Large Area Planar Cell Simulation Tool (DREAM SOFC-PC)

Jerry H. Mason[1,2], Ismail B. Celik[1,3,5], Hayri Sezer[1,4,5], Mohamed A. S. Zaghloul[6], Mohan Wang[6], Michael Buric[1], Zhaoqiang Peng[6], Paul Ohodnicki[6], Shiwoo Lee[1,2], Thomas Kalapos[1,2], Harry Abernathy[1,2], Kevin Peng Chen[6], Gregory A. Hackett[1]

[1]US Department of Energy, National Energy Technology Laboratory, Morgantown, WV/ Pittsburgh, PA/Albany, OR; [2]Leidos Research Support Team, Morgantown, WV/ Pittsburgh, PA/Albany, OR; [3]West Virginia University, Morgantown, WV; [4]Western Carolina University, Cullowhee, NC; [5]Oak Ridge Associated Universities, Oak Ridge, TN; [6]University of Pittsburgh, Pittsburgh, PA

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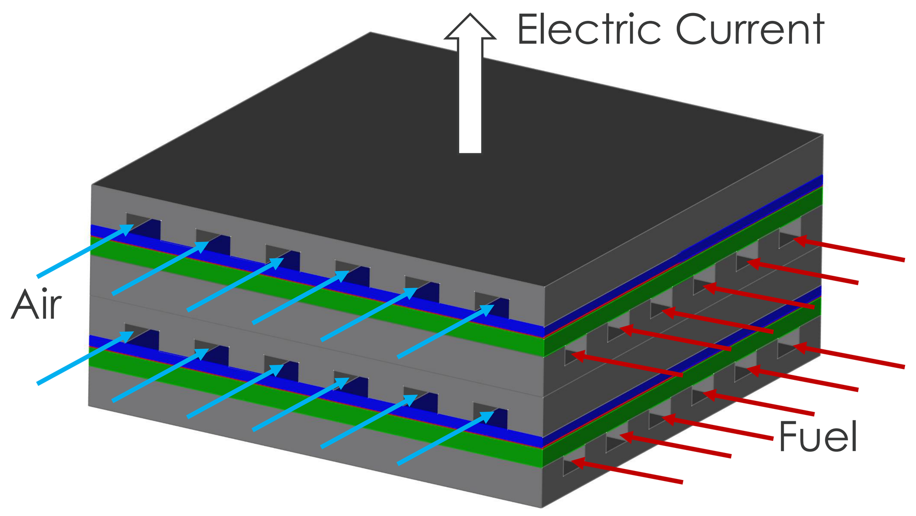
Summary

- In house code, **DREAM SOFC-PC** – applied to simulate performance of large area SOFCs
- Capable of simulating transient cell response, long term degradation and performance metrics of VI and impedance curves using the same simulation tool
- Automatic meshing routine allows for user input of channel and layer dimensions – including cross flow geometry
- Example applications to fuel contaminant degradation and study of the impact of optical fiber temperature sensors are highlighted



Model Equations [1,2]

General Transport equations (3D)

Equations solved via finite volume method throughout the domain using cell-IDs to determine property distributions and source terms

Gas species transport – solve for mass fraction of species j in the pore phase X_p^j:

$$\frac{\partial}{\partial t}\left(\varepsilon_p\rho_p X_p^j\right) = \nabla\cdot\left(\varepsilon_p\Gamma_{p,j}^{eff}\nabla X_p^j\right) + \varepsilon_p\rho_p S_p^j + f_{I_{p,s}}$$

Source term S_p^j includes chemical reactions (i.e. water gas shift, methane reforming) and interface flux $f_{I_{p,s}}$ calculated from Faraday's law.

Heat transfer – solve for enthalpy h, with the assumption that $dh = C_p dT$:

$$\frac{\partial}{\partial t}\left(\rho C_p T\right) + \nabla\cdot(\lambda\nabla T) + \rho S_h$$

Where source term S_h considers heat from Ohmic heating and reactions

Charge transport – derived from Ohm's law

$$\nabla\cdot\vec{I} = \nabla\left(\sigma^{eff}\nabla\varphi\right) = s = \nabla\left[\sigma^{eff}\nabla(E_0 - \eta_{act})\right]$$

Unified potential φ assumed for mixed ionic/electronic conducting phases with source terms applied at electrode/electrolyte interfaces using Butler Volmer:

$$\eta_{act,j} = \frac{RT}{\alpha_j n_j F} ln\left(\frac{i_j}{2i_{0,j}} + \sqrt{\left(\frac{i_j}{2i_{0,j}}\right)^2 + 1}\right)$$

$$i_{0,j} = c_j\left(\frac{Y_{j,int}}{Y_{j,ref}}\right)\exp\left(\frac{E_{j,act}}{RT}\right)$$

Gas channel model (1D)

Gas species transport – 1D Plug flow assumed in the fuel/air channels, reducing to:

$$\frac{\partial}{\partial t}(\rho A X_j) = -\frac{\partial}{\partial z}(A\rho v x_j) + \frac{\partial}{\partial z}\left(A D_{eff}\frac{\partial X_j}{\partial z}\right) - \dot{Q}_j$$

