Numerical Modeling for the Performance of Reversible Solid Oxide Fuel Cell

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Introduction

Background & Motivation

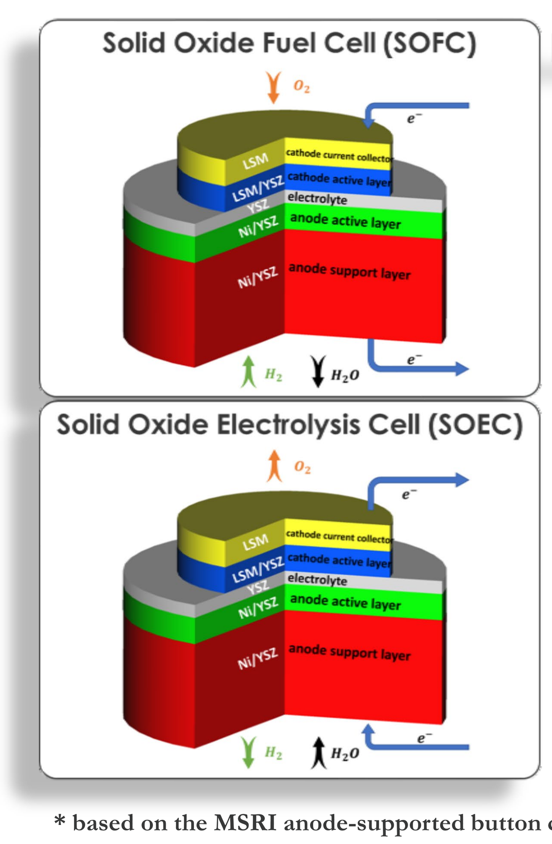
- Different phenomena are observed in various Solid Oxide Electrolysis Cells (SOEC) experiments with different testing conditions.
- A global minimum resistance exists under different working bias conditions.
- Severe performance degradation caused by Ni migration was also reported in the literature.

Purpose of the study

- The performance of solid oxide cells (SOCs) under both electrolysis mode and fuel cell mode is investigated via in-house developed high fidelity multiphysics simulations.

Methodology

Multiphysics modeling



* based on the MSRI anode-supported button cell

basic physical/electrochemical processes:

- Electrochemical reactions
- Chemical reactions
- Charge transport
- Double layer capacitor
- Species consumption/production
- Gas phase diffusion within porous media
- Surface/Bulk diffusion within electrodes
- Gas transport in the channel
- Heat transfer
- Phase change/formation
- Microstructure evolution
- ......

- Mathematically, these highly coupled processes are formulated by sets of partial differential equations

❑ Charge conservation

domain	phase	governing equations
Cathode	LSM	$a_{int,c}C_{DL,c}\frac{\partial}{\partial t}(\varphi_c-\varphi_i)+\nabla\cdot(-\sigma_c\nabla\varphi_c)=i_{Fc}$
	YSZ	$a_{int,c}C_{DL,c}\frac{\partial}{\partial t}(\varphi_i-\varphi_c)+\nabla\cdot(-\sigma_i\nabla\varphi_i)=-i_{Fc}$
Electrolyte	YSZ	$\nabla\cdot(-\sigma_i\nabla\varphi_i)=0$
Anode	YSZ	$a_{int,a}C_{DL,a}\frac{\partial}{\partial t}(\varphi_i-\varphi_a)+\nabla\cdot(-\sigma_i\nabla\varphi_i)=-i_{Fa}$
	Ni	$a_{int,a}C_{DL,a}\frac{\partial}{\partial t}(\varphi_a-\varphi_i)+\nabla\cdot(-\sigma_a\nabla\varphi_a)=i_{Fa}$

❑ Species transportation

$$\varepsilon\frac{\partial\phi}{\partial t}=\nabla\cdot\left(D_\phi^{eff}\nabla\phi\right)-S_\phi$$

