Investigation of Micro- and Macro-Scale Transport Processes for Improved Fuel Cell Performance

Department of Energy Annual Merit Review

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This presentation does not contain any proprietary, confidential, or otherwise restricted information

Project ID # FC092
Overview

Timeline
• Project start date: June 2010
• Project end date: May 2013
• Percent complete: 60%

Barriers
• Barriers addressed
  – C. Performance
  – D. Water Transport within the Stack
  – E. System Thermal and Water Management
  – G. Start-up and Shut-down Time and Energy/Transient Operation

Budget
• Total project funding
  – DOE share: $4.391M
  – Cost share: $1.097M
• Funding received in FY11: $0.6M
• Planned Funding for FY12: $1.3M

Partners
• Project lead: General Motors
• Subcontract Partners:
  ▪ Rochester Inst. of Technology
  ▪ Univ. of Tenn. Knoxville
  ▪ Penn State University
• Other collaborations with material suppliers
Connecting Characterization Techniques with a Validated 1+1D Model

**Approach -**

Baseline Validation Data → AC Validation Data → Year 1

Differential Cell and Parametric In Situ Studies → Year 2

1+1D Model Integration and Validation → Sensitivity Studies

Component Focused In-Situ and Ex-Situ Studies → Sensitivity Studies

Multi-Scale Component Model Dev. and Validation

**Outcome, Year 3**

All component, validation data, and MS Excel based 1+1D model published to a publically available database. (www.pemfcdata.org)

All work streams connected by the transport resistance associated with a component of:

\[ E_{cell} = E_{rev} - \eta_{HOR} - |\eta_{ORR}| - i \cdot R_{tx, e^-} - i \cdot R_{tx, Mem.} - i \cdot R_{tx, H^+} - \eta_{tx, O_2 (Ch)} - \eta_{tx, O_2 (GDL)} - \eta_{tx, O_2 (electrode)} \]

Dry Model Starting Point:


Database: www.PEMFCdata.org

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GM

PENNSTATE

RIT

FUEL CELL

1D Model Including Interfacial Transport

Differential Cell Experiments

Component Studies for Model Refinement

Down-the-Channel Validation
Collaboration

- GM Electrochemical Energy Research Lab (prime): Jon Owejan, Jeffrey Gagliardo, Wenbin Gu, Anu Kongkanand, Paul Nicotera
- Penn State University (sub): Michael Hickner, Jack Brenizer
- Rochester Institute of Tech (sub): Satish Kandlikar, Thomas Trabold
- University of Tennessee (sub): Matthew Mench
- University of Rochester (sub): Jacob Jorne’
- DOE Transport Working Group
- National Institute of Standards and Technology (no cost): David Jacobson, Daniel Hussey, Muhammad Arif
- W.L. Gore and Associates, Inc. (material cost): Simon Cleghorn
- Freudenberg (material cost): Christian Quick
- Engineered Fiber Technologies (material cost): Robert Evans
- Queens University (no cost): Kunal Karan
- Carnegie Mellon University (no cost): Shawn Litster
Core Objectives Addressing DOE Expectations

**Topic 4a - Expected Outcomes:**
- Validated transport model including all component physical and chemical properties
  - Down-the-channel pseudo-2D model will be refined and validated with data generated in the project
- Public dissemination of the model and instructions for exercise of the model
  - Project website to include all data, statistics, observation, model code and detailed instructions
- Compilation of the data generated in the course of model development and validation
  - Reduced data used to guide model physics to be published and described on project website
- Identification of rate-limiting steps and recommendations for improvements to the plate-to-plate fuel cell package
  - Model validation with baseline and auto-competitive material sets will provide key performance limiting parameters

**Characterization and validation data**
Employing new and existing characterization techniques to measure transport phenomena and fundamentally understand physics at the micro-scale is the foundation of this project. Additionally, a comprehensive down-the-channel validation data set is being populated to evaluate the integrated transport resistances. This work will consider a baseline and next generation material set.