- A is the channel cross section area and $\dot{Q}_\phi$ is the flux across channel walls interfaces
- Using mass transfer coefficient k_j as:

$$\dot{Q}_j = k_j A(X_{j,e} - X_{j,c})$$

- Mass is balanced with by setting $\Gamma_{pj}^{eff} = k_j \Delta y_{int}$ at the interface

Velocity is calculated assume constant pressure:

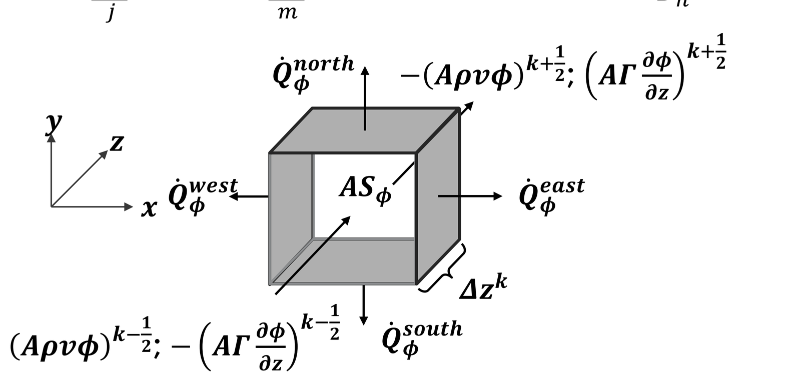
$$v_z = \frac{(\rho v)_{z-\Delta z} + \sum_j Q_j \frac{\Delta z}{\Delta V}}{\rho_z}$$

Heat Transfer – solve for the enthalpy h, with the assumption that $dh = C_p dT$:

$$\frac{\partial}{\partial t}(\rho A C_p T) = -\frac{\partial}{\partial z}(A\rho v C_p T) + \frac{\partial}{\partial z}\left(A\lambda\frac{\partial C_p T}{\partial z}\right) - \dot{Q}_h$$

Flux considers both heat transfer due to mass transport:

$$\dot{Q}_h = \sum_j C_{p,j}\dot{Q}_j T + \sum_m h_m A_m (T - T_m); \quad h_m = \frac{Nu\lambda_m}{D_h}$$



Meshing Routine

Algorithm uses maximum grid expansion ratio (r_{max}) to limit this ratio and iterative process to maintain proper boundaries between cell layers

$r = \frac{\Delta x_1}{\Delta x_{n_x}}$ - ratio between first and last grid size of a layer

↓

$n_x = 2 + \frac{ln(r)}{ln(r_{max})}$ - minimum number of grid points in layer

↓

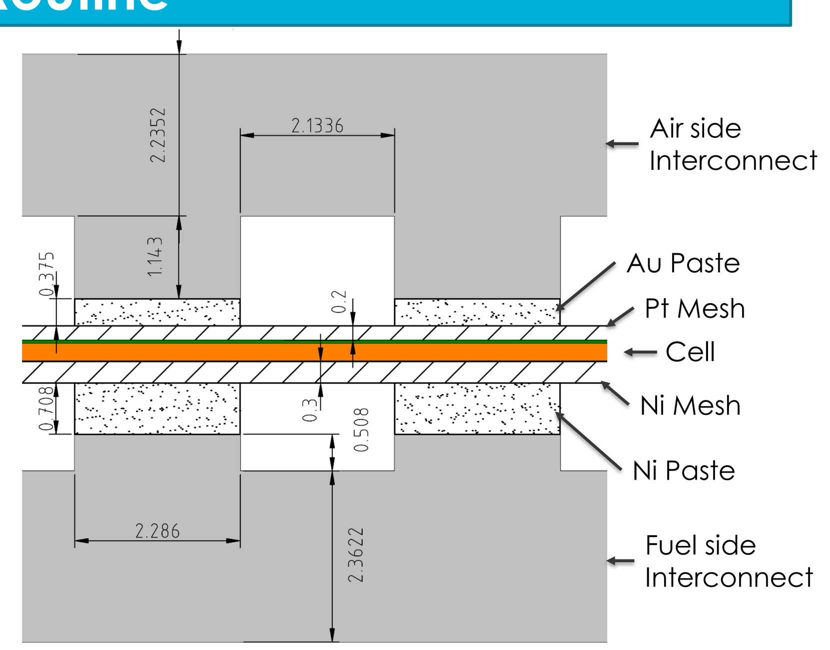
$r_{new} = r^{\frac{1}{n_x - 2}}$ - actual grid expansion ration

