A computational analysis on the performance of a PEM fuel cell with short-side-chain membrane

Wonseok Yang, Dowon Cha, Sungho Yun, Wonhee Cho, and Yongchan Kim

HVAC & Two-phase Flow Laboratory
Department of Mechanical Engineering, Korea University
• PEM fuel cell

• Basic reaction

- **Anode**: \( \text{H}_2 \rightarrow 2\text{H}^+ + 2e^- \)
- **Cathode**: \( \frac{1}{2} \text{O}_2 + 2\text{H}^+ + 2e^- \rightarrow \text{H}_2\text{O} \)

• Advantages of Fuel cell

- High efficiency
- Zero emissions
- Variety of sizes
Short-side-chain PFSA membrane
(e.g. Dow membrane, Hyflon, Aquivion)

INTRODUCTION

- Better proton conductivity
- Higher crystallinity
- Higher glass transition temperature
- Less chance to be exposed to degradation mechanism
Limited research for SSC membrane

**Experimental study**


**Numerical study**

...?
Computational domain of a unit proton exchange membrane fuel cell.

Geometric configuration of the flow field.
§ Governing equation – conservation equation

- **Mass**
  \[
  \frac{\partial}{\partial x_j} (\rho u_j) = S_m
  \]

- **Momentum**
  \[
  \frac{1}{\varepsilon^2} \frac{\partial}{\partial x_j} (\rho u_j u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \mu \frac{\partial u_i}{\partial x_j} \right) + S_u
  \]

- **Species**
  \[
  \frac{\partial}{\partial x_j} (\rho u_j Y_i) = \frac{\partial}{\partial x_j} \left( \rho D_{eff,i} \frac{\partial Y_i}{\partial x_j} \right) + S_k
  \]

- **Energy**
  \[
  \frac{\partial}{\partial x_j} (\rho u_j h) = \frac{\partial}{\partial x_j} \left( k_{eff} \frac{\partial T}{\partial x_j} - \sum_i h_i J_i \right) + u_j \frac{\partial p}{\partial x_i} + S_h
  \]

- **Charge**
  \[
  \frac{\partial}{\partial x_j} \left( \kappa_s \frac{\partial \phi_s}{\partial x_j} \right) + S_{\phi,s} = 0
  \]

  \[
  \frac{\partial}{\partial x_j} \left( \kappa_m \frac{\partial \phi_m}{\partial x_j} \right) + S_{\phi,m} = 0
  \]
### Governing equation – electrochemistry equation

- **Volumetric transfer current**

\[
    j_a = i_a^{ref} A \left( \frac{c_{H_2}}{c_{H_2}^{ref}} \right) \left[ \exp \left( \frac{\alpha_a F \eta_a}{RT} \right) - \exp \left( - \frac{\alpha_c F \eta_a}{RT} \right) \right]
\]

\[
    j_c = i_c^{ref} A \left( \frac{c_{O_2}}{c_{O_2}^{ref}} \right) \left[ \exp \left( \frac{\alpha_a F \eta_c}{RT} \right) - \exp \left( - \frac{\alpha_c F \eta_c}{RT} \right) \right]
\]

- **Reference exchange current density**

\[
    i_a^{ref} = i_{0,a}^{ref} \exp \left[ - \frac{E_{A,a}}{R} \left( \frac{1}{T} - \frac{1}{353.15} \right) \right]
\]

\[
    i_c^{ref} = i_{0,c}^{ref} \exp \left[ - \frac{E_{A,c}}{R} \left( \frac{1}{T} - \frac{1}{353.15} \right) \right]
\]

- **Activation overpotential**

\[
    \eta_a = \phi_s - \phi_m
\]

\[
    \eta_c = \phi_s - \phi_m - V_{oc}
\]
## Geometrical configurations

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Active area (mm$^2$)</td>
<td>2 x 240</td>
</tr>
<tr>
<td>Height of channel (mm)</td>
<td>0.80</td>
</tr>
<tr>
<td>Width of channel (mm)</td>
<td>1.00</td>
</tr>
<tr>
<td>Land width (mm)</td>
<td>0.50</td>
</tr>
<tr>
<td>Thickness of membrane (mm)</td>
<td>0.05</td>
</tr>
<tr>
<td>Thickness of catalyst layer (mm)</td>
<td>0.01</td>
</tr>
<tr>
<td>Thickness of gas diffusion layer (mm)</td>
<td>0.30</td>
</tr>
<tr>
<td>Thickness of collector (mm)</td>
<td>1.80</td>
</tr>
</tbody>
</table>
### Transport properties

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Membrane</th>
<th>Catalyst layer</th>
<th>GDL</th>
<th>Collector</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal conductivity (W/m·K)</td>
<td>0.95</td>
<td>1.5</td>
<td>1.2</td>
<td>150</td>
</tr>
<tr>
<td>Electrical conductivity (S/m)</td>
<td>-</td>
<td>300</td>
<td>500</td>
<td>20,000</td>
</tr>
<tr>
<td>Porosity</td>
<td>-</td>
<td>0.28</td>
<td>0.6</td>
<td>-</td>
</tr>
</tbody>
</table>

