COMSOL CONFERENCE BOSTON 2012

Numerical Simulation of Electrolyte-Supported Planar Button Solid Oxide Fuel Cell

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Excerpt from the Proceedings of the 2012 COMSOL Conference in Boston

Objectives

- **Build a working model of planar button-shaped electrolyte supported SOFC**

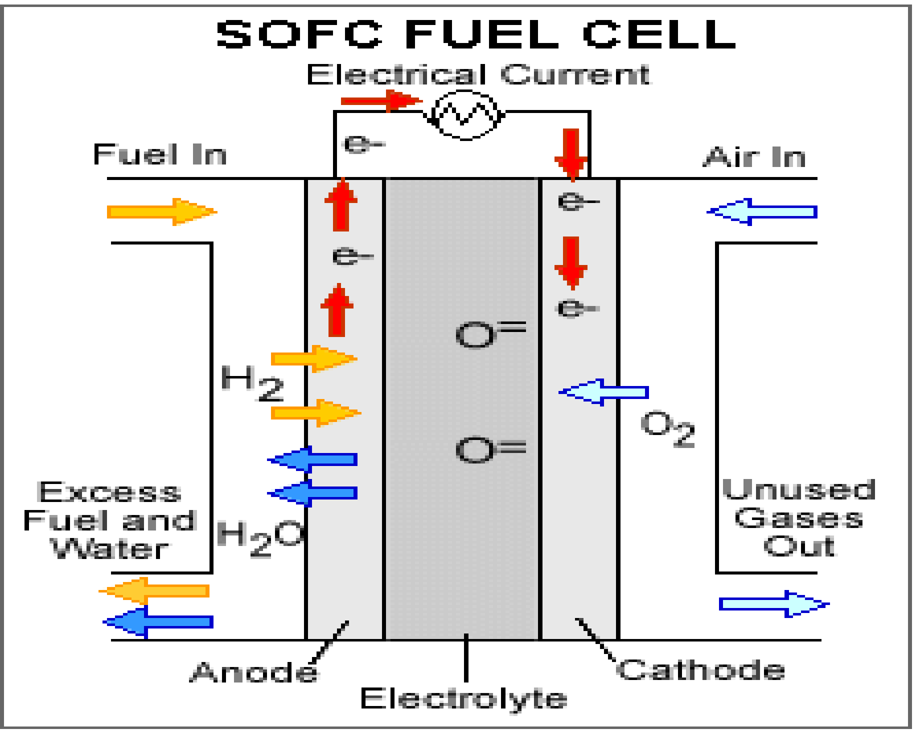
- **Run simulations for several electrolyte material configurations**

- **Study effect of electrolyte on performance**

Solid Oxide Fuel Cell (SOFC)

SOFC

- ✓ Solid electrolyte - Ceramics
- ✓ Operating temperatures (400ºC – 1000ºC)



Picture Source: U.S. Department of Energy website

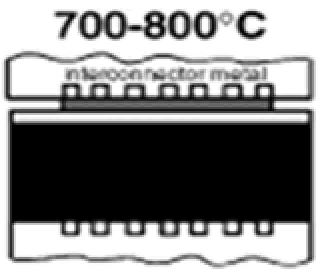
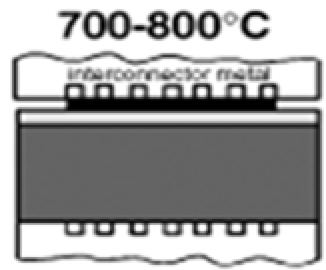
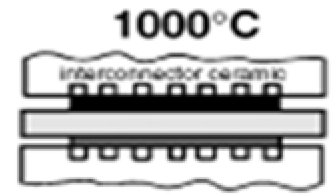
Advantages of SOFC

- ✓ High efficiency (>50%, >80% CHP) [1]
- ✓ Fuel flexibility (H_2, natural gas, biogases, etc.)
- ✓ Combined Heat & Power generation
- ✓ Compatible with gas & steam turbines
- ✓ Power output (W to MW)
- ✓ Relatively higher power density
- ✓ No water flooding issues, unlike PEMFC

$$H_2 \rightarrow 2H^+ + 2e^-$$

$$\frac{1}{2}O_2 + 2H^+ + 2e^- \rightarrow H_2O$$

Types of Planar SOFC

Cathode-supported	*Anode-supported*	*Electrolyte-supported*
		
Cathode: 300 - 1000 µm	**Cathode: 50 µm**	**Cathode: 50 µm**
Electrolyte: < 20 µm	**Electrolyte: < 20 µm**	**Electrolyte: > 100 µm**
Anode: 300 – 1000 µm	**Anode: 500 - 1500 µm**	**Anode: 50 µm**
Activation losses higher than Anode-supported	**Higher Activation losses**	**Higher Ohmic losses**

Source: Mark C. Williams, Joseph P. Strakey and Wayne A. Surdoval, U.S. Department of Energy's Solid Oxide Fuel Cells: Technical Advances, Int. J. Appl. Ceram. Technol., 2 (4) 295–300 (2005)

