COMSOL MULTIPHYSICS

Yuan-Ze University

COMSOL Multiphysics - fuel cell and LED applications

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Outline

- Introduction
- Simulation detail
- FC applications
  - 2D MEA model
  - 3D single cell model
  - FC Stack simulation
- LED applications
- Summary

How fuel cell works

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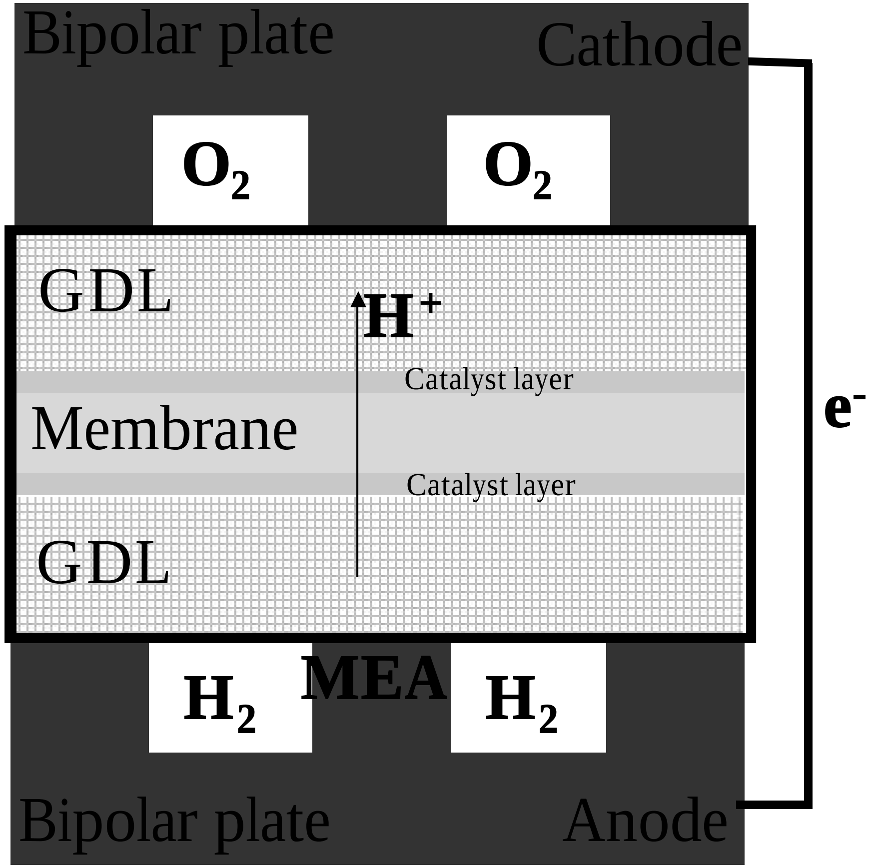
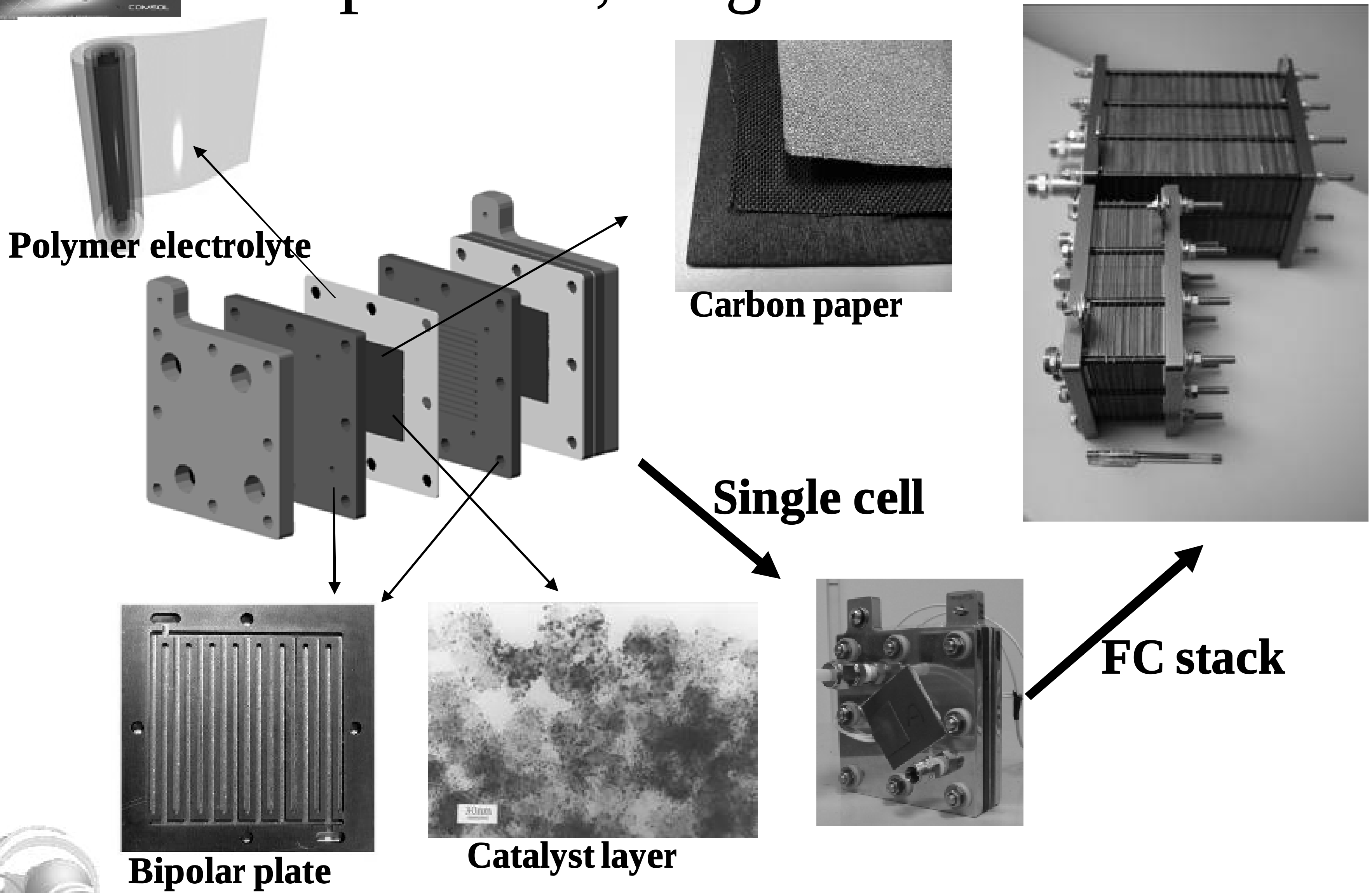


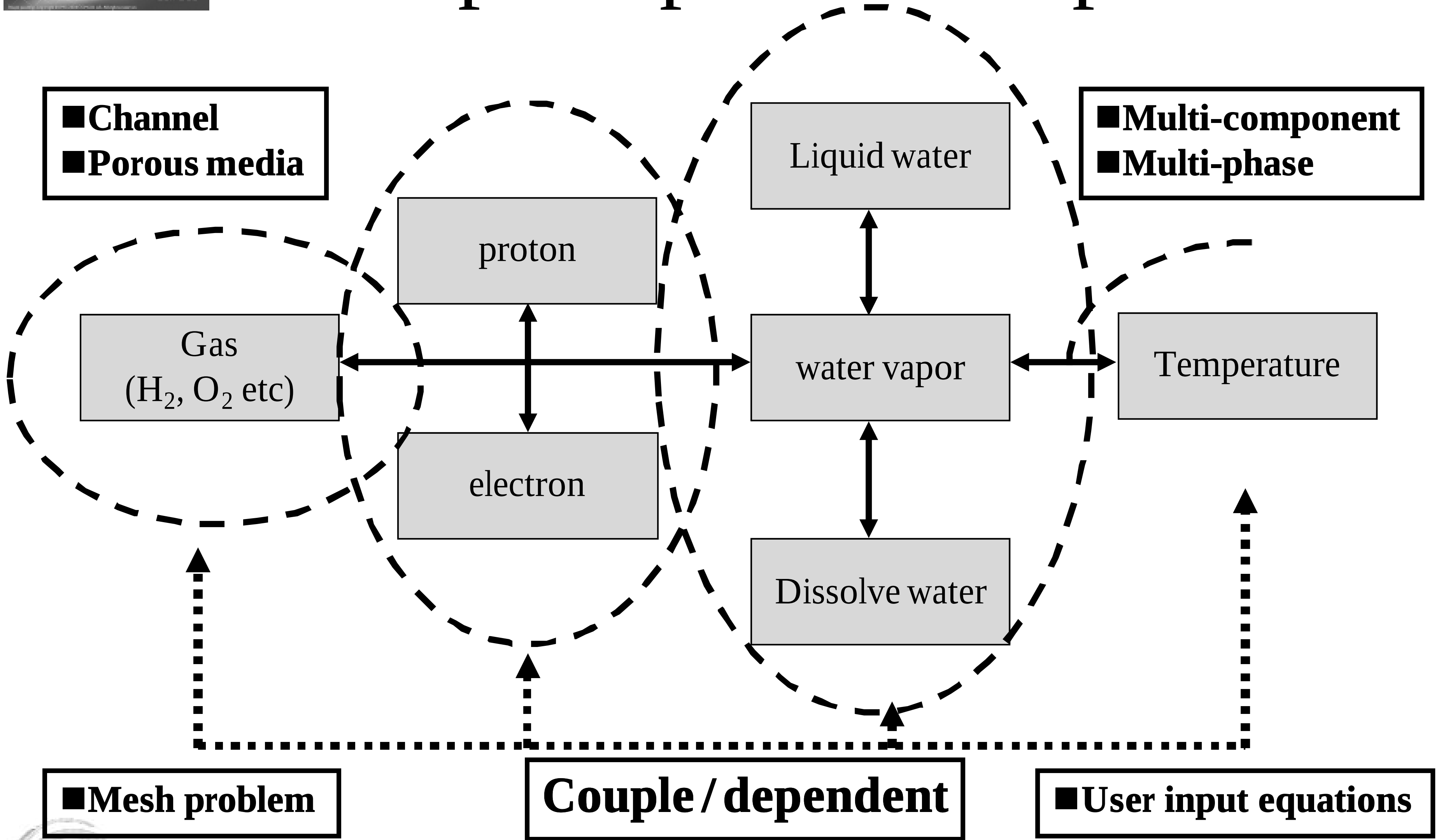
Over all: H_2+O_2? H_2O

- **Bipolar plate** (graphite): ~10000 μm
  electron conduction
- **Gas channel** : ~1000 μm
  gas transport
- **GDL** (Carbon cloth / paper): ~ 250 μm
  electron conduction and gas / water transport
- **CL** (Pt, Carbon, Nafion): ~ 10 μm
  electron conduction, gas / water transport
  proton conduction and chemical reaction
- **Membrane** (Nafion): ~ 100 μm
  proton conduction and water transport

Components, single cell and stack



Complex species transport



Governing equations

- Conservation of species:

$$\nabla\left(-D_{eff,O2}\nabla C_{O2}\right)=S_{O2}$$

$$\nabla\left(-D_{eff,H2}\nabla C_{H2}\right)=S_{H2}$$

$$\nabla\left(-D_{eff,wv}\nabla C_{wv}\right)=S_{wv}$$

$$\nabla\left(-\frac{r_{nafion}}{EW}D_{H2O,eff}^{Naf}\nabla l\right)-\nabla\left(\frac{n_d}{F}s_p^{eff}\nabla f_{electrolyte}\right)=S_l$$

$$\nabla\left(-r_l D_{cap}\nabla s\right)-\nabla\left(r_l\frac{k_{p,l}}{m_l}\nabla p_g\right)=S_l$$