**Multi-Scale component-level models**
Models that consider bulk and interfacial transport processes are being developed for each transport domain in the fuel cell material sandwich. These models will be validated with a variety of in situ and ex situ characterization techniques. One dimensional transport resistance expressions will be derived from these models. This work will consider a baseline and next generation material set.

**1+1D fuel cell model solved along a straight gas flow path**
Consider if a 1+1D simplified model can predict the saturation state along the channel, performance and the overall water balance for both wet and dry operating conditions within the experimental uncertainty of the comprehensive macro-scale validation data sets. Identify shortcomings of 1D approximations.

**Identify critical parameters for low-cost material development**
Execute combinatorial studies using the validated model to identify optimal material properties and trade-offs for low-cost component development in various operating spaces.
**Baseline Material Set**
- Membrane
  - Gore 18 μm
- Anode catalyst layer
  - target loading 0.05 mg Pt cm⁻²
  - 20% Pt/V made with 950EW ionomer I/C 0.6
- Cathode catalyst layer
  - target loading 0.3 mg Pt cm⁻²
  - 50% Pt/V made with 950EW ionomer I/C 0.95
- Microporous layer
  - 8:1:1 carbon-to-PTFE-to-FEP ratio, 30 μm thick
- Gas diffusion substrate
  - MRC 105 w/ 5% wt. PTFE, 230 μm thick w/MPL
- Flow field
  - 0.7 mm wide by 0.4 mm deep channels with stamped metal plate cross-sectional geometry
  - 18.3 mm channel length
  - 0.5 mm cathode land width
  - 1.5 mm anode land width
  - Exit headers typical to a fuel cell stack

**Auto-Competitive Material Set**
- Membrane
  - Gore 12 μm
- Anode catalyst layer
  - target loading 0.05 mg Pt cm⁻²
  - 20% Pt/V with 950EW ionomer I/C 0.6
- Cathode catalyst layer
  - target loading 0.1 mg Pt cm⁻²
  - 15% Pt/V with 950EW ionomer I/C 0.7
- Microporous layer
  - 8:1:1 carbon-to-PTFE-to-FEP ratio, 30 μm thick
- Gas diffusion substrate
  - Anode – prototype high diffusion res, w/ 5% wt. PTFE, 210 μm thick w/MPL
  - Cathode - MRC 105 w/ 5% wt. PTFE, 230 μm thick w/MPL
- Flow field
  - 0.7 mm wide by 0.3 mm deep channels with stamped metal plate cross-sectional geometry
  - 18.3 mm channel length
  - 0.25 mm cathode land width
  - 0.75 mm anode land width
  - Modified exit headers

**Standard Protocol**
4 x 4 x 3 x 3 Factors

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Inlet RH (An/Ca)</th>
<th>Outlet Pressure (An/Ca)</th>
<th>Current Density</th>
</tr>
</thead>
<tbody>
<tr>
<td>20, 40, 60, 80°C</td>
<td>95/95, 0/95, 95/0, 50/50%</td>
<td>150/150, 100/150, 150/100 kPa</td>
<td>0.1, 0.4, 1.5 A/cm²</td>
</tr>
</tbody>
</table>

H₂/Air Stoichiometric Ratios = 1.5 / 2.0 for all experiments
Technical Accomplishments-

Completion of Baseline Validation Dataset

Distributed Data (Case 110)

Error Bar are 95% Confidence Intervals for the Mean

Membrane Water Permeability

Technical Accomplishments-

The device resistance is determined by varying total pressure for different thicknesses of diffusion medium.