Electrolyte Materials – YSZ, SCSZ

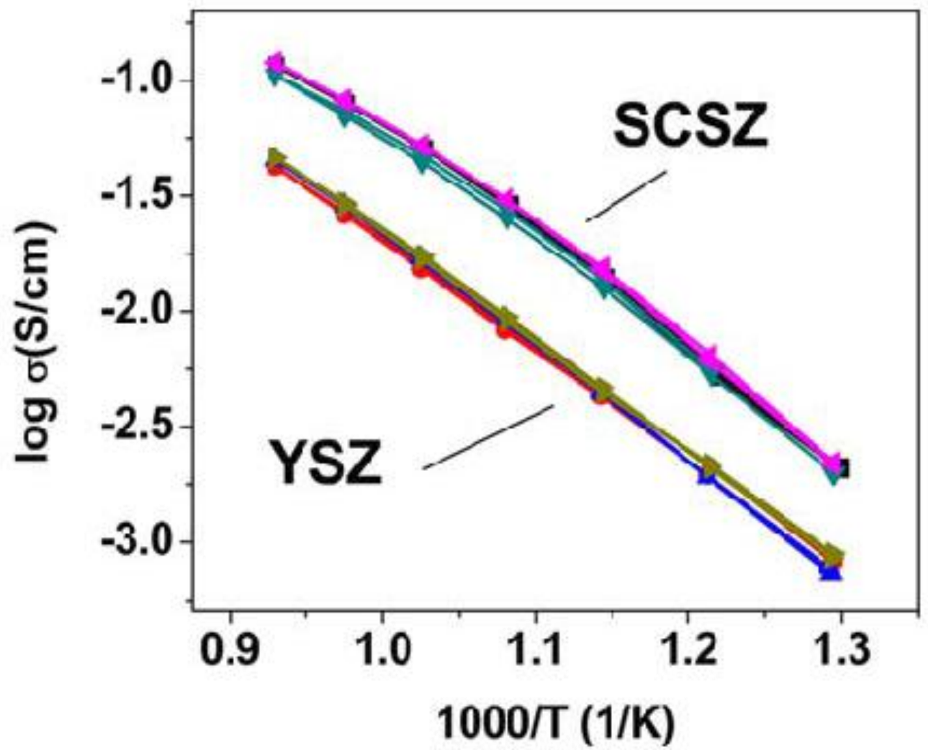
Ideal electrolyte – high ionic conductivity, phase stability, mechanical strength.

SCSZ - $Sc_{0.17}Ce_{0.08}ZrO_2$
YSZ - 8 mol% Y_2O_3 stabilized ZrO_2

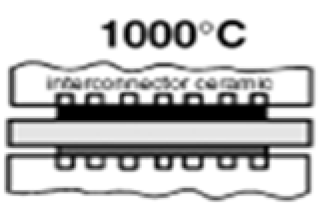
• SCSZ electrolyte will be ideal in terms of conductivity.

• SCSZ undergoes phase transition (cubic to rhombohedral) at 300-500 ^{0}C.

• YSZ is stable in both oxidizing and reducing environments, maintains cubic structure.

