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2014 BOSTON

Rensselaer

CFD Modeling and Analysis of a Planar Anode Supported Intermediate Temperature Solid Oxide Fuel Cell

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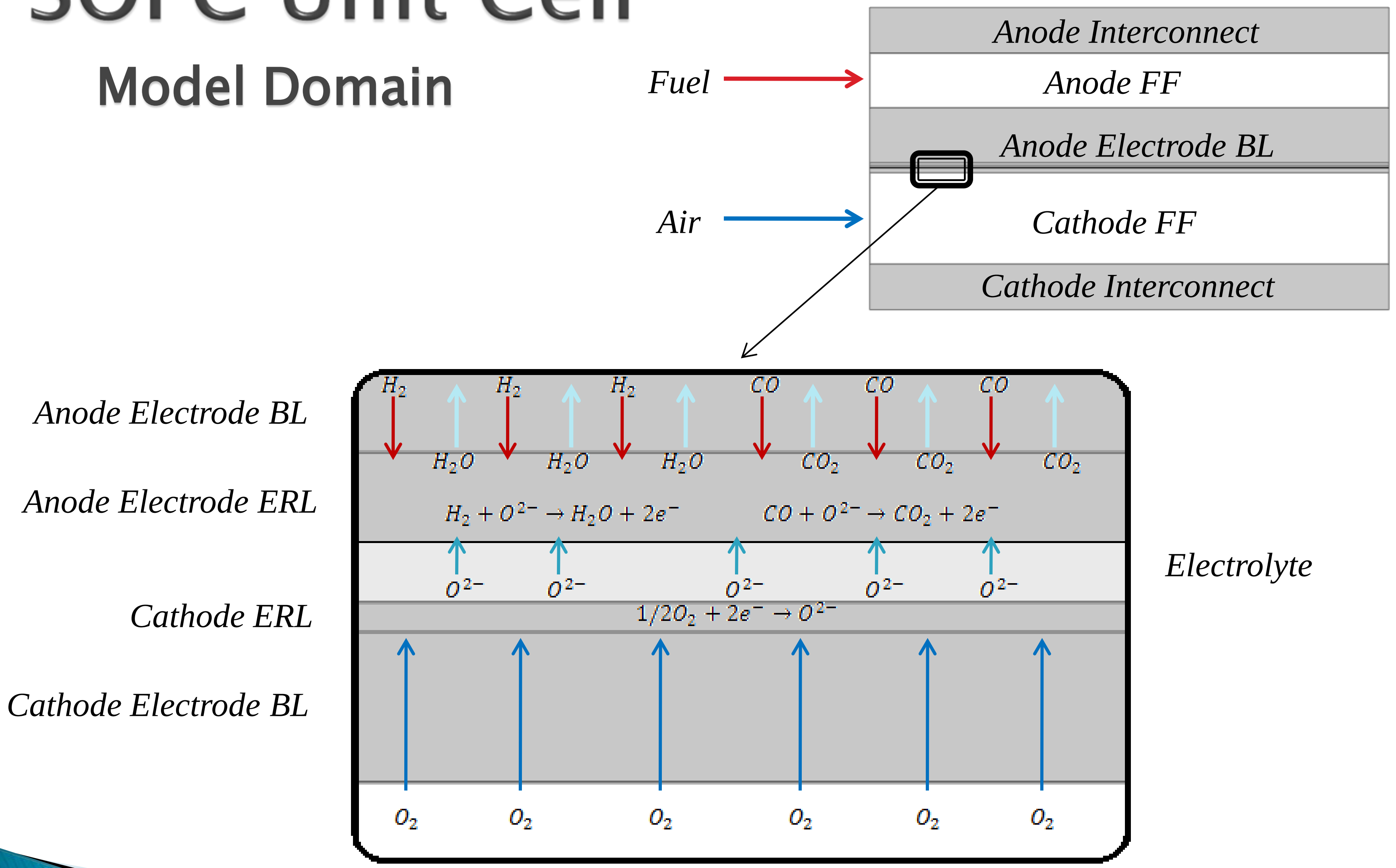
Background

- Solid Oxide Fuel Cells are a class of high temperature fuel cells operating between 600 to 1000C.
- The advantage over other types of fuel cells include the ability to have both the internal reforming of a hydrocarbon fuel and the standard electrochemical reaction both occur simultaneously within the fuel cell.
- To accurately predict and optimize the performance of SOFCs it is necessary to develop reliable multiphysics models.
- In this study, a two-dimensional CFD model of a single cell solid oxide fuel cell was created.
- Using the model, the effects of varying syngas fuel inlet composition on cell performance, species distribution and electrochemistry were analyzed.