\[ R_{CELL} = R_{CH} + R_{DM} + R_{MEM} \]

\[ R_{DEV} = (1 - x_w)R_{\text{dilute}} = \left(1 - \frac{P_{W}}{p}\right)R_{\text{dilute}} = R_{\text{dilute}} - P_{W}\left(\frac{R_{\text{dilute}}}{p}\right) \]

\[ \text{slope} = \frac{\partial R_{\text{dilute}}}{\partial p} = \frac{\partial R_{\text{DEV}}}{\partial p} \]

\[ \text{intercept} = \frac{R_{\text{dilute}}}{p} \]

\[ \frac{D}{D_{\text{eff}}_{DM}} = 2.11 \quad \frac{R_{\text{dilute}}}{p} = 0.0013 \]

Caulk et al., manuscript in preparation, 2012.
Technical Accomplishments -

Membrane Water Permeability

**Diffusion coefficient**

\[ N_w = -D_{MEM} \frac{\partial C_w}{\partial y} = -\frac{\rho}{E W} D_{MEM} \frac{\partial \lambda}{\partial y} \]

**Relationship to permeability**

\[ D_{MEM} = \rho_s \frac{E W}{\rho} \frac{\partial (RH)}{\partial \lambda} P \]

\[ \lambda = \left[ 1 + 0.2325 R H^2 \left( \frac{T - 303}{30} \right) \right] \left( 14.22 R H^3 - 18.97 R H^2 + 13.41 R H \right) \]

Water uptake formula (Mittlesteadt, 2005)

**Nafion® at 30°C**

- Zawodzinski, et al. (1991)
- Morris and Sun (1993)
- Rivin, et al. (2001)
- Ge, et al. (2005)
- Present Experiment

Present experiment gives higher values of D for RH > 50%

Relative error grows with increasing RH if \( R_{DEV} \) is neglected.

Converting to a diffusion coefficient to compare with literature

3-constant representation

\[ P = a \exp \left[ \frac{E}{R \left( \frac{1}{T} - \frac{1}{T_R} \right)} \right] \exp(bR H) \]

\( a = 3.2 \times 10^{-11} \ \text{mol/m}^2\text{s-Pa} \)

\( E = 22 \ \text{kJ/mol} \)

\( b = 3.4 \)

\( T_R = 363 \text{ K} \)

Caulk et al., manuscript in preparation, 2012.
Technical Accomplishments -
Local Pt Transport Resistance at Low Pt Loading

\[
E_{cell} = E_{rev} - \eta_{HOR} - |\eta_{ORR}| - i \cdot R_{tx,e} - i \cdot R_{tx,Mem.} - i \cdot R_{tx,H^+} - \eta_{tx,O2(DM)} - \eta_{tx,O2(electrode)}
\]

Remaining losses occur at the Pt surface - current is normalized by Pt area to consider remaining losses.

- Local oxygen transport limitation?
- Variable kinetics below 700 mV?
- What impact does electrode structure have?
Evaluating Local Transport Resistance with Limiting Current

\[ E_{\text{cell}} = E_{\text{rev}} - \eta_{\text{HOR}} - |\eta_{\text{ORR}}| - i \cdot R_{\text{tx},e^-} - i \cdot R_{\text{tx,Mem.}} - i \cdot R_{\text{tx,H^+}} - \eta_{\text{tx,O2(DM)}} - \eta_{\text{tx,O2(electrode)}} \]

\[ I_{\text{limiting}} = \frac{C_{O_2,\text{channel}} - C_{O_2,\text{Pt}}}{R_{O_2}} \]

Pt roughness factor = loading × HAD area

\[ R_{O_2}^{\text{total}} = \left( R_{O_2}^{\text{DM,bulk}} + R_{O_2}^{\text{electrode,bulk}} \right) + R_{O_2}^{\text{DM,knudsen}} + R_{O_2}^{\text{electrode,knudsen}} + \frac{R_{\text{electrode,local}}}{\text{Pt roughness factor}} \]

By using the same GDL, electrode carbon type, and catalyst layer thickness, the local Pt resistance term can be considered independently.
Technical Accomplishments-
Local Pt Transport Resistance at Low Pt Loading

\[
R_{O_2}^{total} = \left( \frac{R_{DM, bulk} + R_{electrode, bulk}}{R_{O_2}^{bulk} + R_{electrode, knudsen} + R_{O_2}^{electrode, knudsen}} \right) + \frac{R_{O_2}^{electrode, local}}{Pt \text{ roughness factor}}
\]

Plotting \( R_{O_2}^{total} \left( \frac{1}{Pt \text{ roughness factor}} \right) \) isolates the local resistance. This linear model characterizes the data fairly well, thus indicating this empirical relationship is sufficient for the 1+1D model.