- Conservation of energy:

$$\nabla\left(-k_{eff}\ \nabla T\right)=S_T$$

- Conservation of potential:

$$-\nabla\left(s_e^{eff}\nabla j_{Solid}\right)=S_e$$

$$-\nabla\left(s_P^{eff}\nabla j_{electrolyte}\right)=S_p$$

Source terms

Source Terms	AGDL	ACL	PEM	CCL	CGDL
S_{O2} mol/(m^{3}s)				$j_c / 4F$	0
S_{H2} mol/(m^{3}s)	0	$-j_a / 2F$			
S_{wv} mol/(m^{3}s)	$-S_l / M_{H2O}$	$-S_l / M_{H2O} - S_l$		$-S_l / M_{H2O}$	$-S_l / M_{H2O}$
$S_?$ mol/(m^{3}s)		$x_a \frac{r_M}{EW}(l_{eq} - l)$	0	$x_a \frac{r_M}{EW}(l_{eq} - l)$	
S_l (kg/m^{3}s)	S_l	S_l		$S_l - S_l M_{H2O} - \frac{j_c}{4F} M_{H2O}$	S_l
S_e (A/m^3)	0	$-j_a$		$-j_c$	0
S_p (A/m^3)		j_a	0	j_c	
S_T(W/m^3)	$\frac{I^2}{s_e^{eff}} + S_l \Delta h_{lg}$	$\lvert j \rvert \lvert h \rvert + \frac{I^2}{s_{eff}} + S_l \Delta h_{lg}$	$\frac{I^2}{s_p^{eff}}$	$\lvert j \rvert (\lvert h \rvert - \frac{T\Delta S}{nF}) + \frac{I^2}{s_{eff}} + S_l \Delta h_{lg}$	$\frac{I^2}{s_e^{eff}} + S_l \Delta h_{lg}$

Transport parameters

$$D_{H2}^{0} = D_{H2O}^{0} = 1.055\times10^{-4}(T/333)^{1.75}(101325/P)$$

$$D_{H2O}^{0} = 0.2982\times10^{-4}(T/333)^{1.75}(101325/P)$$

$$D_{O2}^{0} = 0.2652\times10^{-4}(T/333)^{1.75}(101325/P)$$

$$D_{O2,nafion}^{0} = 3.1\times10^{-7}\exp(-2768/T))$$

$$D_{H2O,nafion}^{0} = 3.1\times10^{-7}\, l\,(e^{0.28\,l}-1)e^{(-2436/T)} \quad 0 < l < 3$$

$$D_{H2O,nafion}^{0} = 4.17\times10^{-8}\, l\,(161e^{-l}+1)e^{(-2436/T)} \quad 3 \le l \le 17$$

$$H_{O2}^{Nafion} = 1.33\times10^{5}\exp(-666/T)$$

$$s_{p}^{0} = (0.514\,l - 0.326)\exp(1268(\frac{1}{303}-\frac{1}{T})) \quad l \ge 1$$

$$s_{p}^{0} = 0.1879\,l\,\exp(1268(\frac{1}{303}-\frac{1}{T})) \quad l < 1$$

Kinetic parameters

$$h = j_{solid} - j_{electroltye} - j_0$$

$$j_{0,a}^{ref} = i_{0,a}^{ref}\Big|_{343K} (S/V)_0 \exp\left[\frac{E_a^{act}}{R}\left(\frac{1}{343} - \frac{1}{T}\right)\right]$$

$$j_{0,c}^{ref} = i_{0,c}^{ref}\Big|_{343K} (S/V)_0 \exp\left[\frac{E_c^{act}}{R}\left(\frac{1}{343} - \frac{1}{T}\right)\right]$$

$$j_a = j_{0,a}^{ref}\left(\frac{P_{H2}}{P_{H2}^{ref}}\right)\left[\exp\left(\frac{ahF}{RT}\right) - \exp\left(-\frac{ahF}{RT}\right)\right]$$

$$j_c = -4F\frac{P_{O2}}{H_{O2}^{Naf}} x k_h$$

$$f = \frac{r_{agg}}{3}\sqrt{k_h / \left[D_{O2,eff}^{eff}(1 - e_{CL})\right]}$$

$$x = \left[3f\coth(3f) - 1\right]/(3f^2)$$

$$k_h = \frac{1}{4FC_{O2}^{ref}} j_{0,c}^{ref} \exp\left[-\frac{a_c hF}{RT}\right]$$

$$S_l = K_{cond}\Delta P e s r_l : \Delta P \langle 0$$

$$S_l = K_{cond}\Delta P \frac{e(1-s)X_{wv}M_{H2O}}{RT} : \Delta P \geq 0$$

Simulation flow chart

Model geometry ↔
- ✓COMSOL geometry tools
- ✓Import from CAD files

↓

Parameters input ↔
- ✓Constant
- ✓Subdomain expresses

↓

Solve equations ↔
- ✓Direct (UMFPACK)
- ✓Stationary/parametrics
- ✓Adaptive mesh refinement

↓

Post processing ↔
- ✓COMSOL postprocessing tools
- ✓Export according to your own need

- **Convergence**
- **Mesh**

Challenges & solutions

- Convergence
  - Mainly due to coupled equations (8) and lots of variable dependent parameters.
    - ✓Appropriate value of initial value
    - ✓Using RESTART to solve equations step by step
- Mesh
  - Finer or coarser mesh are both possible to solve the problem

Models used in COMSOL

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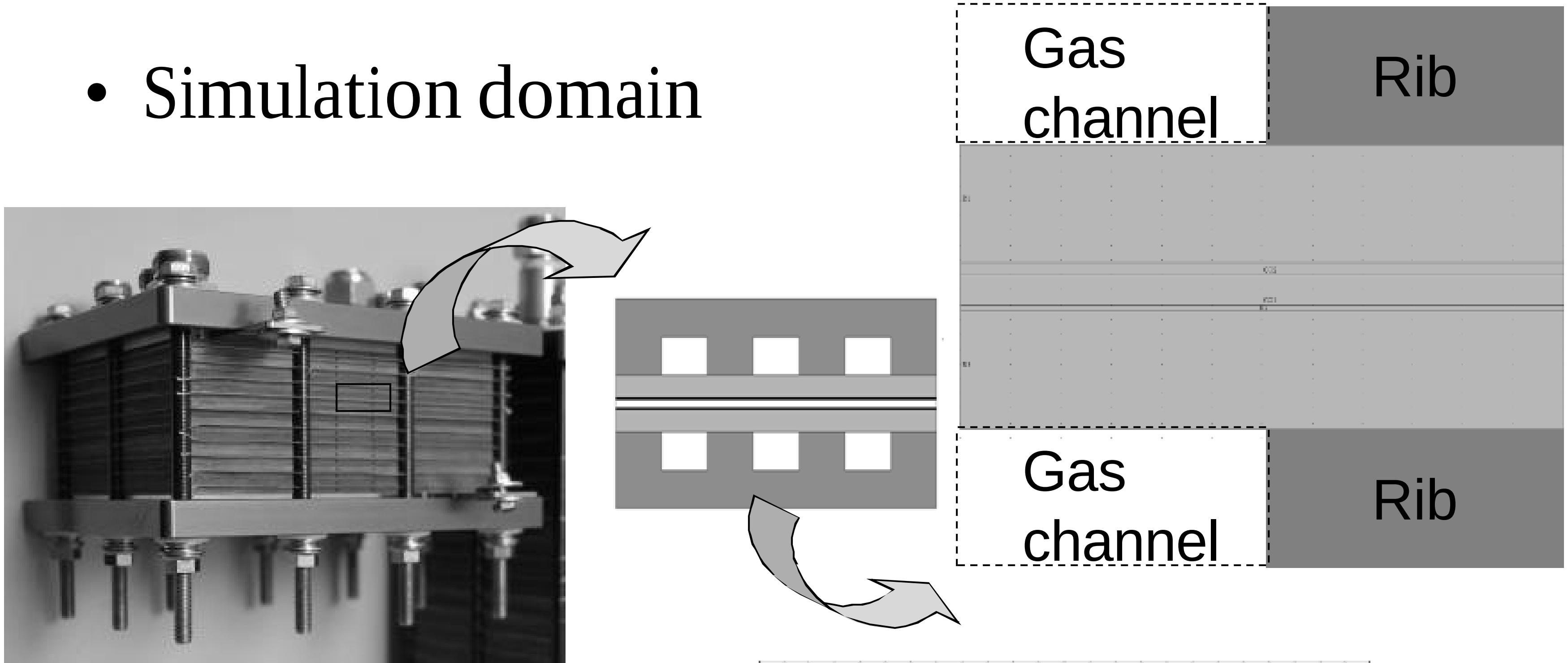
- Chemical Engineering Module
  - Mass Transport → Convection and Diffusion (4)
  - Energy Transport → Convection and Conduction(1)
- AC / DC Module
  - Conductive Media DC (2)
- COMSOL Multiphysics Module
  - PDE, Coefficient Form(1)

All solved variables are dependent

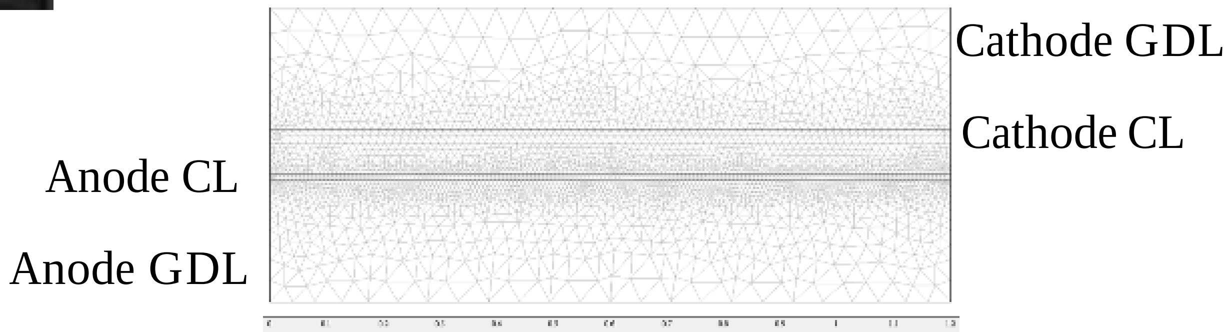
Examples solved by COMSOL - PEMFC & SOFC

2D simulations

- Simulation domain



Cathode GDL: 200µm
Cathode CL: 20µm
Electrolyte: 50µm
Anode CL: 10µm
Anode GDL 200µm



