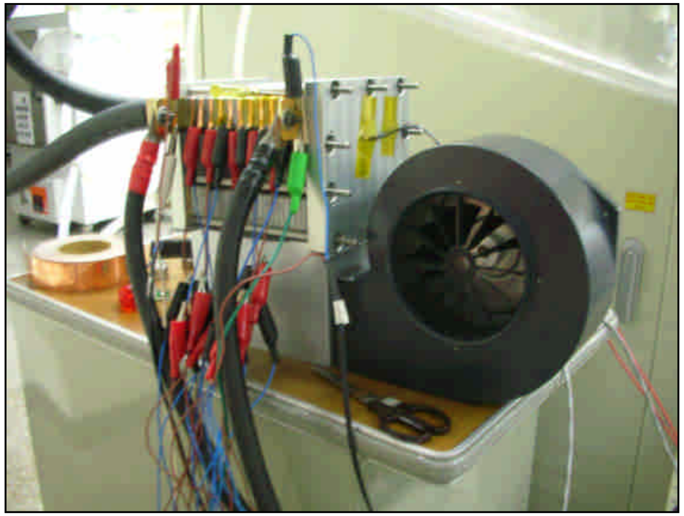
- Modeling gives a sufficient amount of detailed information that is not easily obtained by the experiments.
- Modeling costs much lower.
- Modeling can be readily integrated with numerical optimizer for design of fuel cells.

PEM Fuel Cell Modeling & Experiments



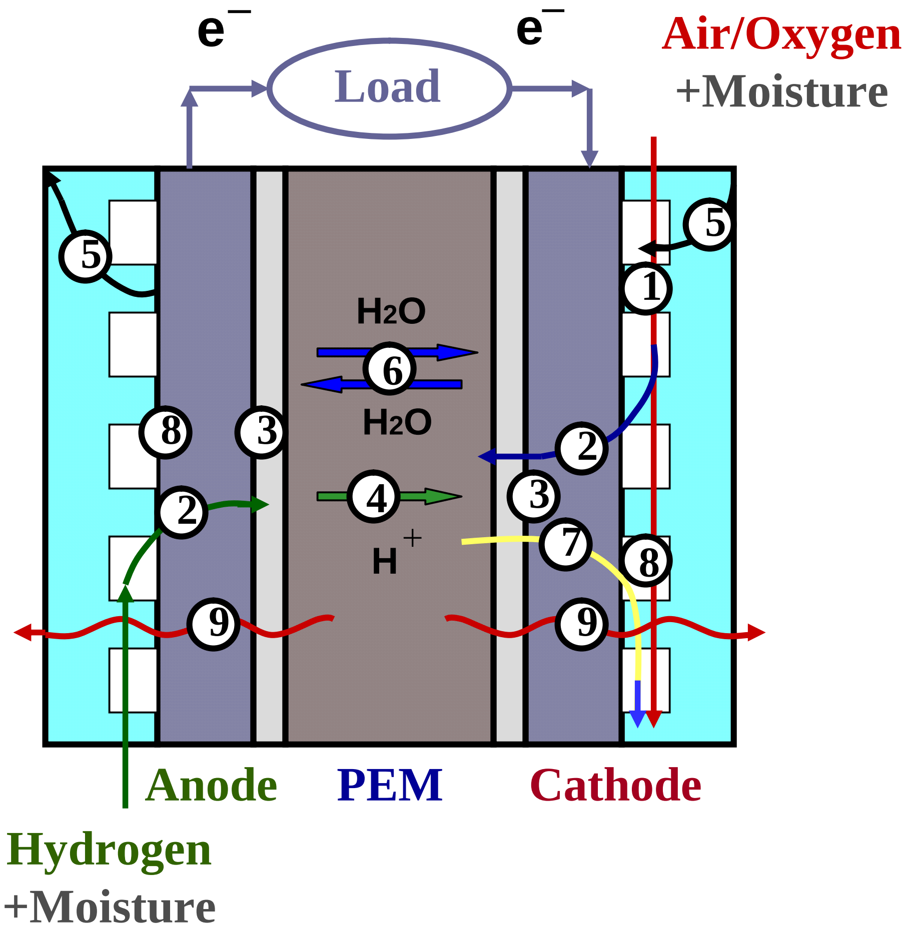




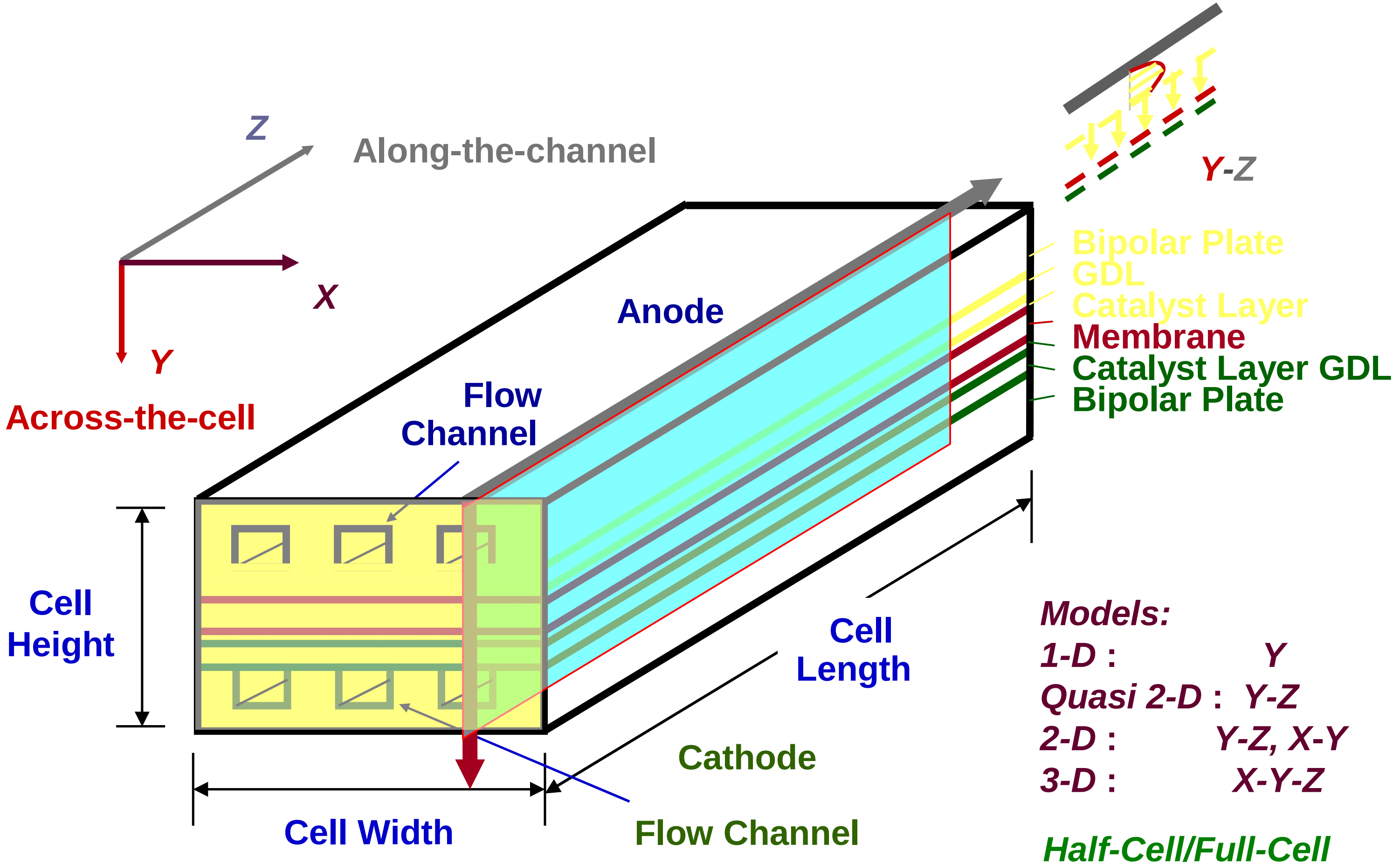


Transport Phenomena in PEMFC

1. Anode Gas Flow
2. Gas Transport
3. Electrochemical Reaction
4. Proton Transport
5. Electron Conduction
6. Water Transport
7. Water Transport
8. Two Phase Flow
9. Heat Transfer (Conduction and Convection)