...but what if we change the structure? Will this resistance remain constant?

<table>
<thead>
<tr>
<th>Pt Loading (mg cm(^{-2}))</th>
<th>Catalyst Type; fraction of catalyst type in overall catalyst wt. fraction</th>
<th>Catalyst Type; fraction of catalyst type in overall catalyst wt. fraction</th>
<th>Carbon wt. Fraction</th>
<th>Thickness (µm)</th>
<th>Agglomerate Cross Sectional Area (µm(^2))</th>
<th>Agglomerate Area Fraction ( \alpha_{Pt, agg} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>15% Pt/V; 0.71</td>
<td>30% Pt/V; 0.29</td>
<td>-</td>
<td>10.4 ± 1.8</td>
<td>0.012</td>
<td>0.5</td>
</tr>
<tr>
<td>0.1</td>
<td>50% Pt/V; 0.42</td>
<td>-</td>
<td>0.58</td>
<td>10.9 ± 0.6</td>
<td>0.016</td>
<td>0.19</td>
</tr>
<tr>
<td>0.05</td>
<td>10% Pt/V; 1.0</td>
<td>-</td>
<td>0.78</td>
<td>11.2 ± 1.1</td>
<td>0.012</td>
<td>0.5</td>
</tr>
<tr>
<td>0.05</td>
<td>50% Pt/V; 0.22</td>
<td>-</td>
<td>0.12</td>
<td>13.1 ± 0.8</td>
<td>0.016</td>
<td>0.14</td>
</tr>
<tr>
<td>0.025</td>
<td>5% Pt/V; 1.0</td>
<td>-</td>
<td>0.01</td>
<td>11.0 ± 1.2</td>
<td>0.015</td>
<td>0.5</td>
</tr>
<tr>
<td>0.025</td>
<td>5% Pt/V; 0.34</td>
<td>10% Pt/V; 0.34</td>
<td>0.33</td>
<td>10.8 ± 0.3</td>
<td>0.015</td>
<td>0.30</td>
</tr>
<tr>
<td>0.025</td>
<td>10% Pt/V; 0.51</td>
<td>-</td>
<td>0.49</td>
<td>10.7 ± 0.5</td>
<td>0.012</td>
<td>0.20</td>
</tr>
<tr>
<td>0.025</td>
<td>15% Pt/V; 0.34</td>
<td>-</td>
<td>0.66</td>
<td>10.4 ± 0.4</td>
<td>0.011</td>
<td>0.16</td>
</tr>
<tr>
<td>0.025</td>
<td>30% Pt/V; 0.18</td>
<td>-</td>
<td>0.82</td>
<td>11.3 ± 0.5</td>
<td>0.013</td>
<td>0.13</td>
</tr>
<tr>
<td>0.025</td>
<td>50% Pt/V; 0.11</td>
<td>-</td>
<td>0.89</td>
<td>12.2 ± 0.8</td>
<td>0.016</td>
<td>0.05</td>
</tr>
</tbody>
</table>
Technical Accomplishments -
Impact of Electrode Structure at Low Pt Loading

With catalyst layer loading, thickness, carbon type, and ionomer content held constant it is observed that the density of platinized aggregates significantly impacts performance. This sensitivity increases with drier operating conditions as well.