SOFC Unit Cell

Model Domain



Governing Equations

Momentum: Continuity and Navier Stokes Equations

- Fuel and Air Channels:

$$\nabla \cdot (\rho \mathbf{u}) = 0 \qquad \rho \mathbf{u} \cdot \nabla \mathbf{u} = \nabla \cdot \left[-p\mathbf{I} + \mu \left((\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I} \right) \right] + \mathbf{F}$$

- Porous Electrode Stokes-Brinkman equations:

$$\nabla \cdot (\rho \mathbf{u}) = 0 \qquad \mathbf{u} \left(\frac{\mu}{\kappa} + S \right) = \nabla \cdot \left[-p\mathbf{I} + \frac{\mu}{\varepsilon} \left((\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2\mu}{3\varepsilon} (\nabla \cdot \mathbf{u}) \mathbf{I} \right) \right] + \mathbf{F}$$

Mass: Maxwell-Stefan Equations

$$\rho y_i (\nabla \cdot \boldsymbol{u}) - \nabla \cdot \left(\rho y_i \sum_j^N \tilde{D}_{ij} \boldsymbol{d}_j \right) = R_i \qquad D_{ij}^{MS} = \frac{1.43x10^{-2} T^{1.75}}{p M_{ij}^{1/2} \left[V_i^{1/3} + V_j^{1/3} \right]^2}$$

- Porous Electrodes: Maxwell Stefan and Knudsen diffusivity

$$D_{ij}^{eff} = \frac{\varepsilon}{\tau_{pore}} \left(\frac{1}{D_{ij}^{MS}} + \frac{1}{D_i^{Kn}} \right)^{-1} = \frac{\varepsilon}{\tau_{pore}} \frac{D_{ij}^{MS} D_{ij}^{Kn}}{D_{ij}^{Kn} + D_{ij}^{MS}}$$

$$D_{ij}^{Kn} = r_{pore} \frac{2}{3} x10^{-4} \sqrt{\frac{8RT}{\pi \bar{M}_{ij}}} = 48.5x10^{-4} \, d_{pore} \sqrt{\frac{T}{\bar{M}_{ij}}}$$

Governing Equations

<u>Heat Transfer: Energy Equation</u>

- Fuel and Air Channels: $$\rho C_p \boldsymbol{u}\nabla T - \nabla(\lambda \nabla T) = Q$$

- Porous Electrodes: $$\rho C_p^{eff} \boldsymbol{u}\nabla T - \nabla(\lambda^{eff} \nabla T) = Q$$

$$\lambda^{eff} = \varepsilon \lambda_{fluid} + (1-\varepsilon)\lambda_{solid}$$

$$C_p^{eff} = \varepsilon C_{p,fluid} + (1-\varepsilon) C_{p,solid}$$

- Electrolyte and Interconnects: $$-\nabla(\lambda \nabla T) = Q$$

- Heat Generation Source Terms:
  - Chemical Reaction
  - Electrochemical Reaction
  - Activation Polarization

$$Q = \sum_{j}^{rxn} -\left(\Delta H_{298}^{rxn} * \dot{r}_{rxn}\right)$$

$$Q = \sum_{i} j_{s,i} A_v \left(\frac{-\Delta H_i}{n_{e,i} F} - E_{cell}\right)$$

$$Q = \eta_{act,s} j_s A_v$$

Governing Equations

Chemical Reactions

- Water Gas Shift Reaction:

$$CO + H_2O \leftrightarrow H_2 + CO_2 \qquad \Delta H_{298} = -41.2\ kJ/mol$$

$$\dot{r}_{WGS}(mol\,m^{-3}s^{-1}) = 0.0171 \exp\left(-\frac{103191}{RT}\right)\left(p_{H_2O}p_{CO} - \frac{p_{H_2}p_{CO_2}}{K_{eq,2}}\right)$$

Electrochemical Reactions

$$H_2 + O^{2-} \rightarrow H_2O + 2e^- \qquad CO + O^{2-} \rightarrow CO_2 + 2e^- \qquad \frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}$$

Ion and Charge Transport $\quad \nabla \cdot (-\sigma_s^{eff}\nabla\phi_s) = j_s A_v$