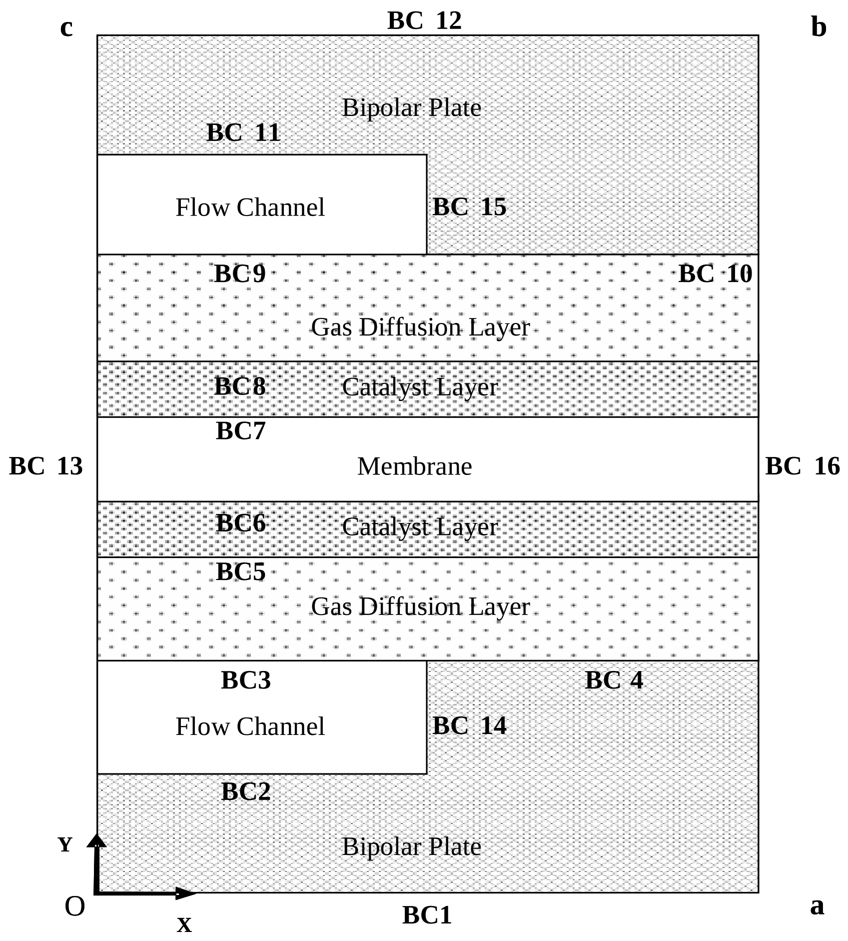
Physical Models of Single Cell

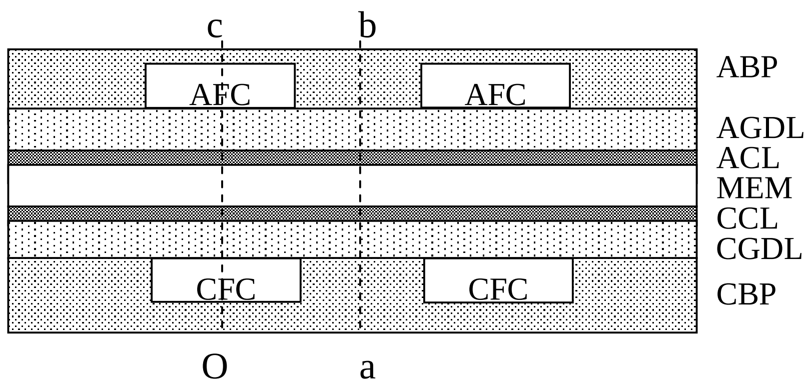


Models:
1-D : Y
Quasi 2-D : Y-Z
2-D : Y-Z, X-Y
3-D : X-Y-Z

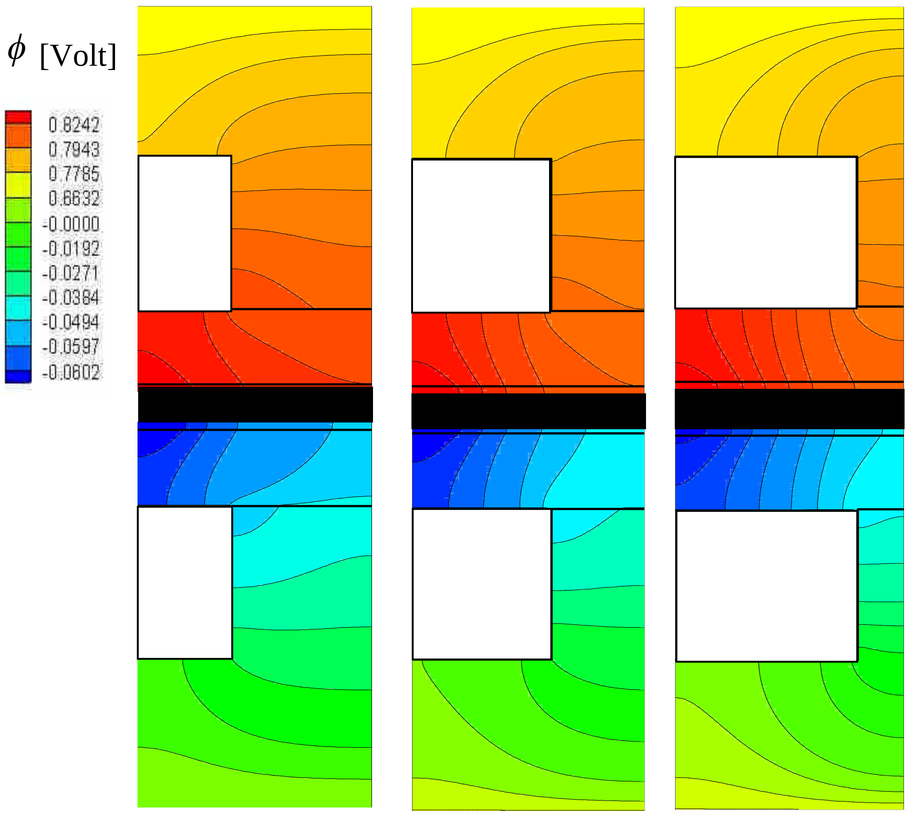
Half-Cell/Full-Cell

Two-Dimensional Single Cell Full Model

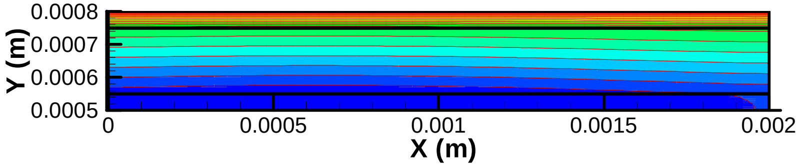




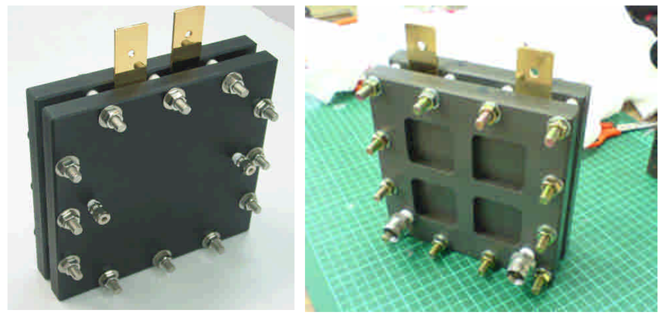
Two-Dimensional Single Cell Full Model

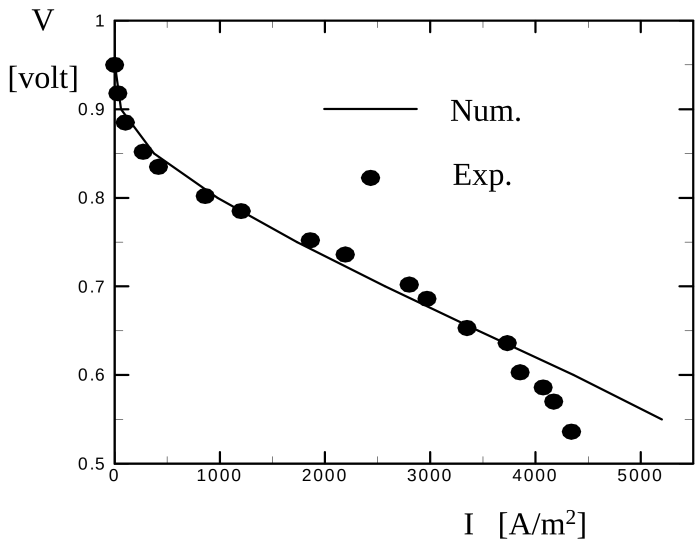


Electron conduction potential

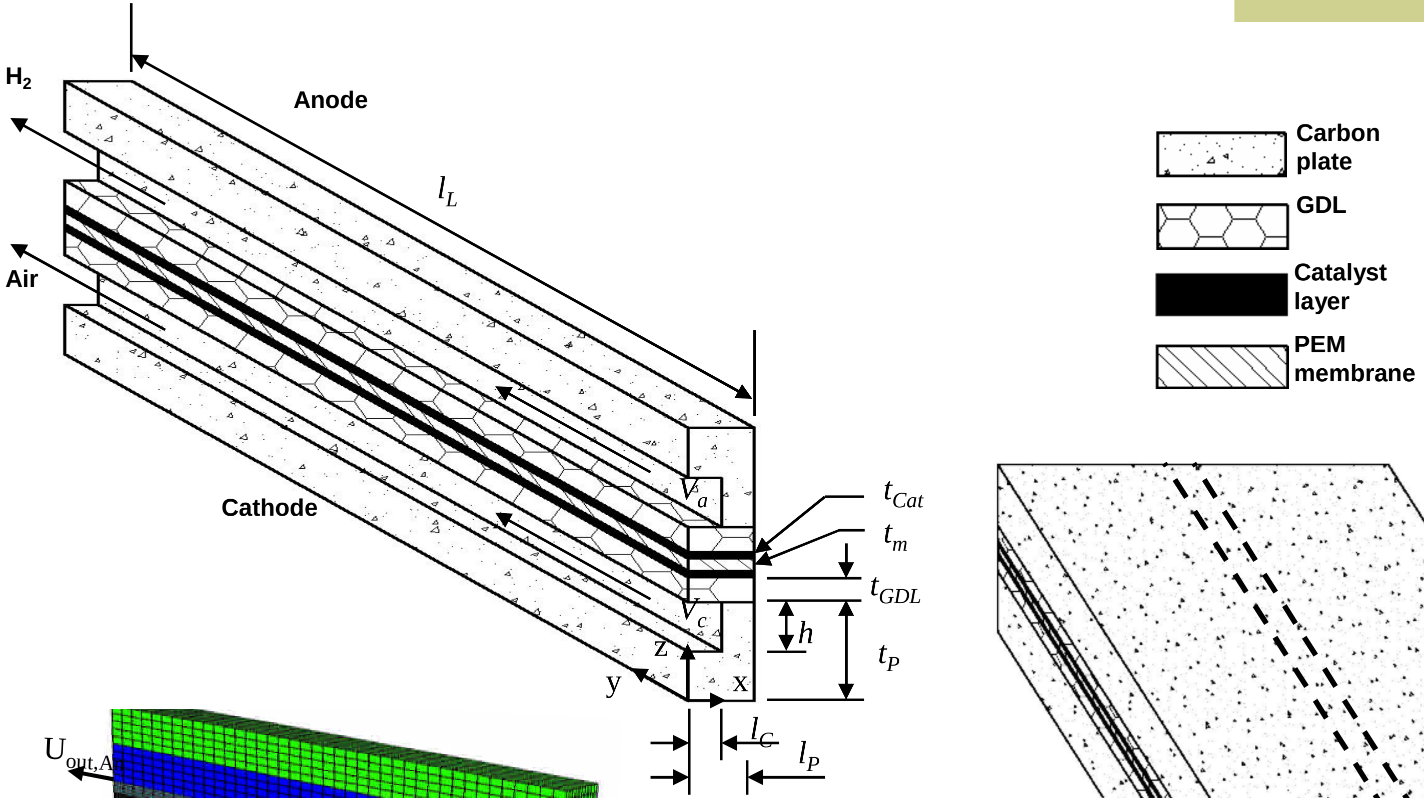


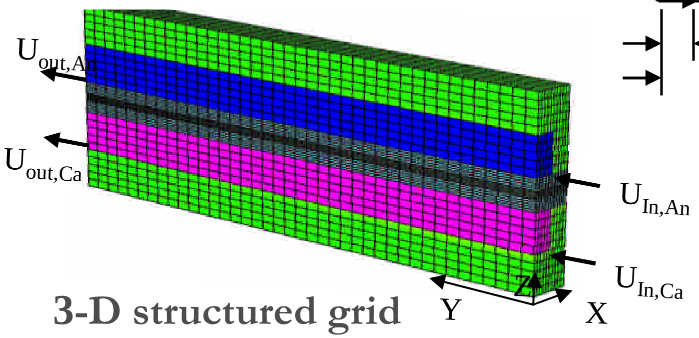
Proton conduction potential



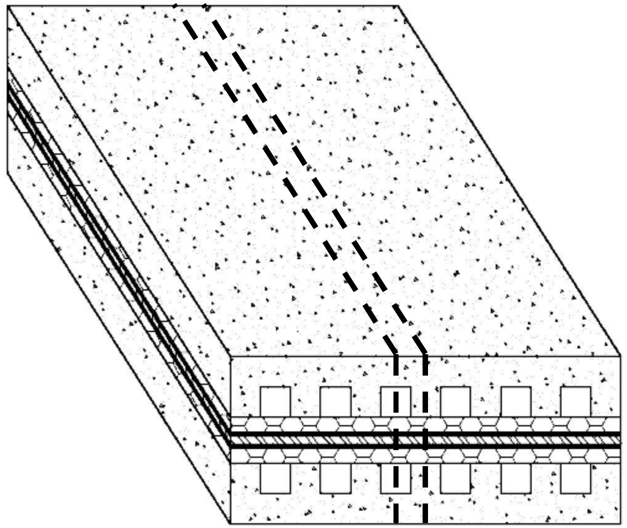


Three-Dimensional Single Cell Full Model (a)