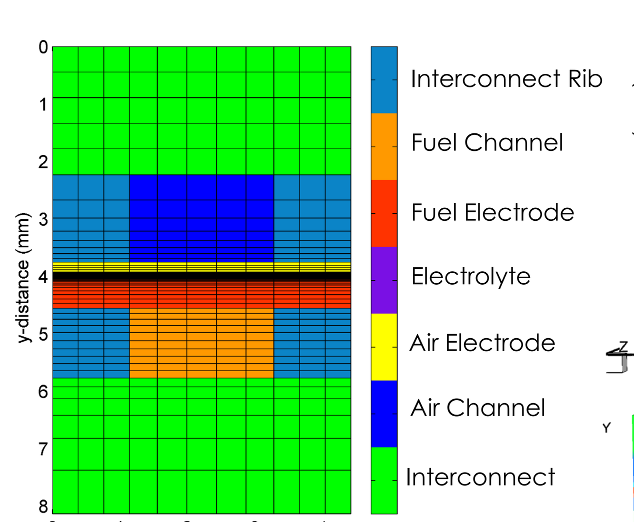
↓

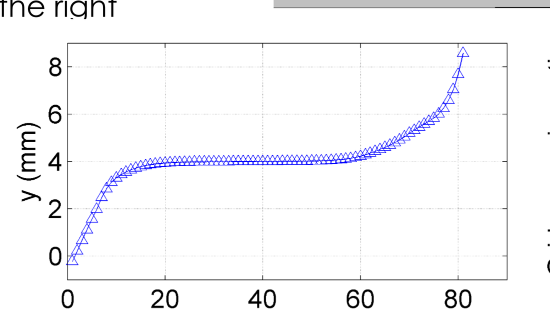
$x^i = x^{i-1} + r_{new}^{i-1} * \Delta x_i$ - produce grid layer ($i = 2$ to n_x)

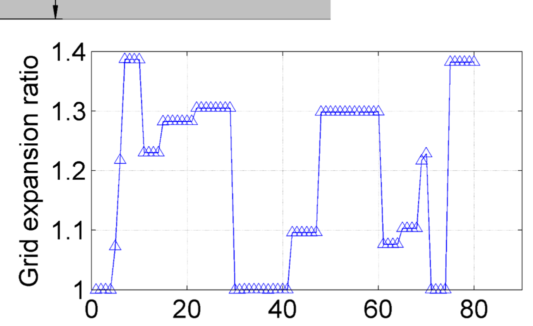
- Repeat for each layer from smallest grid size to largest

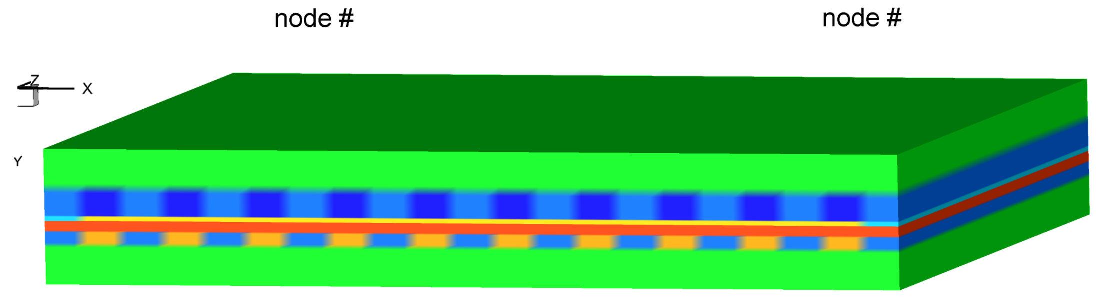
Example: Cell with 250 µm fuel electrode with 10 µm active layer, 40 µm air electrode with 5 µm active layer and 5 µm electrolyte with set up shown to the right