- Relationship between potential and current density determined by Butler-Volmer kinetic equation

$$j = j_o\left[\exp\left(\frac{\alpha_a F\eta_{act}}{RT}\right) - exp\left(\frac{-\alpha_c F\eta_{act}}{RT}\right)\right]$$

$$\eta_{act} = (\phi_{el} - \phi_{io}) - E_{eq}$$

Cell Properties and Parameters

Cell Dimensions (mm)

Cell length	100	Air channel height	1.0
Cell height	3.31	Cathode Backing Layer Height	0.05
Fuel channel height	0.6	Cathode ERL Layer Height	0.01
Anode Backing Layer Height	0.6	Electrolyte Height	0.02
Anode ERL Layer Height	0.03	Interconnect Height	0.5

Operating Conditions

Inlet Temperature (K)	1023
Cathode Inlet Velocity (m/s)	6.5
Anode Inlet Velocity (m/s)	0.5
Outlet Pressure (atm)	1.0
Anode Fuel Feed x_i	Varies
Cathode Air Feed x_i	.21 O_2 .79 N_2
Operating Voltage (V)	0.6 to 1.0

Simulated Fuel Feed Mole Fractions

Case	1	2	3	4	5
H_2	0.30	0.30	0.20	0.30	0.30
H_2O	0.07	0.17	0.27	0.07	0.07
CO	0.50	0.40	0.40	0.40	0.40
CO_2	0.10	0.10	0.10	0.10	0.20
CH_4	0.01	0.01	0.01	0.01	0.01
N_2	0.02	0.02	0.02	0.12	0.02

Cell Properties and Parameters

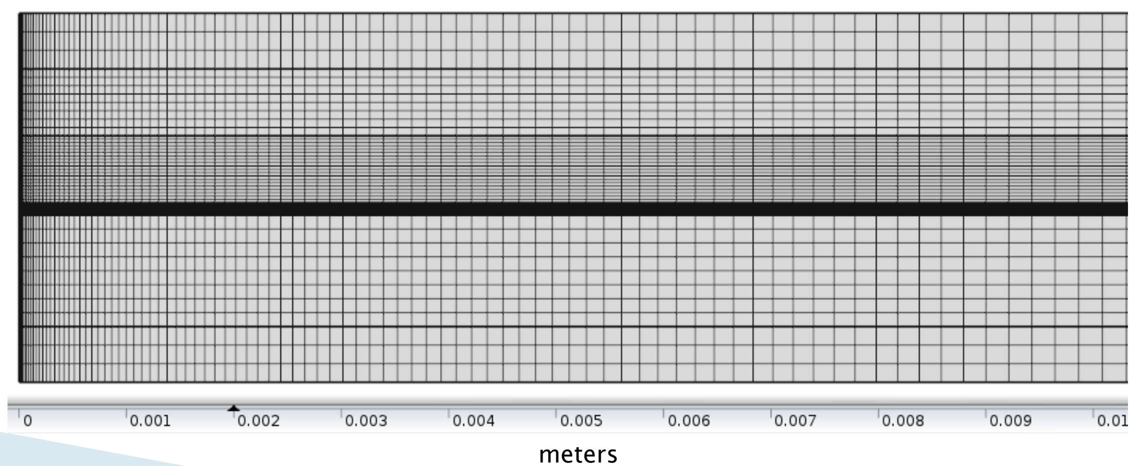
Physical Properties and Parameters*

	Anode	*Cathode*
Permeability (m^2)	2.42×10^{-14}	2.54×10^{-14}
Porosity	0.489	0.515
Pore Diameter (μm)	0.971	1
Electronic/Ionic/Pore Tortuosity	7.53, 8.48, 1.80	7.53, 3.4, 1.80
Electronic/Ionic Volume Fraction	0.257, 0.254	0.232, 0.253
Electronic/Ionic Reactive Surface Area per Unit Volume (m^2/m^3)	3.97×10^{6}, 7.93×10^{6}	3.97×10^{6}, 7.93×10^{6}
Solid Thermal Conductivity (W/m-K)	11	6
Solid Specific Heat Capacity (J/kg-K)	450	430
Solid Density (kg/m^3)	3310	3030
	Electrolyte	Interconnect
Thermal Conductivity (W/m-K)	2.7	20
Specific Heat Capacity (J/kg-K)	470	550
Solid Density (kg/m^3)	5160	3030

