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Effects of Gas Diffusion Layer Porosity on the Location of the Gas-Liquid Interface in a PEM Fuel Cell

Presenter：Chun-I Lee

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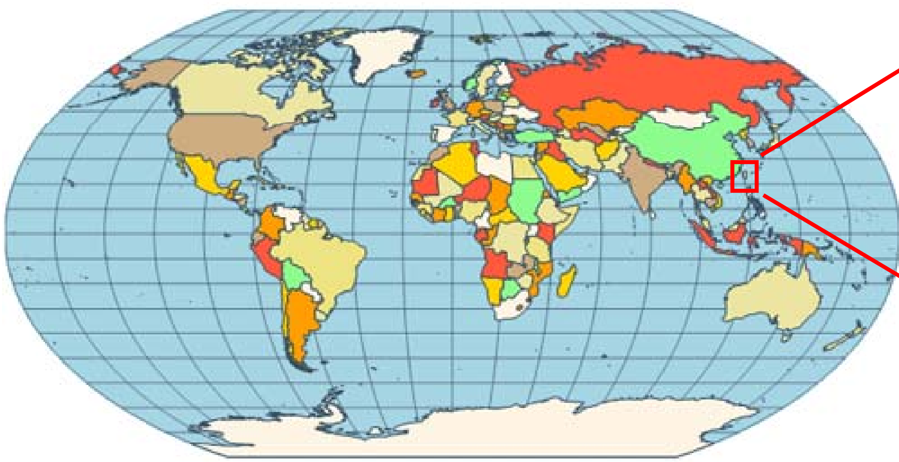
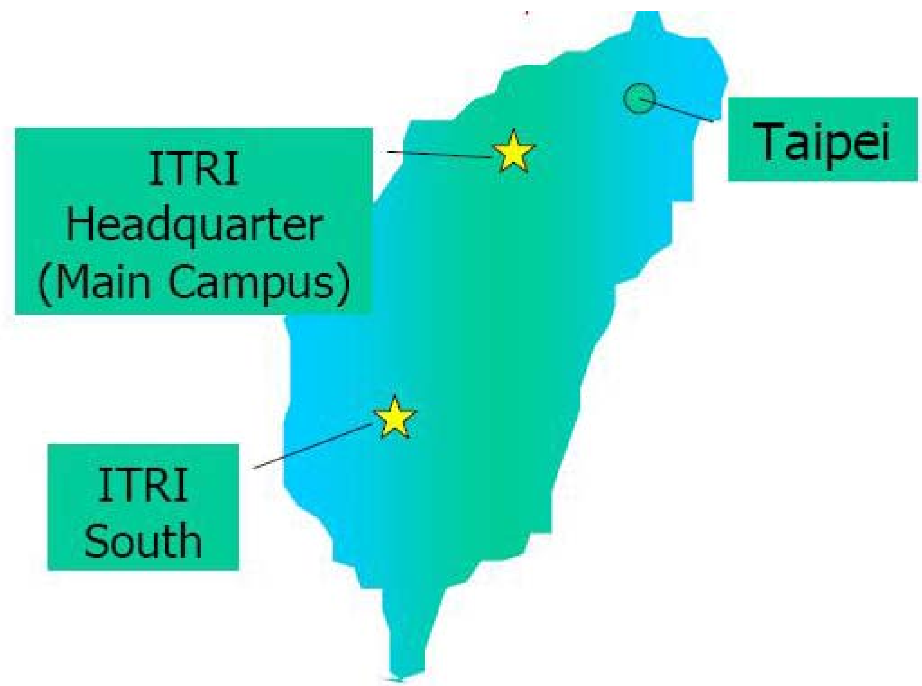
TAIWAN-FORMOSA



ITRI PROFILE

Industrial Technology Research Institute

- Founded in 1973 by the government
- A non-profit R&D organization
- Over 6,000 employees



6 Core Laboratories

- Biomedical Engineering
- Electronics and Optoelectronics
- Energy and Environment
- Information and Communications
- Material and Chemical Research
- Mechanical and Systems

5 Focus Centers

- Display Technology
- Medical Electronics and Devices
- Photovoltaics Technology
- RFID Technology
- SoC Technology

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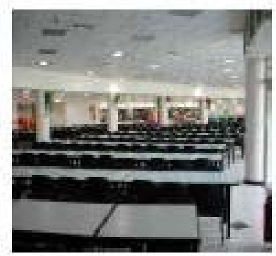
ITRI Innovation Plaza



OUTLINES

- Objective
- Mathematical Modeling
- Results and Discussion
- Conclusions

Objective

- Develop a three-dimensional mathematical model describing the transport phenomena and conjugated water and heat management in a PEMFC.

- Numerically investigate the gas-liquid interface location by effects of the GDL porosity, cathode humidification, humidification temperature, and cell temperature.

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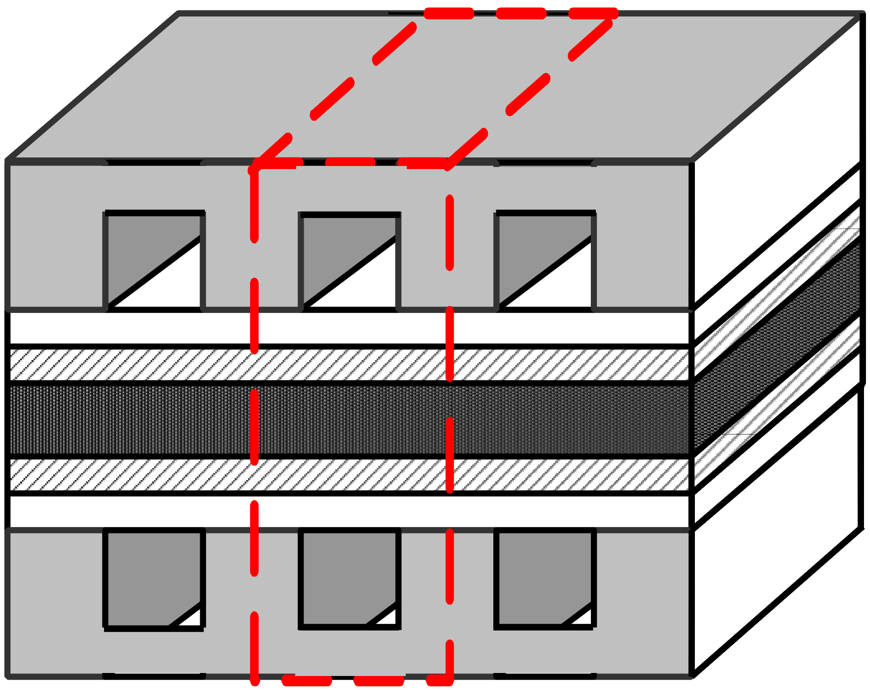
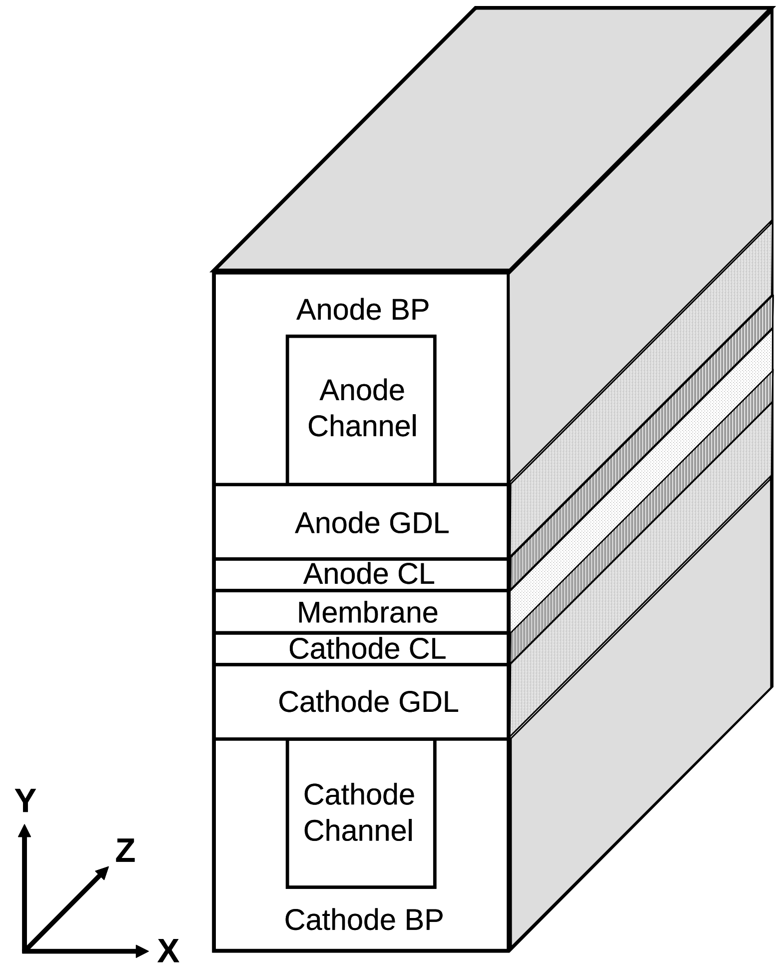
Mathematical Modeling

