A Multi-Dimensional Micro-Scale Model for Oxygen Reduction on LSM-YSZ Cathode

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Introduction

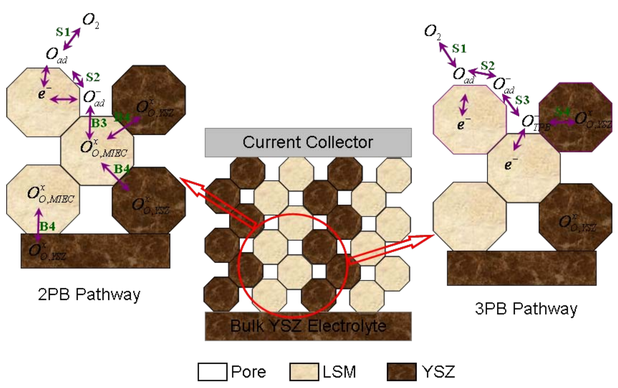
- Cathode performance limits the overall efficiency of SOFCs.
- Knowledge of the kinetics of oxygen reduction will lead to better cathode designs
- Performance of the cathode is also dependent on the microstructure.
- Oxygen reduction on LSM-YSZ cathode is known to occur through parallel pathways.
  - 2PB pathway and 3PB pathway.
- A three dimensional computational model needed for oxygen reduction on LSM/YSZ.

Model Description

- Micro-scale dynamic model for charge and mass transfer inside the cathode.
- A multi-step charge transfer reaction mechanism with parallel 2PB and 3PB pathways.
- Averaged microstructural parameters obtained from reconstructed cathode using SEM images.

Reaction Mechanism:

$$(S1)\quad \frac{1}{2}O_2 + S \leftrightarrow O_{ad}$$
$$(S2)\quad O_{ad} + e^- \leftrightarrow O_{ad}^-$$
$$(S3)\quad O_{ad}^- \leftrightarrow O_{TPB}^-$$
$$(S4)\quad O_{TPB}^- + e^- + V_{O,YSZ}^{**} \leftrightarrow O_{O,YSZ}^{x} + S$$
$$(B3)\quad O_{ad}^- + V_{O,MIEC}^{**} + e^- \leftrightarrow O_{O,MIEC}^{x}$$
$$(B4)\quad O_{O,MIEC}^{x} + e^- + V_{O,YSZ}^{**} \leftrightarrow O_{O,YSZ}^{x} + V_{O,MIEC}^{**}$$



Model Equations

Gas species transport (O_2)

$$\varepsilon \frac{\partial n_{O_2}}{\partial t} = \nabla\left(D_{O_2}^{eff} \nabla n_{O_2}\right) - r_{ads}$$

Coverages Transport (O, O^-,O^-_{TPB})

$$\frac{\partial \theta_i}{\partial t} = \nabla\left(D_{\theta_i}^{eff} \nabla \theta_i\right) + r_i$$

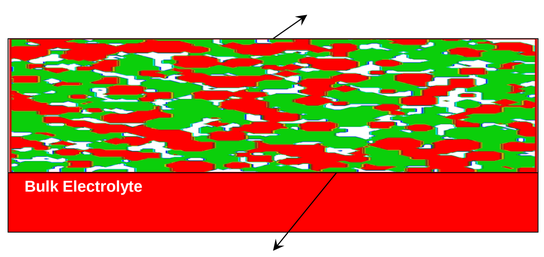
Vacancies Transport ($C_{V,MIEC}$, $C_{V,YSZ}$)

$$\frac{\partial C_V}{\partial t} = \nabla\left(D_{C_V}^{eff} \nabla C_V\right) + r_{C_V}$$

Charge Transport

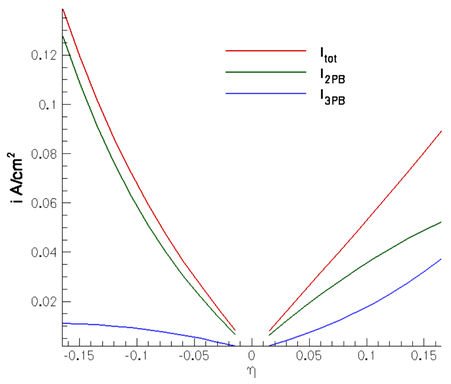
$$C_{DL}\frac{\partial(\Delta\varphi)}{\partial t} = \nabla\cdot\left(\sigma_i \nabla(\Delta\varphi)\right) - i_F$$

