In-House Developed Multiphysics Simulation for the Performance of Solid Oxide Cells (SOCs)

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Introduction

Background and Motivation

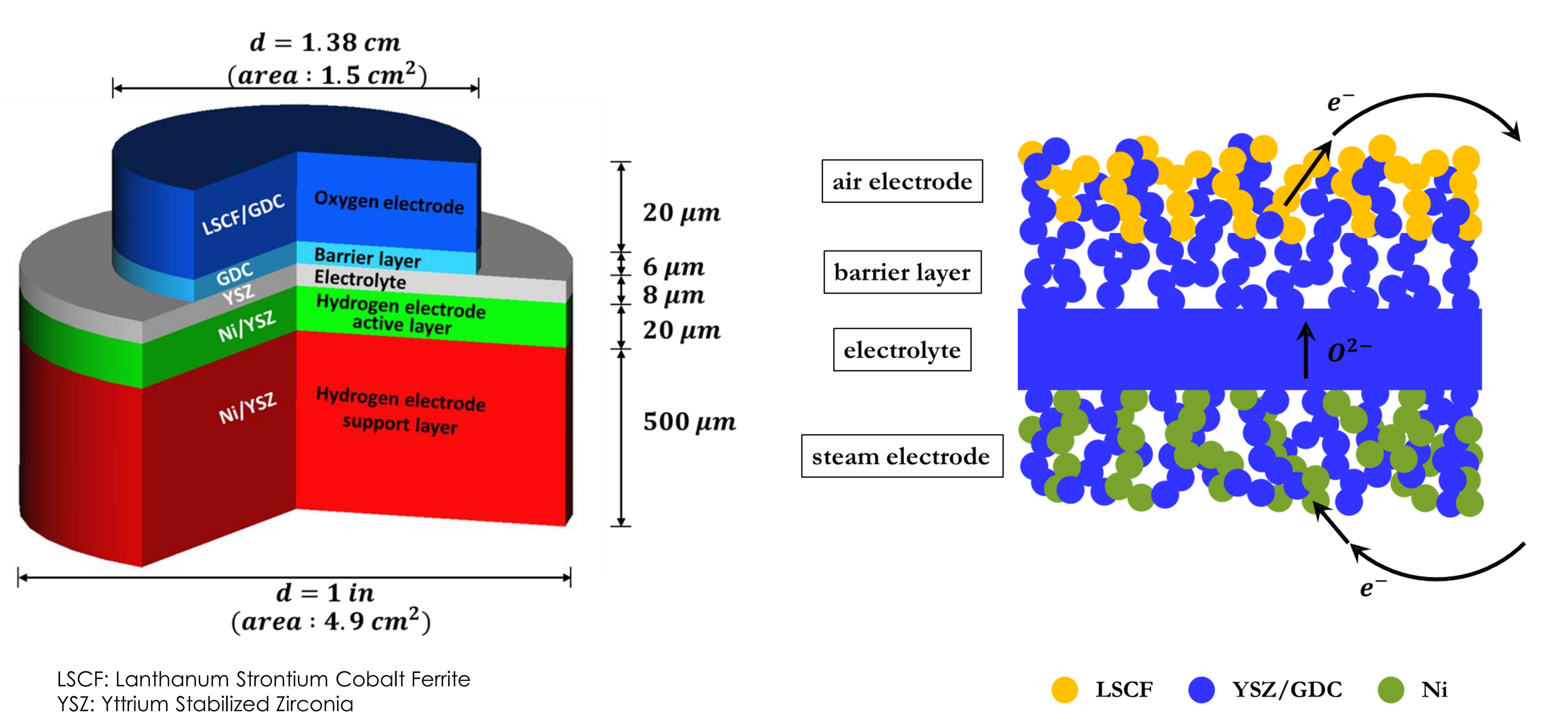
- Reversible solid oxide cells(r-SOCs) are an enabling energy storage/production technology for a dynamic grid environment. Reversible operation requires strong working knowledge of fuel cell (SOFC) and electrolyzer (SOEC) operation.
- Performance degradation of SOECs has been observed; however, the details of physical processes related to the performance degradation remain unknown.

Purpose of the Study

- Multiphysics simulations were performed to investigate the performance degradation of solid oxide electrolysis cells under various working conditions.