- Physical domain





Mathematical Modeling

- Assumptions
  - The system operates in a steady state.
  - The gas mixtures at the anode and cathode are ideal gases.
  - The mixture flow field is laminar as its velocity is low under normal operating conditions.
  - The properties of the porous medium are isotropic and homogeneous.
  - Thermodynamic and electrochemical properties of the gases and the solid materials of the fuel cell components are assumed constant.

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Mathematical Modeling

- Governing equations
  - Mass conservation

$$\nabla \cdot \left(\varepsilon_{eff} \rho \vec{u} \right) = 0$$

$$\varepsilon_{eff} = \varepsilon (1 - s)$$

  - Momentum conservation

$$\nabla \cdot \left(\rho \varepsilon_{eff} \vec{u} \vec{u} \right) = -\varepsilon_{eff} \nabla P + \nabla \cdot \left(\varepsilon_{eff} \mu_{eff} \nabla \vec{u} \right) + S_m$$

$$S_m = -(\vec{F}_{Darcy} + \vec{F}_{Forch})$$

$$\vec{F}_{Darcy} = \frac{\varepsilon_{eff}^{\ 2} \mu_{eff} \vec{u}}{K} \qquad \vec{F}_{Forch} = \frac{\varepsilon_{eff}^{\ 3} C_F \rho}{\sqrt{K}} \left| \vec{u} \right| \vec{u}$$

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Mathematical Modeling

- Species conservation

$$\nabla \cdot \left(\varepsilon_{eff}\vec{u}C_k\right) = \nabla \cdot \left(D_{k,eff}\nabla C_k\right) + S_c$$

$$S_c = \begin{cases} H_2 : -\dfrac{1}{2FC_a} j_a \\ O_2 : -\dfrac{1}{4FC_c} j_c \\ H_2O : \dfrac{1}{2FC_c} j_c \end{cases}$$

$$j_a = Aj_0^{ref}\left(\frac{C_{H_2}}{C_{H_2}^{ref}}\right)\left[e^{(\alpha_a F/RT)\eta} - \frac{1}{e^{(\alpha_c F/RT)\eta}}\right]$$

$$j_c = Aj_0^{ref}\left(\frac{C_{O_2}}{C_{O_2}^{ref}}\right)\left[e^{(\alpha_a F/RT)\eta} - \frac{1}{e^{(\alpha_c F/RT)\eta}}\right]$$

- Energy equation

$$\nabla \cdot \left(\varepsilon_{eff}\rho C_p\vec{u}T\right) = \nabla \cdot \left(k_{eff}\nabla T\right) + S_T$$

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Mathematical Modeling

- Charge conservation
  - For electrons

$$\nabla \cdot \left(\sigma_{eff} \nabla \phi_e \right) + S_{\phi_e} = 0$$

$$S_{\phi_e} = \begin{cases} -j_a & \text{at anode} \\ j_c & \text{at cathode} \end{cases}$$

  - For protons

$$\nabla \cdot \left(\kappa_{eff} \nabla \phi_p \right) + S_{\phi_p} = 0$$

$$S_{\phi_p} = \begin{cases} j_a & \text{at anode} \\ -j_c & \text{at cathode} \end{cases}$$

$$\kappa_{eff}(T) = (05139\psi - 0.00326)\exp\left[1268\left(\frac{1}{303} - \frac{1}{T}\right)\right]$$

$$\psi = \begin{cases} 0.043 + 17.81a - 39.85a^2 + 36.0a^3 & 0 < a \le 1 \\ 14 + 1.4(a-1) & 1 < a \le 3 \end{cases} \qquad a = \frac{x_w P}{P_{sat}}$$

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Mathematical Modeling

- Liquid water transport

$$\nabla \cdot \left(\varepsilon_{eff} \rho \vec{u} \lambda_l (s) \right) = \nabla \cdot \left(\varepsilon_{eff} D^c \nabla s - \frac{K k_{rl} k_{rg} (\rho_l - \rho_g) g}{k_{rl} \nu_g + k_{rg} \nu_l} \right) + S_l$$

$$S_l = \begin{cases} M_l r_{con} \dfrac{\varepsilon_{eff} x_w}{RT} (x_w P - P_{sat}), & if \quad x_w P > P_{sat} \\ r_{eva} \varepsilon_{eff} s \rho_l (x_w P - P_{H_2O}), & if \quad x_w P < P_{sat} \end{cases}$$

$$\log_{10} P_{sat} = -2.1794 + 0.02953T - 9.1837 \times 10^{-5} T^2 + 1.4454 \times 10^{-7} T^3$$

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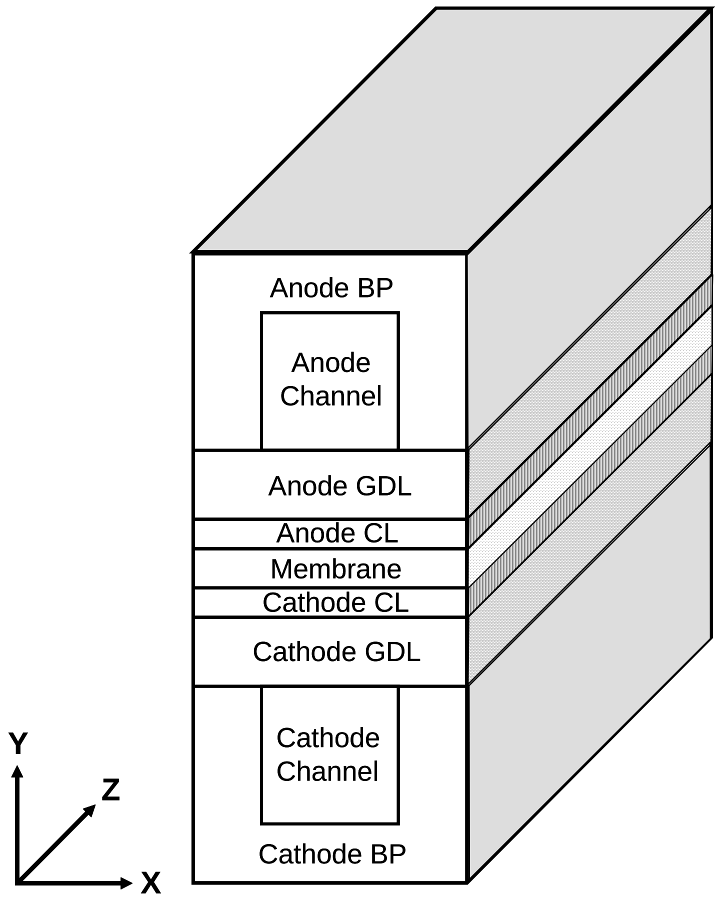
Mathematical Modeling

Boundary conditions

- Inlet boundary

$$u_{a,in} = \xi_a \frac{I_{ref}}{2F} A_m \frac{RT_{a,in}}{P_{a,in}} \frac{1}{x_{O_2}} \frac{1}{A_{ch}}$$

$$u_{c,in} = \xi_c \frac{I_{ref}}{4F} A_m \frac{RT_{c,in}}{P_{c,in}} \frac{1}{x_{H_2}} \frac{1}{A_{ch}}$$