*Reference 1

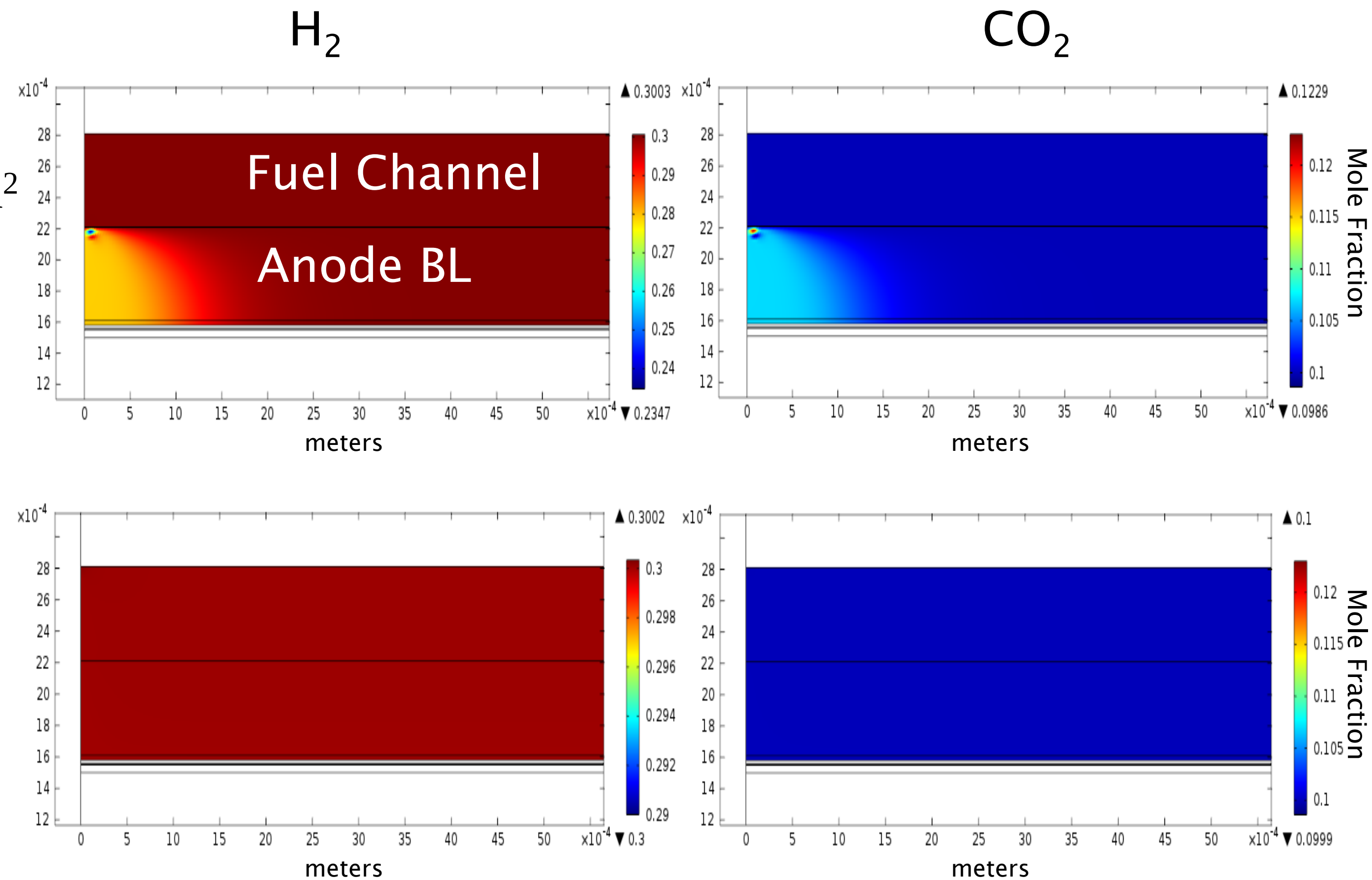
Solution Method

- COMSOL Multiphysics FEM Modeling Software
- Domain
  - 34,400 elements–varied distribution horizontally
- Segregated Pardiso Solver with parametric voltage steps
- Dampening Factor 0.05% applied to electrochemical species and heat generation source terms