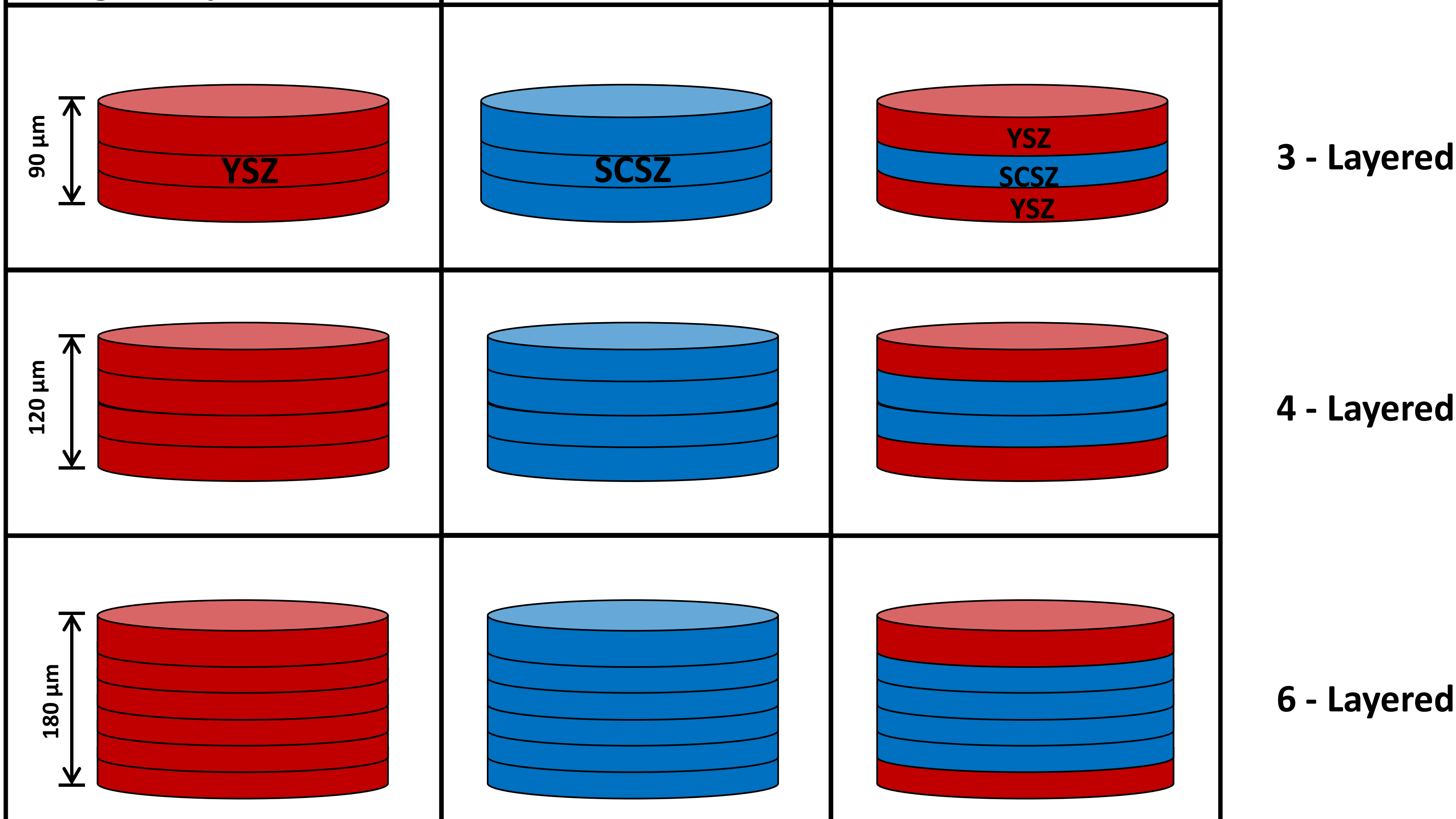


Electrolyte Supported Design



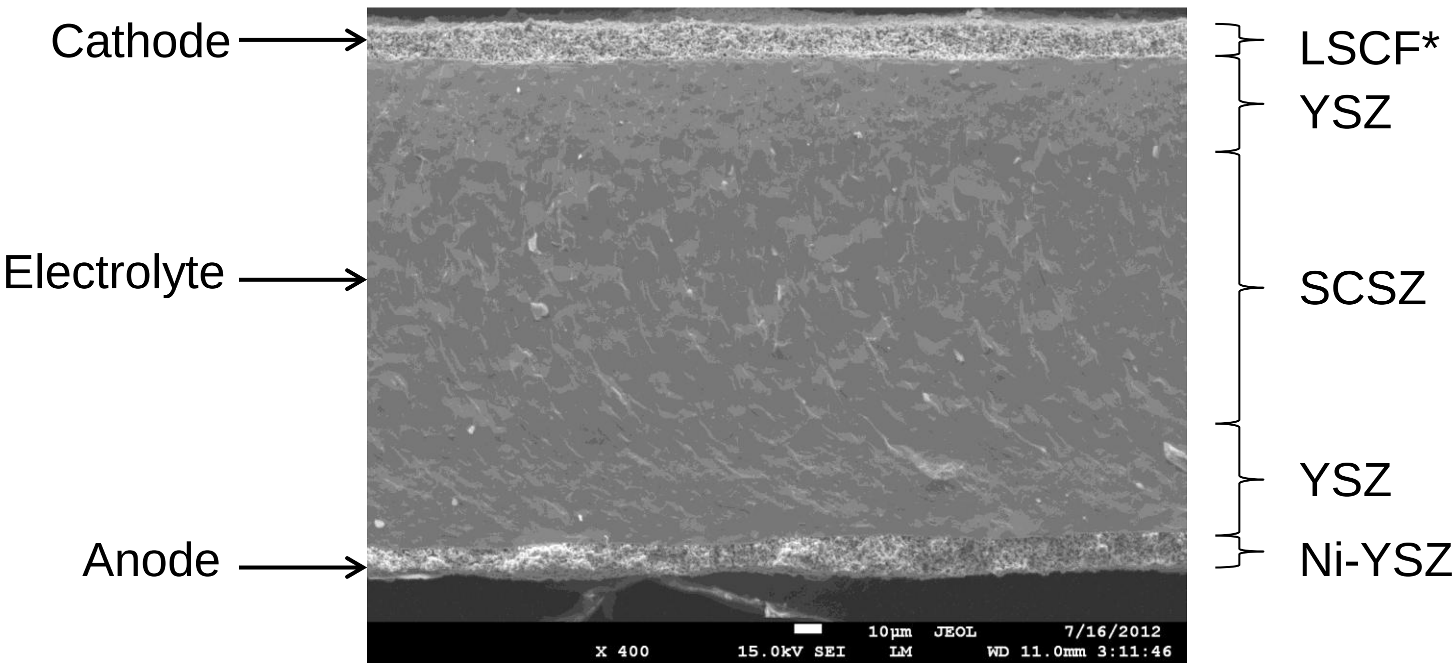
Layered SOFC Electrolytes

YSZ only	SCSZ only	YSZ-xSCSZ-YSZ
Phase stability at high temperatures	High ionic conductivity	