- Outlet boundary

Neumann conditions

Mathematical Modeling

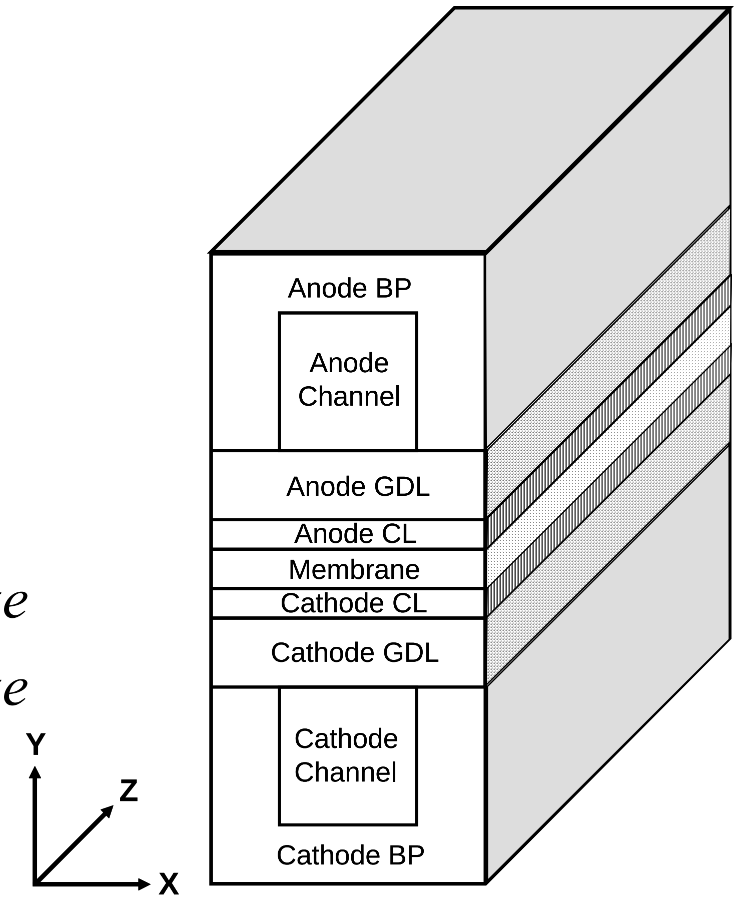
- Wall

  No-slip conditions

- Symmetric boundary

- Electronic Phase potential boundary

$$\begin{cases} \phi_e = 0 & at \quad anode \quad bipolar\ plate \\ \phi_e = \eta_{cell} & at \quad cathode \quad bipolar\ plate \\ \dfrac{\partial \phi_e}{\partial y} = 0 & otherwise \end{cases}$$



Mathematical Modeling

- Geometrical and operating parameters

Quantity	Value
Gas channel depth/width	0.762 / 0.762 mm
Shoulder width	0.381 mm
GDL thickness	0.3 mm
Catalyst layer thickness	0.01 mm
Membrane thickness	0.03 mm
Fuel cell height/length	1.534 / 71.12 mm
Anode/cathode pressure	1 / 1 atm
Stoichiometry, at ξ_a / ξ_c at 1.0 A/cm^2	1.5 / 3
Porosity of diffusion and catalyst layers	0.4 / 0.4

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Mathematical Modeling

Quantity	Value
Porosity of membrane	0.28
Permeability of diffusion and catalyst layers	1.76×10^{-11}/ 1.76 x 10-11 m^2
Permeability of membrane	1.8×10^{-18} m^2
Transfer coefficient at anode/cathode	0.5 / 1.5
Condensation rate constant	100 s^{-1}
Evaporation rate constant	100 $atm^{-1}s^{-1}$
Tortuosity of the diffusion and catalyst layers	1.5
Tortuosity of the membrane	3
Surface tension , ζ	0.0625 Nm^{-1}

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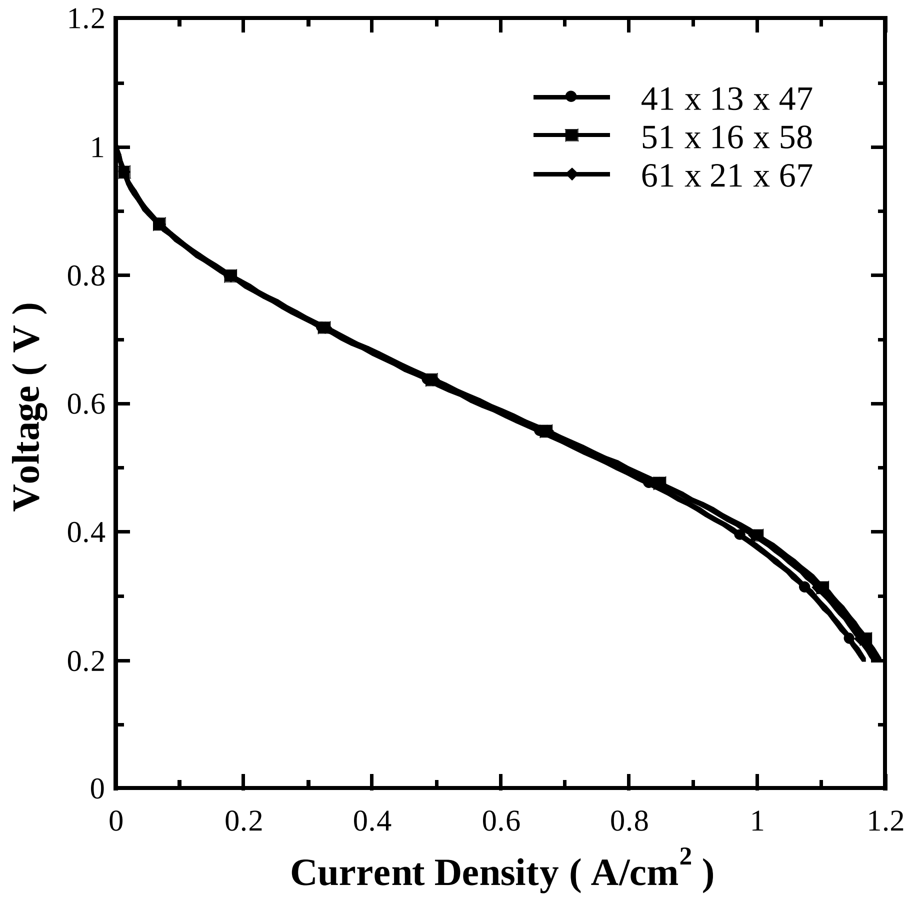
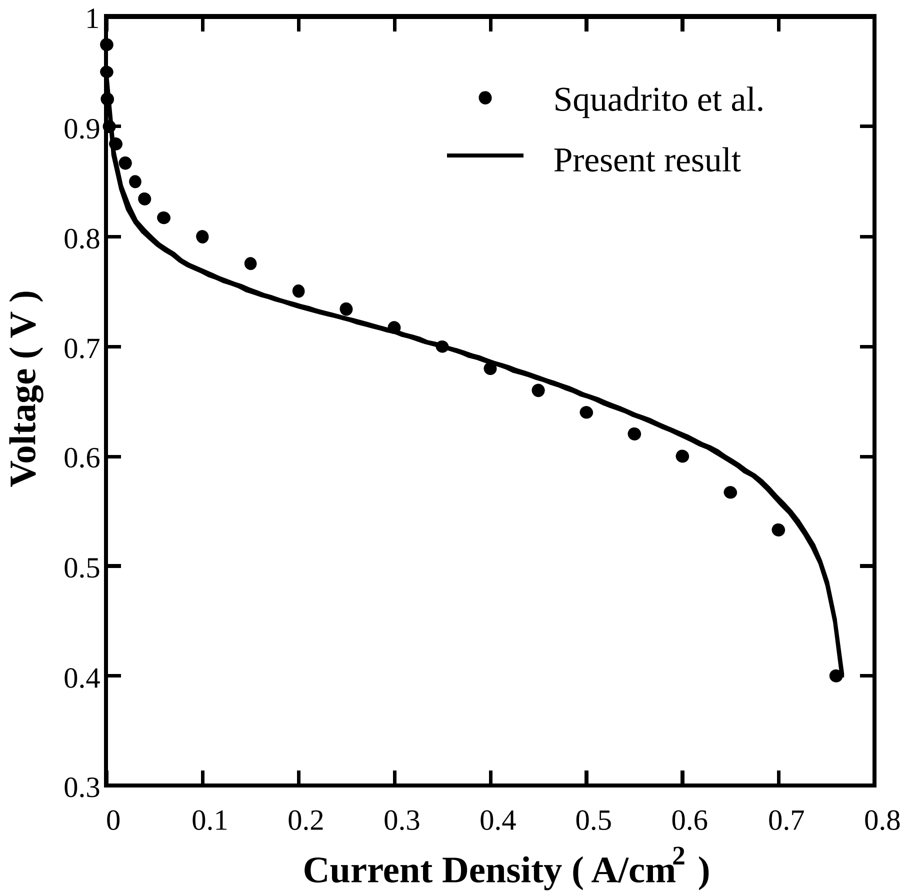
Grid Test