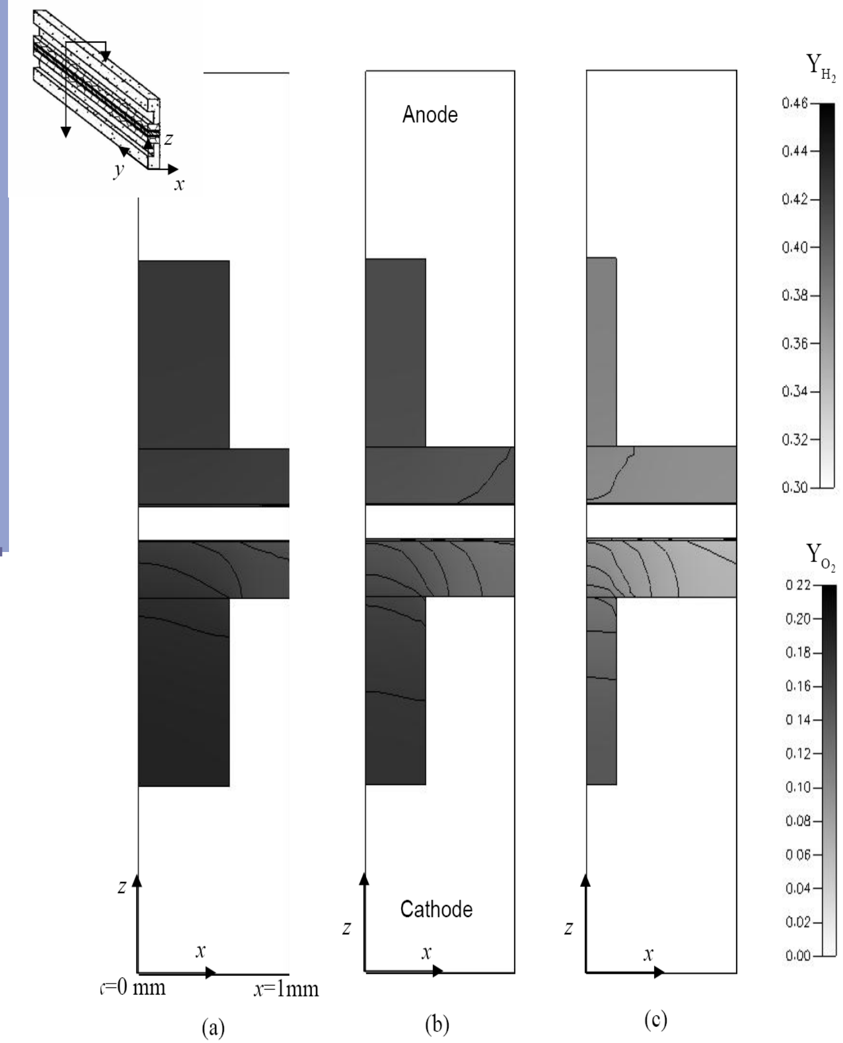


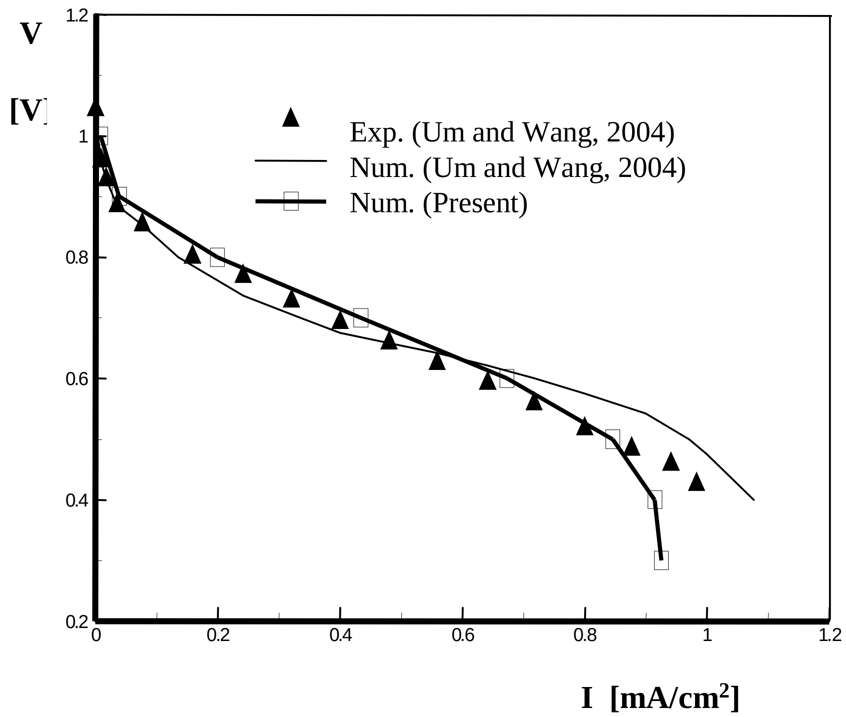


3-D structured grid

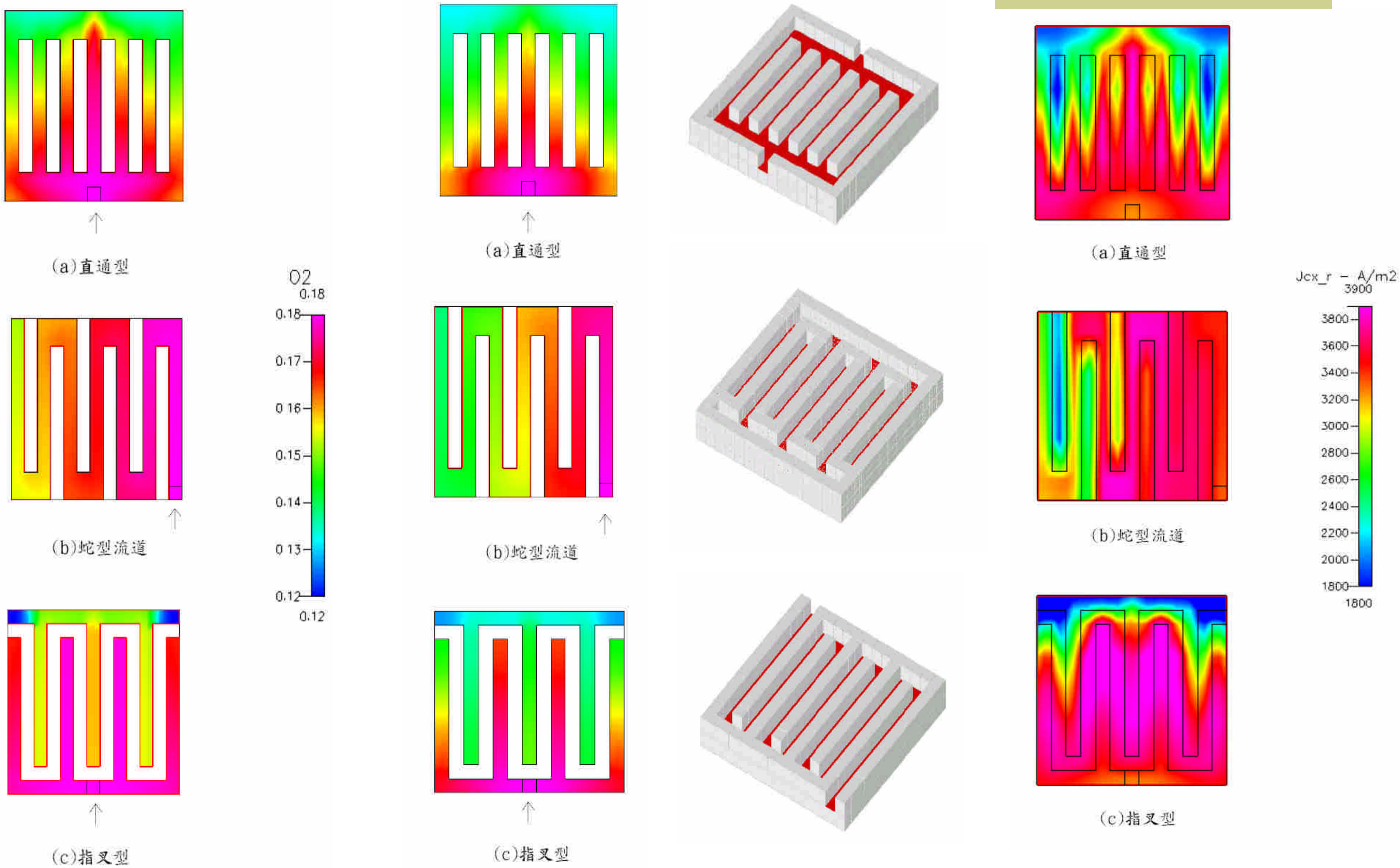


Three-Dimensional Single Cell Full Model (a)

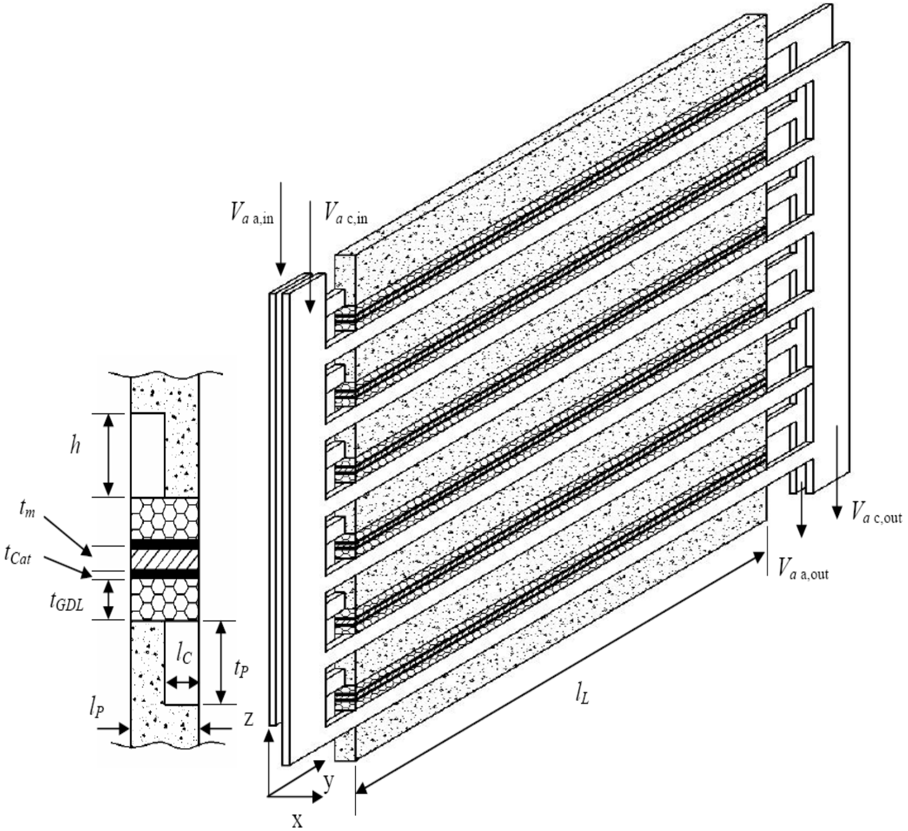


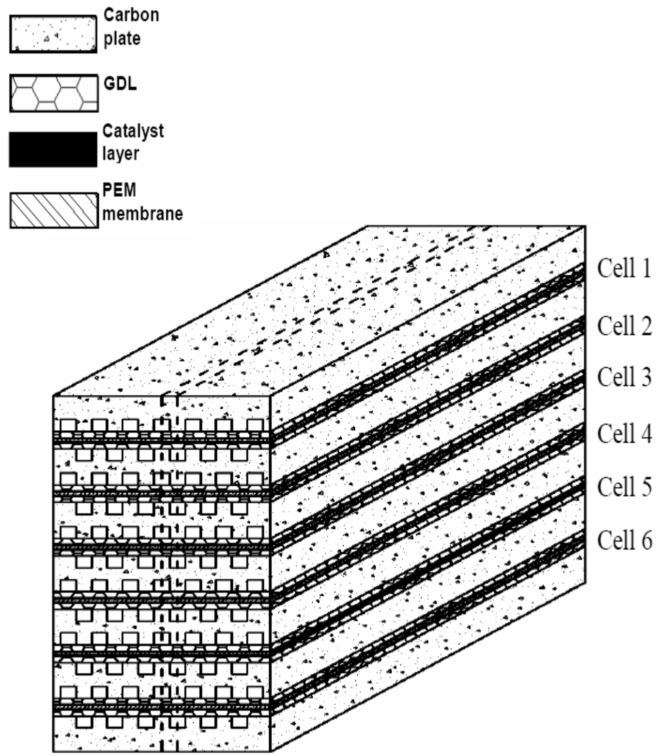


Three-Dimensional Single Cell Full Model (b)