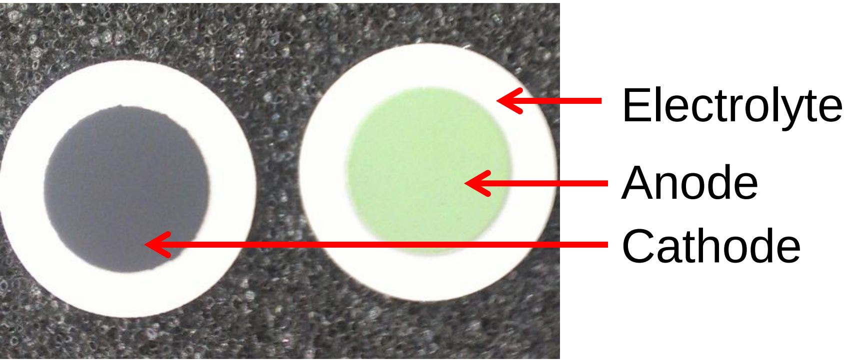
SOFC Material Properties

	Anode – Ni-YSZ	Cathode - LSCF	Electrolyte – YSZ	Electrolyte - SCSZ
Ionic Conductivity [S/m]	1	5.15	4.24 – 4.62	10.58 – 11.93
Electronic Conductivity [S/m]	650000	2300	negligible	negligible
Porosity	40 %	40 %	0	0