Multiphysics Modeling

Cell configuration & working conditions



LSCF: Lanthanum Strontium Cobalt Ferrite
YSZ: Yttrium Stabilized Zirconia
GDC: Gadolinium-doped Ceria

Governing equations

- **Charge conservation** (electron-conducting phase)

$$\underbrace{a_{int}C_{DL}\frac{\partial}{\partial t}(\varphi_e-\varphi_i)}_{\text{double layer capacitor}} + \underbrace{\nabla\cdot(-\sigma_e\nabla\varphi_e)}_{\text{charge transport}} = \underbrace{i_F}_{\text{electrochemical reactions}}$$

- **Species transport**

$$\varepsilon\frac{\partial\phi}{\partial t} = \underbrace{\nabla\cdot\left(D_\phi^{eff}\nabla\phi\right)}_{\text{diffusion}} - \underbrace{S_\phi}_{\text{consumption/production rate}}$$

- **Electrochemical model** (Butler-Volmer model in this study)

Steam electrode:

$$i_{F,S} = i_{0,S}(P_{H_2}^{\infty})^{a}(P_{H_2O}^{\infty})^{b}\left\{\frac{P_{H_2}}{P_{H_2}^{\infty}}\exp\left[\frac{(1-\alpha)nF\eta_S}{RT}\right]-\frac{P_{H_2O}}{P_{H_2O}^{\infty}}\exp\left[-\frac{\alpha nF\eta_S}{RT}\right]\right\}$$

Air electrode:

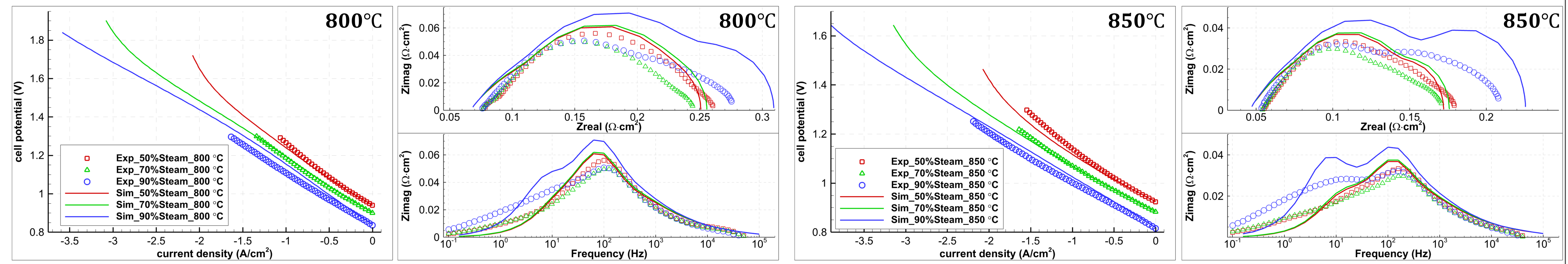
$$i_{F,A} = i_{0,A}(P_{O_2}^{\infty})^{m}\left\{\frac{P_{O_2}}{P_{O_2}^{\infty}}\exp\left[-\frac{\alpha nF\eta_A}{RT}\right]-\exp\left[\frac{(1-\alpha)nF\eta_A}{RT}\right]\right\}$$

References

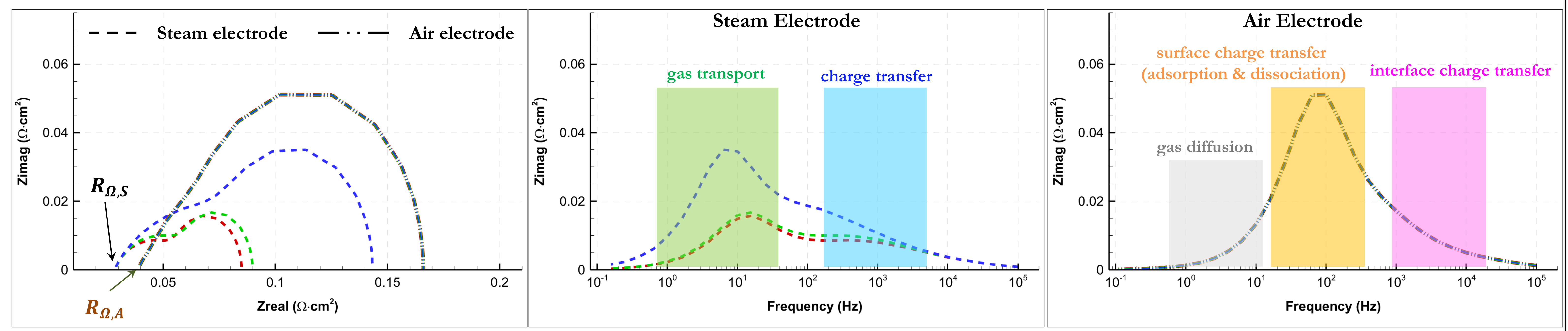
1. T. Yang et al., International Journal of Hydrogen Energy, 2022.
2. T. Yang et al., Journal of The Electrochemical Society, 166(8), pp F448-F457, 2019.
3. T. Yang et al., International Journal of Hydrogen Energy, 43(32), pp 15445-15456, 2018.
4. T. Yang et al, Physical Chemistry Chemical Physics, 19(45), pp 30464 – 30472, 2017.
5. T. Yang et al., International Journal of Electrochemical Science, 12, pp 6801-6828, 2017.