Comparison of predictions on the three different grid systems

Modeling Validation



Comparison of the predicted *I*–*V* curve and the experimental data

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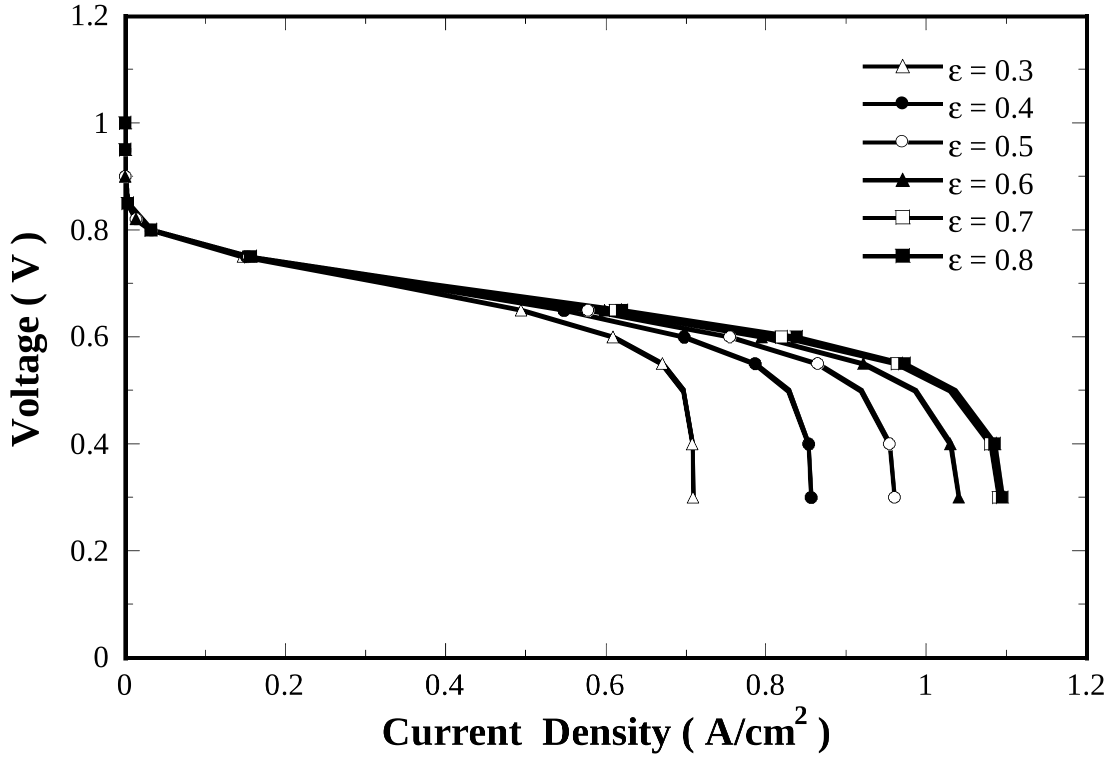
Results and Discussion

- Effects of GDL porosity



The polarization curves at V = 0.7V and RH_{ca} = 80%

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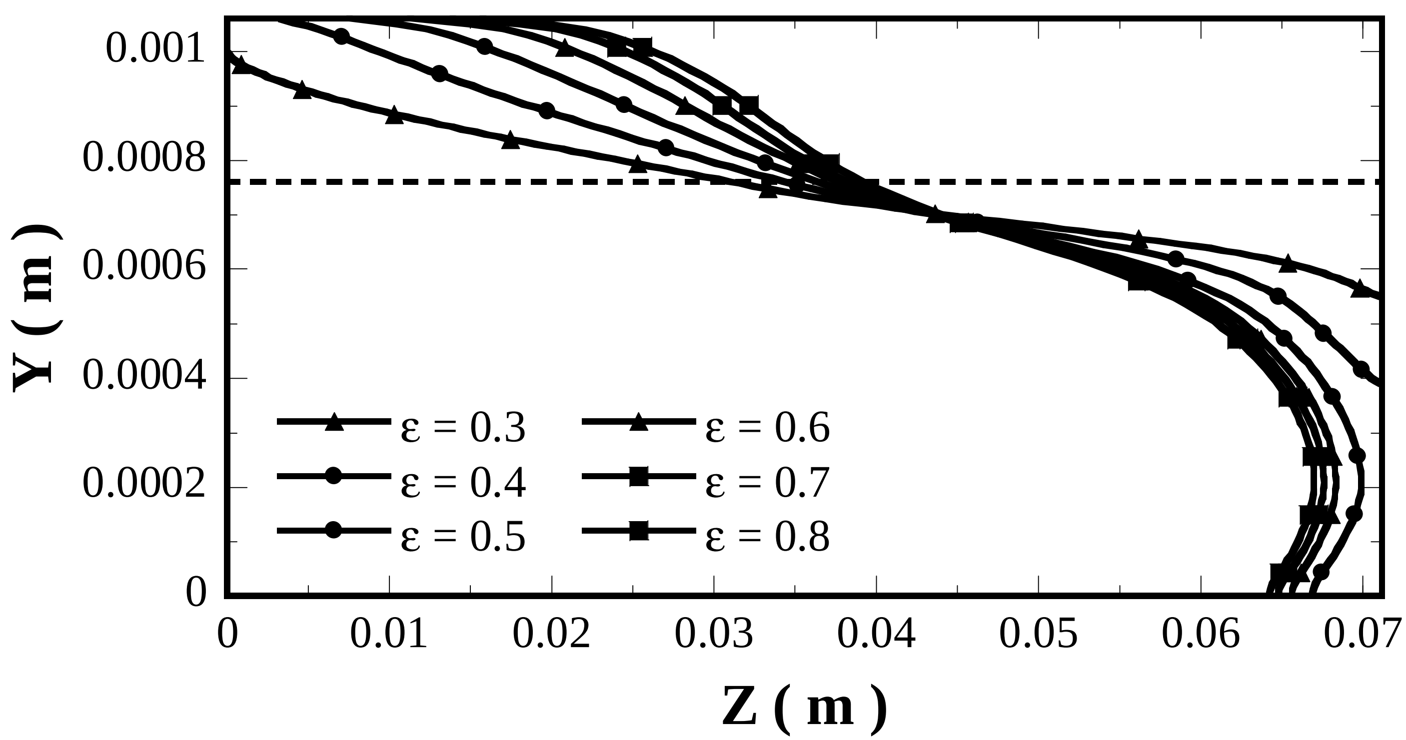
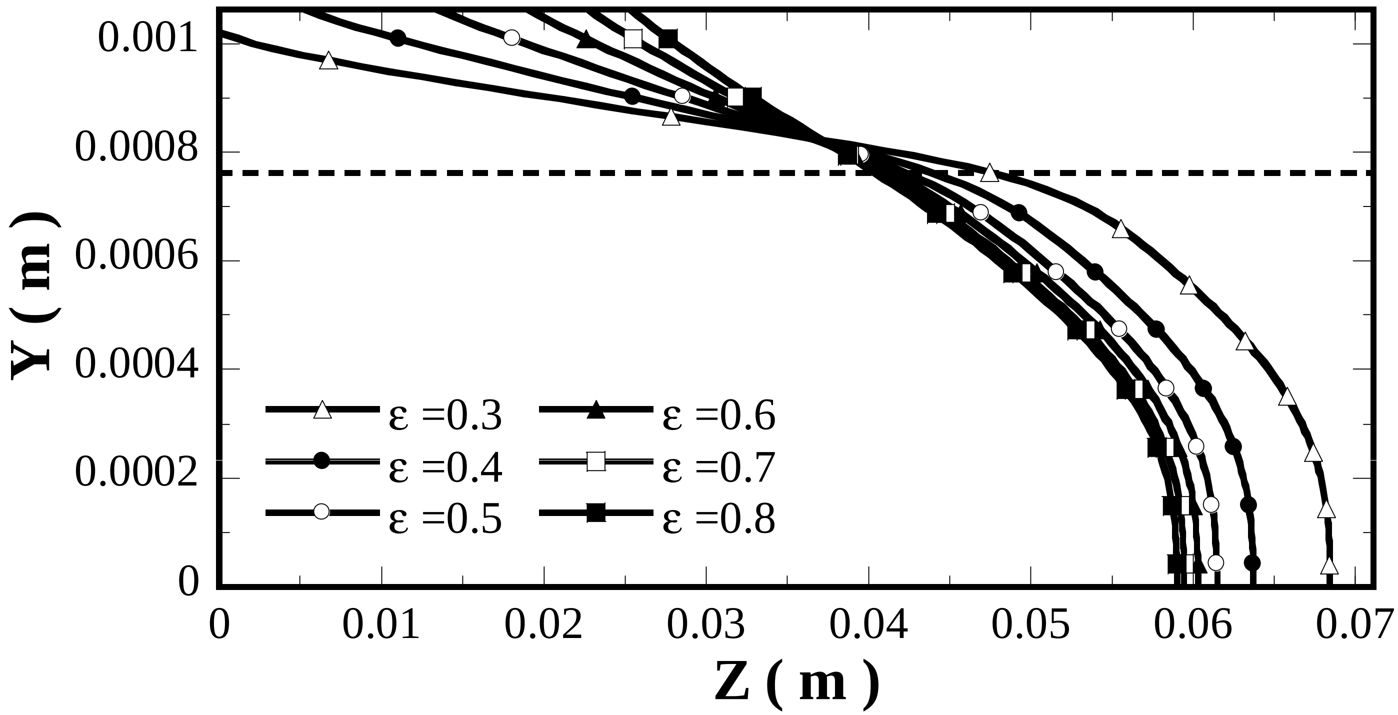
Results and Discussion