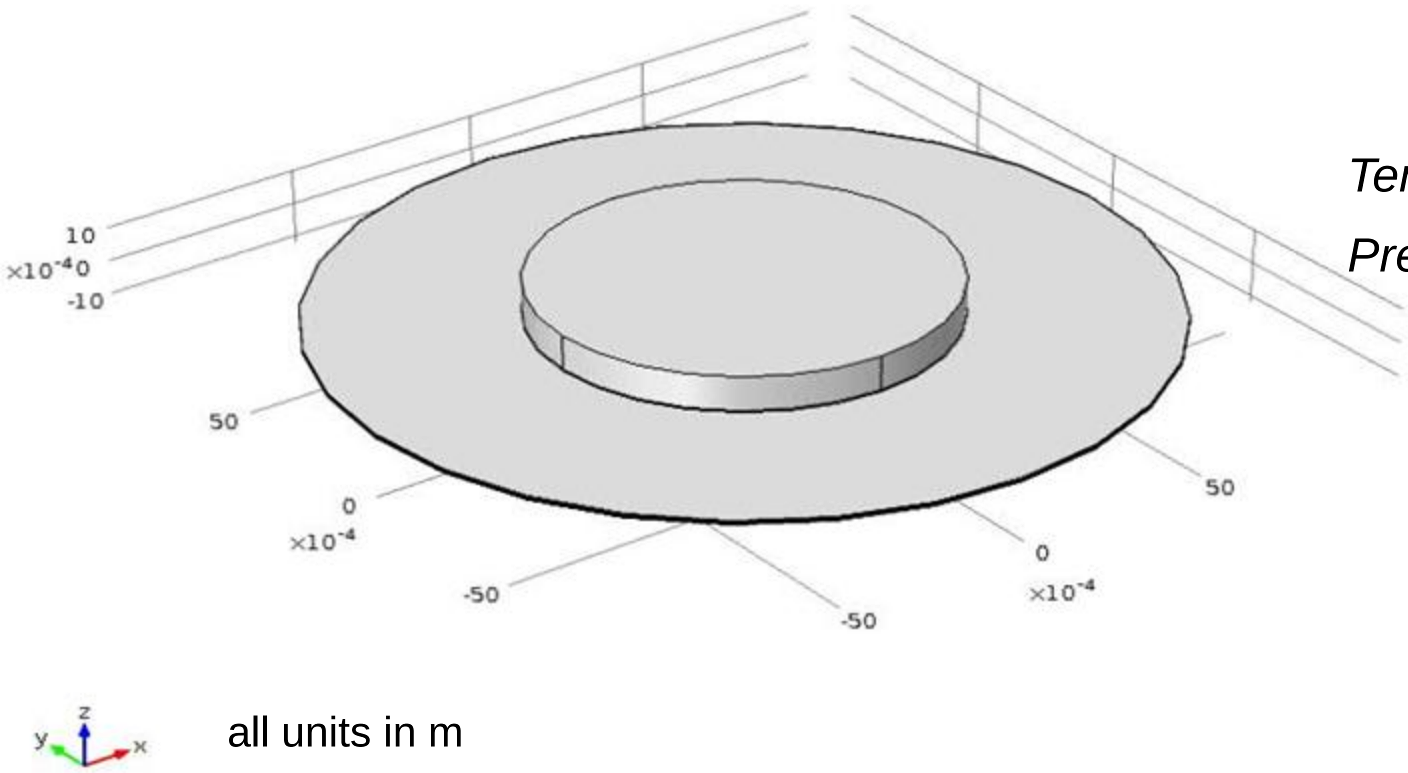


LSCF* - $(La_{0.6}Sr_{0.4})_{0.95\text{-}0.99}Co_{0.2}Fe_{0.8}O_3$

SOFC Geometry: Top View

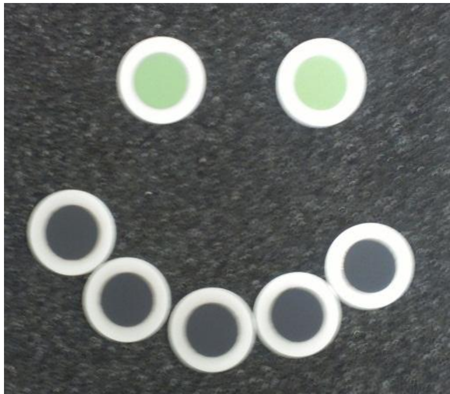


Physics involved:	Electrochemistry & Fluid dynamics
Mesh:	Unstructured
# of Mesh elements:	116,000 to 1,035,000

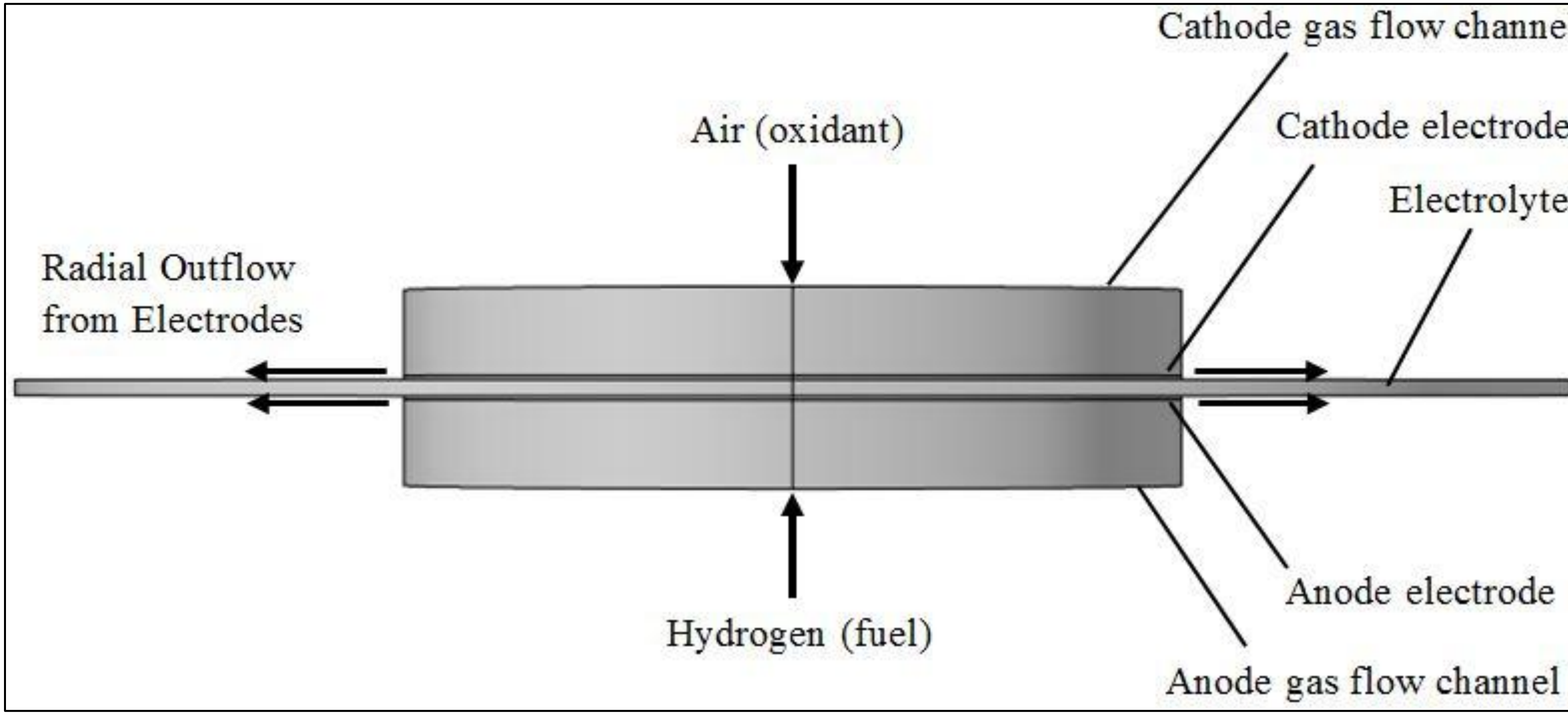


Temperature:	800 °C
Pressure:	1 atm

all units in m



SOFC Geometry



Anode & Cathode thickness	50 μm
Electrolyte layer thickness	30 μm
Anode & Cathode diameter	10 mm
Electrolyte diameter	20 mm
Gas flow channel height (Anode & Cathode)	1 mm
Gas flow channel diameter (Anode & Cathode)	10 mm