C/Air interface
Ionic current = 0, Electronic potential prescribed, Oxygen concentration prescribed, and flux of all Other species (coverages and vacancies) is zero

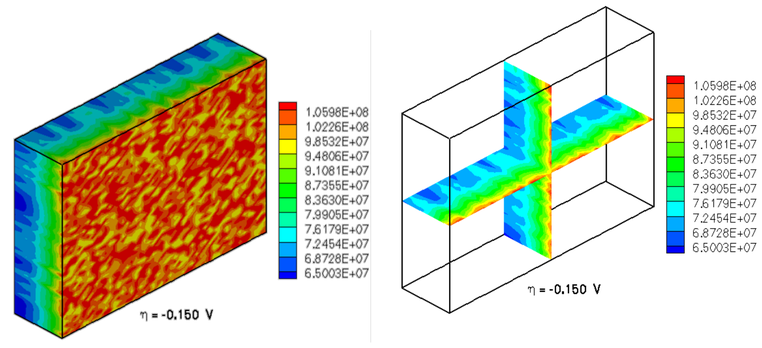


C/E Interface
Electronic current = 0, Ionic potential prescribed, YSZ oxygen vacancy production as a function of current, all other fluxes are zero

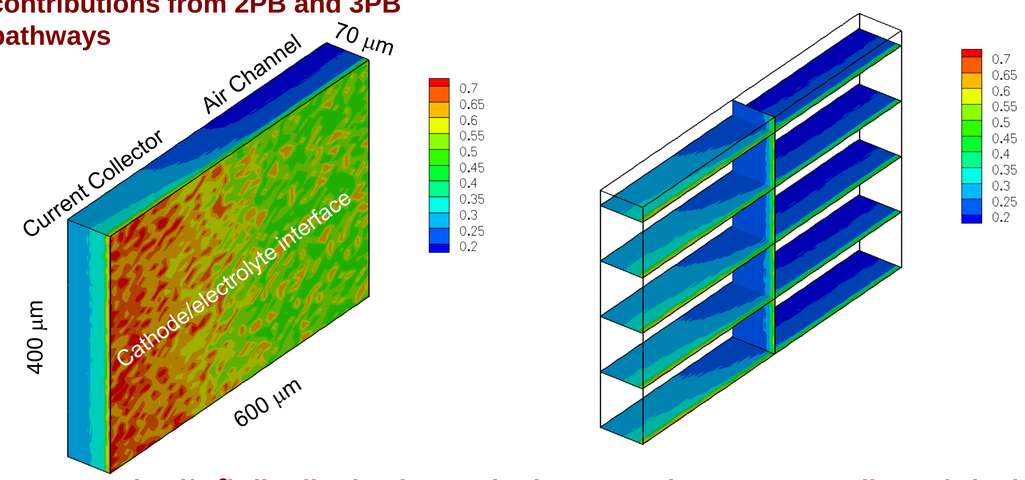
Results



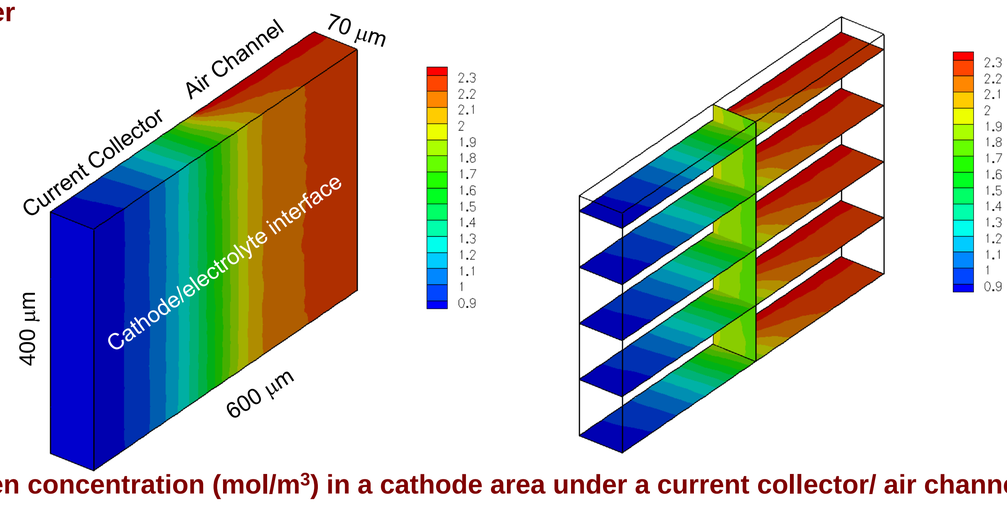
Polarization curve and the contributions from 2PB and 3PB pathways