Refined study of C dilution impact at 0.025 mgPt cm\(^{-2}\)

No dilution impact observed in pure oxygen. (see supplemental slides)
Impact of Electrode Structure at Low Pt Loading

Technical Accomplishments—

Local transport resistance is significantly impacted by the number of Pt agglomerates. Need a geometric scaling factor to account for increased flux through ionomer.

\[ \alpha_{pt,\ agg} + \alpha_{C,\ agg} + \phi = 1 \]

\( \phi = \text{Electrode Porosity} \)

(see table in slide 13)

With geometric correction:

\[ R_{O_2}^{electrode,\ local} = 4.4 \text{ s/cm for all data} \]

Image analysis of FESEM

All types—diluted and non-diluted
Thickness-dependent properties have been resolved using a photoacid dye. The proton dissociation is suppressed in thinner films indicating less bulk water in thin films. This change in water motion is likely related to higher activation energy and lower conductivity in thin films as well as oxygen diffusion.

Ratio of deprotonated (435 nm) to protonated (512 nm) peak of pyranine dye (HPTS) in PFSA film shows proton transfer dynamics were suppressed in thinner films. Provides fundamental information on water confinement and transport properties.
Technical Accomplishments - Potential Dependent Pt Oxide Coverage

Repeated at: $P_{O_2} = 204, 104, 64, 33, 15 \text{ kPa}$

$\theta = \frac{\text{oxide area}}{\text{HAD area}}$

$\theta = \frac{1}{[1 + e^{a(b - E)}]}$

N. P. Subramanian et al., JECS, 159 (2012)
Technical Accomplishments -

Oxide Dependent Kinetics for Low Pt Loading

- Negligible bulk transport overpotential (<= 5mV): Pure O₂, 100%RH, low i (<= 0.4 A/cm²geo)
- Operation at low potential: Vary $P_\text{O}_2$ via operation in vacuum!!

5-cm², differential cell, Pt/C, 80C, 50%Pt/V

Simple Tafel Kinetics

\[
\frac{1}{\text{Tafel Slope}} = \left( \frac{\partial \log i}{\partial E_{\text{IR-free(RHE)}}} \right)_{P_\text{O}_2,T} = \frac{aF}{2.303RT} \left( \frac{1}{1-\theta} + \frac{\omega}{RT} \right) \left( \frac{\partial \theta}{\partial E_{\text{IR-free(RHE)}}} \right)
\]

Cathode Loading ~ 0.4 mgPt/cm²geo

\[i = i_0 \left( \frac{P_{\text{O}_2}}{P_{\text{O}_2,\text{ref}}} \right)^\gamma \exp \left( -\frac{\alpha F \eta}{RT} \right)\]

\[\alpha = 1, \gamma = 0.58, i_0 = 2.1e-8 \text{ A/cm}^2_{\text{Pt}}\]

Coverage-dependent ORR

\[i = i_0 \left( \frac{P_{\text{O}_2}}{P_{\text{O}_2,\text{ref}}} \right)^\gamma (1-\theta) \exp \left( -\frac{\alpha F \eta}{RT} \right) \exp \left( -\frac{\omega \theta}{RT} \right)\]

\[\alpha = 0.5, \gamma = 0.7, \omega = 3.0 \text{ kJ}, i_0 = 3e-5 \text{ A/cm}^2_{\text{Pt}}\]

Symbols: Data
Dashed Line: Data Trend
Solid Line: Model

Coverage-dependent kinetic model provides a good fit of the experimental data in the range ~0.9-0.72 V. Relationship is extrapolated to 140 mV/dec at $\theta = 0$.

N. P. Subramanian et al., JECS, 159 (2012).
Transport resistance in the GDL increases proportionally with saturation. For the 1+1D model a linear approximation of the transition region is used. Through-plane neutron radiography is used to determine max saturation and slope.
Technical Accomplishments-

GDL Thermal Conductivity Dependence on Saturation

At RH > 100%, GDL thermal conductivity impacts saturation level at higher operating temperatures as condensation increases with lower average GDL temperature. Additionally, the GDL thermal conductivity increases with saturation...