Modeling Methodology

COMSOL:
Electrochemistry – Current distribution & Transport of chemical species

Current distribution	Transport of chemical species

Current distribution

$$\nabla \cdot j = Q$$

$$j = \sigma \nabla \Phi$$

$$\eta_m = \Phi_s - \Phi_l - E_{eq,m}$$

Butler-Volmer equation:

$$j = j_o \left[\left(\frac{c}{c_0} \right)_R exp\left\{ \frac{n\alpha F}{RT} \eta \right\} - \left(\frac{c}{c_0} \right)_P exp\left\{ \frac{-n(1-\alpha)F}{RT} \eta \right\} \right]$$

j = i/area [A/m^2], current density vector
Q – source or sink term
Φ_l, Φ_s - electrolyte and electrode potential respectfully [V]
σ - electrolyte conductivity [S/m]
η – activation overpotential [V]
$E_{eq,m}$ - equilibrium potential for the m reaction
c_R,c_P – concentration of reactants & products respectfully
j_0 – reference current density
n: number of charges transferred
α : transfer coefficient

Transport of chemical species

Maxwell-Stefan diffusion model:

$$\frac{\partial}{\partial t}(\rho \omega_i) + \nabla \cdot (\rho \omega_i u) = \nabla \cdot m_i + R_i$$

$$m_i = \rho \omega_i \sum_{k=1}^{Q} \widetilde{D}_{ik} d_k + D_i^T \frac{\nabla T}{T}$$

ρ: mixture density (kg/m^3)
u: mass average velocity (m/s)
ω_i: mass fraction
j_i: mass flux relative to the mass average velocity (kg/(m^{2}s))
R_i: consumption or production rate (kg/(m^{3}s))
T: temperature (K)
D_i^T: thermal diffusion coefficients (kg/(ms))
d_k: diffusional driving force acting on species k (1/m)
$\widetilde{D}_{ik}$: multicomponent Fick diffusivities (m^2/s)

Modeling Methodology

Fluid mechanics – Brinkman equations (porous media)

Continuity equation:

$$\frac{\partial}{\partial t}(\varepsilon_p \rho) + \nabla \cdot (\rho u) = Q_{br}$$

For incompressible fluids:

$$\rho \nabla \cdot \mathrm{u} = \mathrm{Q}_{\mathrm{br}}$$

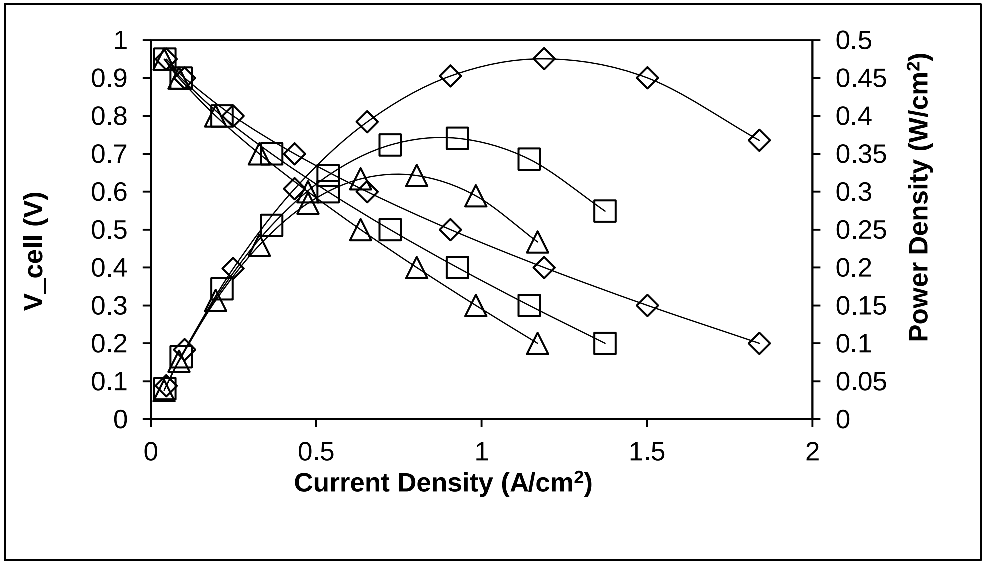
Momentum equation:

$$\frac{\rho}{\varepsilon_p}\left(\frac{\partial u}{\partial t} + (u \cdot \nabla)\frac{u}{\varepsilon_p}\right) = -\nabla p + \nabla \cdot \left[\frac{1}{\varepsilon_p}\left\{\mu(\nabla u + (\nabla u)^T) - \frac{2}{3}\mu(\nabla \cdot u)I\right\}\right] - \left(\frac{\mu}{k} + Q_{br}\right)u + F$$