O_2/H_2 consumption

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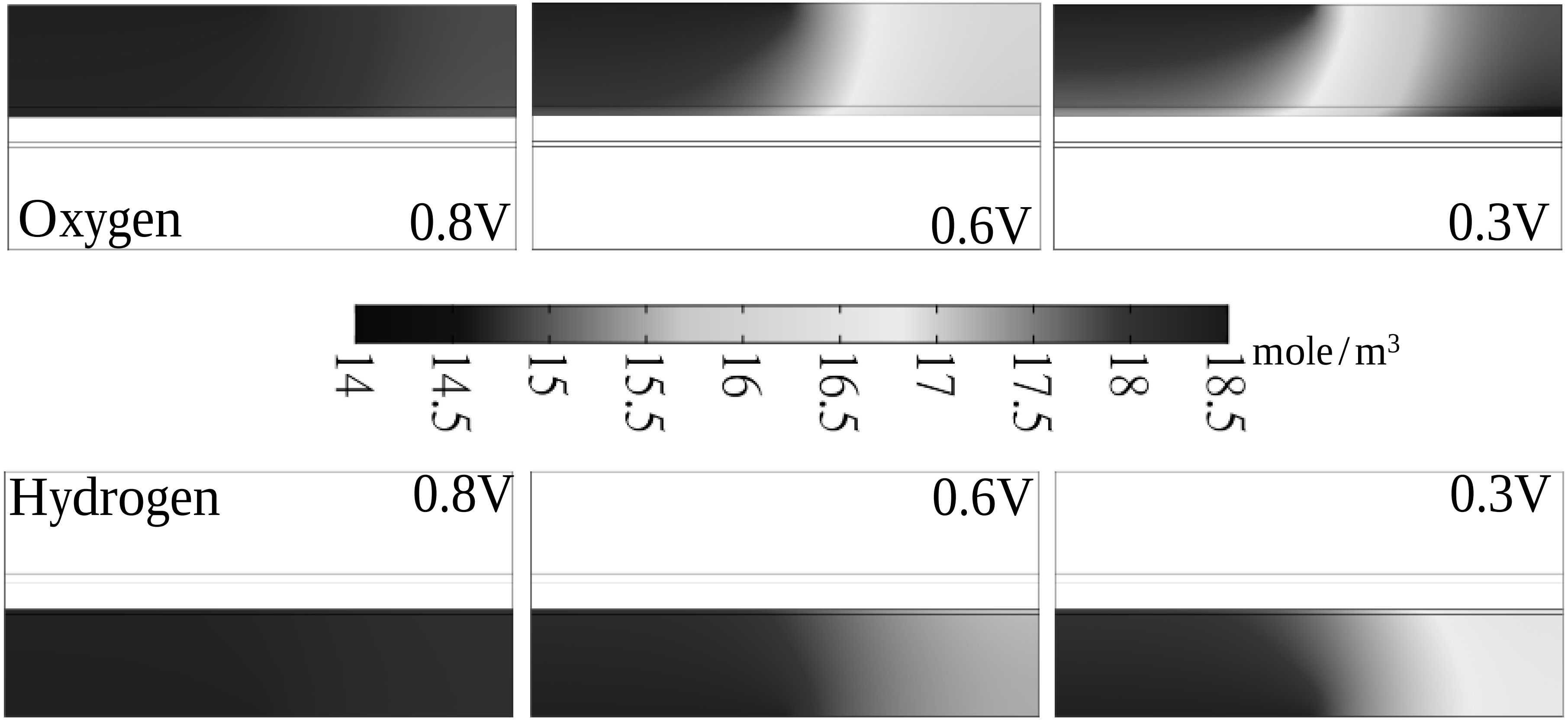
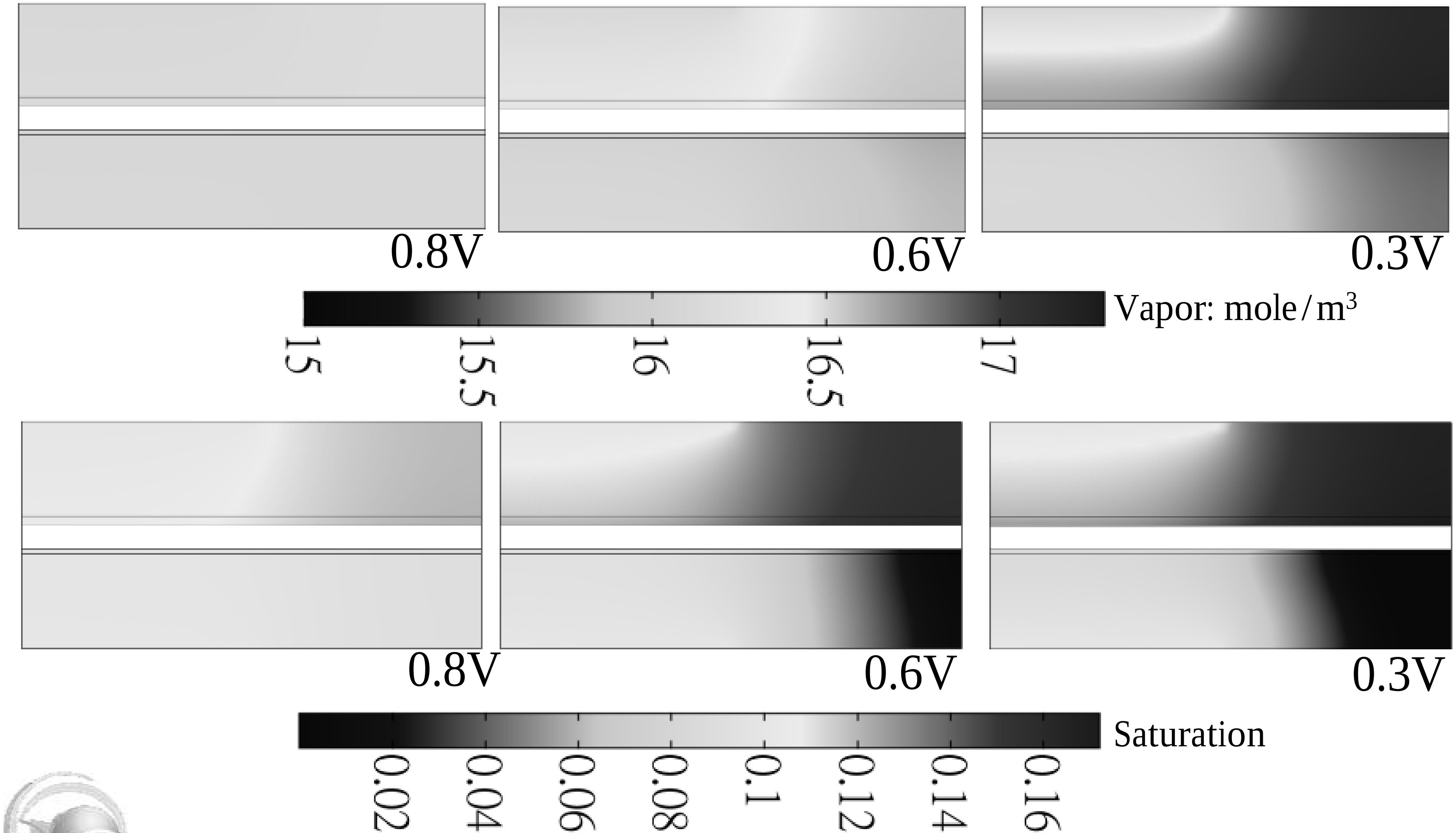
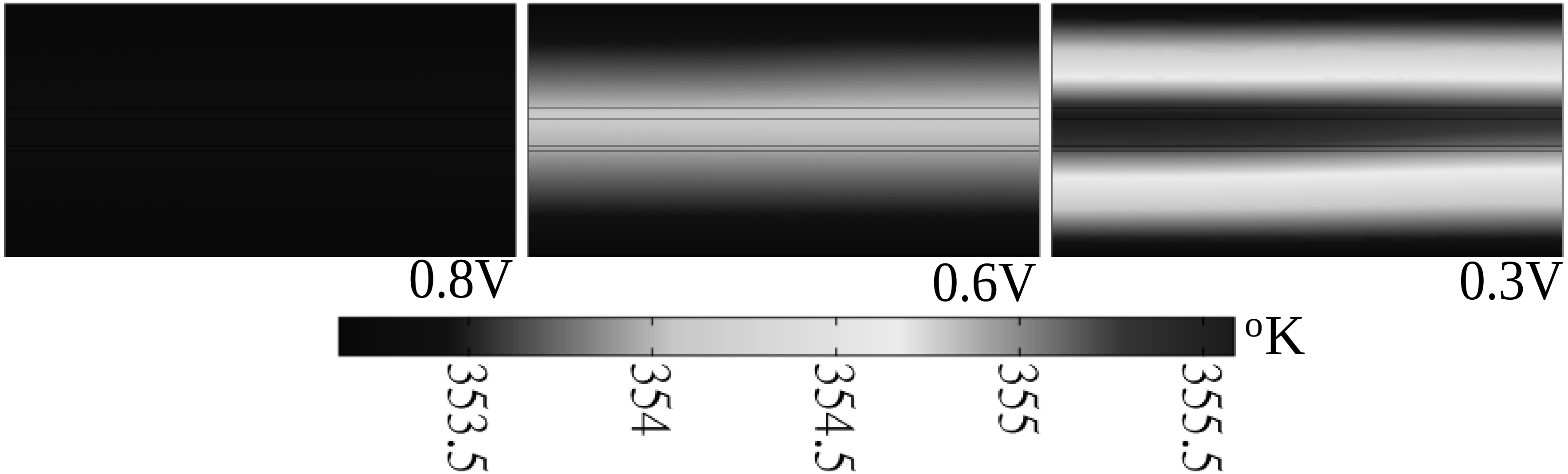
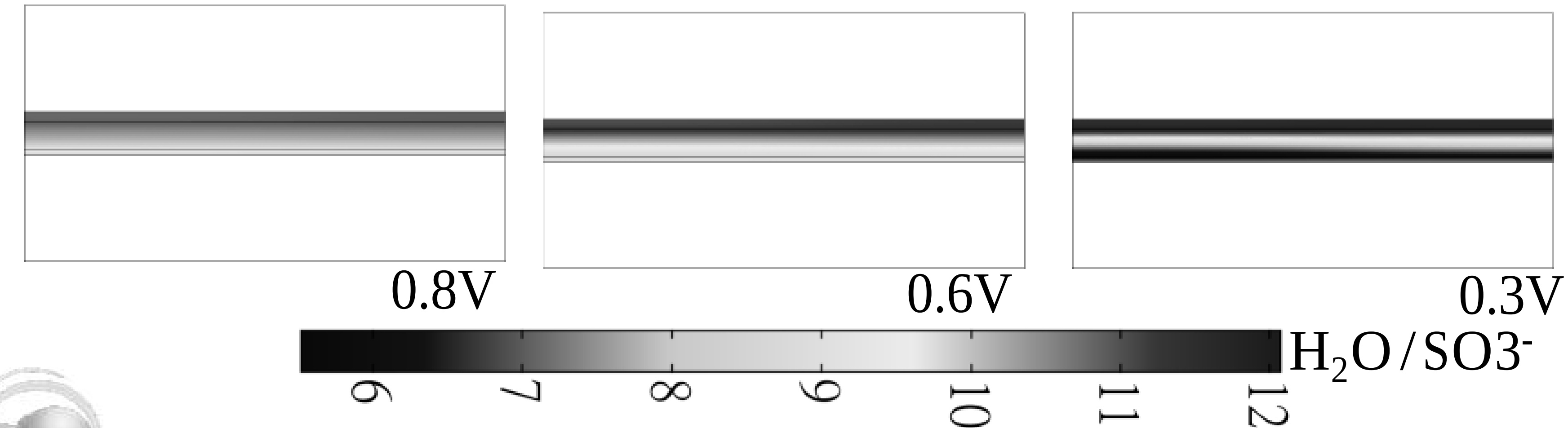


Water (vapor & liquid)



Temp. / water content plot





Validation with exp

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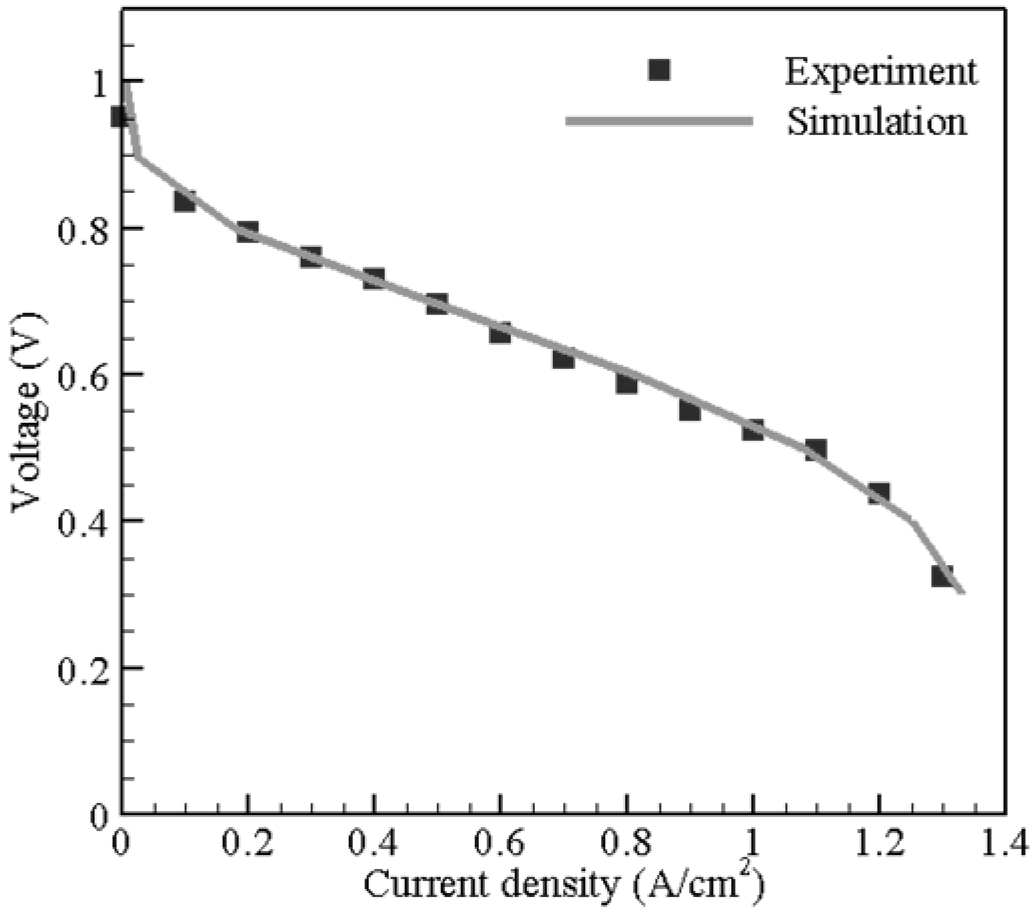
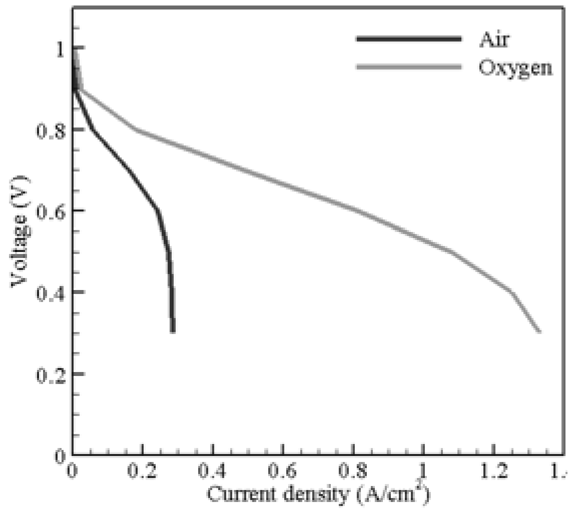
✓Performance curve
✓Operation condition
✓Parameter sensitivity