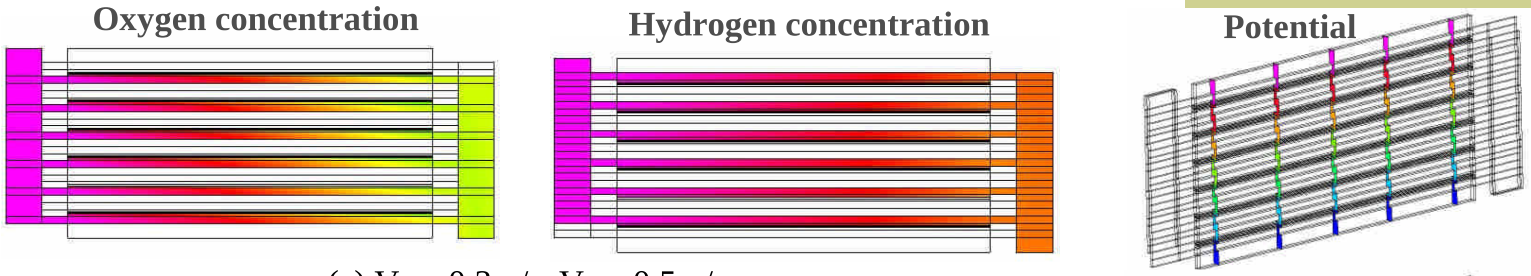


Three-Dimensional Stack Full Model

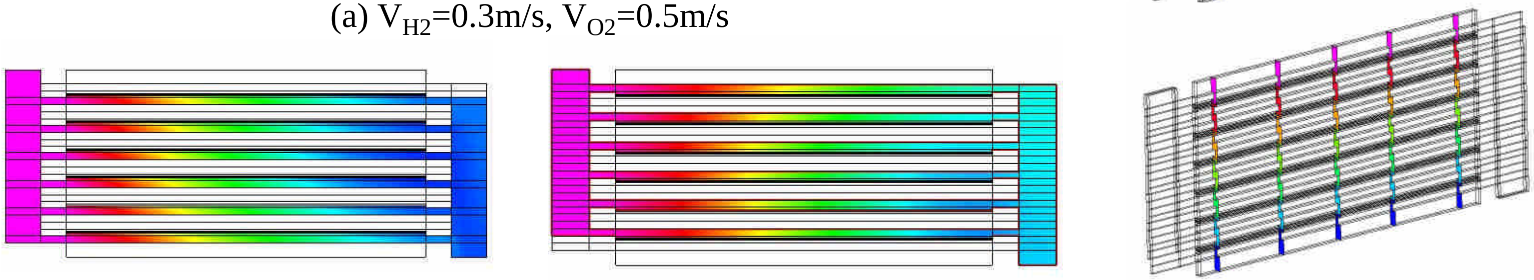




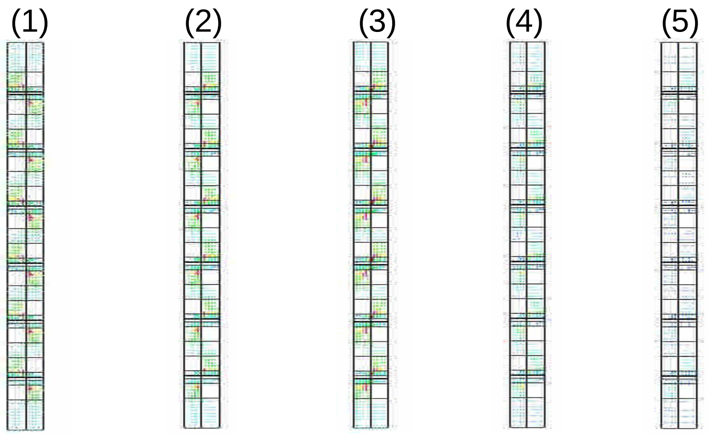
Three-Dimensional Stack Full Model



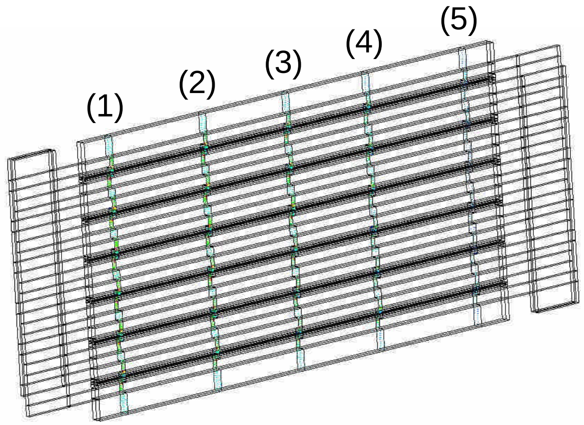
(a) V_{H2}=0.3m/s, V_{O2}=0.5m/s



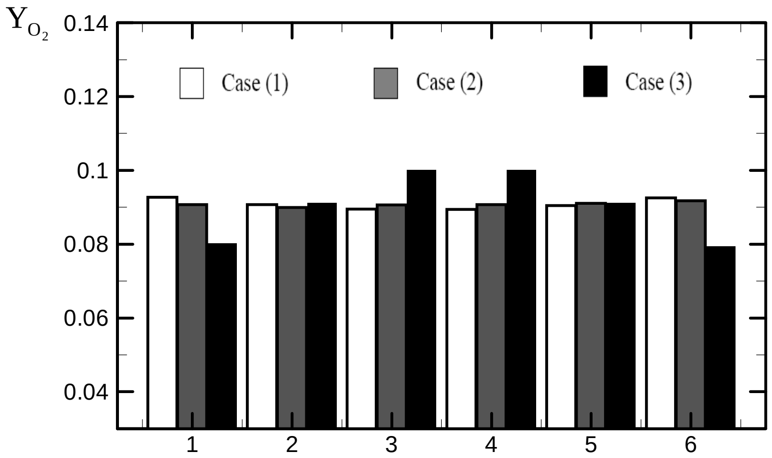
(b) V_{H2}=0.1m/s V_{O2}=0.18m/s

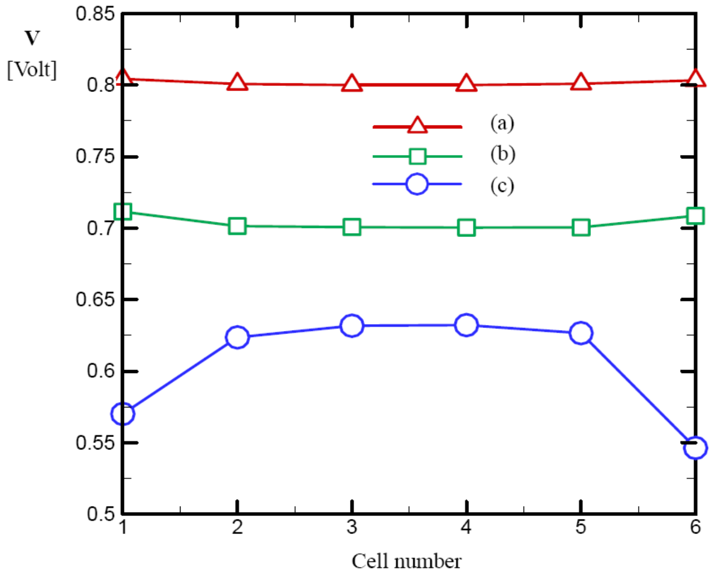


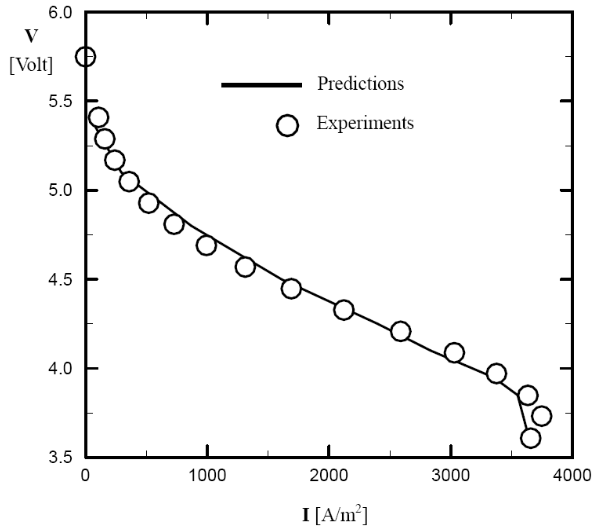
Current flow



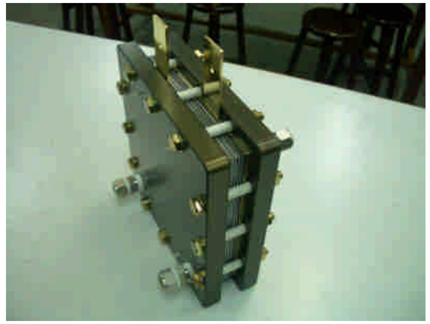
Three-Dimensional Stack Full Model



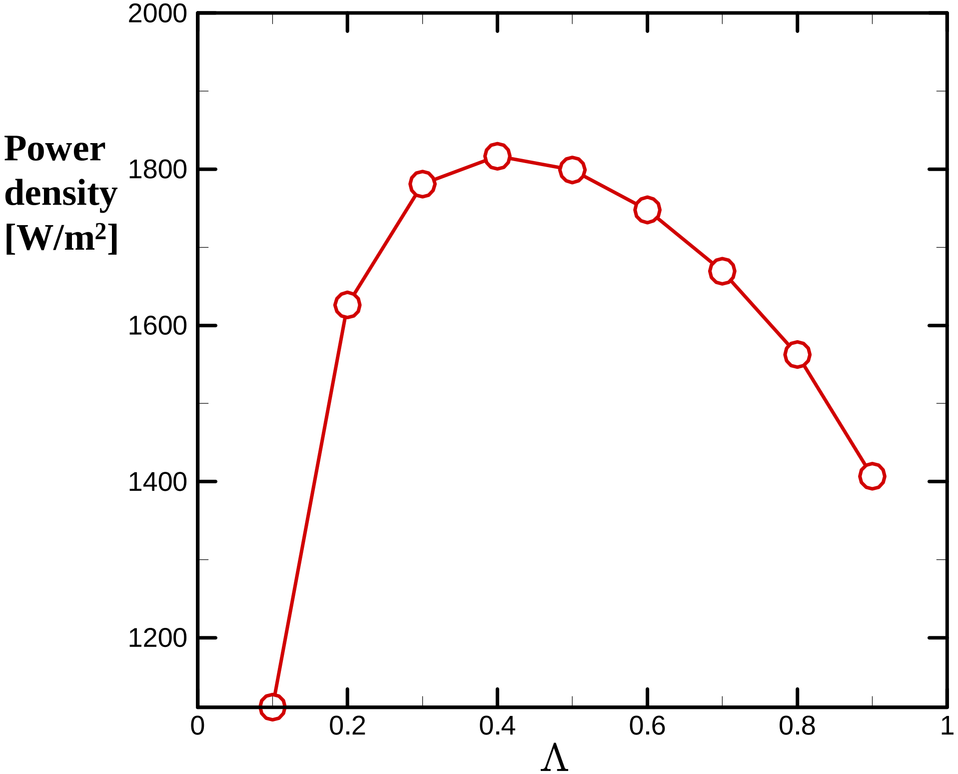




Six-cell short stack O_2/H_2

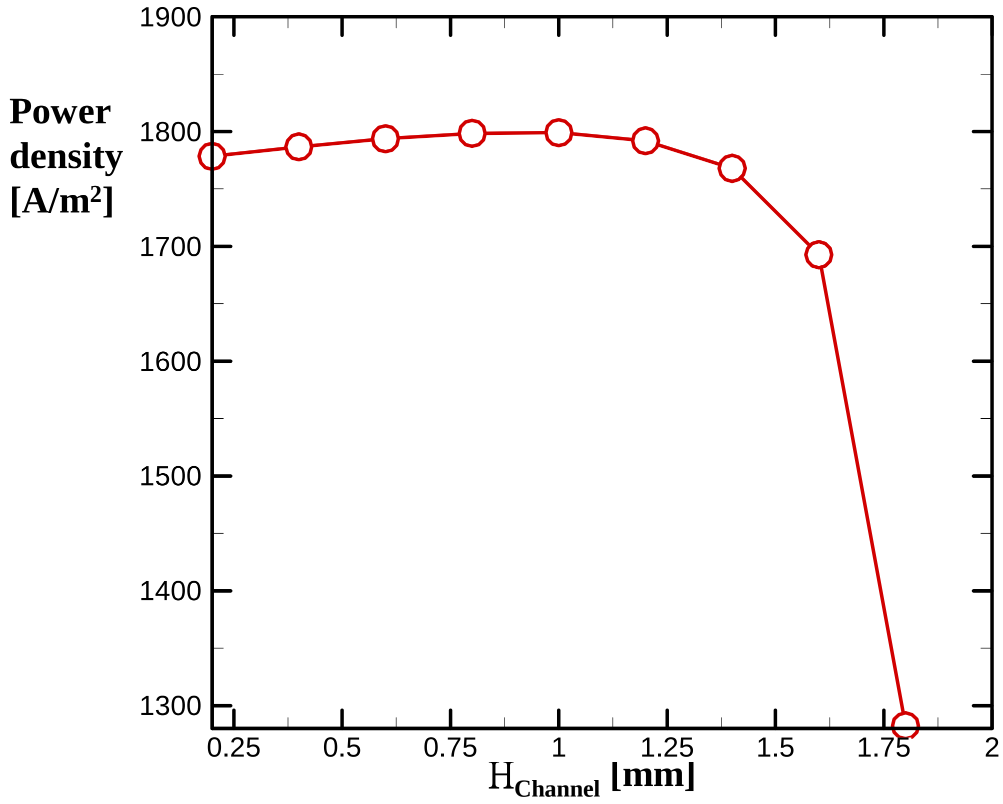


Parametric Study – channel width fraction



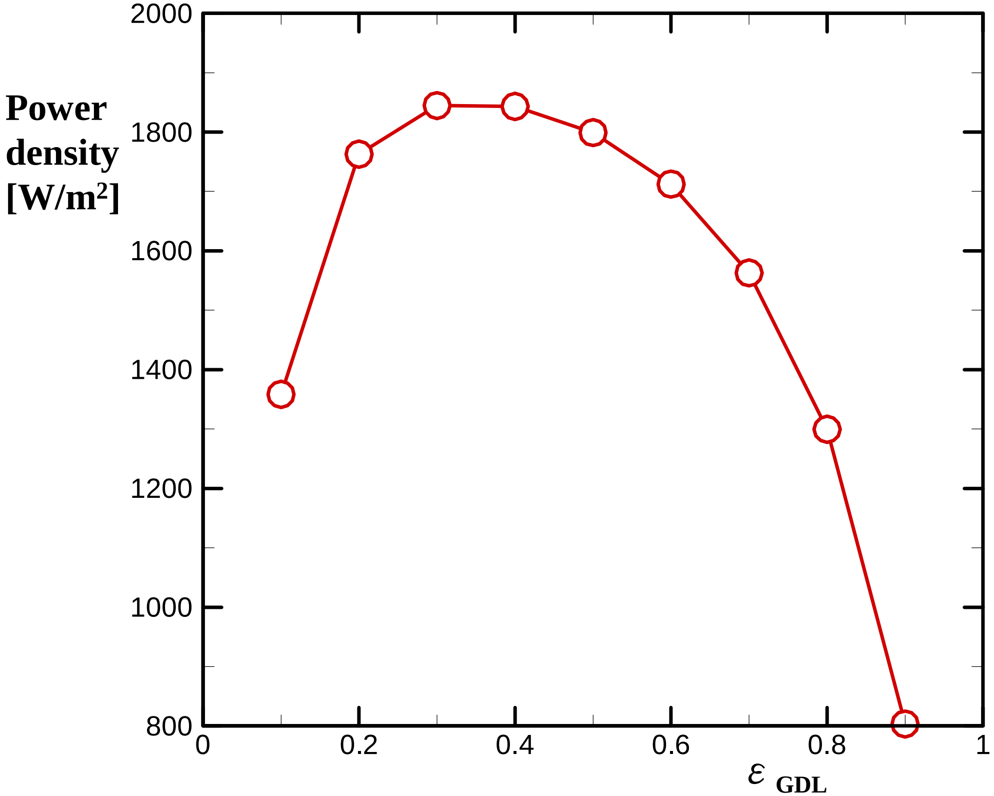
V_o=0.7V, ε_{GDL}=0.5, $\varepsilon_{V,Cat}$=0.112, $\varepsilon_{N,Cat}$=0.3, $H_{Channel}$=1mm, t_{GDL}=300 μm, t_{Cat}=10 μm, t_{Mem}=178μm.