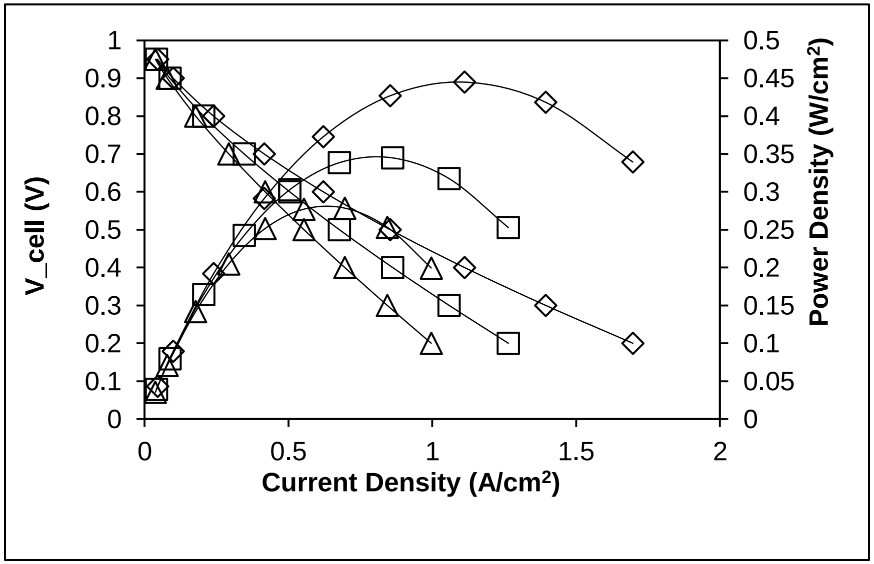
μ : dynamic viscosity of the fluid (Pa·s)
u : velocity vector (m/s)
ρ : fluid density (kg/m^3)
p : pressure (Pa)
ε_p : porosity
k : permeability of porous medium (m^2)
Q_{br} : mass source or mass sink (m^3/s)
F : volume forces vector (kg/m^2s^2)