Without considering the water saturation effect, the catalyst layer temperature would be over-predicted, resulting in lower than realistic GDL water saturation and mass transport loss.
Liquid water in the anode subsystem has a negative impact on efficiency and cold start performance. This material change significantly shifts the water balance toward the cathode without changing performance. Additionally, the “AC GDL” consists of lower cost precursor materials combined with a lower carbonization temperature. This material has an estimated cost reduction of 40% in comparison with typical GDL materials.
Currently the overall dP (from validation data) is an input parameter, however the active area pressure is corrected based on a two-phase relationship of the flow field outlet. Next, two-phase channel dP and liquid water slug stagnation relationships will be added.
Technical Accomplishments and Progress - Current Status of Wet 1+1D Model Prediction

Model Comparison for 1.5 A/cm² Test Cases, Baseline Material Set

- Cell Potential
- Cell Water Balance
- Dry Model Potential
- Wet Model Potential
- Dry Model Water Balance
- Wet Model Water Balance

Error Bars are 95% Confidence Intervals for the Mean

80°C; 100% RH; 170 kPa

Wet model is still in development, relationships to be added in 2012:
- Channel transport resistance (currently using 2-phase dP with single phase mass transfer coef. and no interfacial resistance).
- Interfacial resistance due to slug coverage.

Distributed Data (Case 110)

See back-up slides for HFR
Summary

• Baseline validation data set is complete with 95% confidence intervals
  — 95% confidence intervals for the mean established for performance metrics by 3 separate experimental runs of the project standard protocol.
• Several 1-D relationship have been established and integrated to the 1+1D model
  — New steady membrane permeability relationship with RH establishes a higher water flux at high RH.
  — Pressure independent local transport resistance is shown to scale with platinized agglomerate surface area, further isolating oxygen diffusivity as root cause of increased resistance near the Pt surface.
  — Oxide coverage-dependent kinetic relationship improves overpotential prediction at less than 750 mV.
  — GDL transport resistance transition from dry to wet is refined with a critical saturation value and thermal conductivity as a function of saturation.
  — Dry entrance and two-phase exit relationships isolate active area pressure drop.
• Down-the-channel 1+1D model improved with new relationships integrated
  — Performance and water balance prediction improved based on a comparison to baseline validation data.
• Database updated
  — Visit www.PEMFCdata.org (development will continue throughout the project).

Future Work

• Complete auto-competitive down-the-channel validation
  — Provide a second validation dataset with key parametric variations the exercise the model.
• Continue component characterization
  — Continue on-going work of directly measure oxygen diffusivity in thin ionomer films.
  — Complete round-robin comparison of water uptake in thin films (GM, PSU, Queens).
  — Complete validation of ex situ oxygen diffusion resistance f(saturation) measurements.
  — Execute a design of experiments study to optimize the auto-competitive GDL.
  — Apply all characterization techniques to the auto-competitive material set.
  — Use characterization techniques to study sensitivity parametric variations (particularly ones that are not included in the model).
• Finalize wet 1+1D model
  — Add two-phase channel pressure drop, mass transfer coefficient, and GDL surface coverage.
  — Currently liquid water in the GDL is assumed to be evenly distributed through-plane. This approximation will be improved by predicting the location of the saturation front.
  — Currently liquid water in the catalyst layer imposes no additional transport resistance. We intend to implement a capillary tube relationship with a film-to-slug transition in the electrode pores.
• Continue development of component models
  — Multi-scale component models are being developed to fundamentally describe the measured transport resistances in the 1+1D model.
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- Susan Reid
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- Michael Manahan

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- Yiuxu Liu
Current Status of Wet 1+1D Model Prediction