The gas-liquid interface location at V= 0.7V and RH_{ca} = 80%

Results and Discussion



Oxygen fraction distribution at V = 0.7V and RH_{ca} = 80 %

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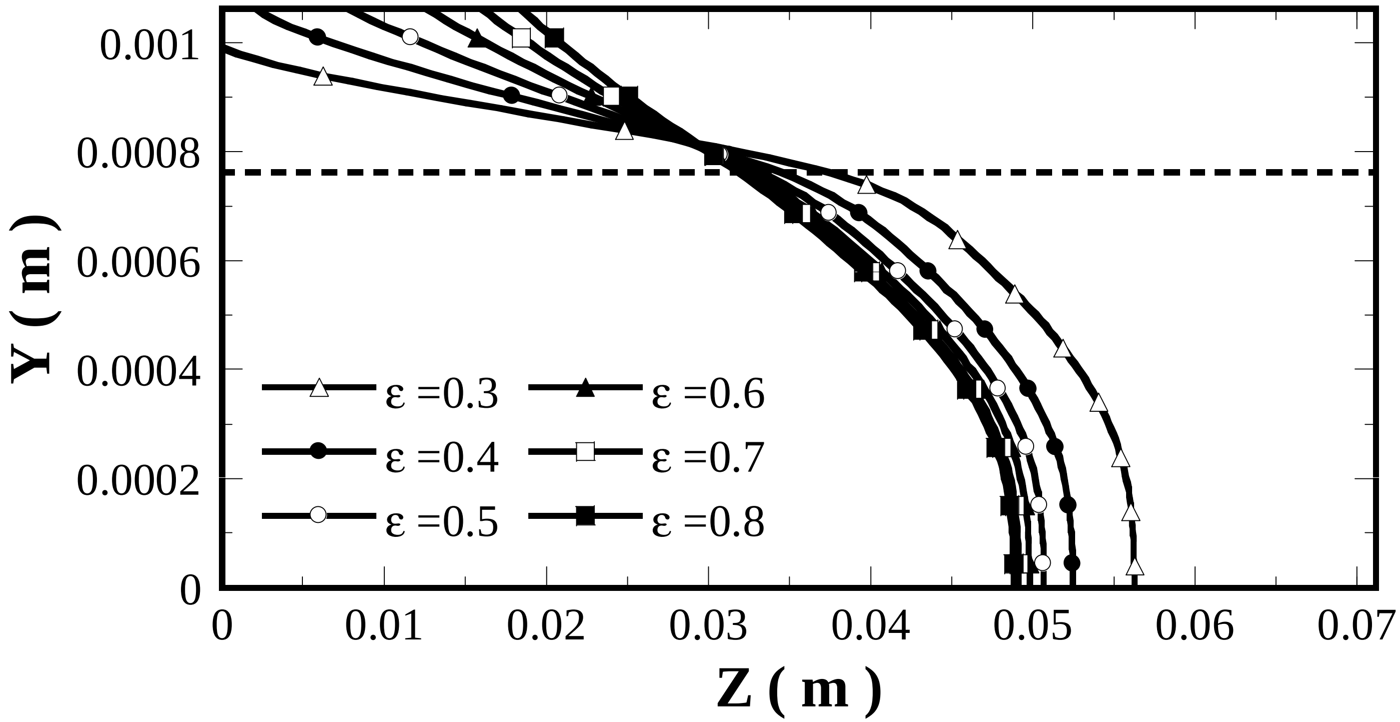
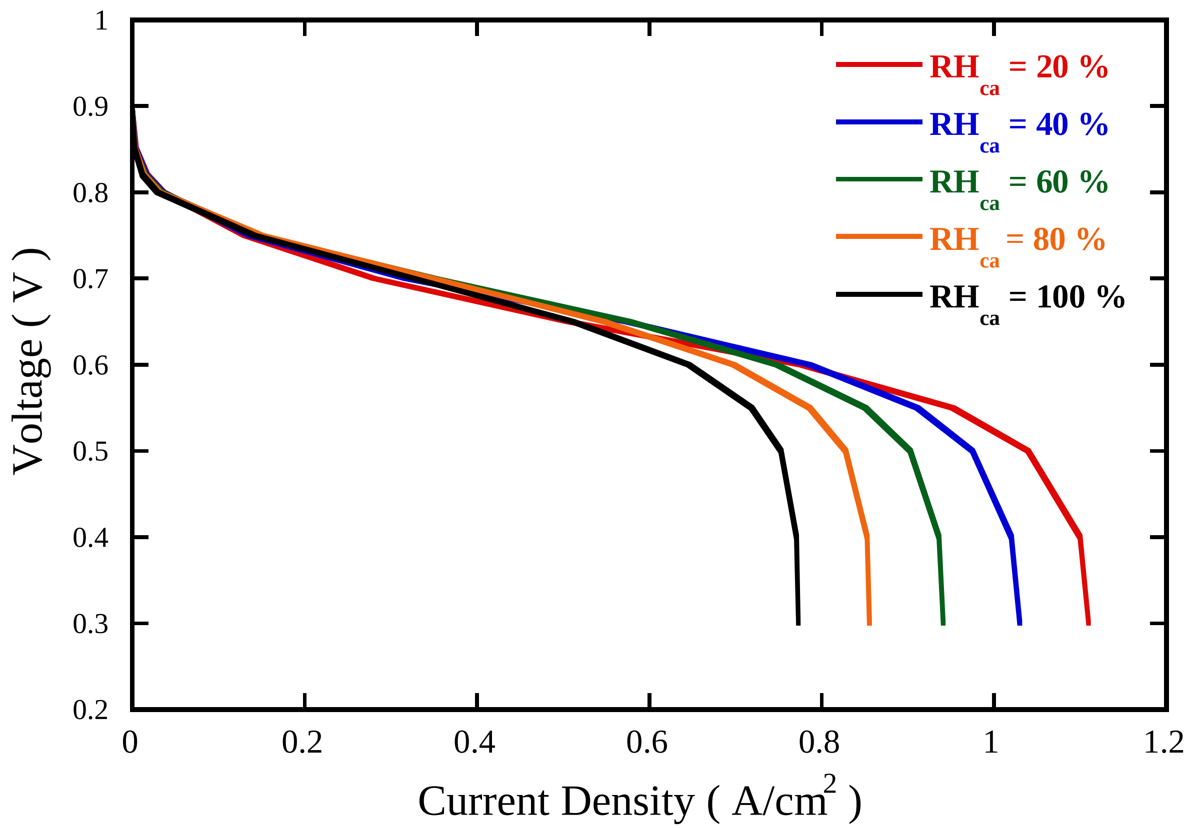
Results and Discussion