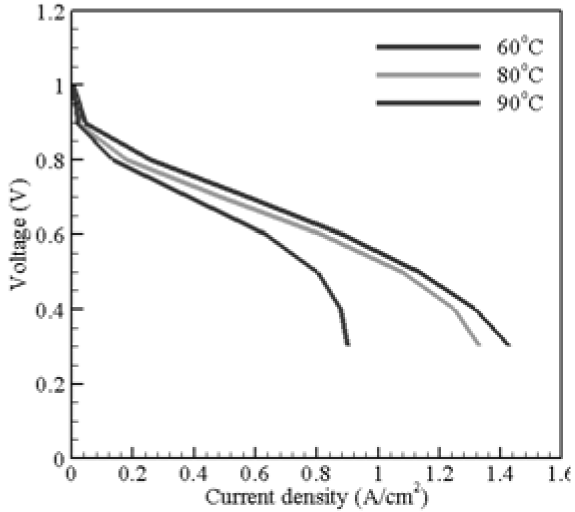


Operation conditions

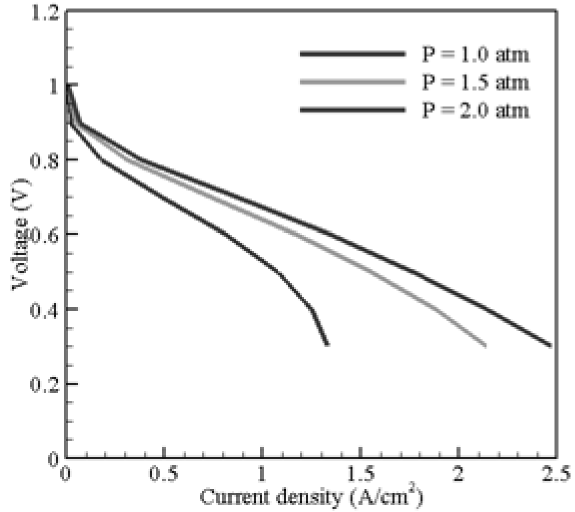
- O_2 / Air



- Temperature effect



- Pressure effect



INCREASE
CL performance

REDUCE
CL cost

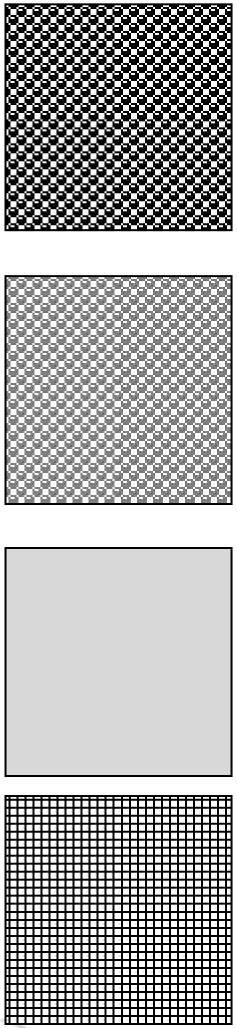
- ✓Pt loading
- ✓Nafion content
- ✓Pt/C wt%
- ✓Support material
- ✓CL thickness
- ✓Alternative catalyst material

CL with d

Perfo

Cost can be reduced!

Different CL design



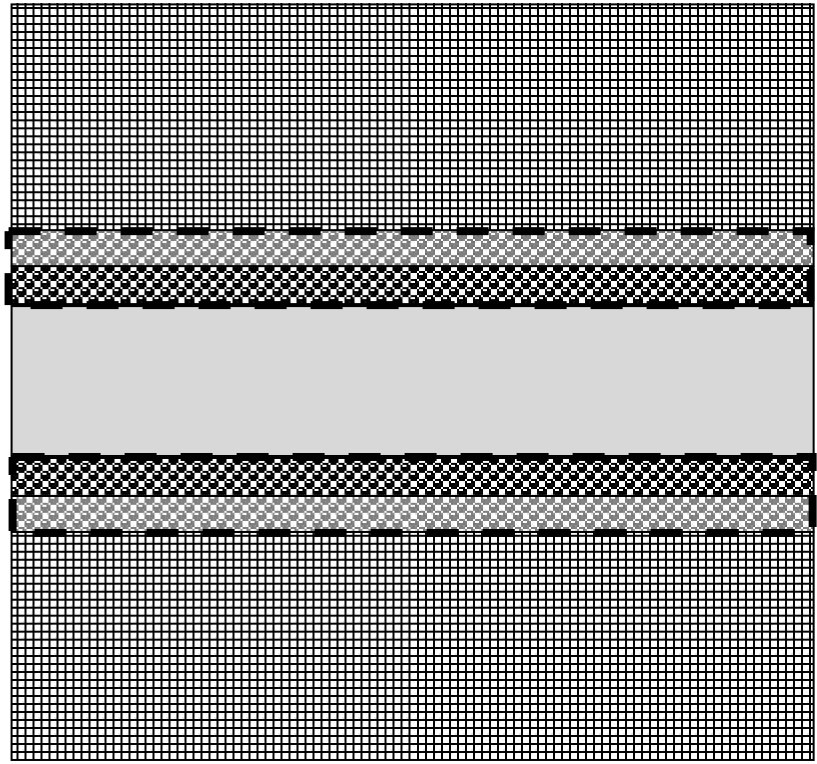
Pt/C: 80wt%

Pt/C: 40wt%

Mem(Nafion)

Gas diffusion layer

Non-uniform composition of Pt/C ratio



MEA structure

Case studied

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•Cathode: 1.0 mg/cm²

MEA#	**1**	**2**	**3**	**4**
Pt/C 80wt	0	0.1	0.2	0.4
Pt/C 40wt	1.0	0.9	0.8	0.6
Total	1.0	1.0	1.0	1.0

unit: mg/cm^2

•Anode: 0.5 mg/cm²

MEA#	**1**	**2**	**3**	**4**
Pt/C 80wt	0	0.05	0.1	0.2
Pt/C 40wt	0.5	0.45	0.4	0.3
Total	0.5	0.5	0.5	0.5

unit: mg/cm^2

Content of Pt/C 80wt% increase?

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Experimental validation

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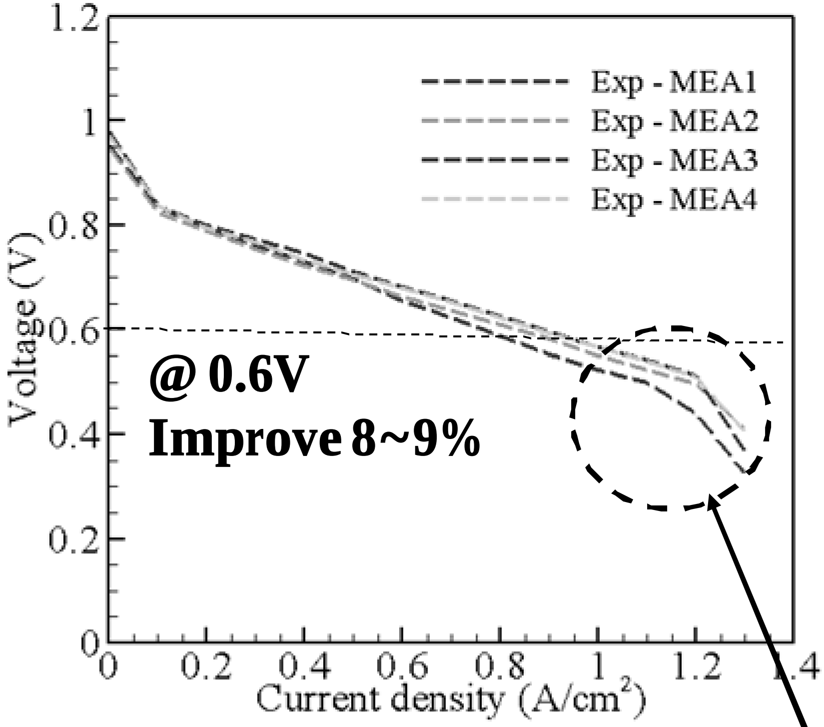

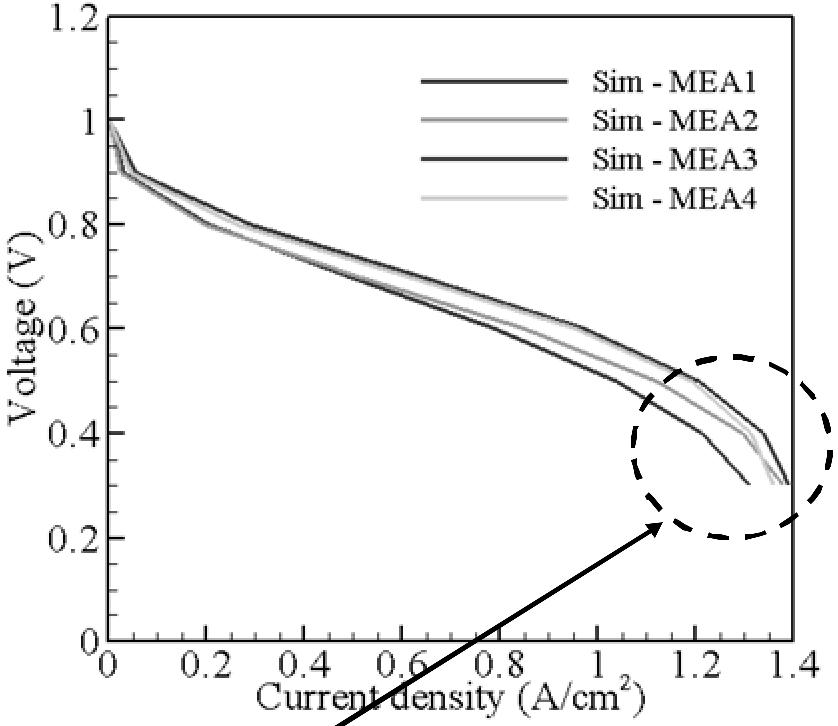

Variation of the performance is reproduced!
MEA3>MEA4>MEA2>MEA1

Trend of mass transport limit region is reproduced!