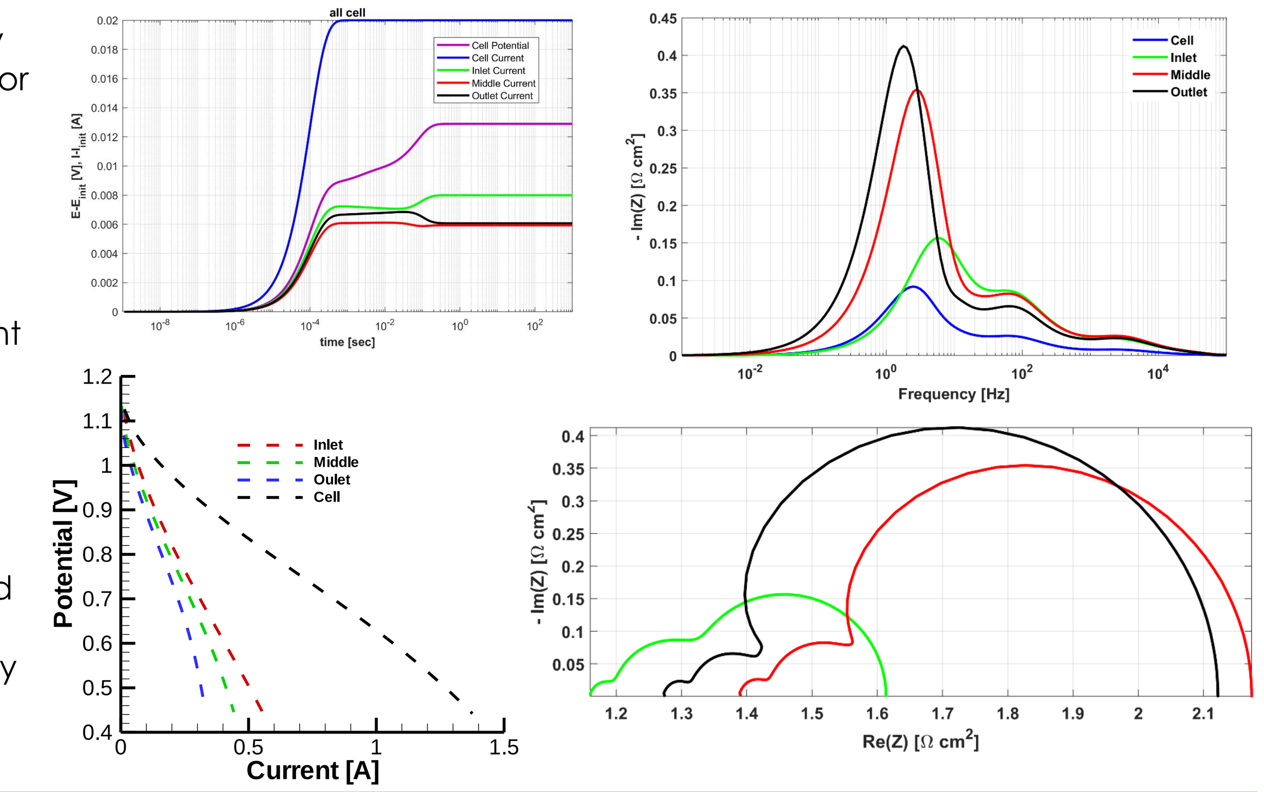






Performance Evaluation Metrics

- **VI Curve** produced by holding either current or potential constant, scanning through applied loads at user input interval
- **Impedance curve** produced using current interruption method (Bessler [3]) applying interpolation in frequency space
- **Location dependent performance** obtained by considering cell sections independently



Application I: Degradation due to fuel contaminants[4][5]

Model assumptions:

- Impurity molecules chemically react to form secondary phases, these secondary phases(contaminant coverage) are assumed to block the active sites of catalytic material.
  - Decreases the reaction rate of the half cell reaction
- Contaminant coverage and secondary phase formation is believed to block pores
  - Decreases the effective diffusion of the fuel
  - Decreases the reaction rates of the half cell reaction

Monolayer adsorption mechanism

$$H_2 + 2Ni \underset{k_{b,H_2}}{\overset{k_{f,H_2}}{\rightleftarrows}} 2(Ni - H)$$

$$X + Ni \underset{k_{b,X}}{\overset{k_{f,X}}{\rightleftarrows}} Ni - X$$

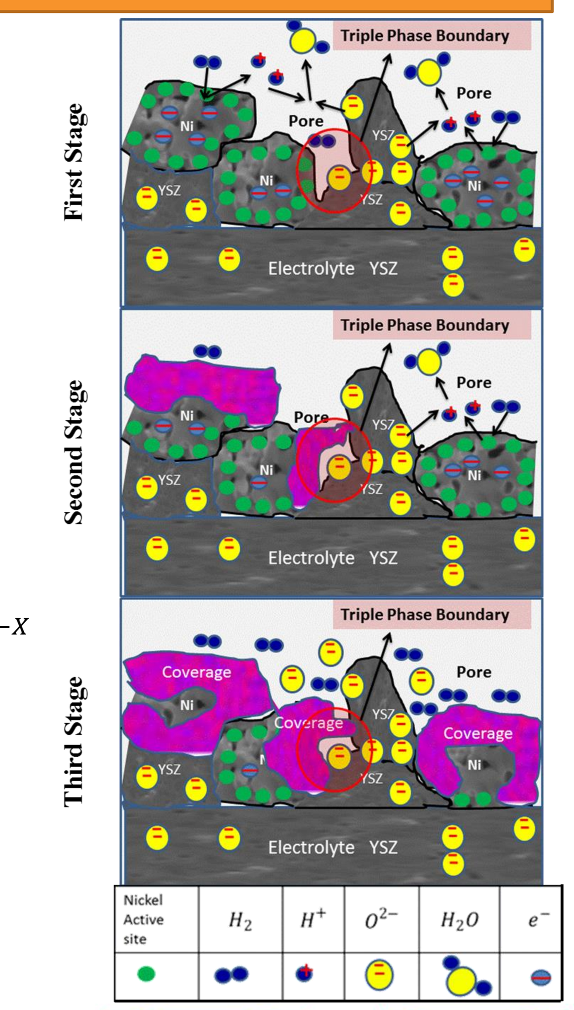
Transport of surface coverage

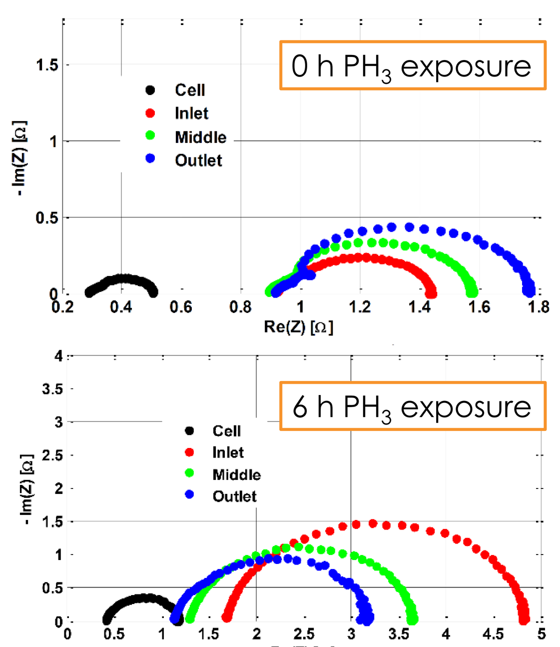
$$\frac{\partial\theta_i}{\partial t} = D_\theta\nabla^2\theta_i + \omega_{\theta_i}$$