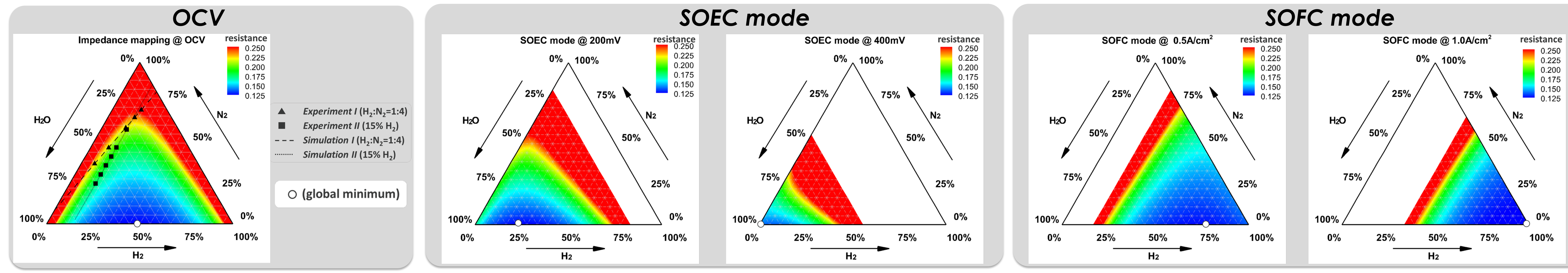
- Exchange current densities (i_{Fc}, i_{Fa}) and species consumption/production rate (S_ϕ) are coupled via the electrochemical model (i.e., Butler-Volmer model).

References

- T. Yang et al., *Journal of The Electrochemical Society*, 166(8), pp F448-F457, 2019.
- T. Yang et al., *International Journal of Hydrogen Energy*, 43(32), pp 15445-15456, 2018.
- T. Yang et al, *Physical Chemistry Chemical Physics*, 19(45), pp 30464 – 30472, 2017.
- T. Yang et al., *International Journal of Electrochemical Science*, 12, pp 6801-6828, 2017.

Results

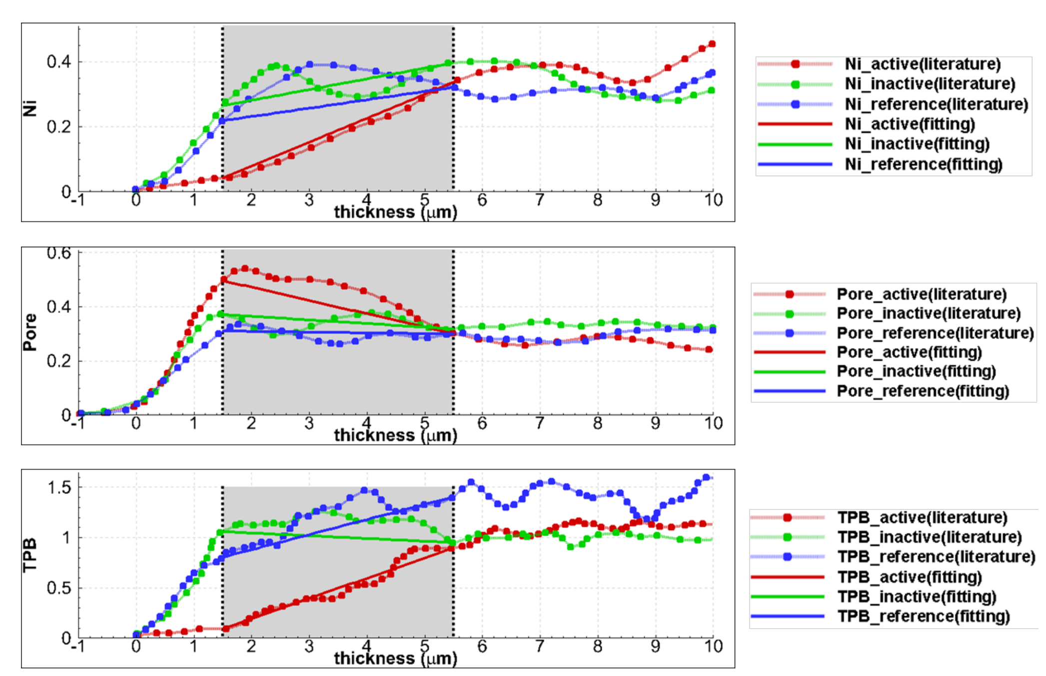
Parametric study of cell performance under practical working conditions (fuel/steam supply conditions & working loads)



Mapping of impedance behavior under different working loads and fuel/steam supply conditions