Experimental data: T. F. Yang et al, 2010, JPS Vol. 195 pp. 7359

Key parameters in CL model

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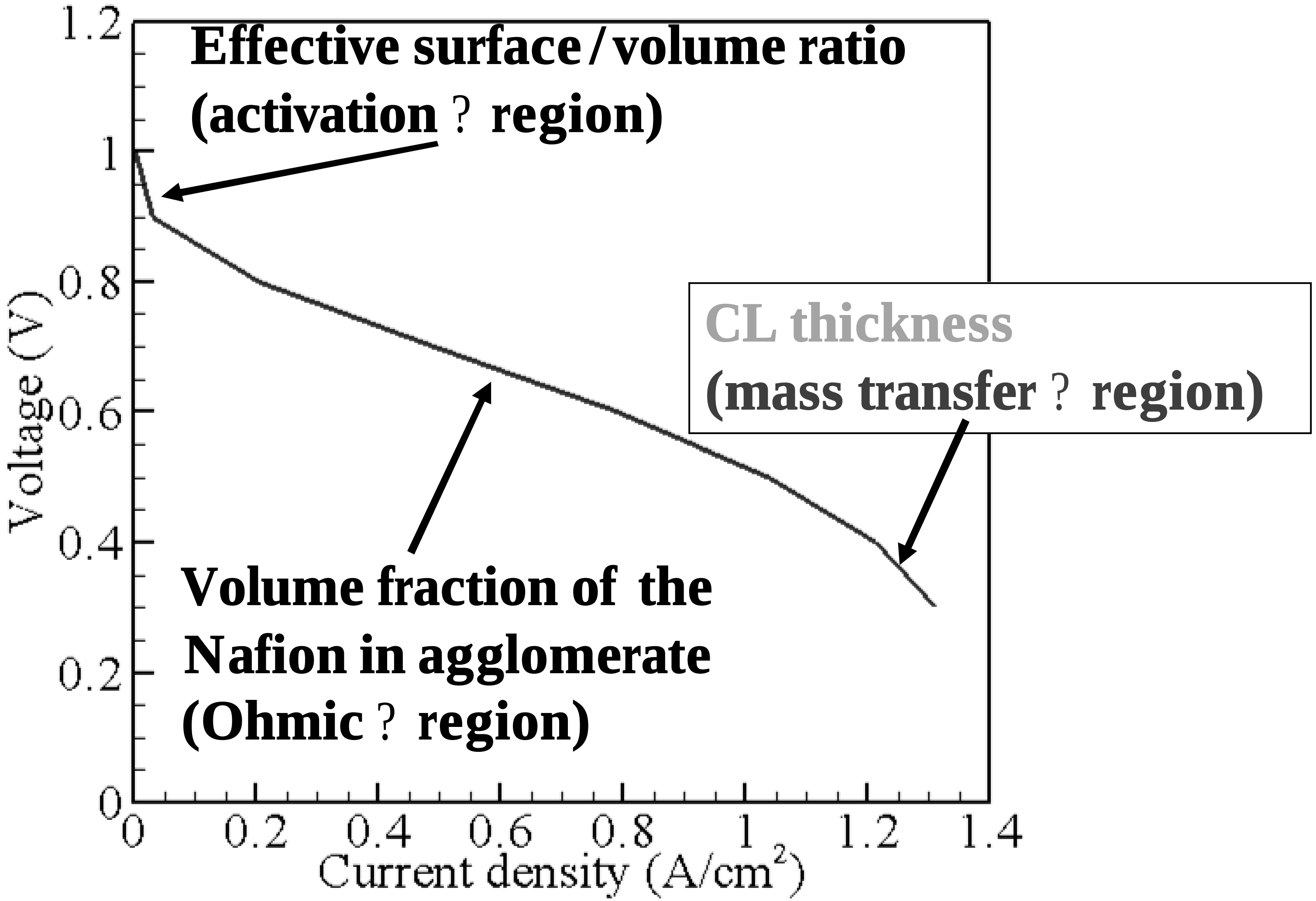
- When Pt/C wt% changes... ...
  - Porosity
  - **CL thickness**
  - **Volume fraction of the Nafion in agglomerate**
  - Volume fraction of the Pt/C in agglomerate
  - Thickness of the Nafion cover on the agglomerate
  - **Effective surface to volume ratio**

Dominate factors



Effects of different CL sub-layer

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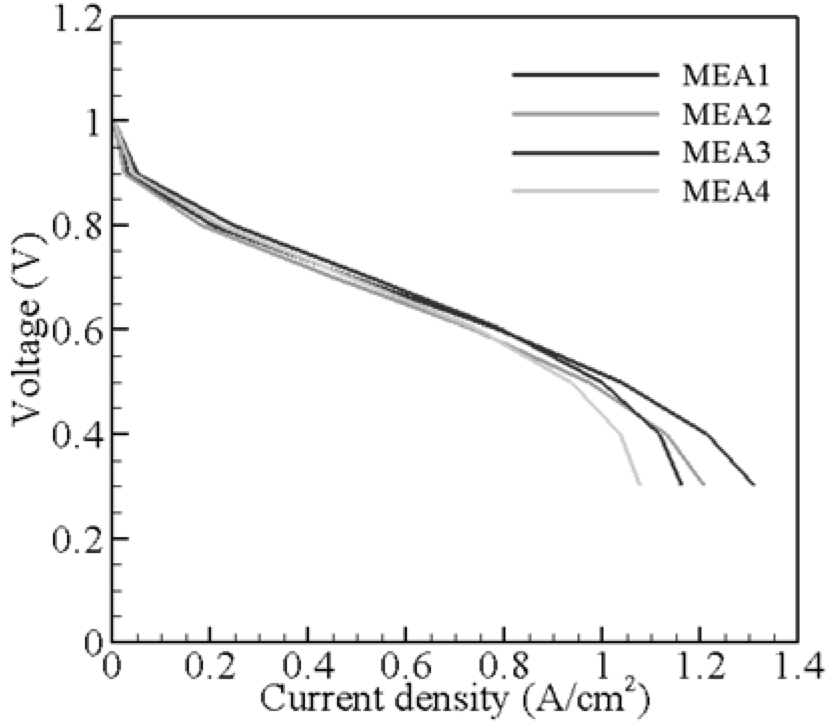
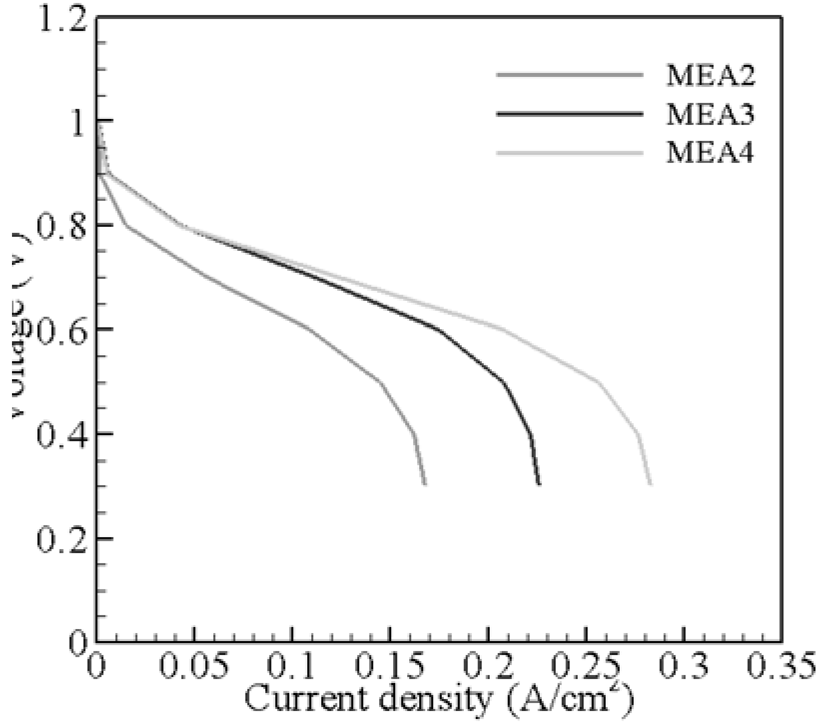
•**Sub-layer with Pt/C 40wt%**



MEA1>MEA2>MEA3>MEA4

-0.1 A/cm²   -0.04 A/cm²   -0.09 A/cm²

•**Sub-layer with Pt/C 80wt%**



MEA1<MEA2<MEA3<MEA4

+0.167 A/cm²   +0.057 A/cm²   +0.057 A/cm²

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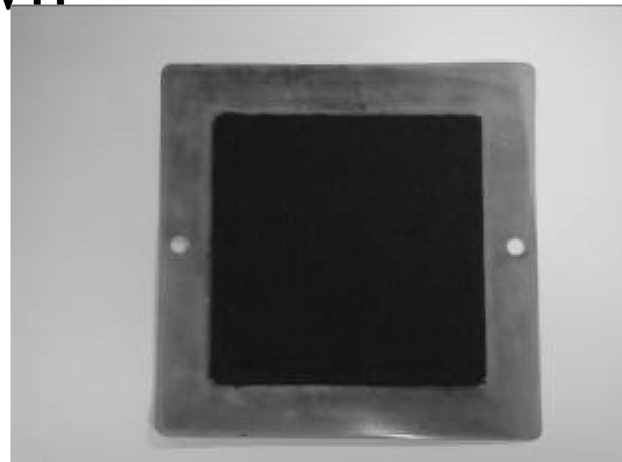
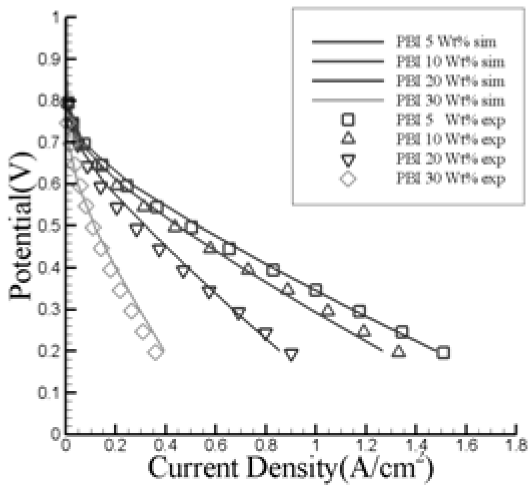
PBI based HT-PEMFC

- Operation temperature can be raised to ~180^{o}C
- No water management is required
- Higher electrode kinetics
- Acid doping level is important
- Best CL composition is unknown