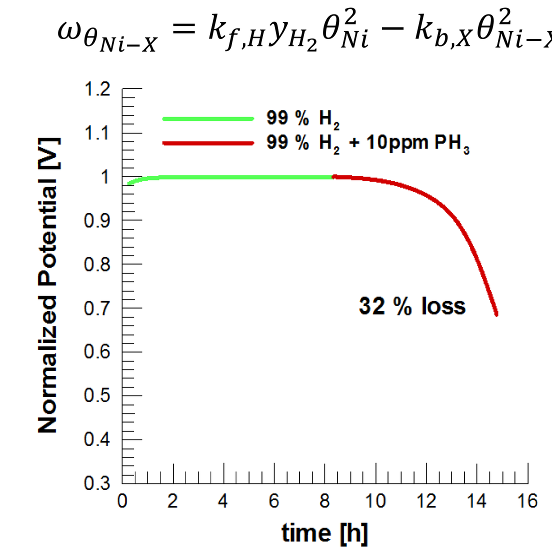
$$\theta_{Ni-X} + \theta_{Ni-H} + \theta_{Ni} = 1$$

$$\omega_{\theta X} = k_{f,X} y_X \theta_{Ni} - k_{b,X}\theta_{Ni-X}$$

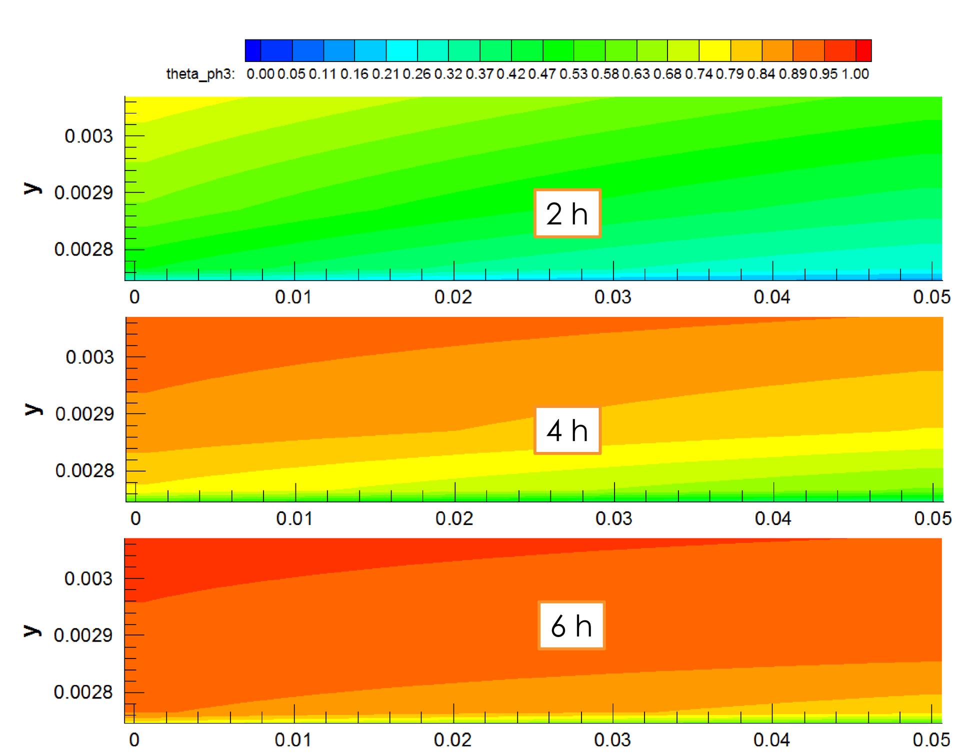
$$\omega_{\theta_{Ni-X}} = k_{f,H} y_{H_2}\theta_{Ni}^2 - k_{b,X}\theta_{Ni-X}^2$$