Faradaic current (A/m³) distribution inside the cathode under polarization



LSM vacancy (mol/m³) distribution in a cathode area under a current collector/ air channel corner



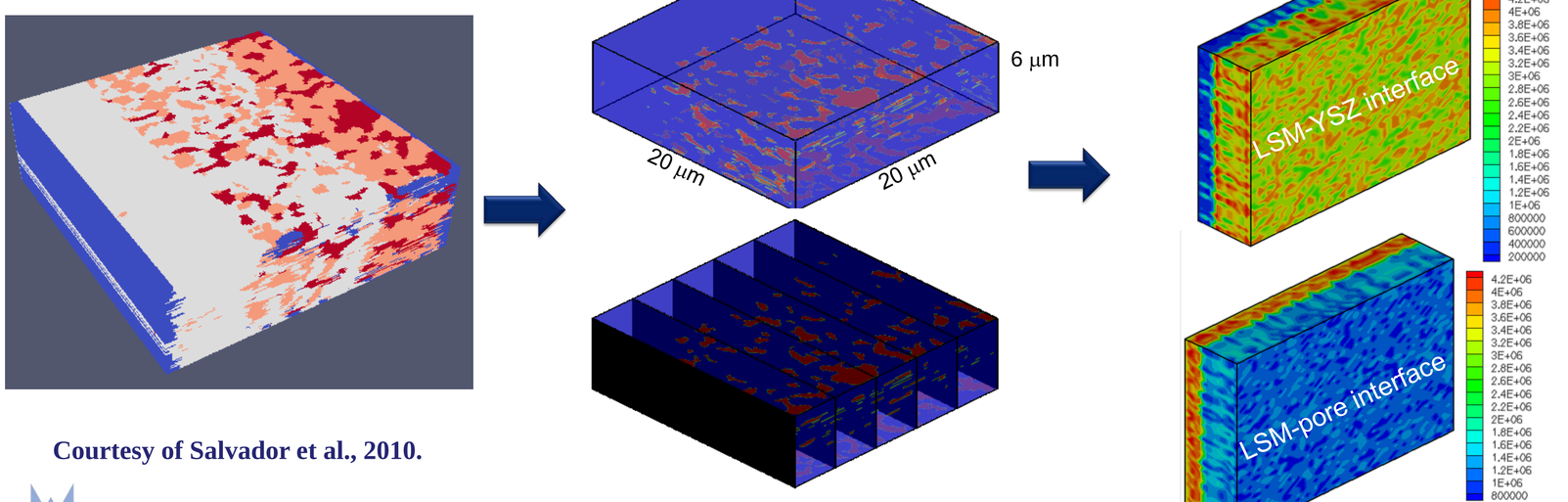
Oxygen concentration (mol/m³) in a cathode area under a current collector/ air channel corner

Conclusions

- A multi-dimensional micro-scale model is developed for SOFC cathodes using multistep reaction mechanism and micro-structure information.
- Microstructure data is obtained from real cathodes using image analysis.
- Model predicts separate contributions from 2PB and 3PB pathways to the total current.
- Model also resolves the effect of microstructure on the local distributions.

Microstructure Properties

Cathode Reconstruction Procedure:



Courtesy of Salvador et al., 2010.

ACKNOWLEDGEMENT

This technical effort was performed in support of the National Energy Technology Laboratory's on-going research in the area of Fundamental Transfer Processes in Solid Oxide Fuel Cells under the RDS contract DE-AC26-04NT41817. The microstructure images are provided by Dr. Paul Salvador's research group.

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