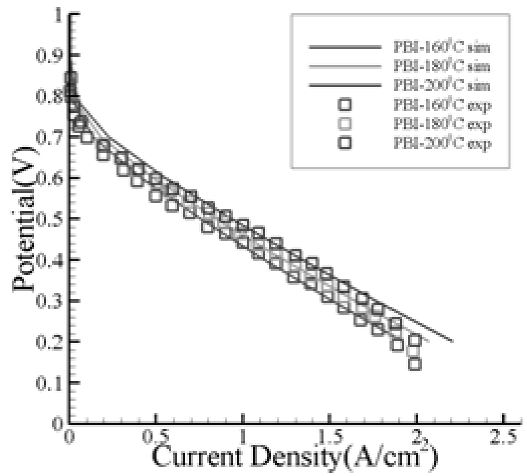


PBI wt% % Temp effect

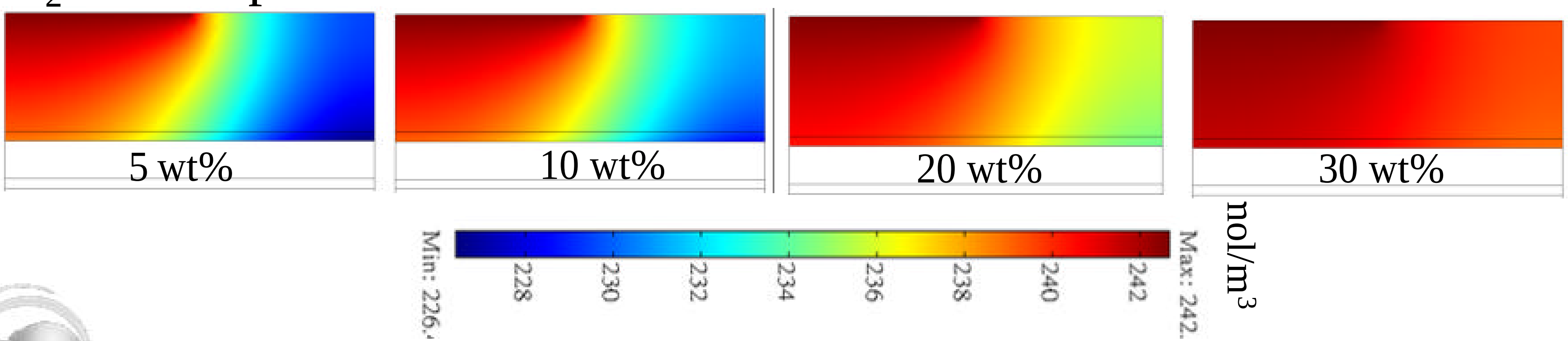
PBI wt% effect



Temperature effect



O_2 consumption



Temp. distribution

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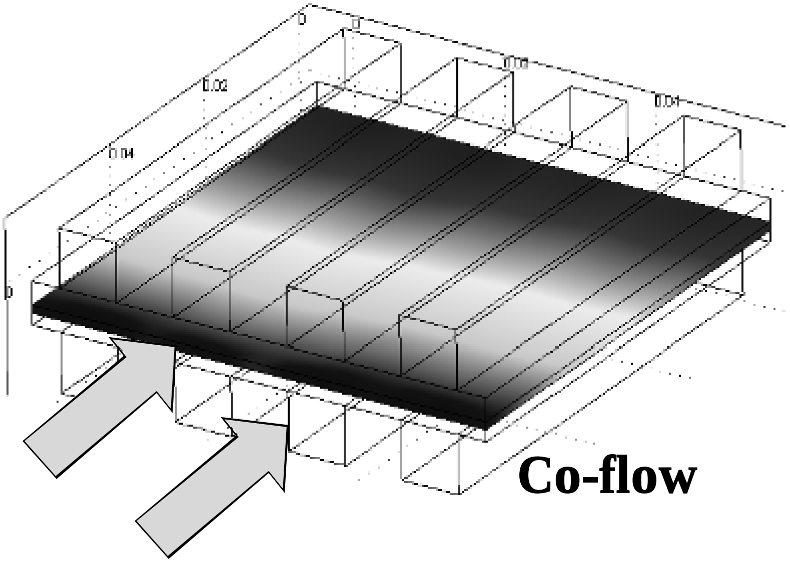
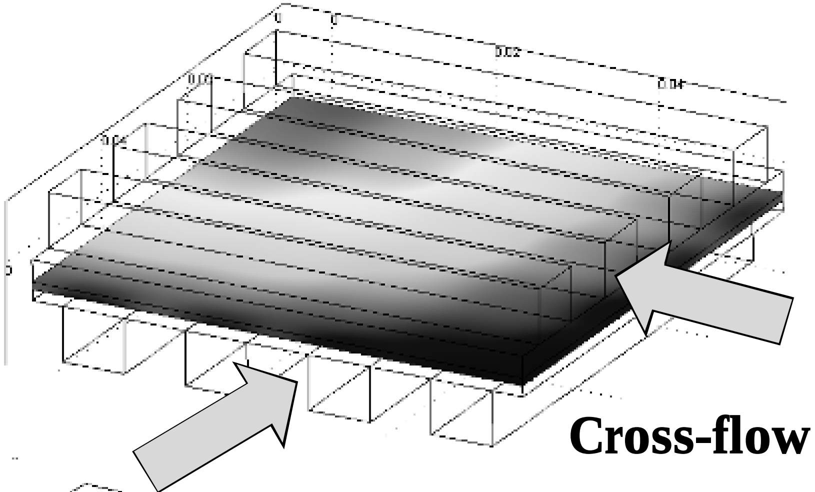
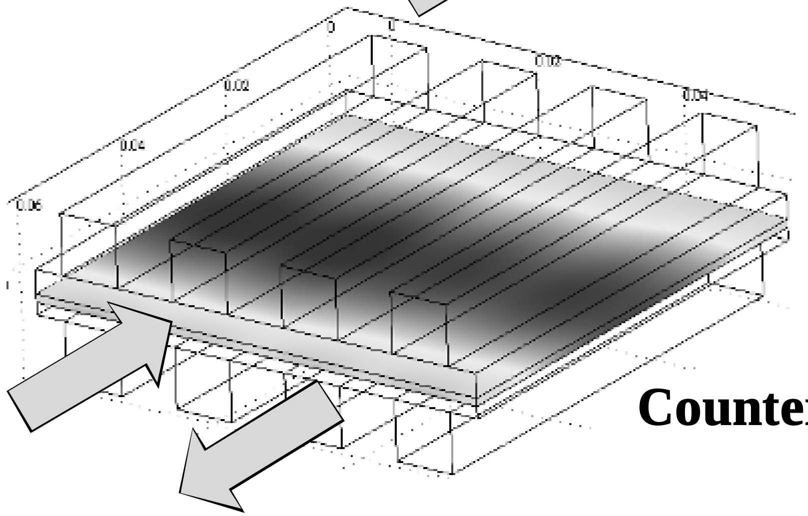


Co-flow



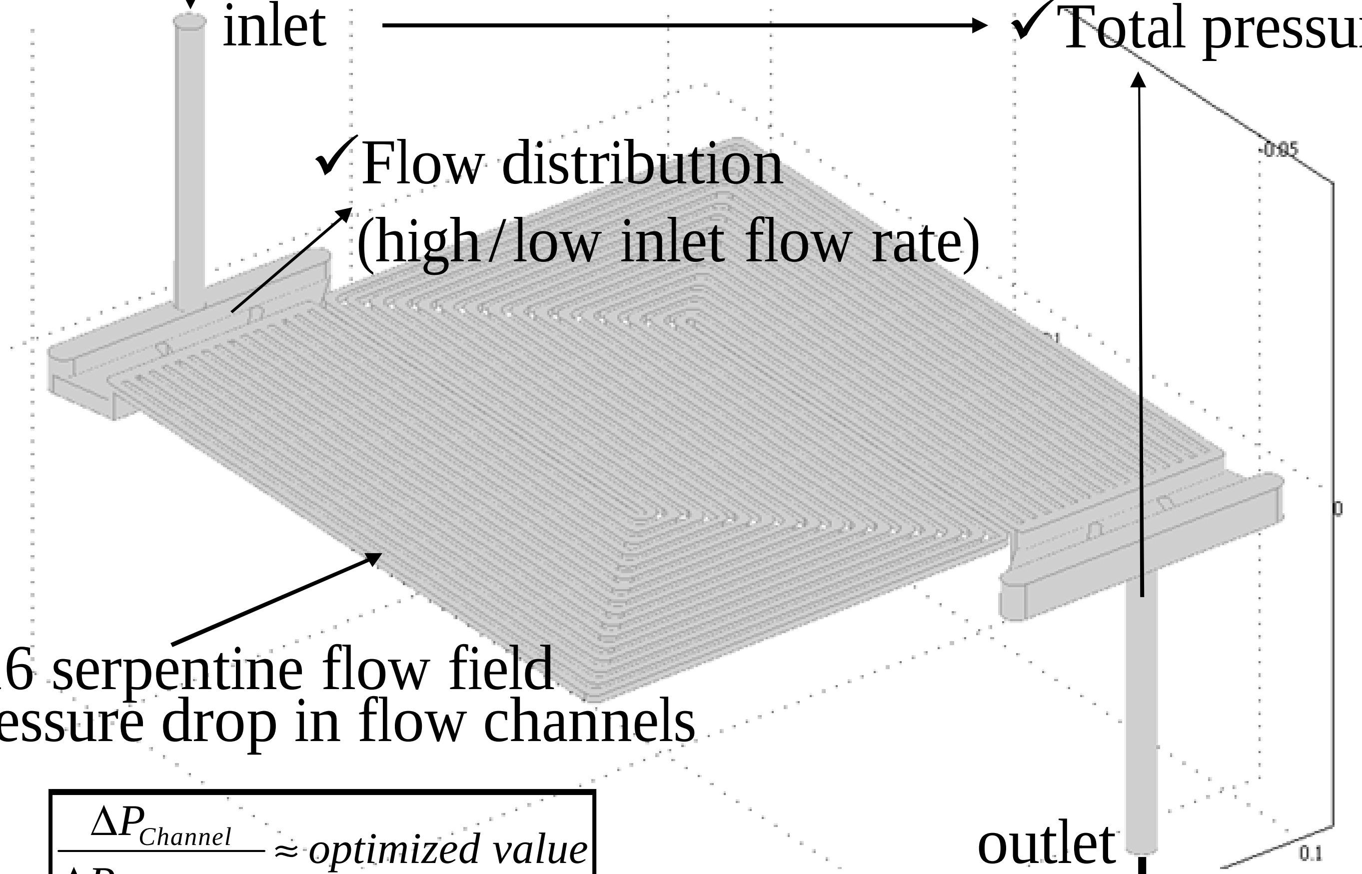
Cross-flow

Temperature distribution is highly non-uniform on the electrolyte



Counter-flow

FC stack simulation



inlet → ✓Total pressure drop

✓Flow distribution
(high/low inlet flow rate)