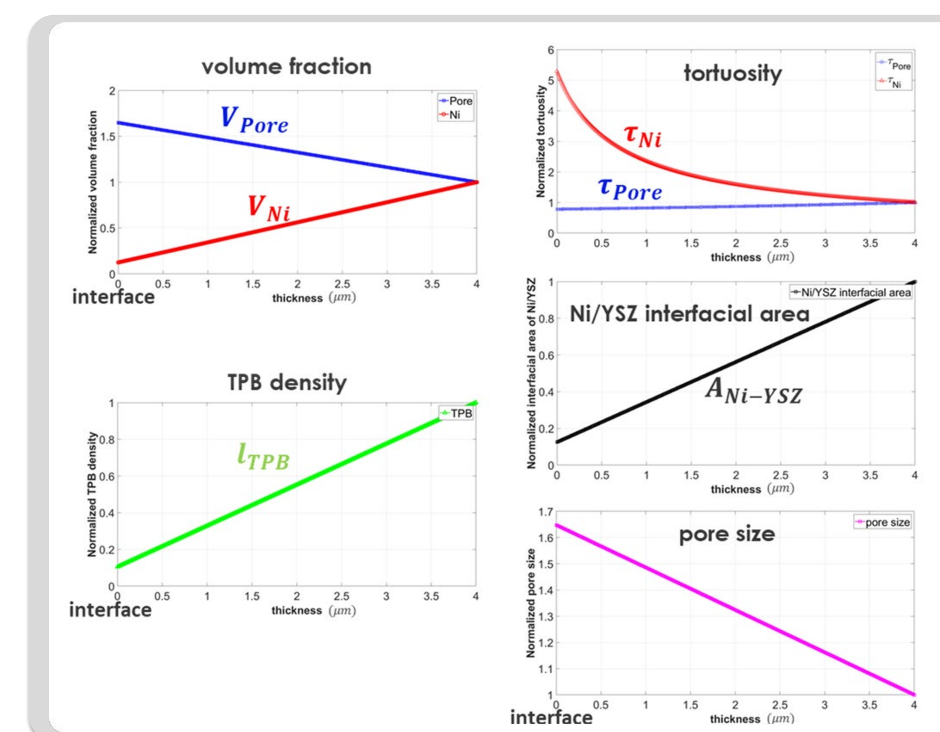
Performance Degradation due to Ni Redistribution

- ***microstructural properties change***



- F. Monaco et al., *ECS Transactions*, 91(1), pp. 653-64. (2019)
- F. Monaco et al., *Journal of the Electrochemical Society*, 166(15), pp. F1229-F1242. (2019)

Properties extracted from literature



Properties calculated based on empirical formula

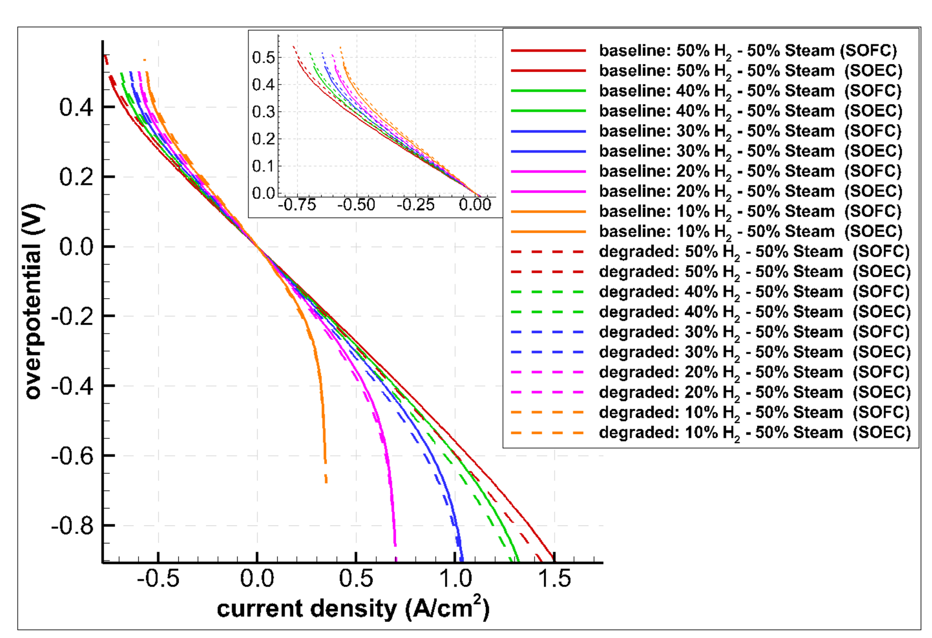
Reference properties (PFIB)

	anode active layer	cathode active layer
ϵ	0.2	0.36
f_{Ni} or f_{LSM}	0.34	0.35
f_{YSZ}	0.45	0.29
l_{tpb} (m/m^{-3})	5.97×10^{12}	6.72×10^{12}
D_{pore} (μm)	0.44	0.44
D_{Ni} or D_{LSM} (μm)	0.57	0.57
D_{YSZ} (μm)	0.35	0.35
$A_{Ni/YSZ}$ or $A_{LSM/YSZ}$ (m^2/m^{-3})	1.0×10^6	0.95×10^6