Water fraction distribution at V = 0.7V and RH_{ca} = 80 %

Results and Discussion

- Effects of cathode humidification



The polarization curves at various cathode humidifications

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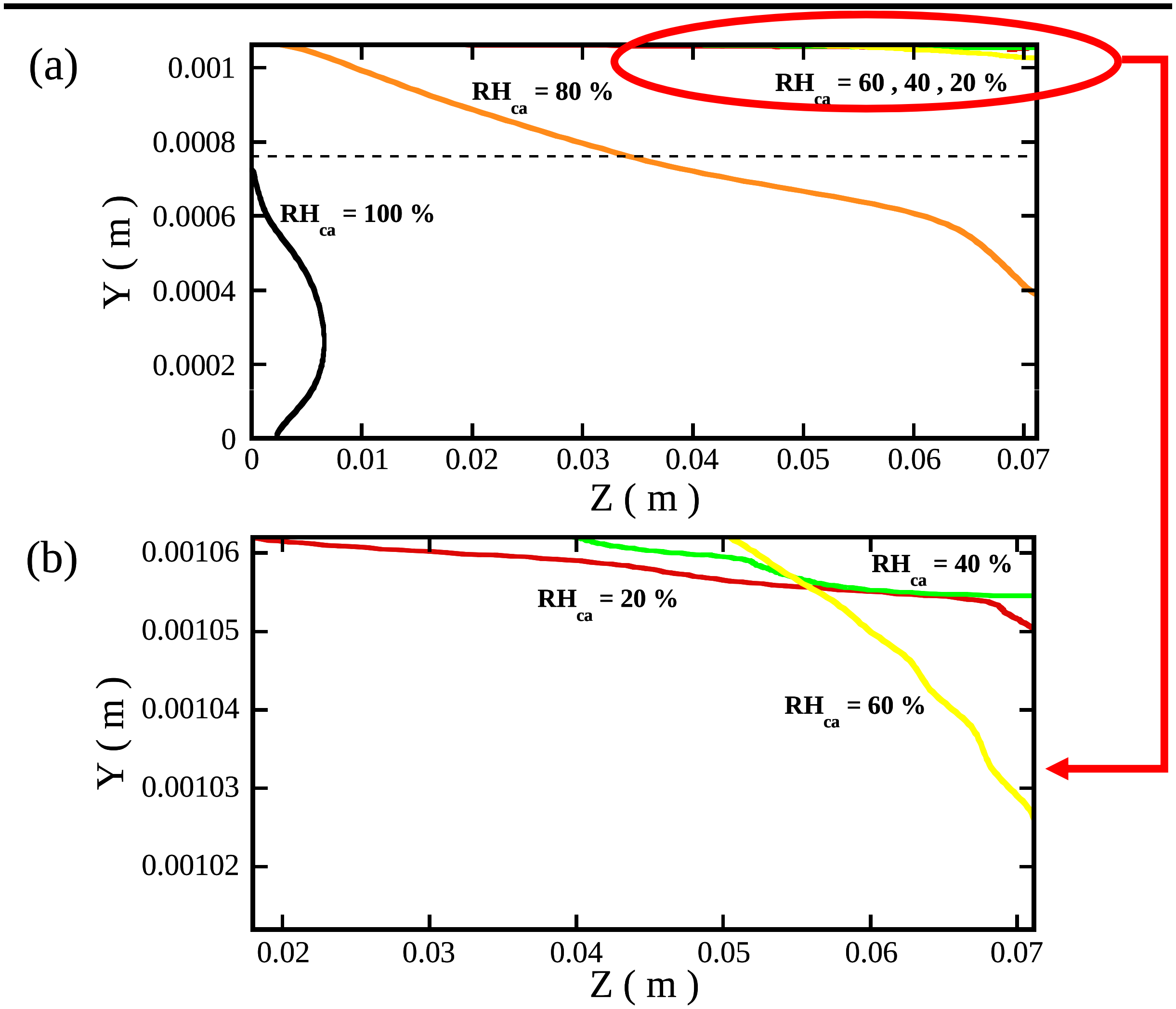
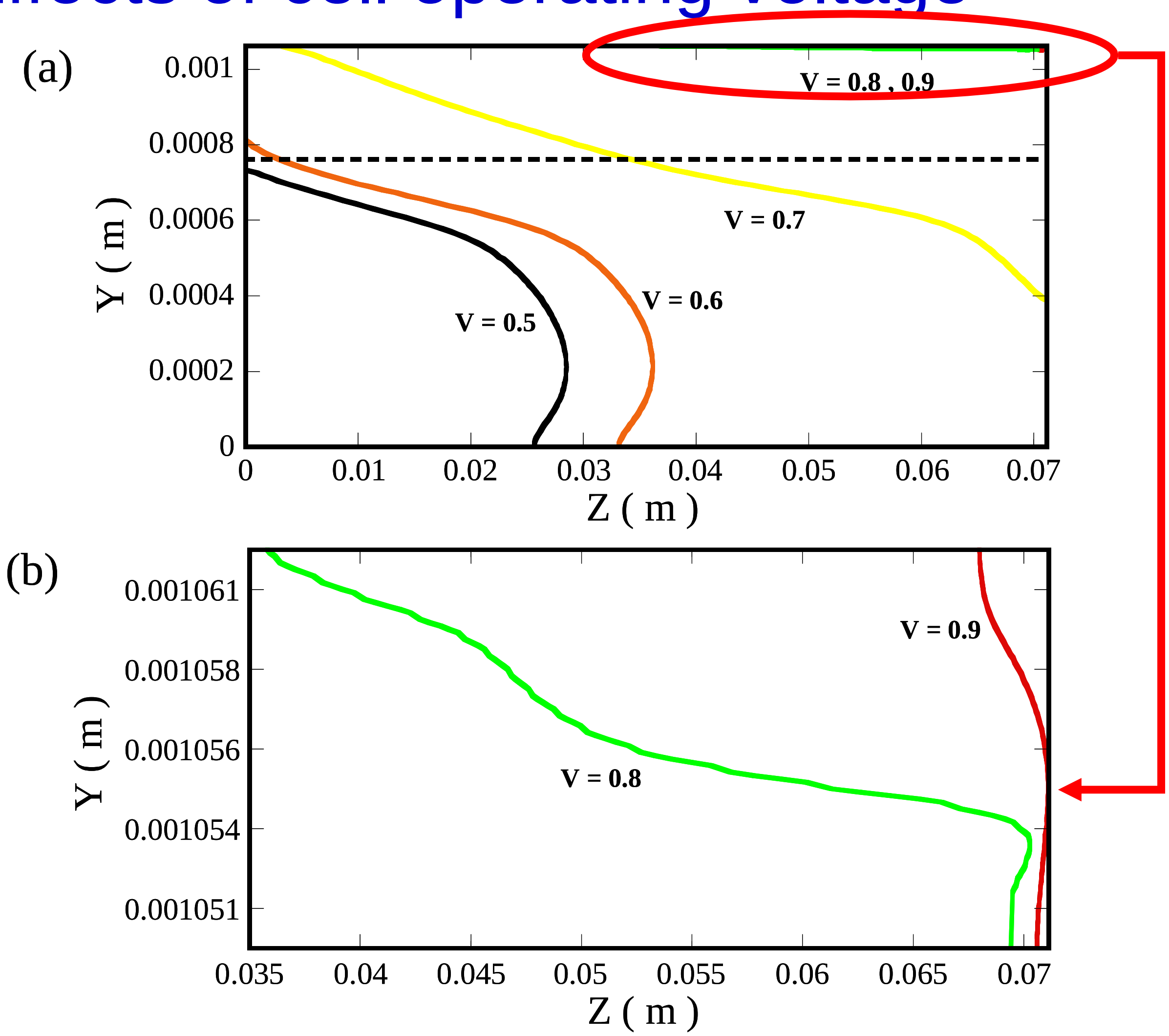
Results and Discussion