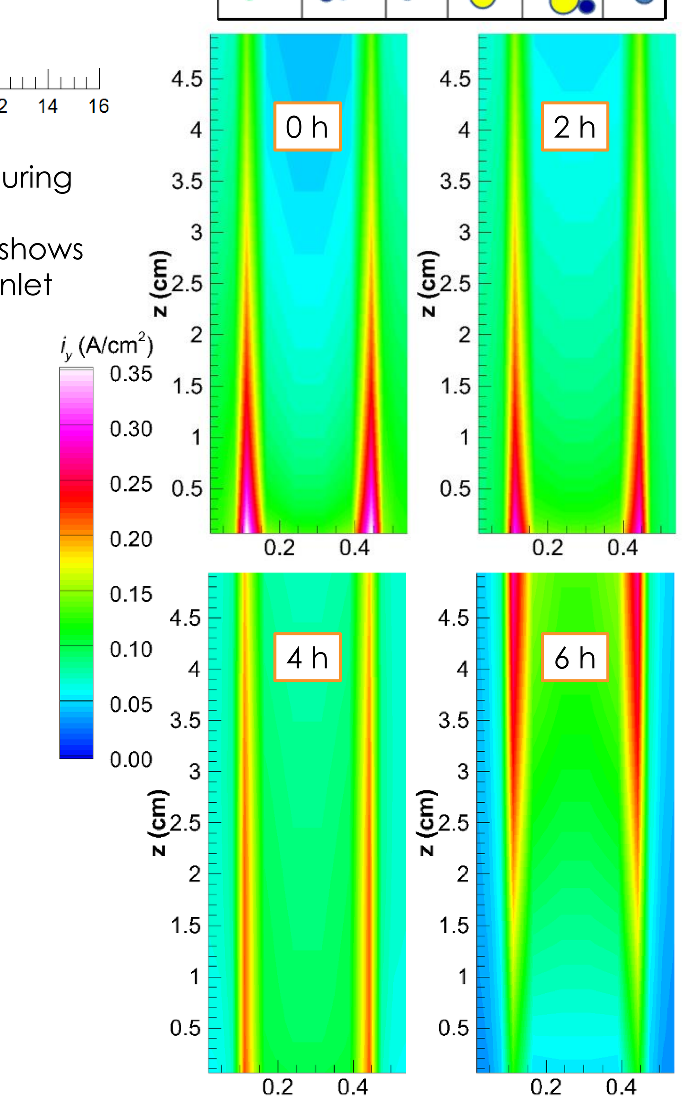




- Cell voltage drops ~32% during phosphine exposure
- Location specific analysis shows degradation worse near inlet



- Contours of phosphine coverage at x/2 (y-z plane) taken at 2, 4 and 6 hours of phosphine exposure
- Anode/electrolyte interface at y = 0, fuel inlet at z = 0
- Coverage most significant near fuel channel/electrode interface near fuel inlet, propagates towards electrolyte/outlet

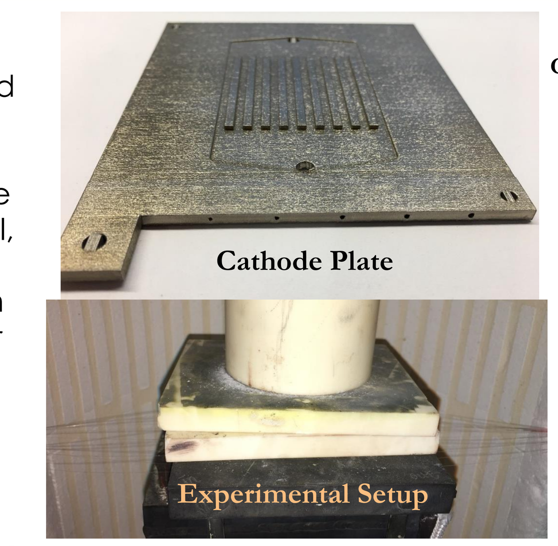


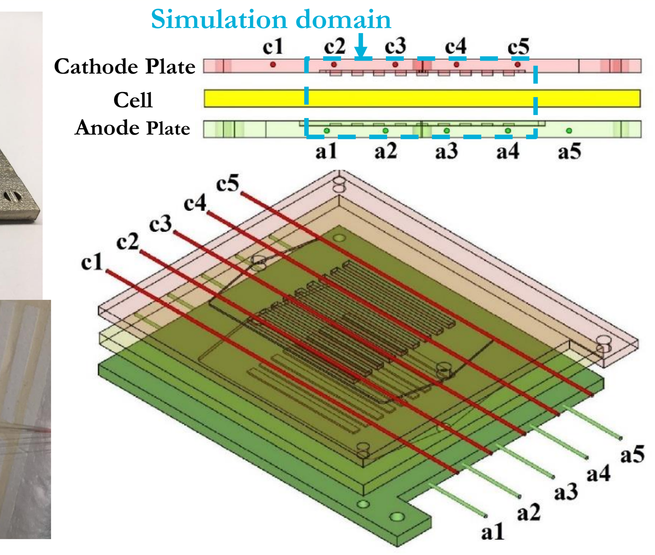
- Contours of current density at anode electrolyte interface shows shift of peak current from inlet to outlet as coverage promulgates

Application II: Optical fiber sensors[6]

Experiment

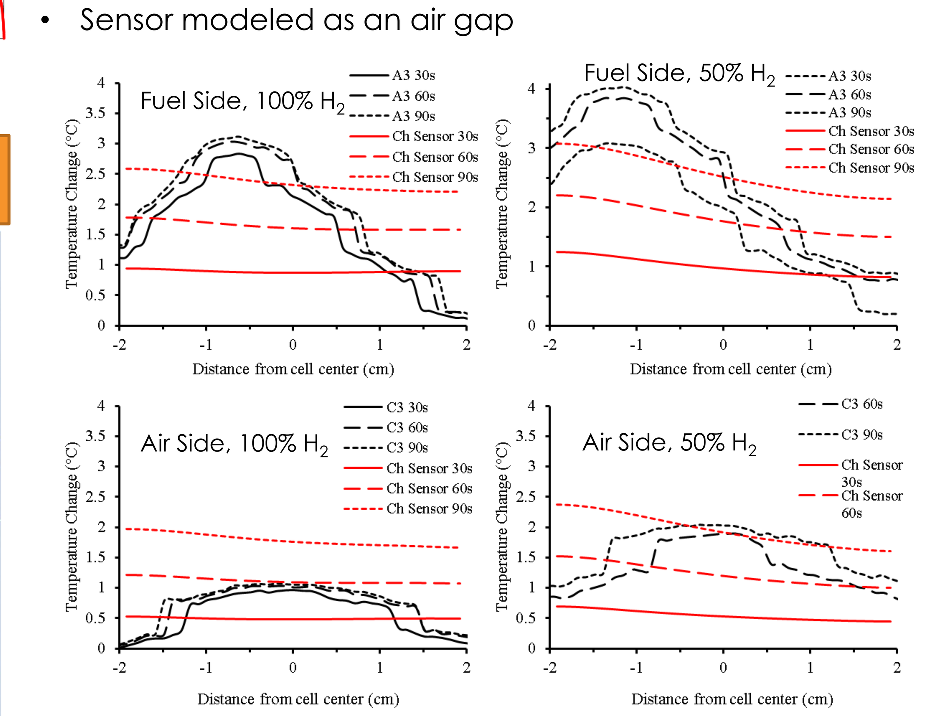
- Current collector plates 3D printed with 750 µm holes for sensors
- Femtosecond laser irradiation to stabilize Rayleigh scattering profile
- Measurements with ~4 mm spatial, ~0.1°C temperature resolution
- Cell operated at 750°C, 100 sccm flow rates for fuel and air, counter flow
- Temperature transients measured during first 90s of applied current, different fuel mixtures compared