Permeability Comparison

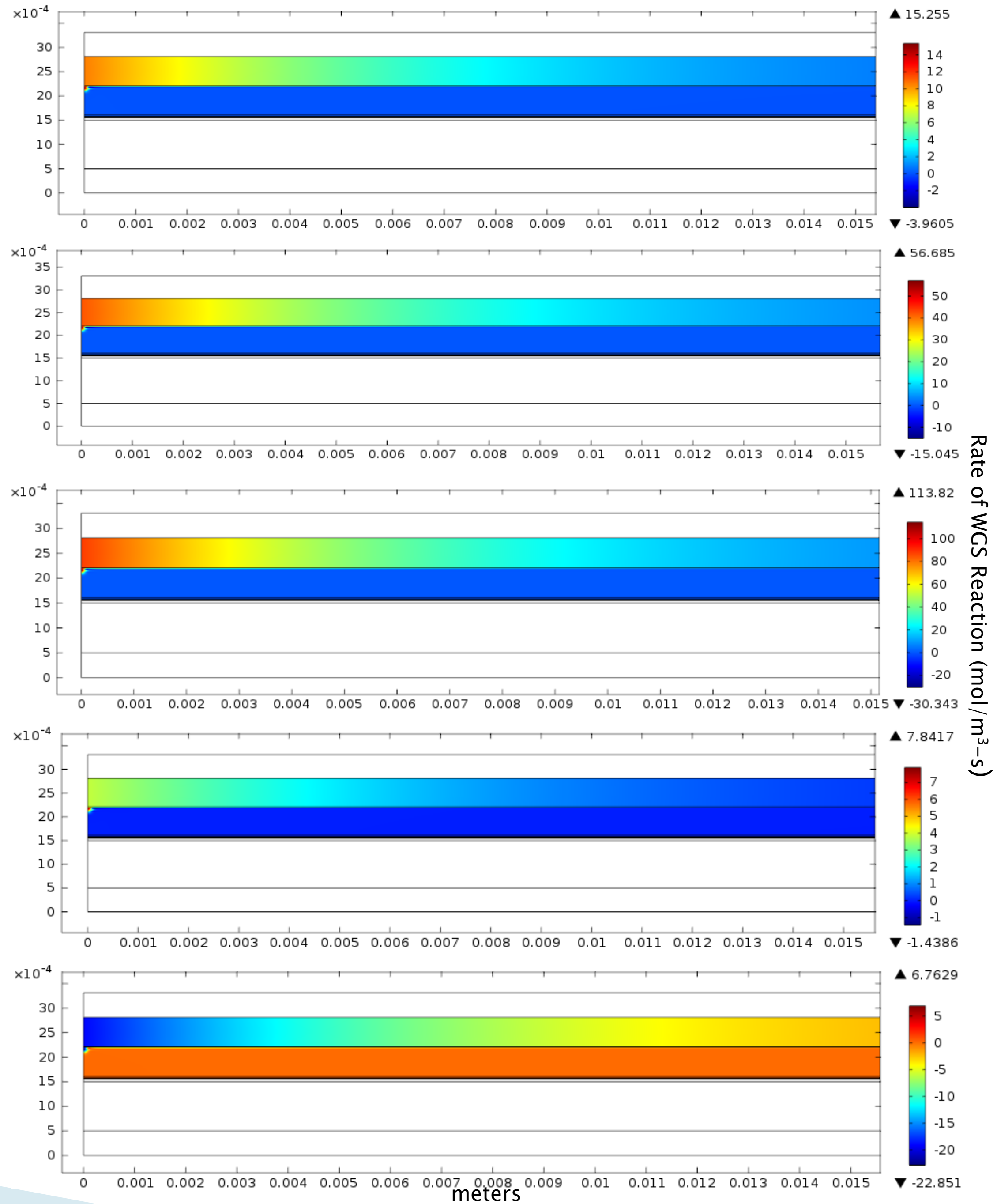
- Case 1 Anode: No reactions, $\kappa = 2.42 \times 10^{-14}\ m^2$
- Case 1 Anode: No reactions, $\kappa = 2.42 \times 10^{-5}\ m^2$