Parametric Study – channel depth



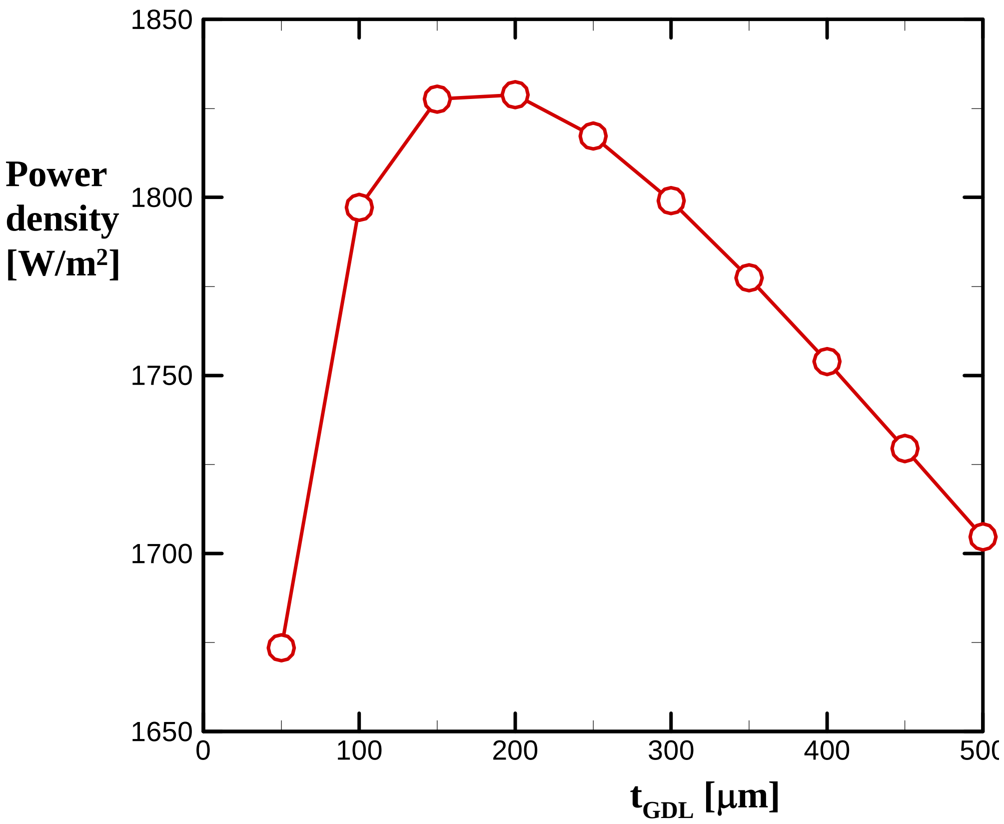
V_o=0.7, Λ =0.5, ε_{GDL}=0.5, $\varepsilon_{V,Cat}$=0.112, $\varepsilon_{N,Cat}$=0.3, t_{GDL}=300 μm, t_{Cat}=10 μm, t_{Mem}=178μm.

Parametric Study – porosity of GDL



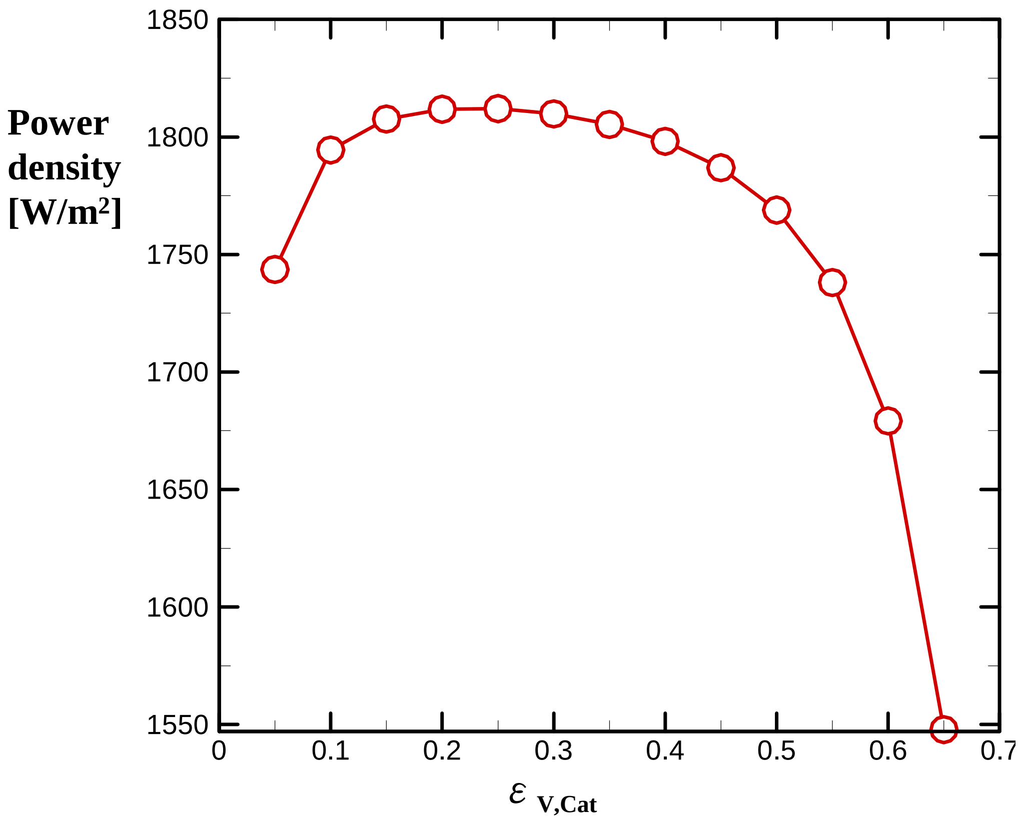
V_o=0.7, Λ =0.5, H=1mm, $\varepsilon_{V,Cat}$=0.112, $\varepsilon_{N,Cat}$=0.3, t_{GDL}=300 μm, t_{Cat}=10 μm, t_{Mem}=178μm.

Parametric Study – thickness of GDL



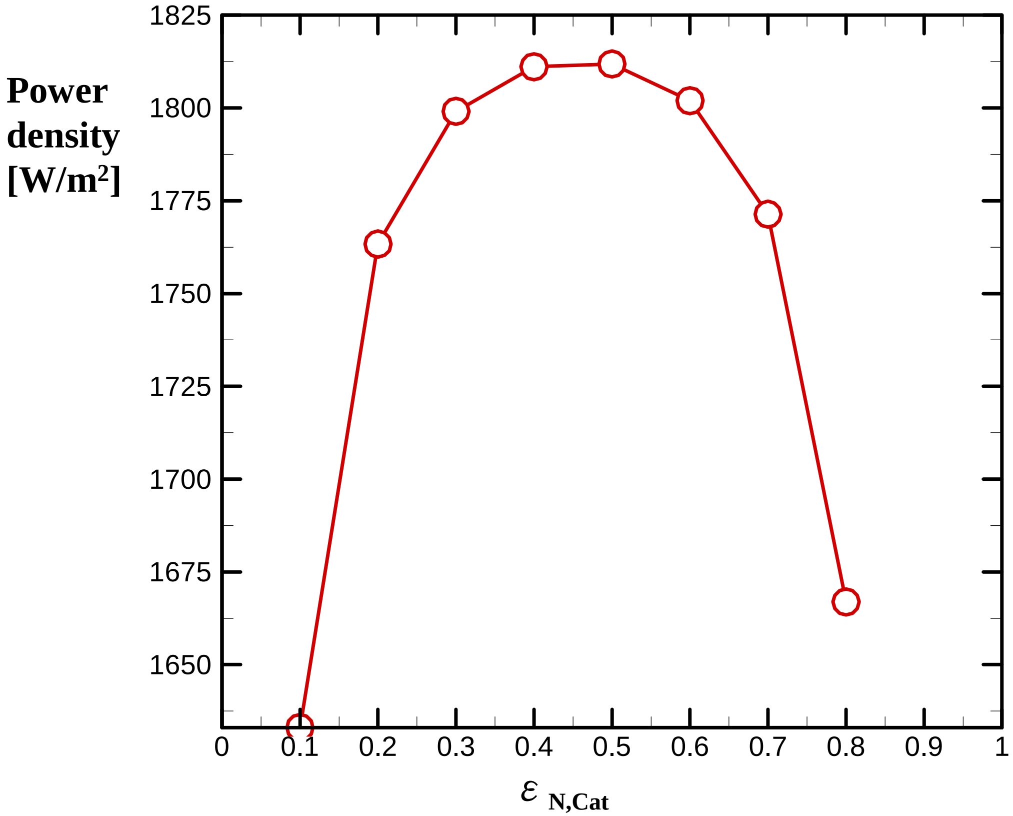
V_o=0.7, Λ =0.5, H=1mm, $\varepsilon_{V,Cat}$=0.112, $\varepsilon_{N,Cat}$=0.3, ε_{GDL}=0.5, t_{Cat}=10 μm, t_{Mem}=178μm.

Parametric Study – porosity of catalyst layer



V_o=0.7, Λ=0.5, H=1mm, $\varepsilon_{N,Cat}$=0.3, ε_{GDL}=0.5, t_{Cat}=10 μm, t_{GDL}=300 μm, t_{Mem}=178μm.

Parametric Study – volumetric fraction of Nafion loading



V_o=0.7, Λ=0.5, H=1mm, $\varepsilon_{V,Cat}$=0.112, ε_{GDL}=0.5, t_{Cat}=10 μm, t_{GDL}=300 μm, t_{Mem}=178μm.

