Numerical Modeling for the Performance of Reversible Solid Oxide Fuel Cell

**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**

  - **Basic physical/ electrochemical processes:**
    - Electrochemical reactions
    - Chemical reactions
    - Charge transport
    - Double layer capacitance
    - 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**
      - Cathode
      - Anode
    - **Phase**
      - LSM
    - **Governing equations**
      - \( \frac{\partial}{\partial t} (\rho \cdot \Phi) - \nabla \cdot (\rho \cdot \mathbf{J}) = \dot{\rho} \)

  - **Species transportation**
    - Exchange current densities \( \dot{\rho} \) and species consumption/production rate \( \dot{\rho} \) are coupled via the electrochemical model (i.e., Butler-Volmer model).

- **Performance degradation**
  - 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.

- **Summary**
  - Multiphysics simulations can provide guidance for the design of efficient reversible solid oxide fuel cells (r-SOFC) systems.