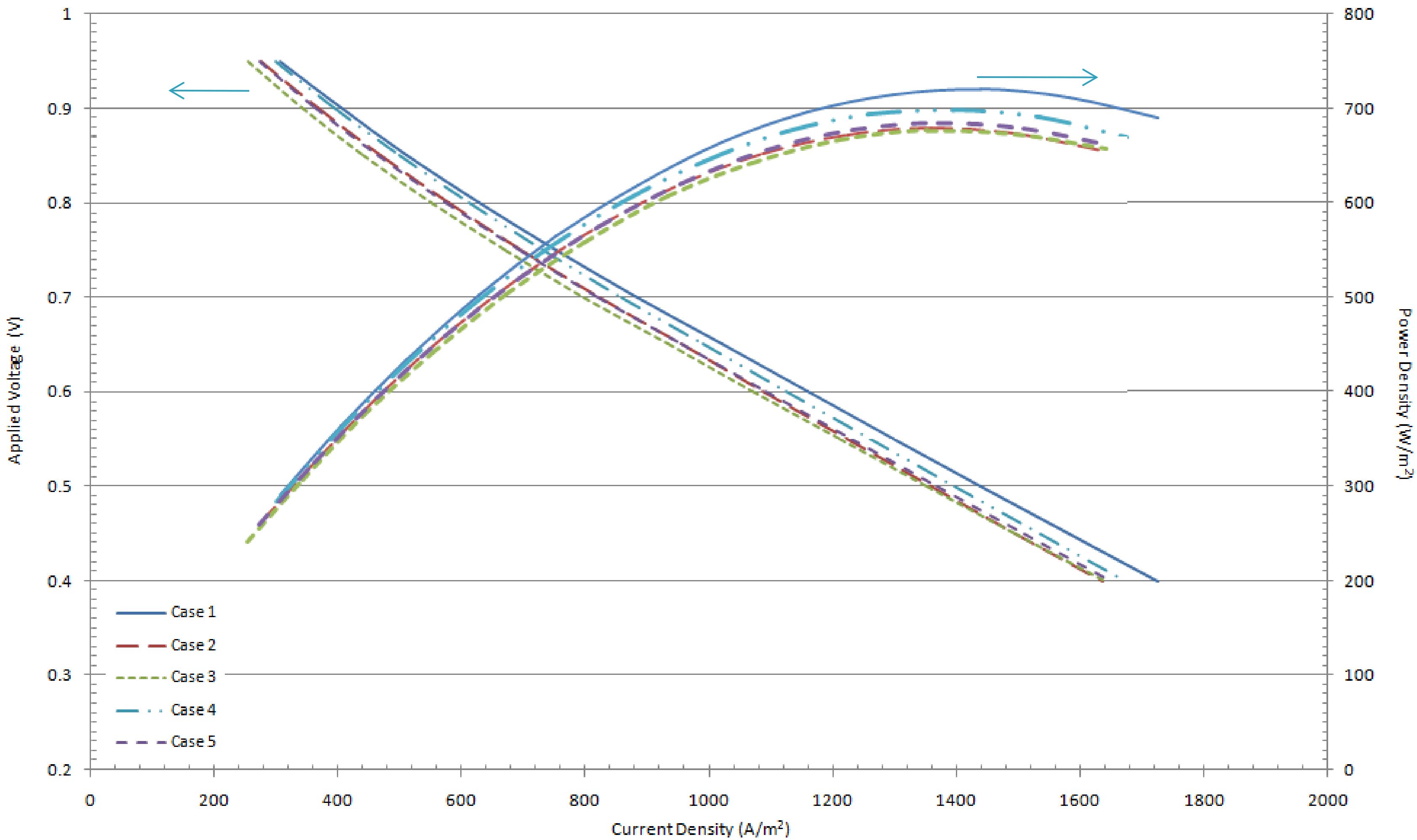
- Decreased permeability resulted in visible inlet effects due to mass diffusion limitations. However they were only present in the initial 0.2% of cell length.

Water Gas Shift Reaction

- Highest WGS rate observed with largest concentration of H_2O in fuel (Case 3)
- Increased CO_2 in fuel results in negative reaction rate in FF (Case 5)
- Increased CO in fuel increases WGS rate (Case 1)