Model Comparison for 1.5 A/cm² Test Cases, Baseline Material Set

- Cell HFR
- Dry Model HFR
- Wet Model HFR

- 150/150 kPa
- 150/100 kPa
- 100/150 kPa

- 100/100 %RH
- 50/50 %RH
- 100/0 %RH
- 0/100 %RH

- 20°C
- 40°C
- 60°C
- 80°C

HFR (Ohms-cm²)

Case 30  Case 36  Case 42  Case 48  Case 54  Case 60  Case 66  Case 72  Case 78  Case 84  Case 93  Case 99  Case 105  Case 111  Case 117  Case 129  Case 138  Case 144

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Electrode Dilution Study – Impact of Operating Conditions

100% O₂; 100% RH; 80°C; 150 kPa

50% O₂; 100% RH; 80°C; 150 kPa

80°C; 100% RH; 170 kPa (Wet)

93.5°C; 65% RH; 250 kPa (Dry)
Capillary flow versus saturation relationships have been developed for baseline materials. Using method of standard porosimetry*

Fitting equations can be used directly in model.

Much more data are available, including pore size distribution, interfacial effects, and composite material relationships.

Work is now being summarized in journal submission and for online project website.

Ex-Situ Characterization of Two-Phase Flow Resistance

Channel Transport Resistance
- Channel ΔP & GDL Coverage
  - Uniform water introduction along flow length
  - Transparent flow field
  - Video processing for water quantification

GDL Coverage Quantification Method
- Video Processing Algorithm for GDL coverage

GDL Coverage represents inactive GDL surface area fraction due to water saturation

Flow field Geometry Investigation

Simulating O₂ Diffusion Resistance
- Diffusion resistance $\propto$ boundary layer thickness
  - Boundary layer thickness is numerically obtained using experimental channel water saturation
  - Sherwood number expressed in terms of channel water saturation
Summary of 1+1D Model Updates

Potential-dependent ORR kinetics

\[ i = i_0 \left( \frac{P_{O_2}}{P_{O_2,ref}} \right)^\gamma (1 - \theta) \exp \left( -\frac{\alpha F \eta}{RT} \right) \exp \left( -\frac{\omega \theta}{RT} \right) \]

\( \theta \) - PtOH coverage - strong function of potential

Local oxygen transport resistance

\[ R_{O_2,local}^e = \frac{\delta_{equiv}}{K_{O_2}RT} \]

\[ \frac{i}{4F} = \frac{P_{O_2,cathode}^e - P_{O_2,cathode}^\theta}{RT} \left( \frac{\delta}{K_{O_2}RT} + \frac{R_{O_2,local}^e}{L_{Pt}A_{Pt}} \right) \]

\( K_{O_2} \) - oxygen permeability in bulk ionomer as a function of T and RH
\( \delta_{equiv} \) - equivalent ionomer film thickness accounting for the measured local oxygen transport resistance at reference temperature and RH

Channel pressure drop

\[ \Delta P_{AA} = \Delta P_{Input} - \Delta P_{dry,ER} - \Delta P_{(s), OR} \]

Currently use \( \Delta P_{AA} \approx \Delta P_{Input} \)
Next step: incorporate measured \( \Delta P_{dry,ER} \) and \( \Delta P_{(s), OR} \)

Water saturation dependent DM thermal conductivity

\[ T_{CL} = T_{CH} + (z_H \Delta H) \frac{\delta_{DM}}{k_{DM,s=0} \exp (0.97s)} \]

Without considering the water saturation effect, catalyst layer T would be over-predicted, resulting in lower than realistic DM water saturation and mass transport loss.

Average RH based Membrane Permeability

\[ P = a \exp \left[ \frac{E}{R} \left( \frac{1}{T} - \frac{1}{T_R} \right) \right] \exp (bRH) \]

\( a = 3.2 \times 10^{-11} \text{ mol m}^{-1} \text{ Pa}^{-1} \text{ s}^{-1}, \quad E = 22 \text{ kJ mol}^{-1}, \quad b = 3.4, \quad T_R = 363 \text{ K} \)