1. Geometrical Parameters Optimization

Iterative Regularization Method

Designed variables: Λ, t_{GDL}, h, …

Objective function: $J = 1/(I \times V)$ (minimized)

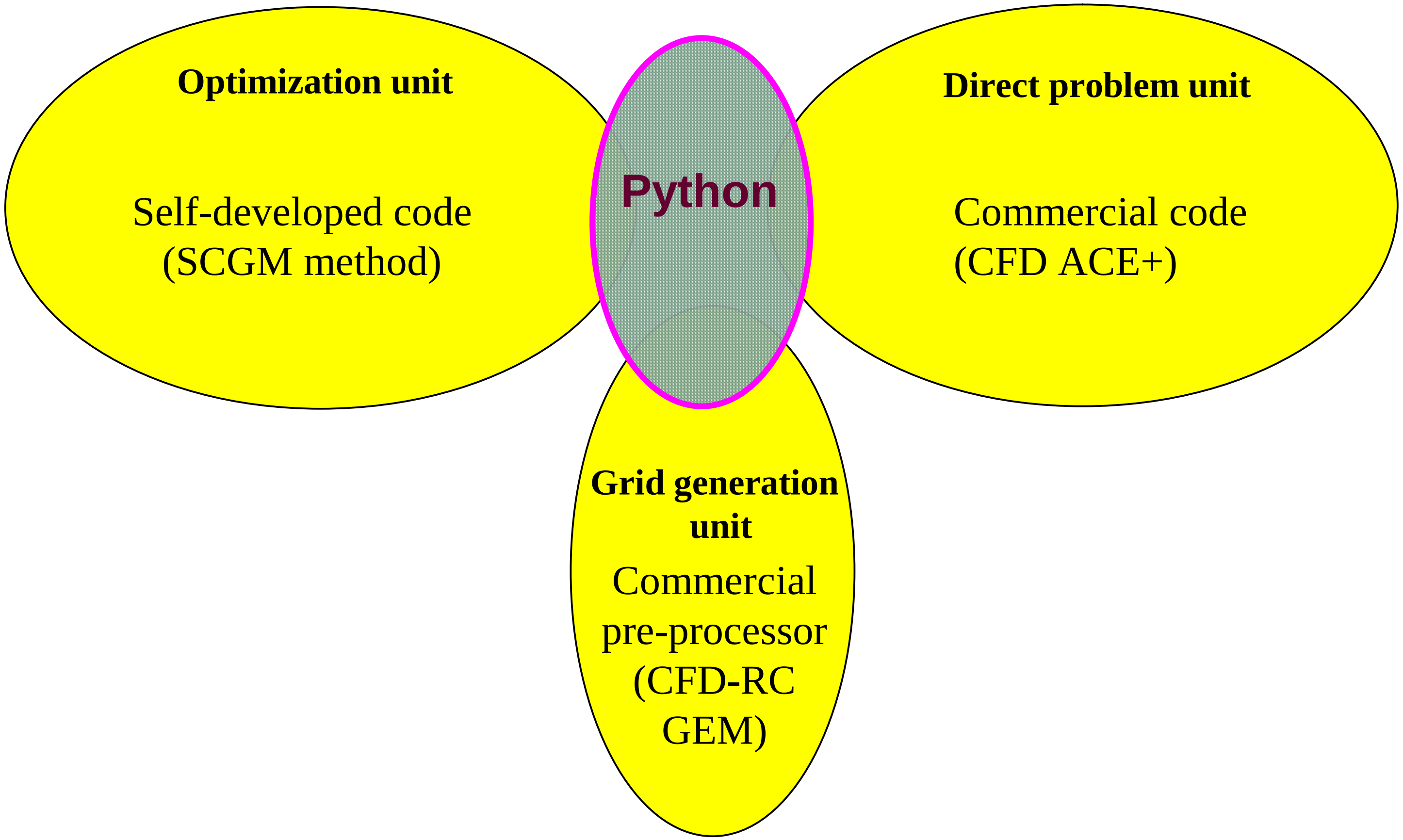
Direct Problem Solver: CFD ACE+

Sensitivity Analysis: Direct differentiation

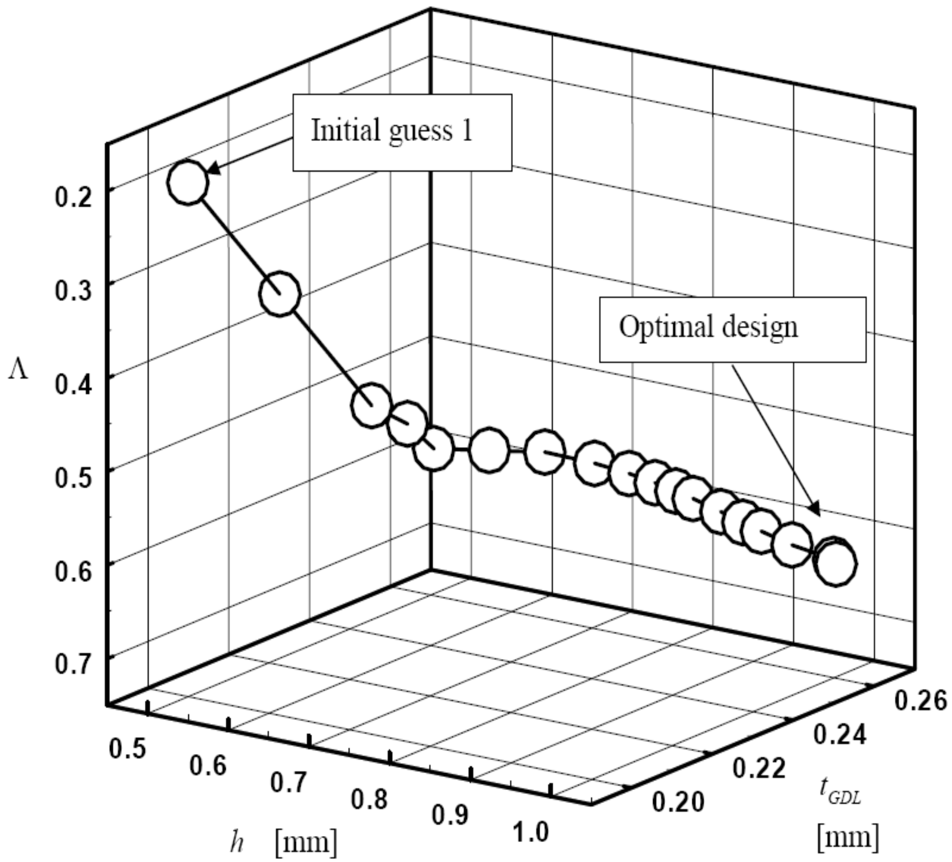
Optimization Process: SCGM method

1. Geometrical Parameters Optimization

PEM Fuel Cell Optimizer

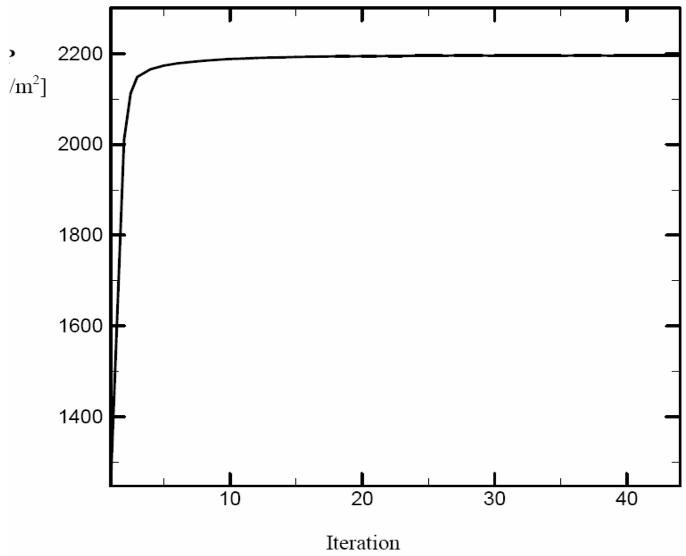


Optimal Design

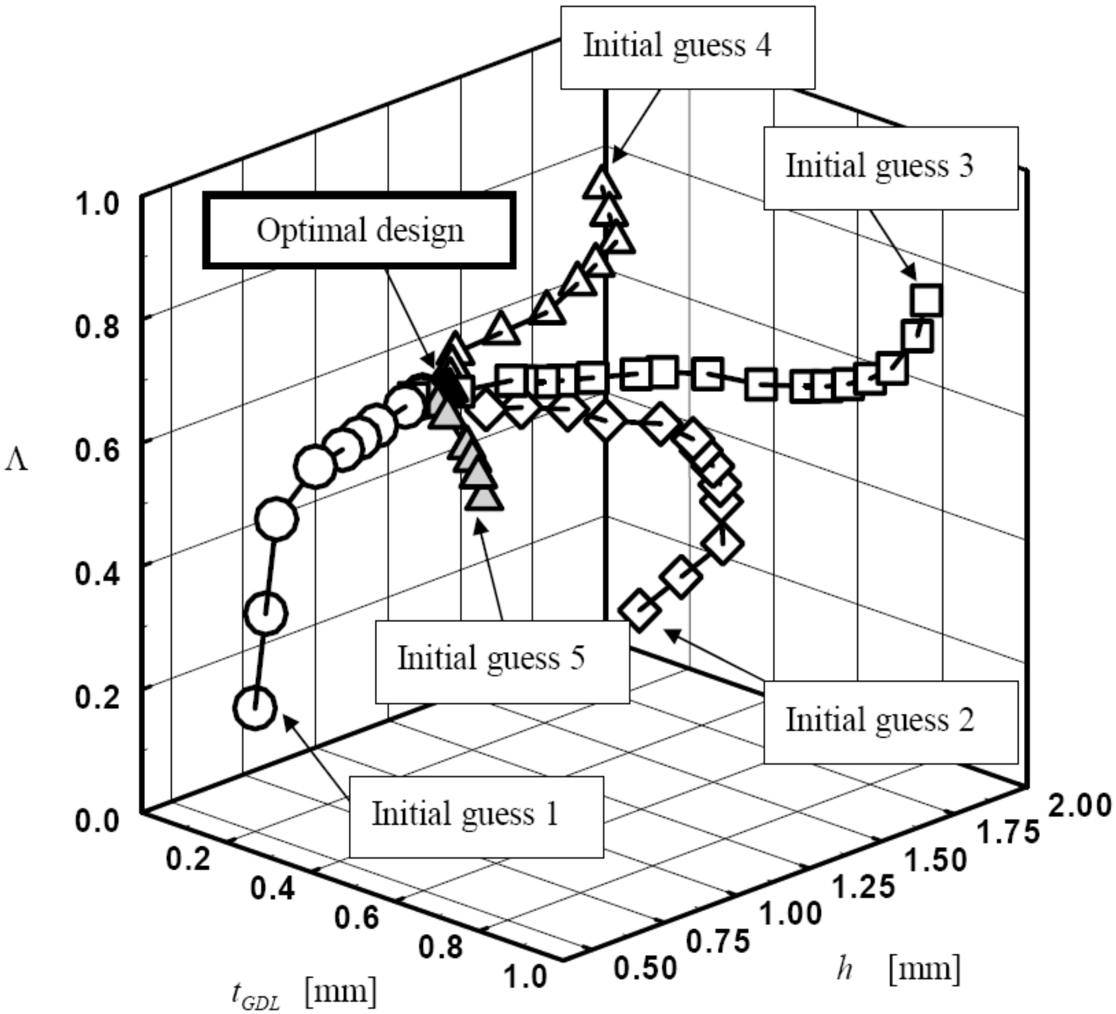


Optimal design: increase 457W/m^2 (75%)

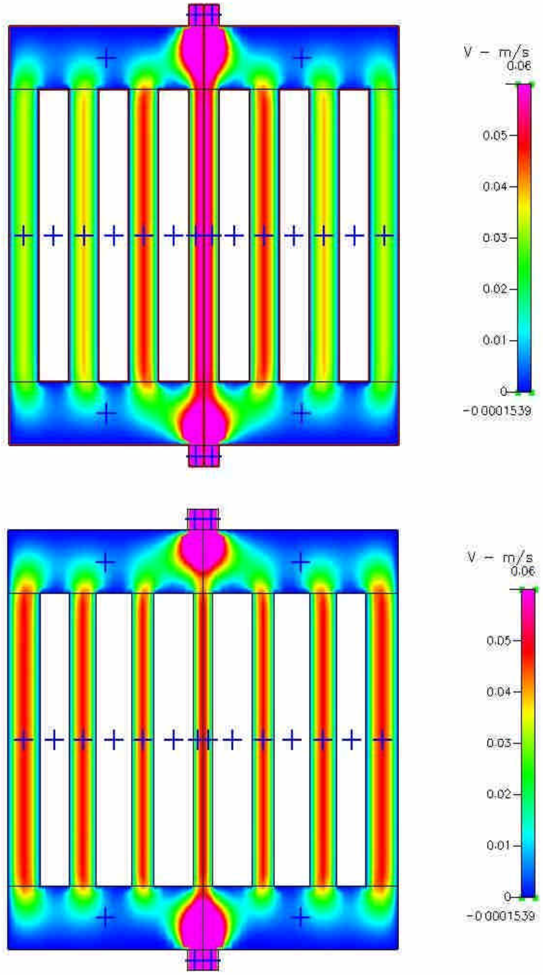
Λ = 0.635, t_{GDL} = 0.263 mm , h = 1.0 mm