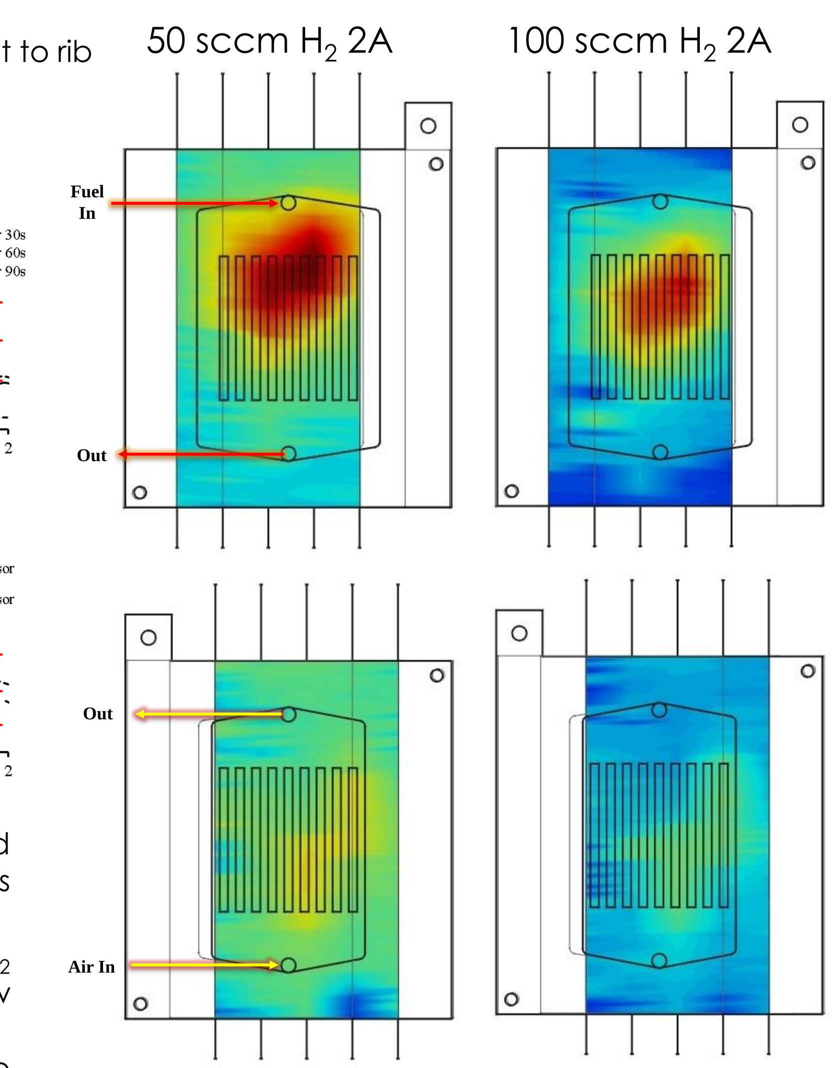


Model

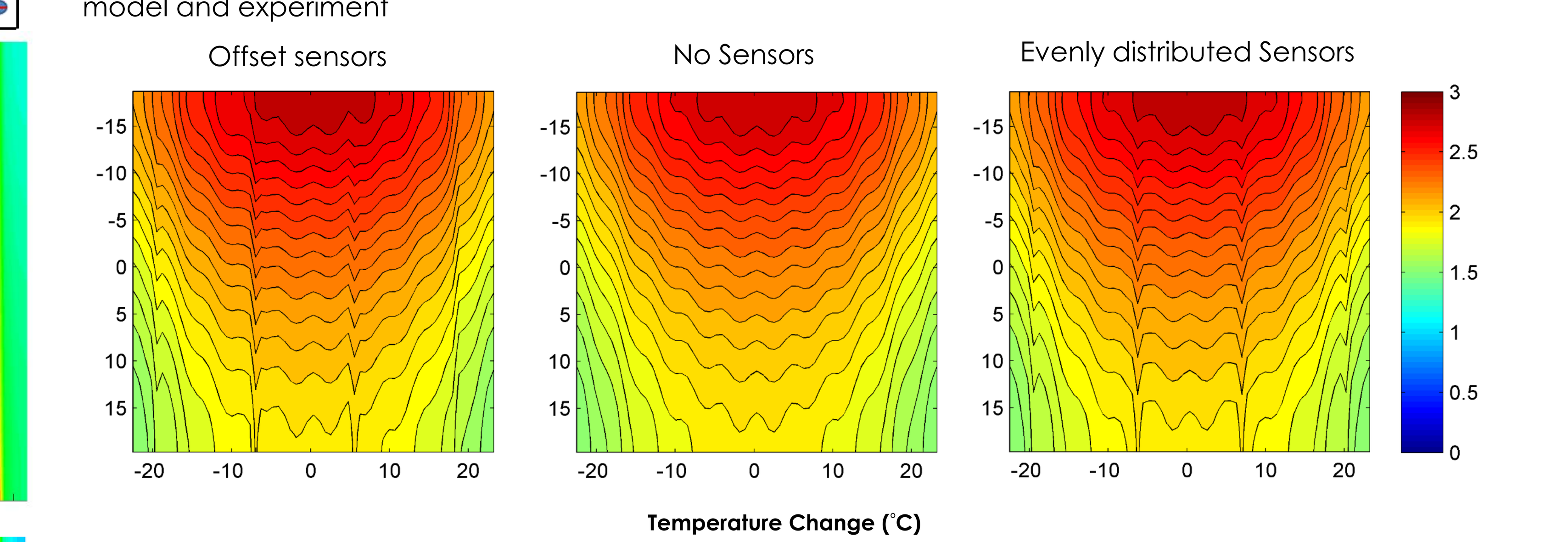
- Single channel simulations with sensors located adjacent to rib and channel as well as full cell simulations performed
- Sensor modeled as an air gap



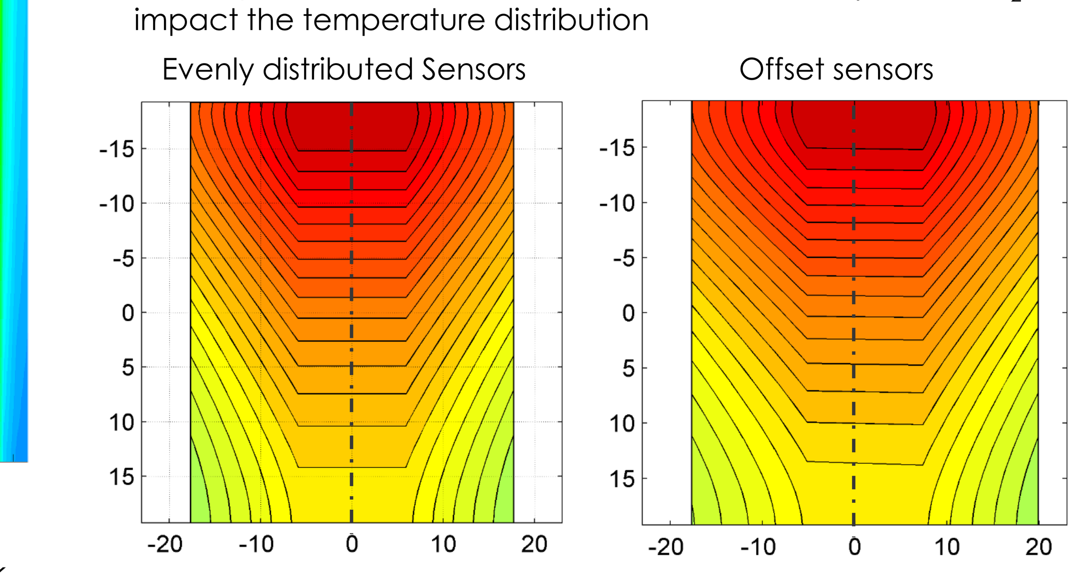
- Temperature distributions plotted from the anode, and cathode sensors a3 and c3, respectively. Model results in red, experiments in black
- The peak on the anode side, appears closer to the H_2 gas inlet and shifts closer to the fuel inlet as the H_2 flow rate is reduced.
- Cathode side temperature ~1°C lower, peak in the center from experiment, toward fuel inlet in the simulations
- Highest peak 50% molar H2 case (~4°C in experiment, ~3°C in simulation)
- Overall, temperature magnitudes similar between model and experiment



- 2D temperature contours constructed for anode (top) and cathode (bottom) from sensor data (90 s data shown here)
- Peak temperature occurs near cell center, fuel inlet, **contour is skewed to one side** consistently



- 2D temperature contours from full cell simulations (50 sccm H_2/50 sccm N_2 case at 90s) show sensors will impact the temperature distribution



- Reconstructed contours from sensor locations show offset sensors will result in artificial asymmetry in measured temperature distribution

Conclusions

- Reasonable agreement between model and experiments on temperature gradient magnitude indicates results are reasonable
- Simulation results show that asymmetric temperature distribution measured experimentally might be due to sensor presence
- Overall, sensors have minor impact on temperature distribution, but should be distributed evenly to reduce bias
- Result comparison can be used to improve model assumptions while also informing future sensor experiments and application techniques

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