Results

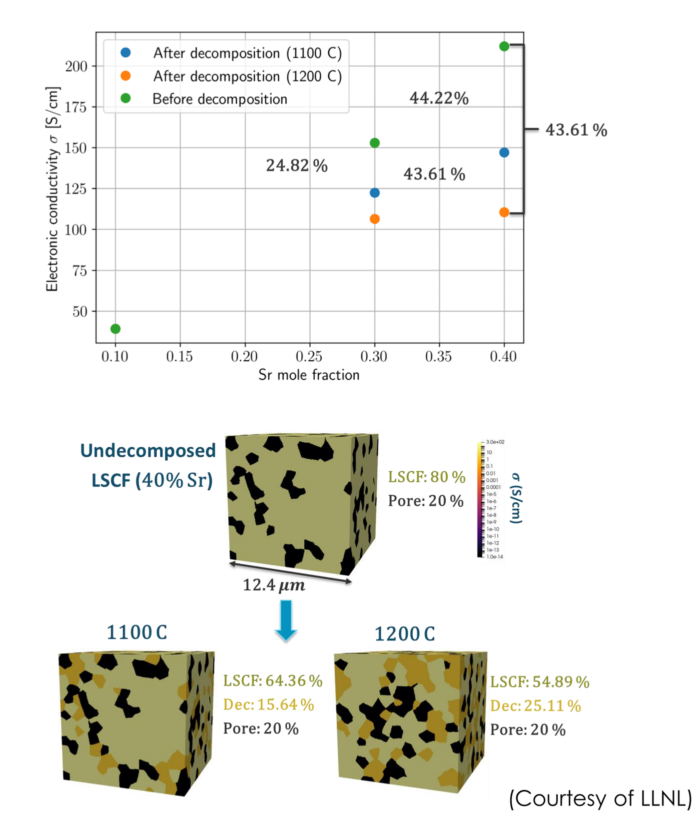
Calibration of the multiphysics simulation



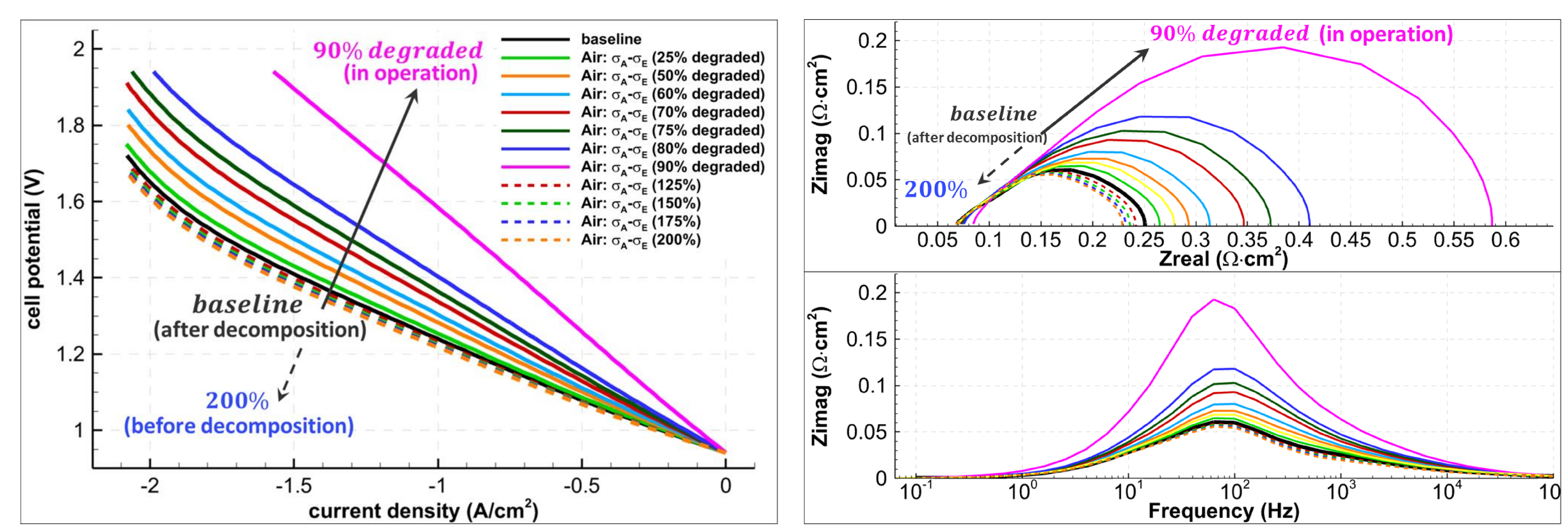
Resistance of electrodes (800℃)



Effects of electrical conductivity on the cell performance



Effective electronic conductivity of the porous LSCF electrode is lowered by the formation of the spinel phase



Summary & Future Work

- Multiphysics simulations were performed to study the degradation of solid oxide electrolysis cells under various working conditions.
- Resistance components of steam electrode and air electrode were extracted from simulated impedance behavior.
- The effects of electrical conductivity of air electrode (decomposition) on the performance was investigated, which can also be related to performance degradation during operation.