The gas-liquid interface location at V = 0.7V
(a) RH_{ca} = 20~100% (b) RH_{ca} = 20~60%

Results and Discussion

- Effects of cell operating voltage



The gas-liquid interface location at RH_{ca} = 80% (a) V= 0.5~0.9V (b) V=0.8~0.9V

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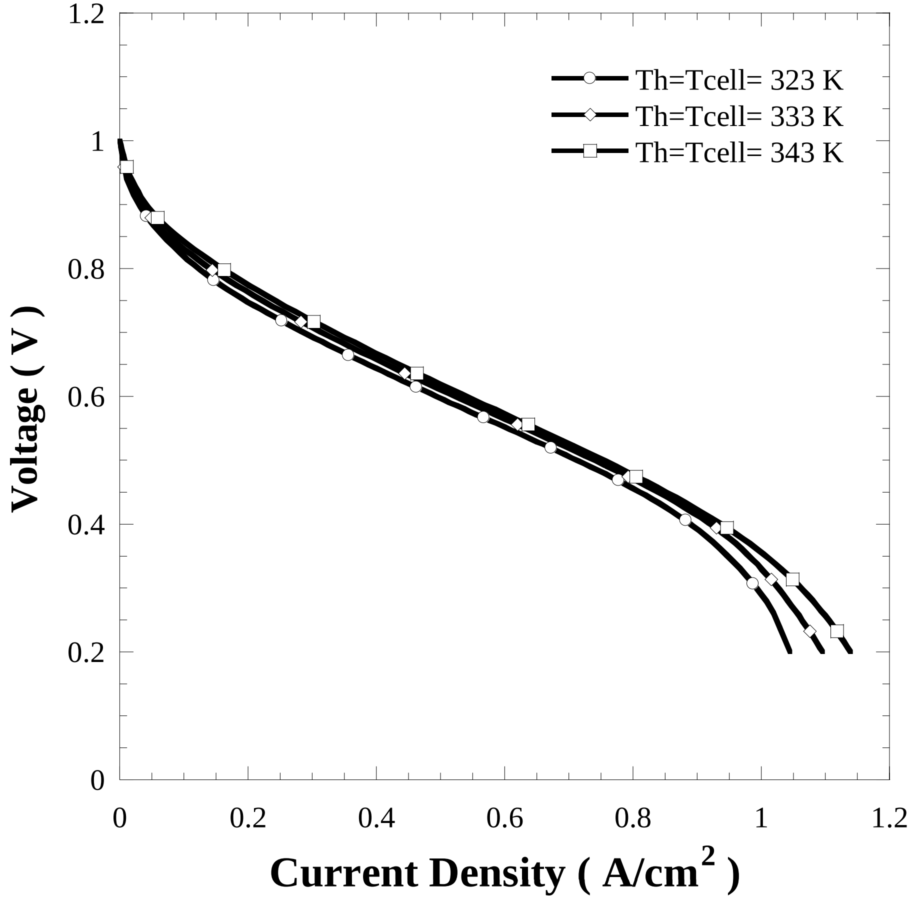
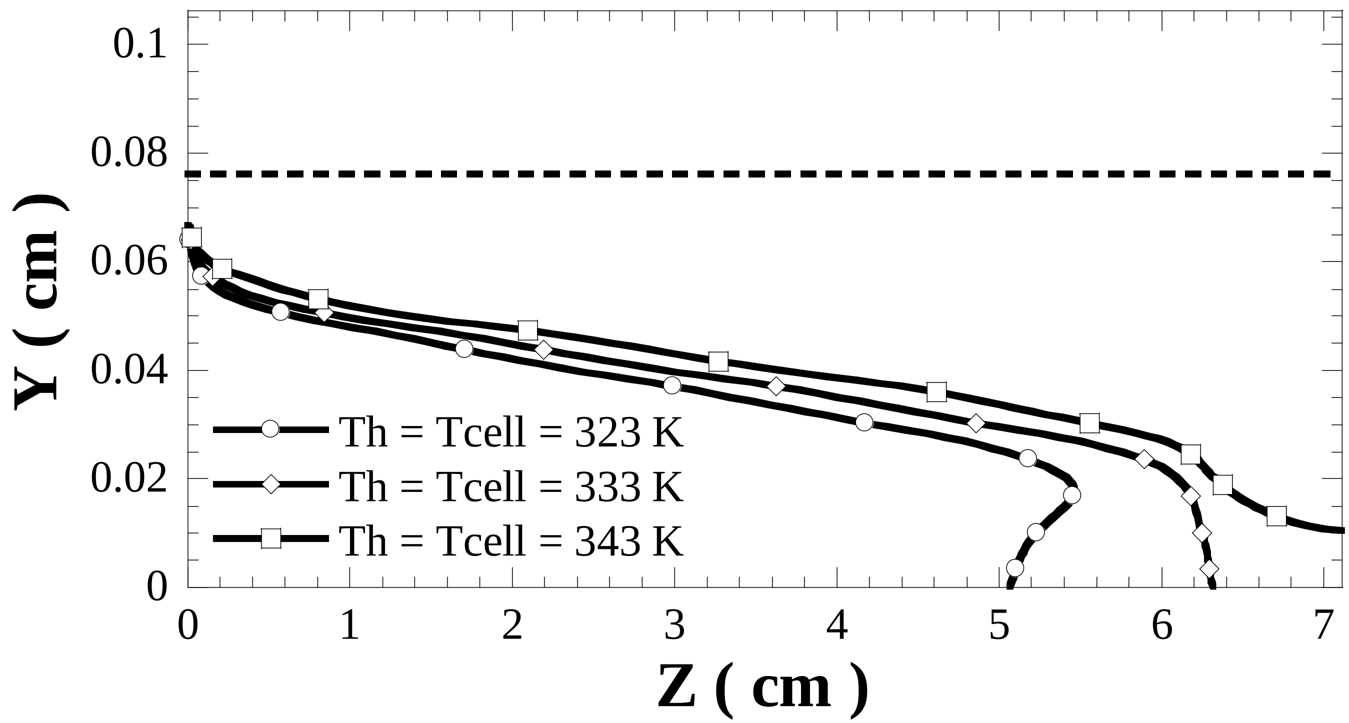
Results and Discussion