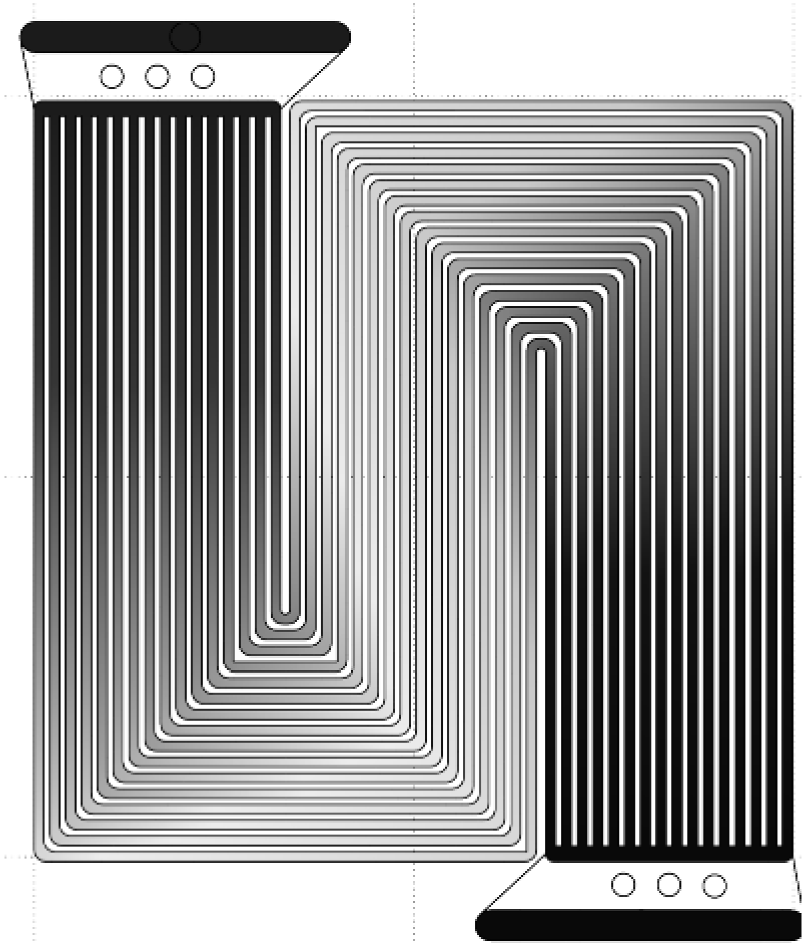
16 serpentine flow field

✓Pressure drop in flow channels

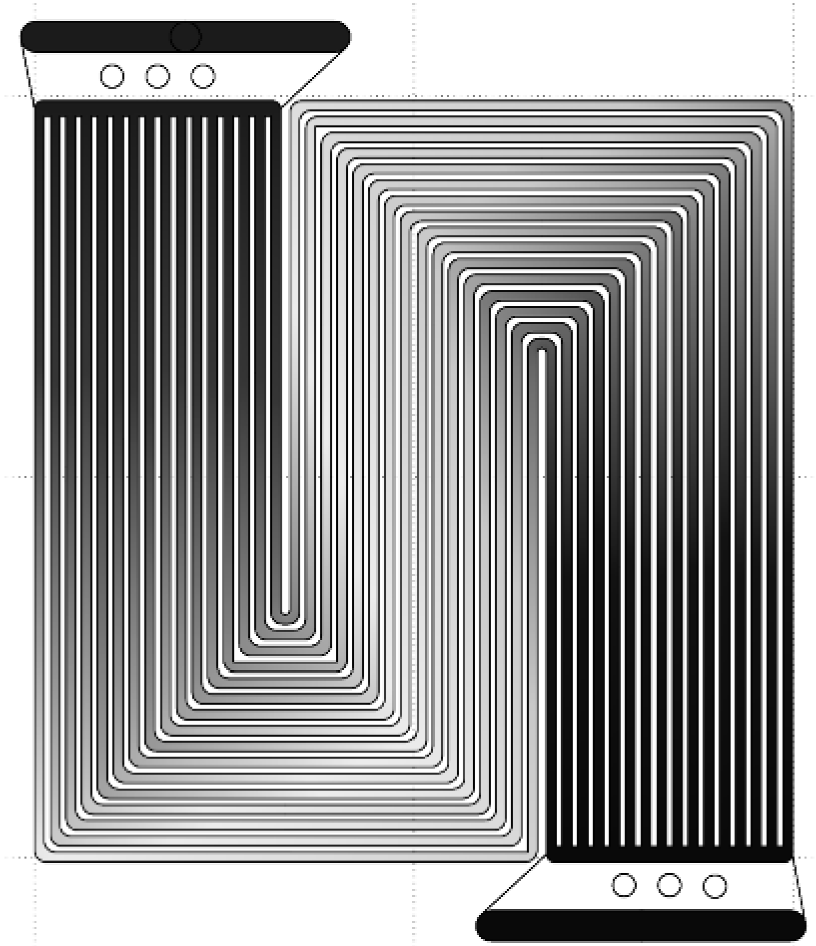
outlet

$$\frac{\Delta P_{Channel}}{\Delta P_{Inlet\_Header}} \approx optimized\ value$$

Pressure drop

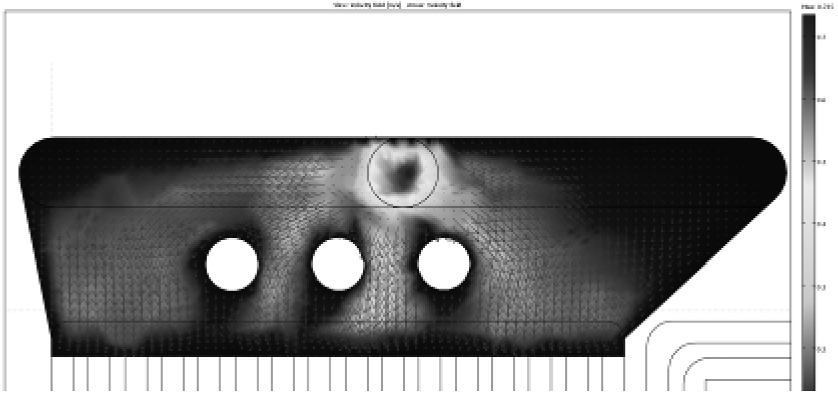


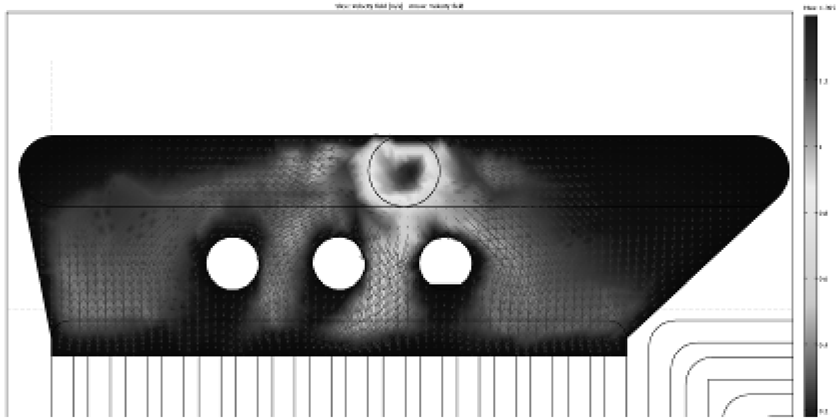
High flow rate $\Delta P \sim 155 Pa$



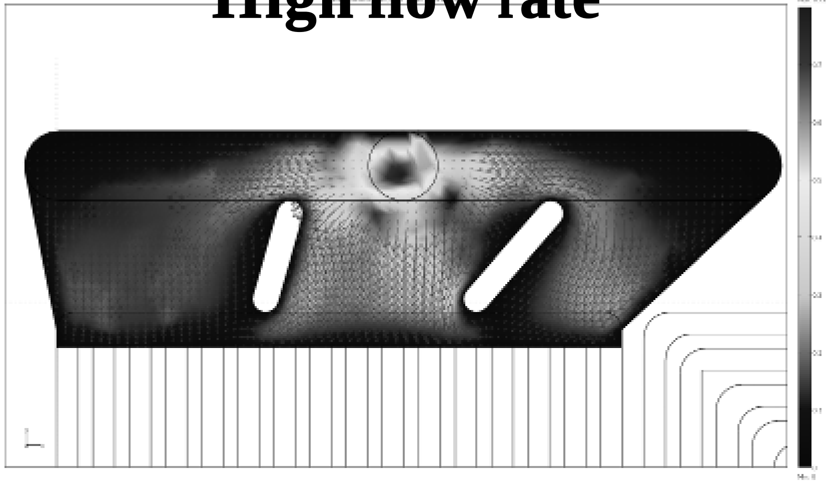
Low flow rate $\Delta P \sim 63 Pa$

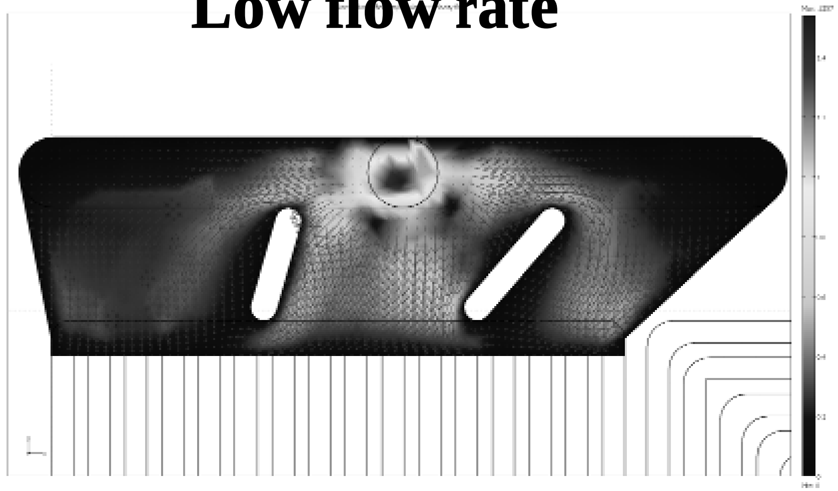
Flow distributor effect



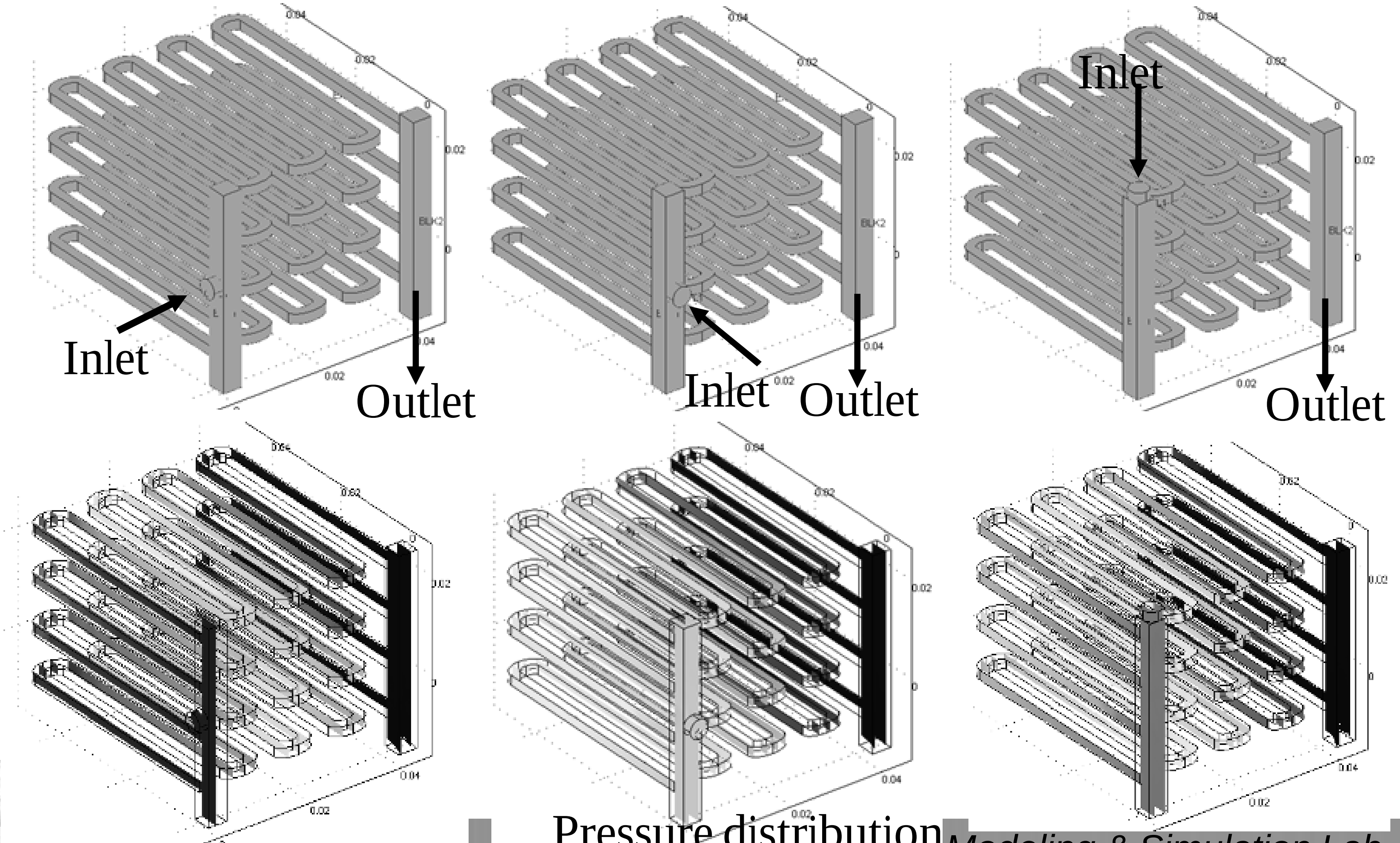


High flow rate | **Low flow rate**





FC stack simulation



Pressure distribution

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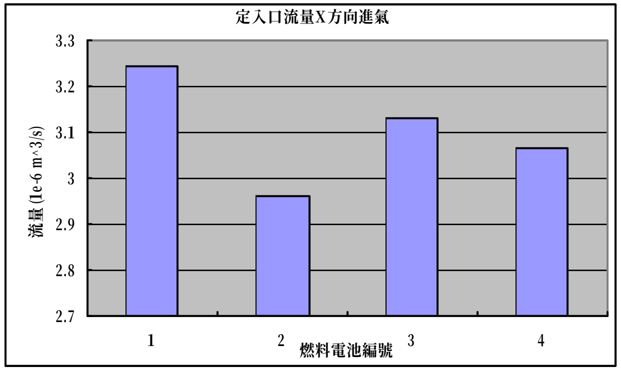
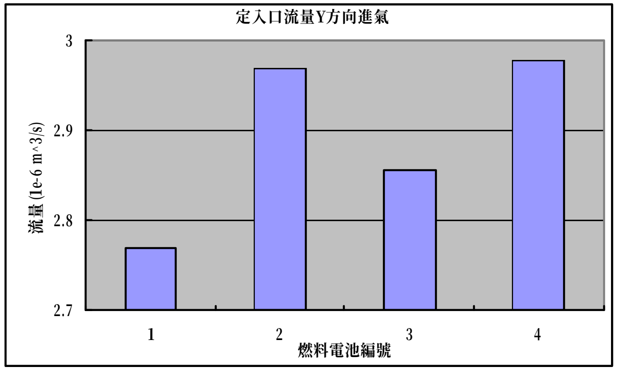
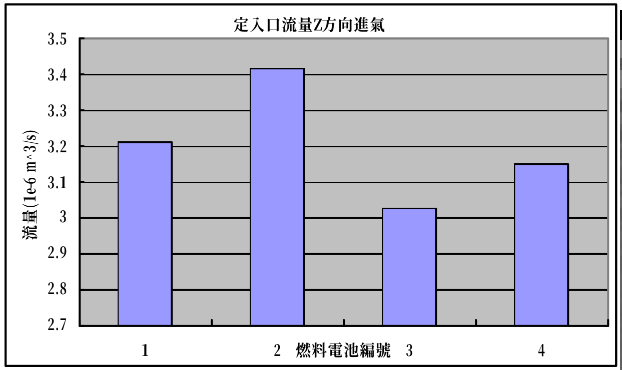
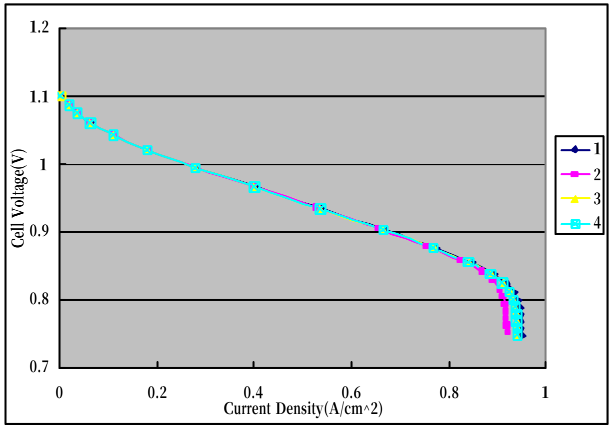
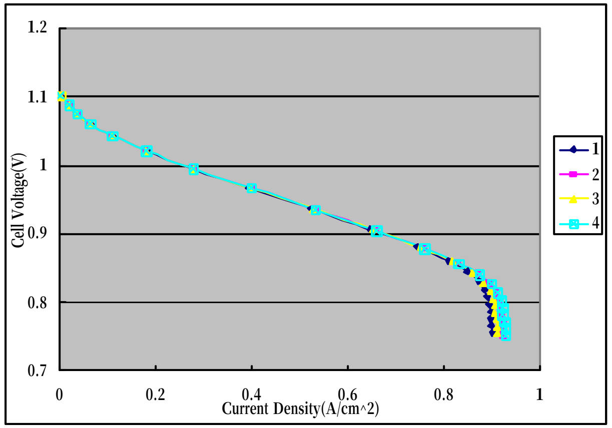
Flow distribution