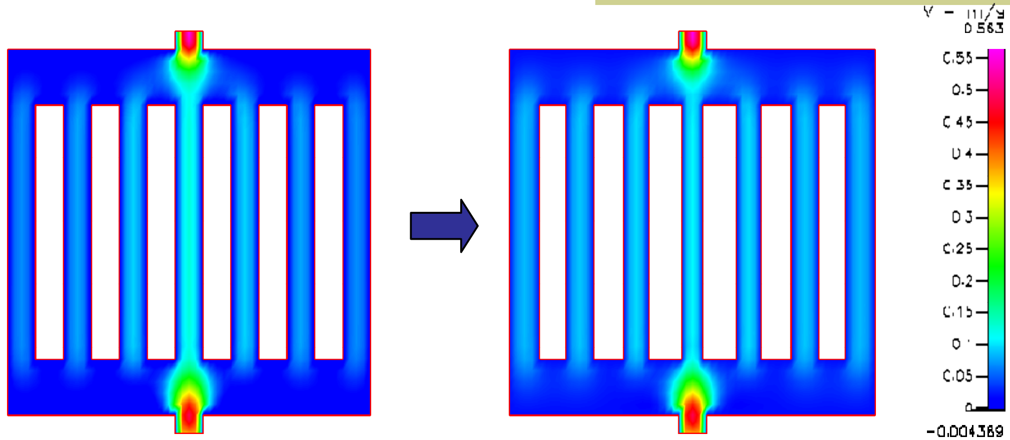
1. Geometrical Parameters Optimization

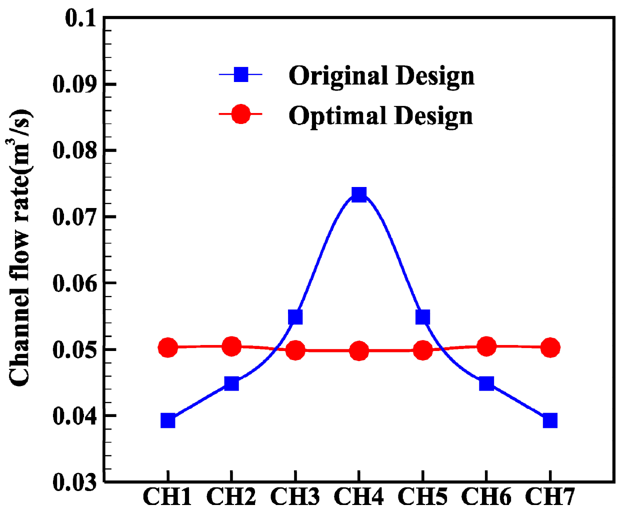


2. PEM Fuel Cell Channel Width Optimization



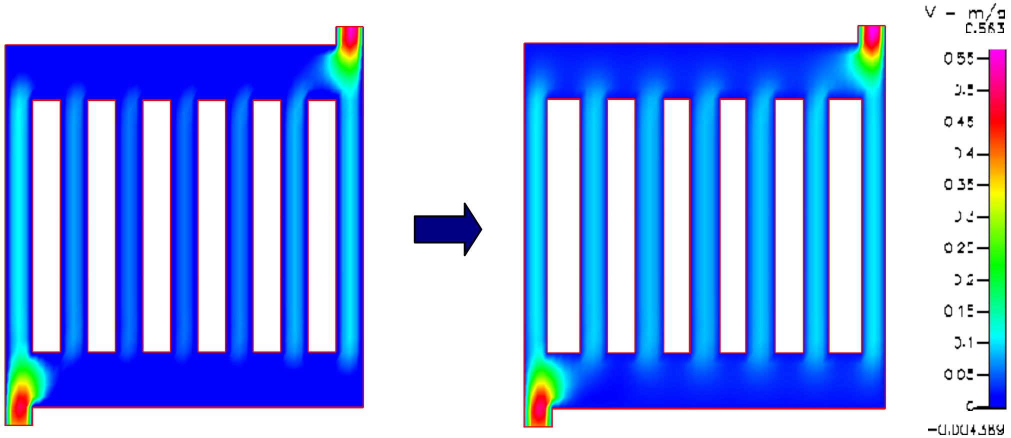
Uniform Velocity

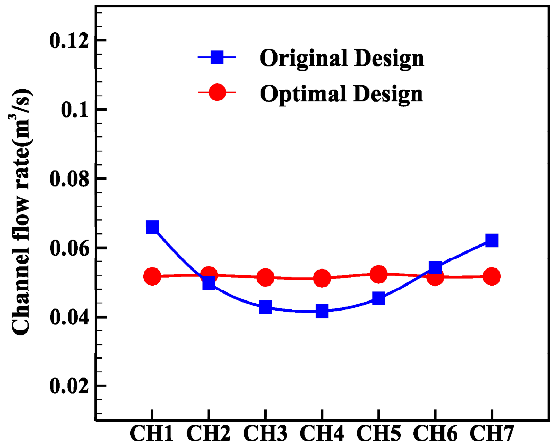


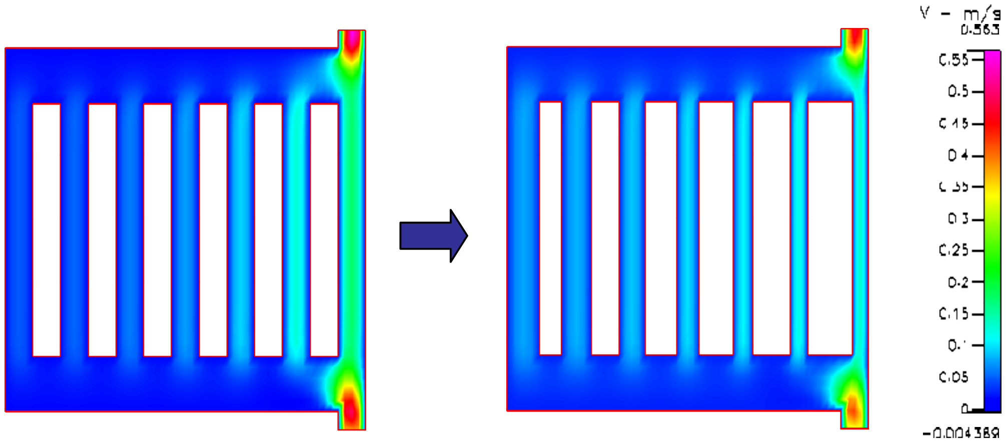


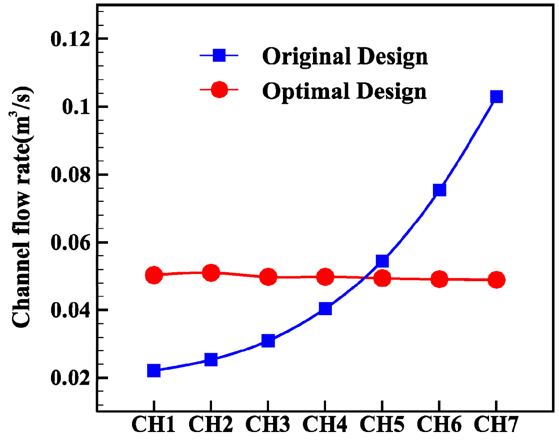
Uniform Flow Rate

2. PEM Fuel Cell Channel Width Optimization

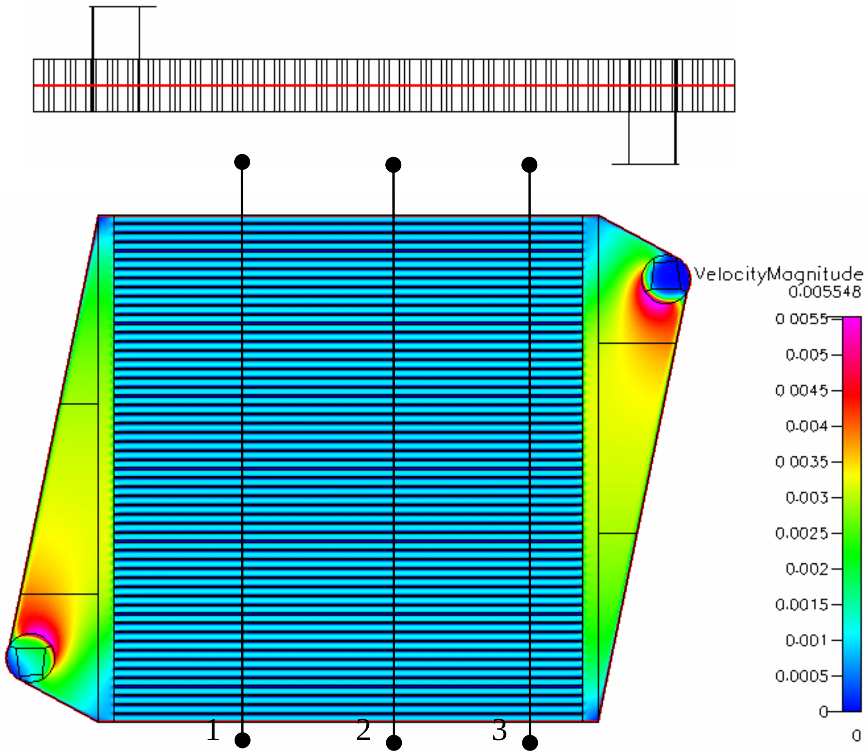


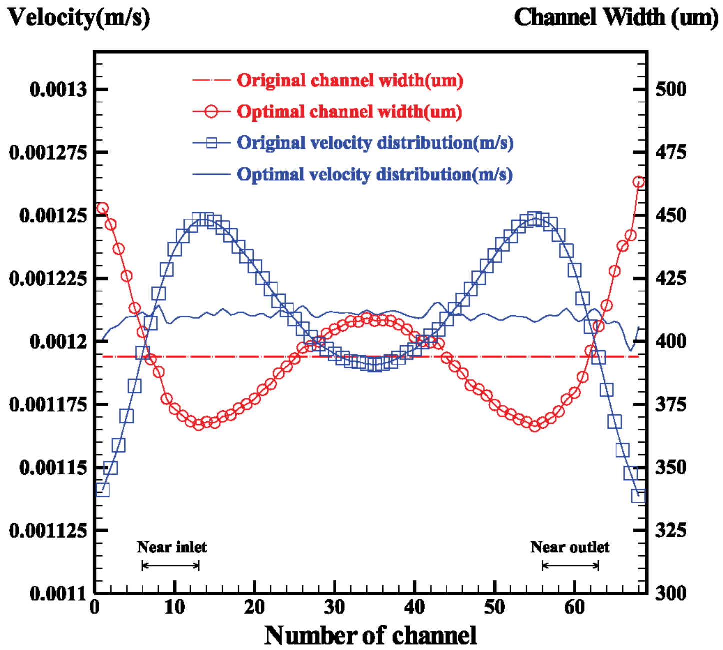






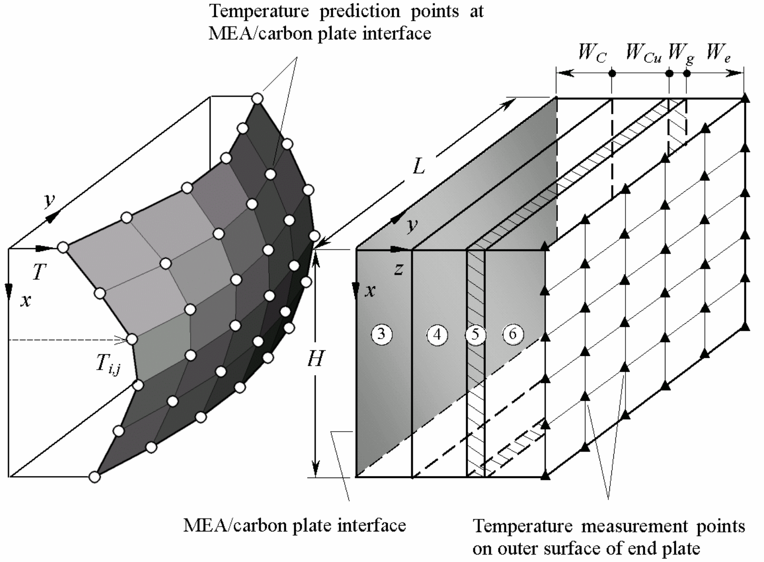
3. Micro-reformer Channel Width Optimization