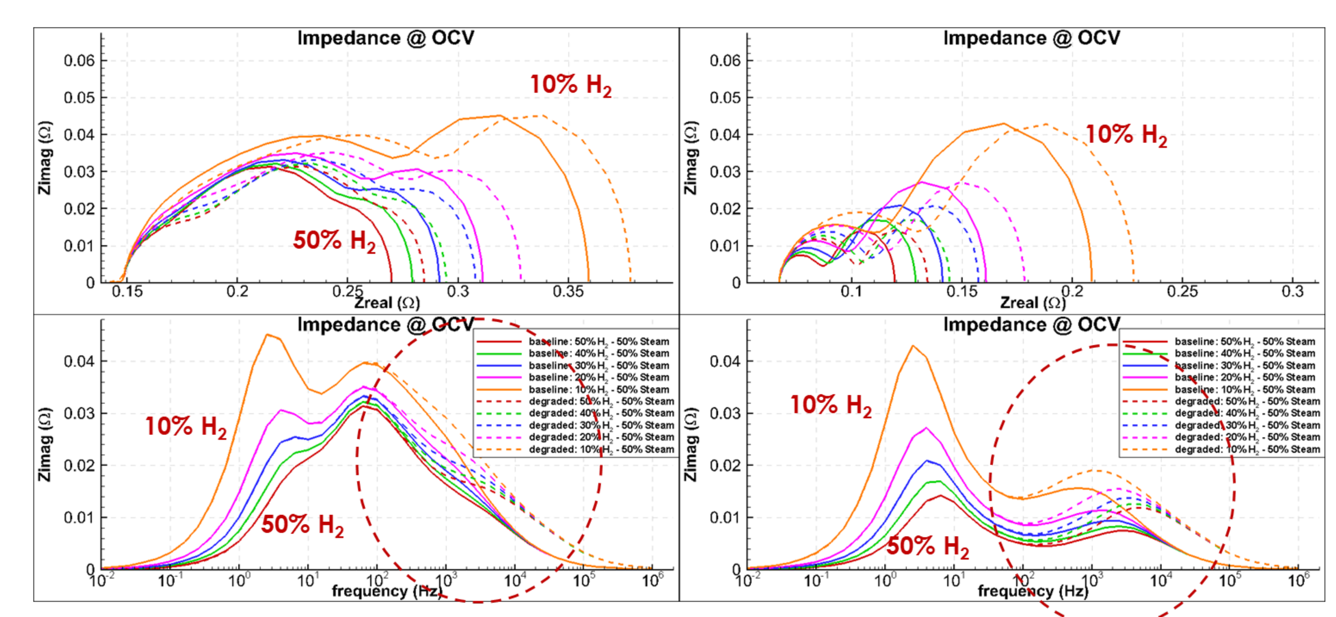
- T. Hsu et al., *Journal of Power Sources*, 386, pp. 1-9. (2018)
- R. Mahbub et al., *ECS Transactions*, 78, pp. 2159-70. (2017)

Reference properties from PFIB datasets

- ***Performance degradation***



V-I curves



Impedance behavior

Main performance degradation occurs on the high frequency range (> 1000 Hz), indicating that the Ni redistribution inside the active layer mainly affects the charge transfer processes in the hydrogen/steam electrode.

Summary

- Multiphysics simulations are developed for the performance investigation of solid oxide cells under both SOFC and SOEC operation mode.
- The full parameter space (various fuel/steam supply conditions) is explored to better understand the trends of cell performance under practical working conditions. For each specific working loads, a global minimum resistance is found, but the conditions for the global minimum resistance shift for different working loads under different working modes.
- The performance degradation due to the Ni redistribution is predicted and investigated based on the changes of reaction sites and microstructural properties. The charge transfer processes in the hydrogen/steam electrode are mainly affected by Ni redistribution.
- This study can provide guidance for the design of efficient reversible solid oxide fuel cell (r-SOFC) systems.

U.S. DEPARTMENT OF ENERGY

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