- Effects of temperature



The polarization curves at RH_{ca}= RH_{an}=100%

Results and Discussion



The gas-liquid interface location at V= 0.7V and RH_{ca}= RH_{an}=100%

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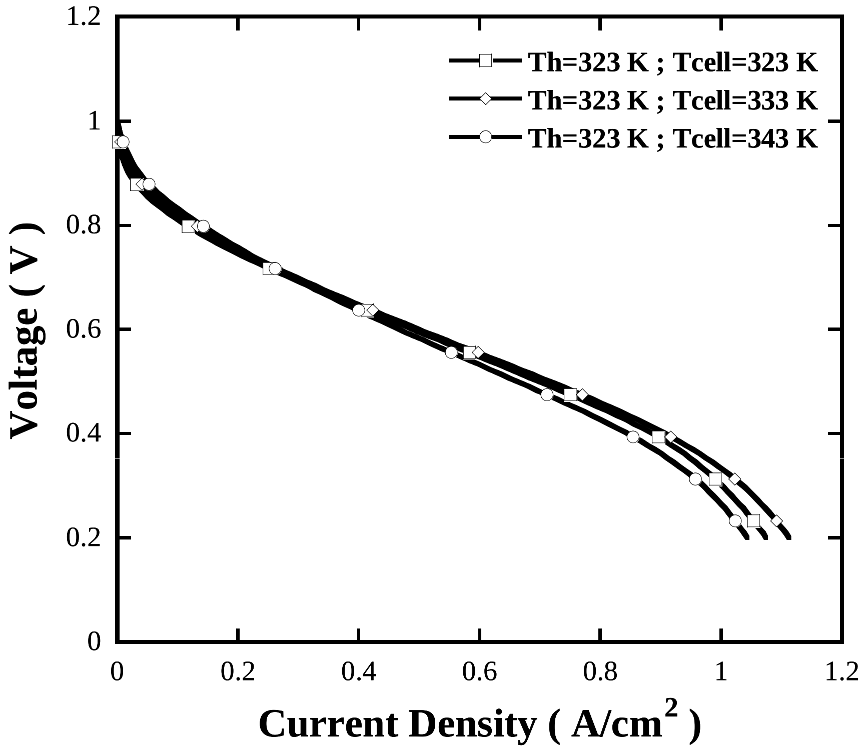
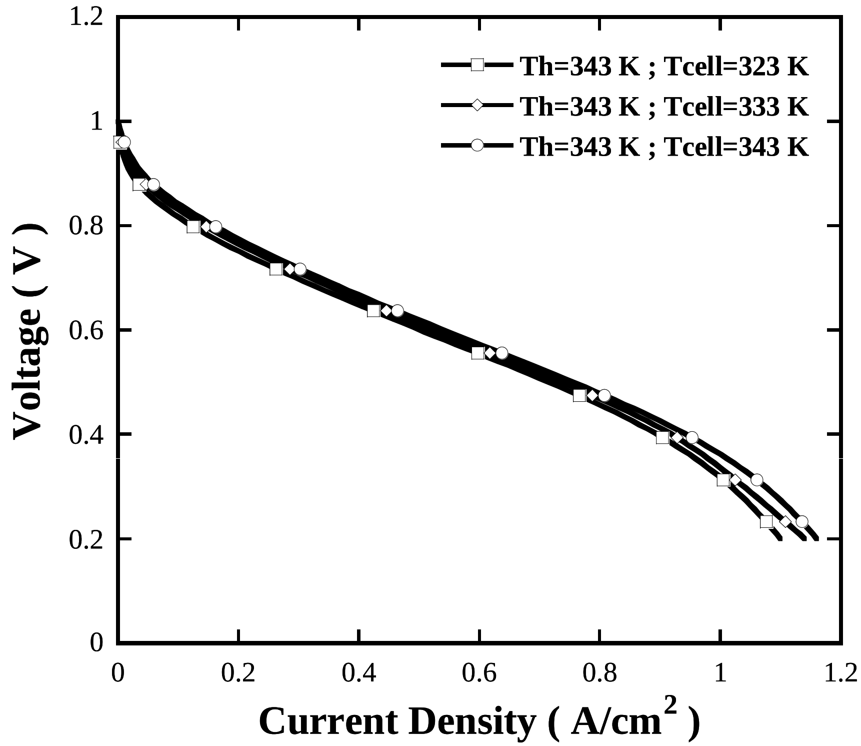
Results and Discussion

(a)



(b)



The polarization curves at V = 0.7V and RH_{ca}= RH_{an}=100%
(a) Th= 323K (b)Th= 343K

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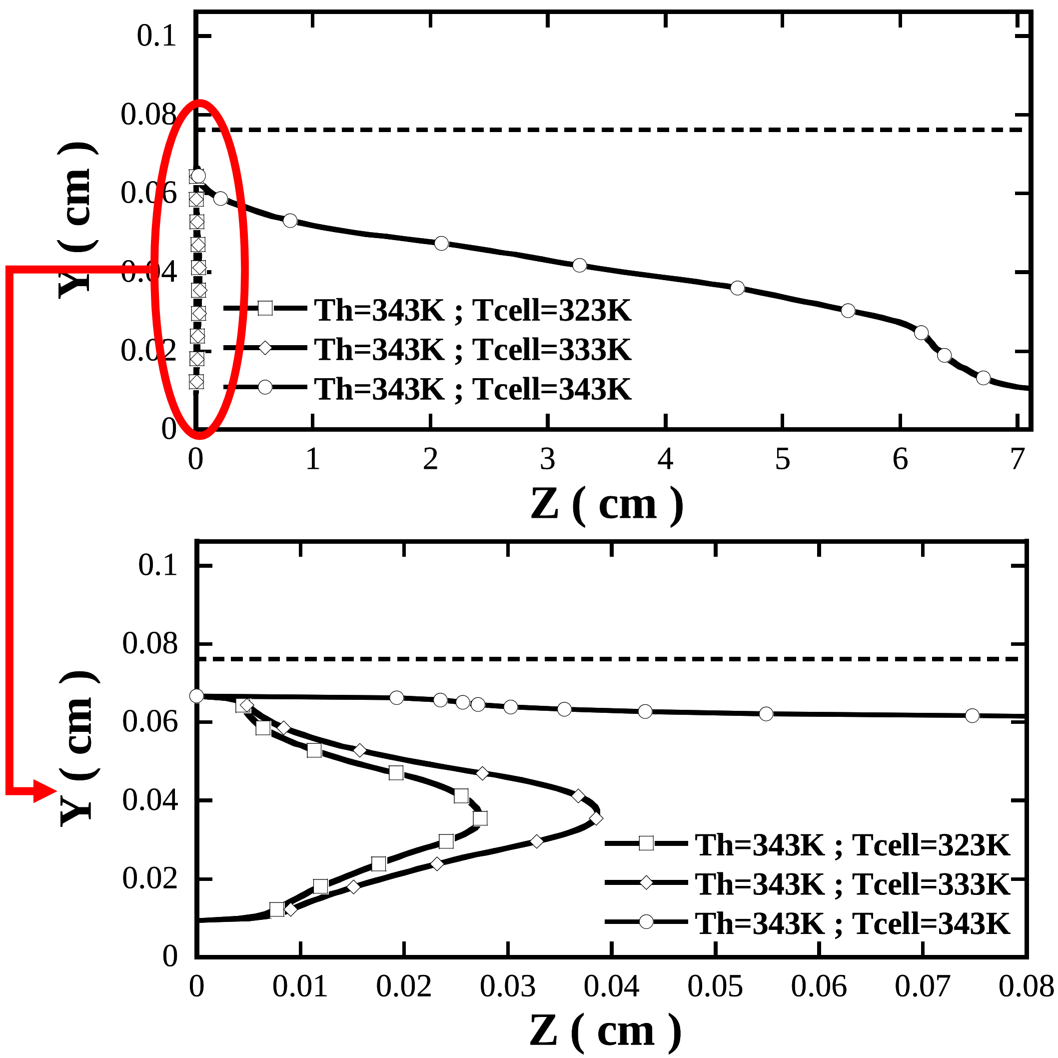
Results and Discussion



The gas-liquid interface location at V= 0.7V, Th=343K, and RH_{ca}= RH_{an}=100%

Conclusions

- Comprehensive investigations of the transport phenomena in PEMFCs with three-dimensional, multi-component and two-phase are achieved by using the multi-physics modeling and CFD algorithm.

- The developed model is successfully adopted to study the cell performance and electrochemical reaction subjected to various water and thermal operating schemes.

Conclusions

- The location of gas–liquid interface is affected by cathode humidification, GDL porosity, operating voltage, and temperature.

- The cell performance is affected by the gas–liquid interface.

- Proper cathode humidification level improves concentration polarization at high reaction rate.

- As the condensed water in the pores of the porous media blocks the transport of fuel gas, the cell performance and power density decrease.

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Conclusions

- The diffusion transport of the reactant gas to the cathode catalyst layer and the production of water via the gas diffusion layer to the flow channel increases with increasing the GDL porosity.

- The cell performance is influenced by the operating temperature.

- As the anode and cathode humidification temperatures are equal to or higher than the cell temperature, the gas-liquid interface moves toward the flow channel inlet as the temperature is decreased.

Thank you for your attention

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