Results

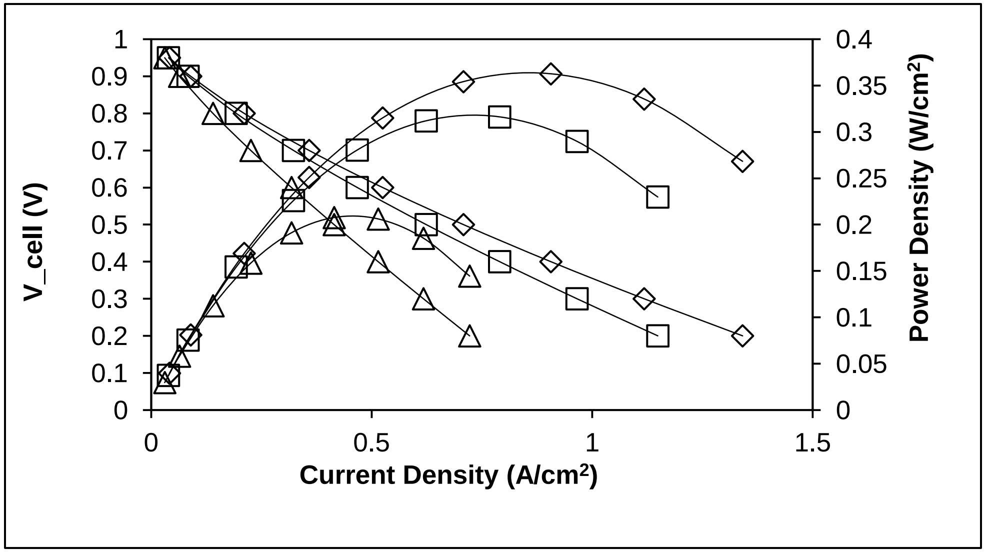
3 - Layered Electrolyte



4 - Layered Electrolyte

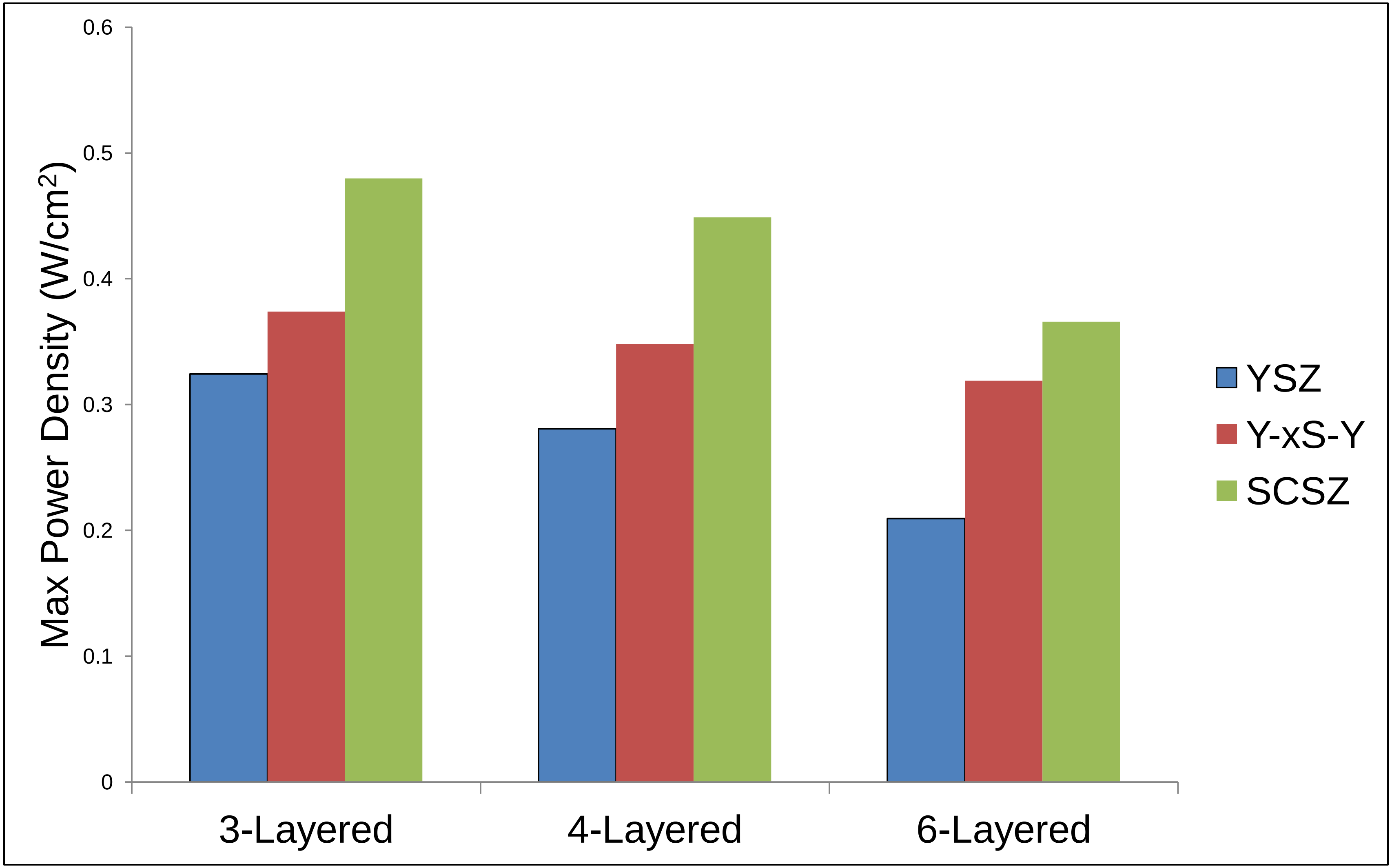


6 - Layered Electrolyte



- ***Pure SCSZ electrolytes had highest power***
- ***Lower ohmic losses***

Comparison of YSZ, YSZ-SCSZ Layered, and SCSZ Single Cell Performance



Conclusion & Future Work

- **Using SCSZ as the electrolyte material yields the best performance, i.e., the maximum power and current density.**
- **As the number of electrolyte layers increases, the performance decreases (higher ohmic losses).**
- **Future work will include incorporating heat transfer physics.**
- **Compare and match the i-V plot and other experimental results when the SOFCs are produced and tested in the lab.**
- **Use model to calculate parameters (α, j_o) by curve fitting with experimental results.**
- **Finite Element Modeling of SOFC electrolyte to find relationship between load, fracture strength and deflection.**

Questions?
Thank you!

References

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[5] *Processing Microstructure Property Correlation of Porous Ni-YSZ Cermets Anode for SOFC Application*. S.K. Pratihar, et al.

[6] *Introduction of A-site deficiency into La0.6Sr0.4Co0.2Fe0.8O3–d and its effect on structure and conductivity*. Mineshige, et al.

[7] *High temperature properties of La0.6Sr0.4Co0.8Fe0.2O3-d phase structure and electrical conductivity*. Wang, et al.

[8] *The ionic conductivity, thermal expansion behavior, and chemical compatibility of La0.54Sr0.44Co0.2Fe0.8O3-d as SOFC cathode material*. Fan, et al.

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[10] *Structure and electrical properties of La, _.,Sr,Co, _,Fe,O,. Part 2. The system La, _.,SrxCo0.2Fe0.803*. Tai, et al.