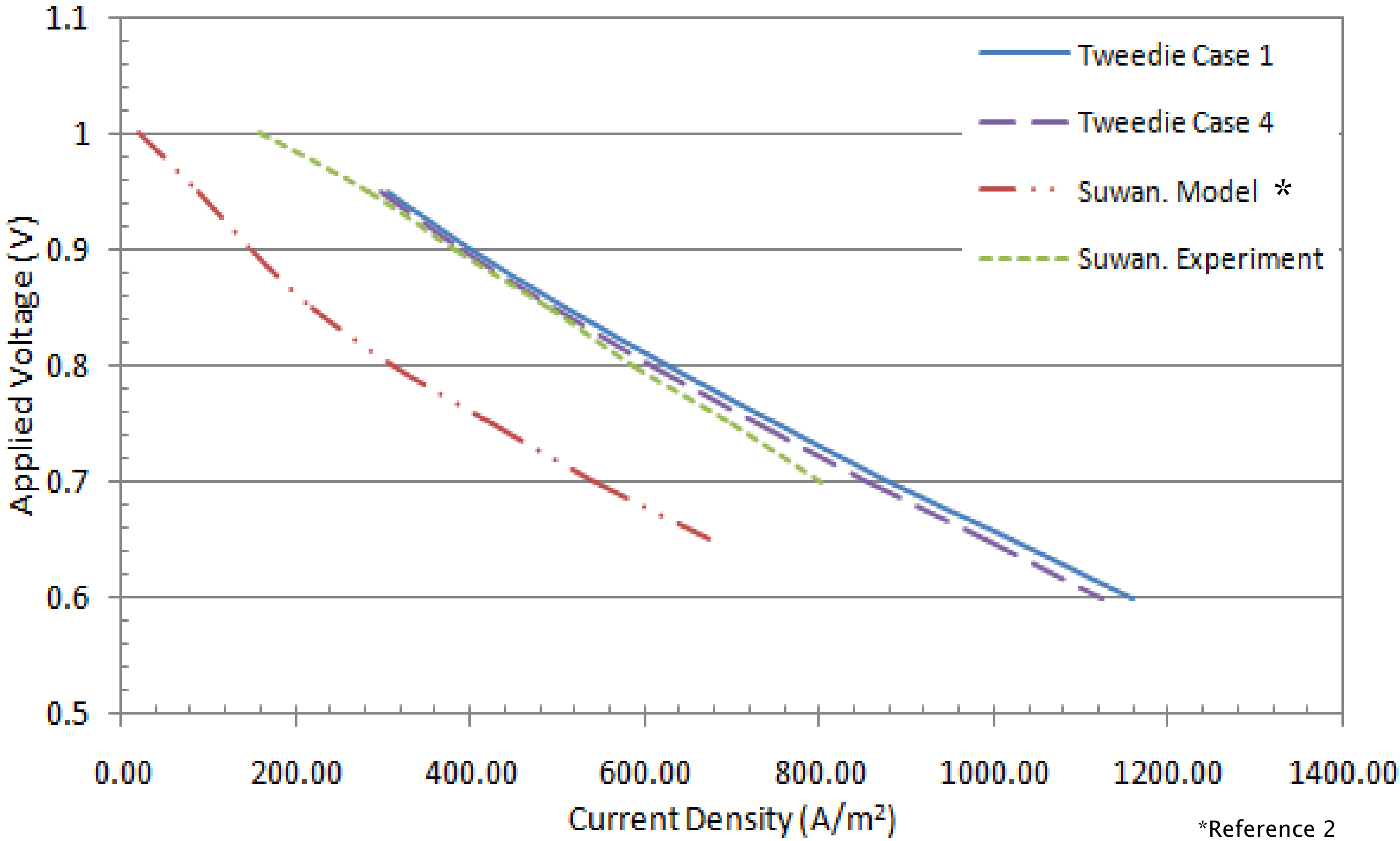


Characteristic Polarization Curves



Case 1 Max Power Density: 720 W/m^2

Comparison vs Experiment Data



*Reference 2

Conclusions

- Model agrees reasonably well with experimental data.
- Case 1 shows the best performance with a max power density 720W/m^2, Case 4 has the 2nd best performance.
- WGS rate increases with higher reactant species concentration, reverses with higher product species concentration in fuel.
- No carbon formation observed under operating conditions using syngas fuel at voltages below 0.95V.
- Proper selection of microstructural parameters (permeability) is important.
- Complexity of model allows for significant future study of parameters, optimization, etc.

References

1. M. Tweedie Thesis. CFD Modeling and Analysis of a Planar Anode Supported Intermediate Temperature Solid Oxide Fuel Cell. Rensselaer Polytechnic Institute, May, 2014.
2. R. Suwanwarangkul et al., "Experimental and Modeling Study of Solid Oxide Fuel Cell Operating with Syngas Fuel," *Journal of Power Sources*, vol. 161, pp. 308–322, 2006.