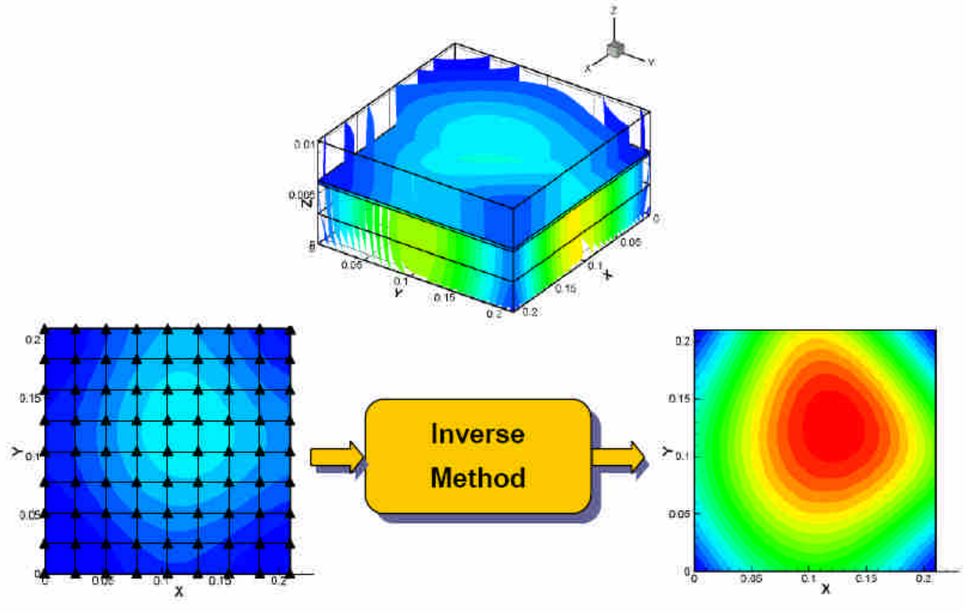




4. Non-destructive Method for Determination of Internal Temperature Distribution

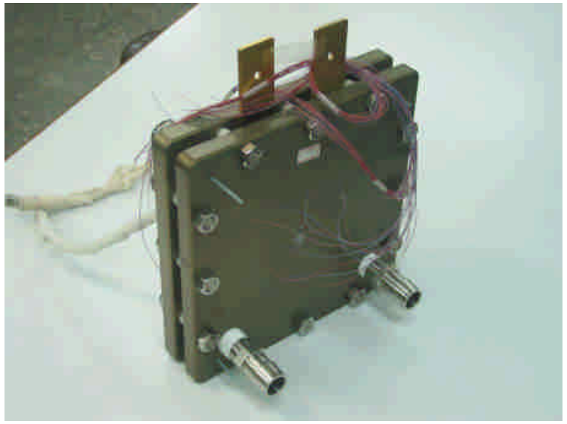
PEM Fuel Cell Optimization





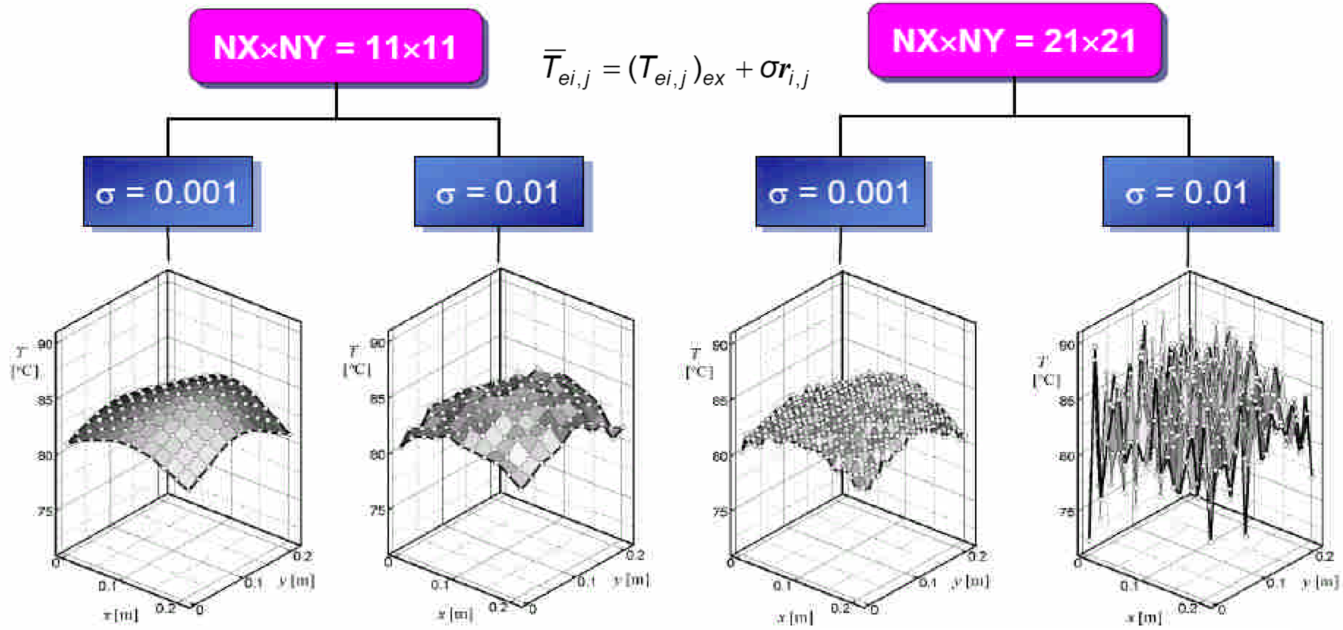
Surface temperature of end plate

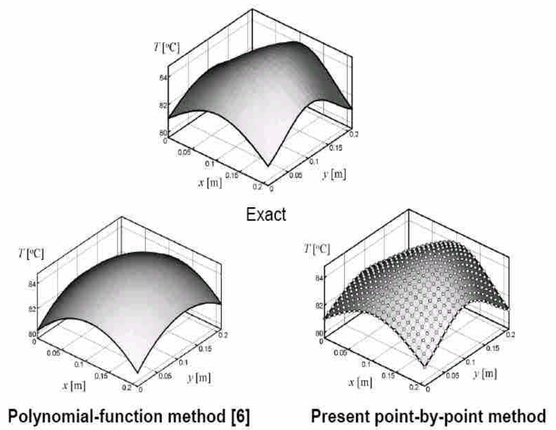
MEA/carbon temperature

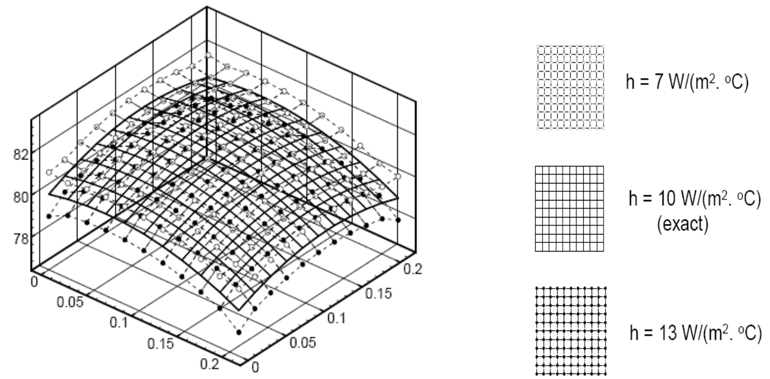


4. Non-destructive Method for Determination of Internal Temperature Distribution

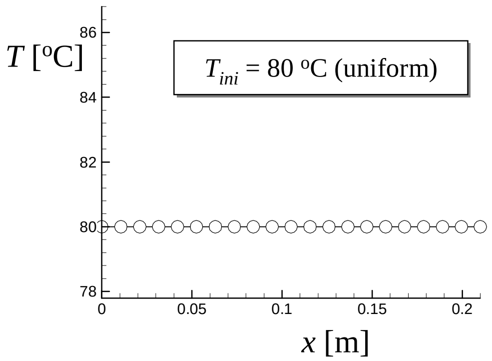
$$\overline{T}_{ei,j} = (T_{ei,j})_{ex} + \sigma r_{i,j}$$



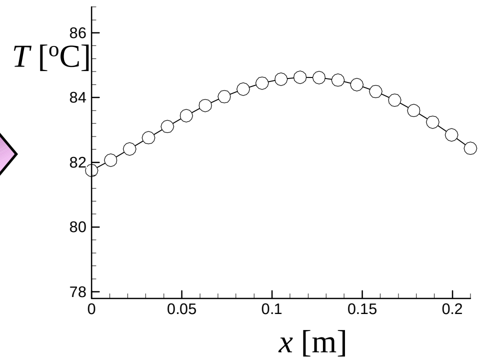




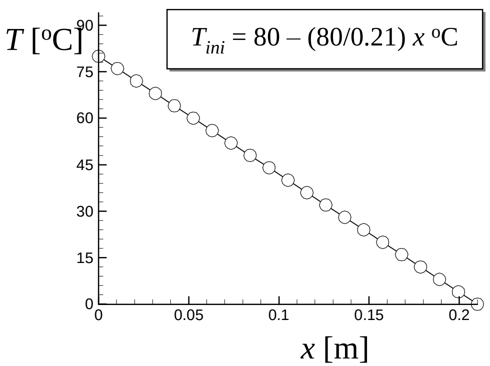
4. Non-destructive Method for Determination of Internal Temperature Distribution

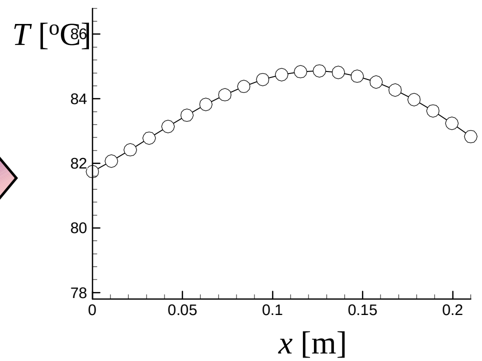


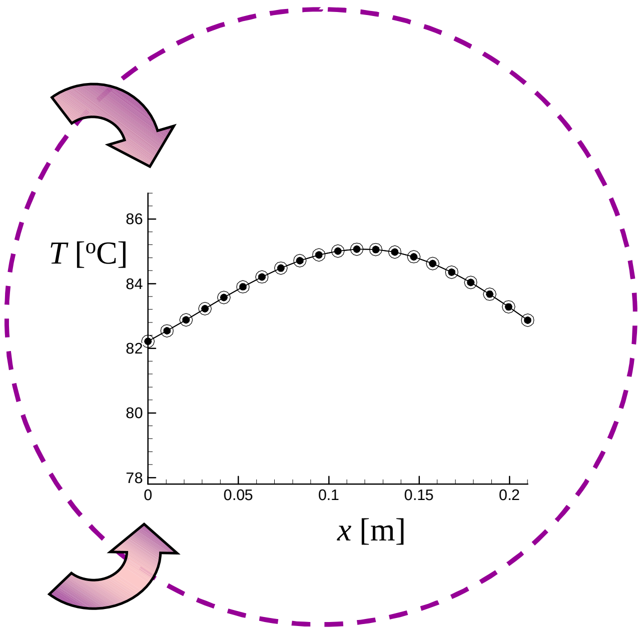
Initial guess



Final iteration

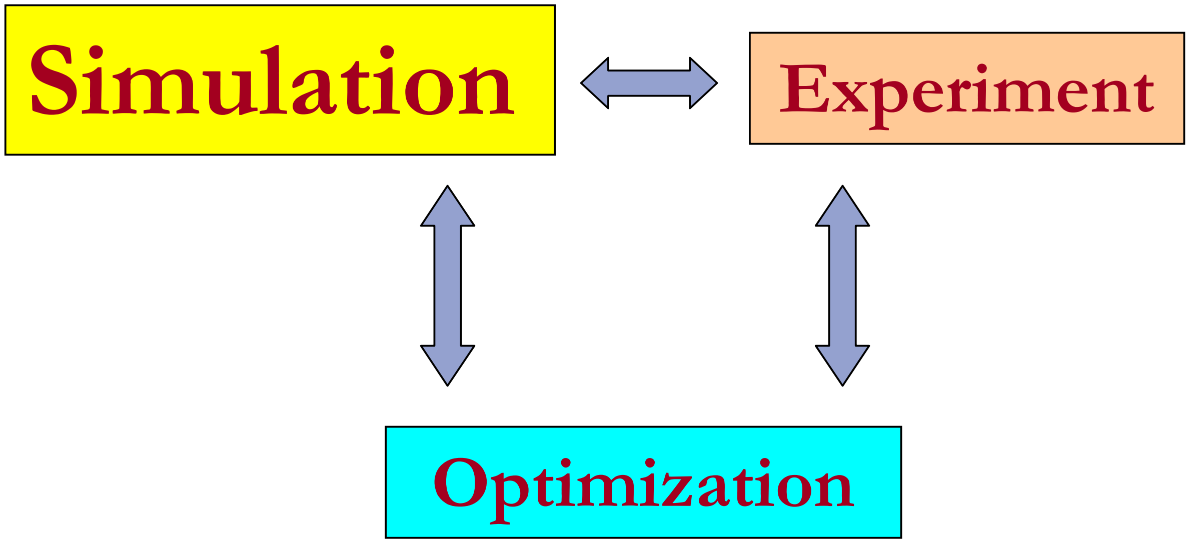






Final solution
(Exact solution)

Concluding Remarks



Thank you !

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