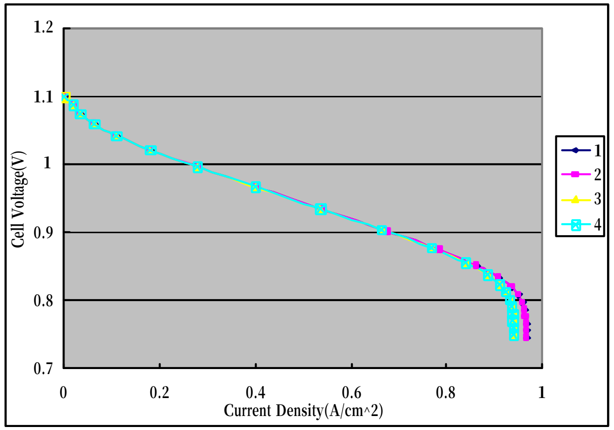




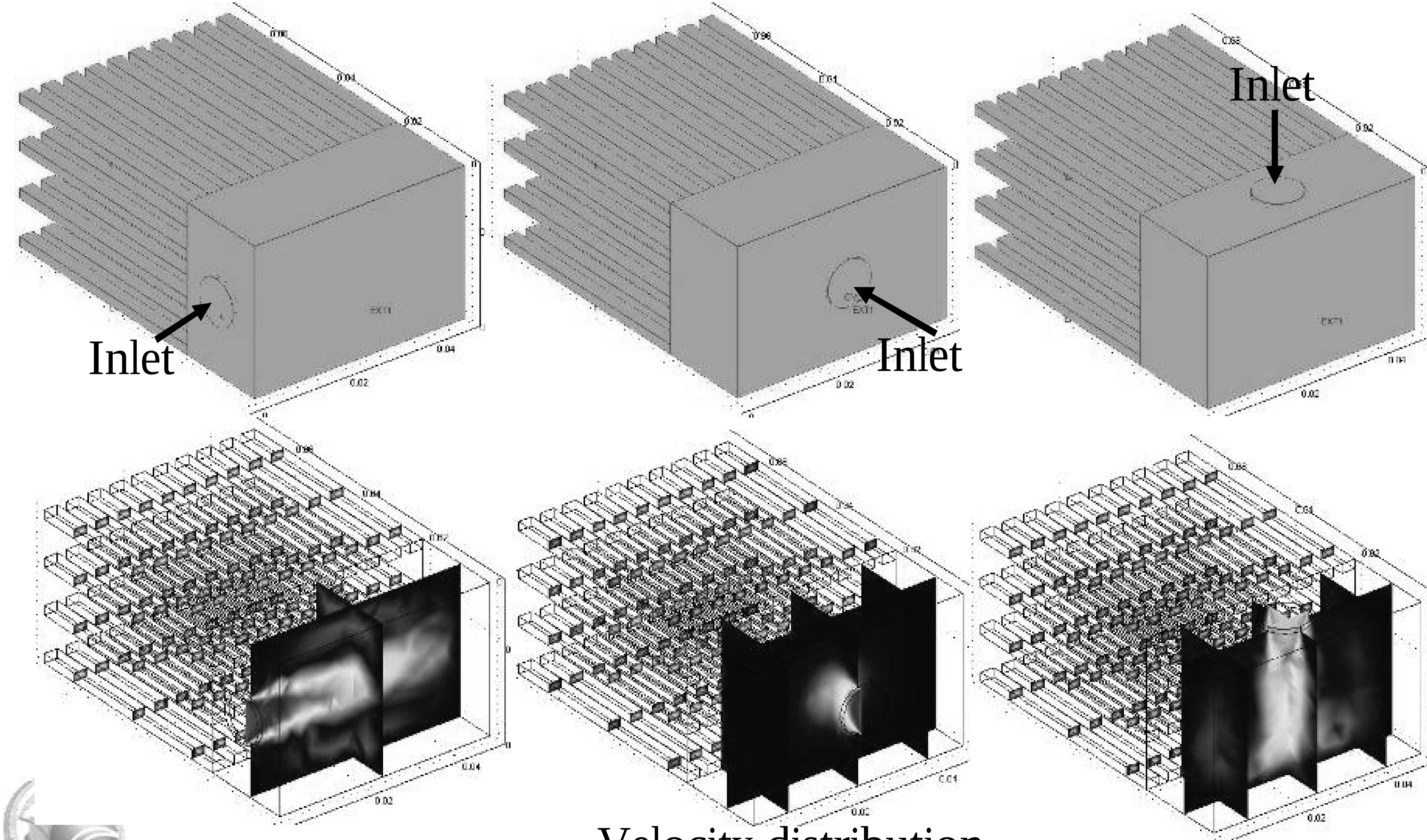








FC stack simulation



Velocity distribution

Flow distribution

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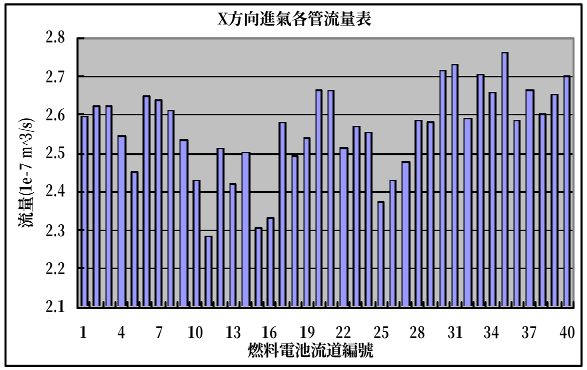

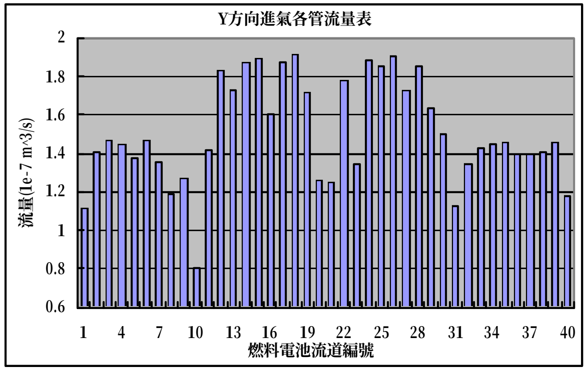

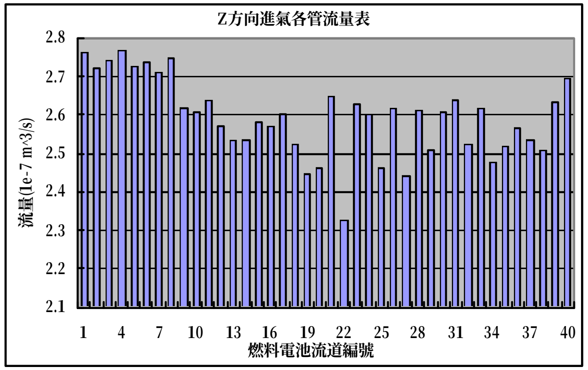

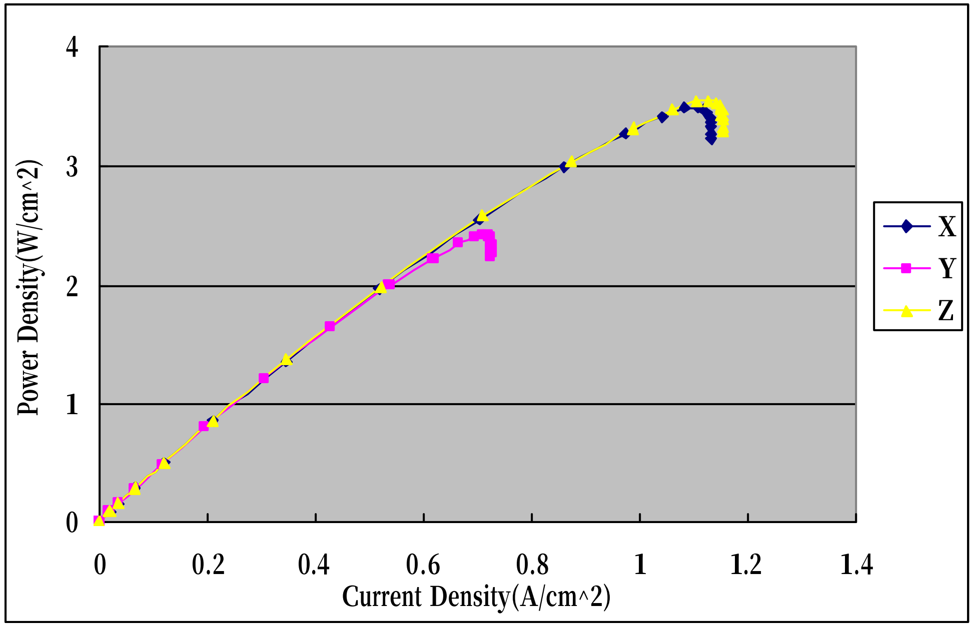

Heat transfer in LED

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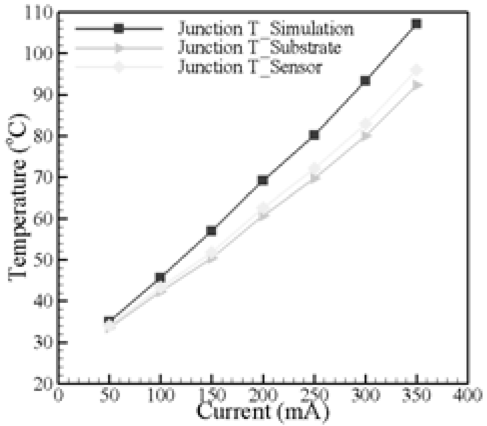
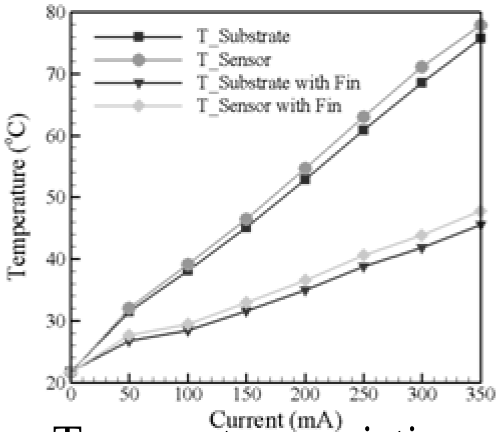
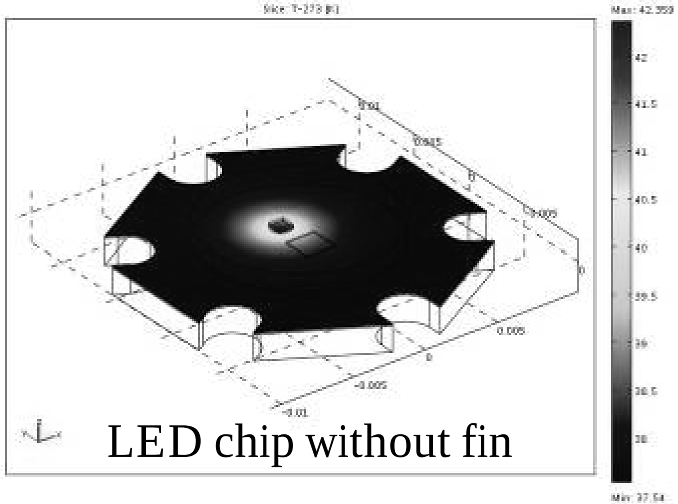


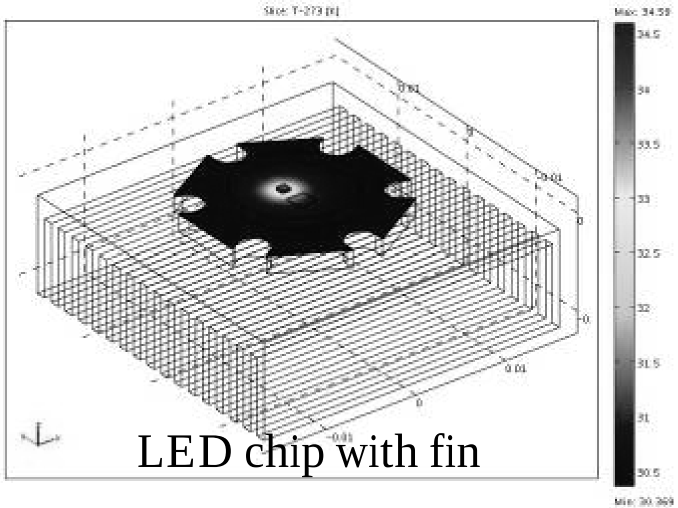
Junction temperatures at various current input



Temperature variation at different current input



LED chip without fin



LED chip with fin

Summary

- COMSOL Multiphysics is good at complex coupling problems
  - Different models can be integrated easily
  - Friendly user input interface

- It has been shown that modeling/simulation of fuel cells (component, single cell or stack) & LED is feasible.

Thanks for your attention!

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