### Electrochemical properties

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Anode</th>
<th>Cathode</th>
</tr>
</thead>
<tbody>
<tr>
<td>Activation energy(E_{A,a}) (J/mol)</td>
<td>12000</td>
<td>66000</td>
</tr>
<tr>
<td>Reference exchange current density at reference temperature(i_{0,a}^{\text{ref}}) (A/cm²)</td>
<td>0.500</td>
<td>0.1e-04</td>
</tr>
<tr>
<td>Reference concentration (kmol/m³)</td>
<td>5.64e-02</td>
<td>3.39e-03</td>
</tr>
<tr>
<td>Transfer coefficient</td>
<td>0.5</td>
<td>1.0</td>
</tr>
<tr>
<td>Open circuit voltage (V)</td>
<td>1.0</td>
<td></td>
</tr>
</tbody>
</table>
Water content

\[
\lambda = 0.043 + 17.18a - 39.85a^2 + 36a^3; \quad 0 < a \leq 1
\]

\[
\lambda = 14 + 1.4(a - 1); \quad 1 < a
\]

Water sorption for Aquion 850, Nafion 1100 and Nafion 1000 as functions of water activity
(ref. “Mechanical Properties of Perfluoro Sulfonated Acids: The Role of Temperature and Solute Activity”)
Proton conductivity of Dow 858 and Dow 1084 as a function of water uptake and temperature
(ref. “Short-side-chain proton conducting perfluorosulfonic acid ionomers: Why they perform better in PEM fuel cells”)

\[
\sigma_T = \exp \left[ 1059.5 \left( \frac{1}{303} - \frac{1}{T} \right) \right]
\]

\[
\sigma = (-8.48 + 2.31\lambda - 0.084204\lambda^2 + 0.0010423\lambda^3)\sigma_T ; \ 5 \leq \lambda
\]

\[
\sigma = (0.219\lambda)\sigma_T ; \ 0 < \lambda < 5
\]
**MODEL VALIDATION**

- **Validation at 75°C**
  - Error range: ~3.5%

- **Validation at 90°C**
  - Error range: ~3.4%

- **Membrane**: Aquivion® E87-05S
## OPERATING CONDITION

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Operating pressure (atm)</td>
<td>2.0 (absolute)</td>
</tr>
<tr>
<td>Inlet flow rate (kg/s)</td>
<td></td>
</tr>
<tr>
<td>$H_2$</td>
<td>$1.66 \times 10^{-7}$</td>
</tr>
<tr>
<td>St 1.5 under 2 A/cm$^2$</td>
<td></td>
</tr>
<tr>
<td>Air</td>
<td>$5.67 \times 10^{-7}$</td>
</tr>
<tr>
<td>St 2.5 under 2 A/cm$^2$</td>
<td></td>
</tr>
<tr>
<td>Operating temperature (°C)</td>
<td>45 / 60 / 75 / 90</td>
</tr>
<tr>
<td>Inlet relative humidity (%)</td>
<td>25 / 50 / 75 / 100</td>
</tr>
<tr>
<td>Membrane equivalent weight (g/eq)</td>
<td>870</td>
</tr>
</tbody>
</table>

- **Simulation tool**
  - ANSYS Fluent release 17.0
RESULT & DISCUSSION

- Performance with temperature variation (RH100%)
  - Polarization curve
  - Power density curve

- Performance increased with temperature
- Large concentration polarization loses at 90°C
RESULT & DISCUSSION

- Effect of $O_2$ concentration
  - Contours for $O_2$ concentration at the cathode channel/GDL interface

✓ Lower $O_2$ concentration at 90°C $\rightarrow$ concentration polarization loss
RESULT & DISCUSSION

- **Effect of H$_2$O concentration**
  - Contours for H$_2$O concentration at the cathode channel/GDL interface

  ![Contour Plot](image)

  - 75°C 2.0 A/cm$^2$
  - 90°C 1.95 A/cm$^2$

  ✓ Higher H$_2$O concentration at 90°C → water flooding
RESULT & DISCUSSION

- Performance with relative humidity variation (90°C)
  - Polarization curve
  - Power density curve

- Performance increased with relative humidity
- Large differences between 75% and 50%
RESULT & DISCUSSION

- Effect of water content
  - Contours for water content in the middle plane of the membrane (0.8 A/cm²)

✓ Higher water content at 75RH \(\rightarrow\) higher proton conductivity
RESULT & DISCUSSION

- Effect of proton conductivity
  - Contours for proton conductivity in the middle plane of the membrane (0.8A/cm²)

✓ Higher proton conductivity at 75RH → better performance
RESULT & DISCUSSION

- Effect of temperature in humidity control
  - Performance with RH variation at 0.8 A/cm²
  - Activity and conductivity change at 30% RH

- Higher performance with decrease of temperature at low RH
- Decrease of water activity and conductivity with increase of Temperature in low RH condition
- Increased effect of relative humidity with increase of temperature
CONCLUSION

- Effect of temperature increase on the cell performance
  - Increase of exchange current density and Improved mass transport properties
  - Very high temperature results in concentration polarization loss

- Effect of relative humidity increase on the cell performance at high temperature
  - Increase of membrane water content and proton conductivity
  - Large deference between 50% and 75% due to membrane property

- Optimal relative humidity exists in each operating temperature
Thank you