Seeking minimum entropy production for flow-field patterns and geometries in fuel cells

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30.08.2019
Summary

• Aim:
  – Optimize tree-shaped flow field pattern for PEMFCs by minimizing the entropy production (EP).
  – Find design criteria

• Method:
  – 1D calculations using analytic pressure drop and EP in MATLAB
  – 3D simulations with OpenFoam’s simpleFoam solver

• Results:
  – Larger width scaling parameters than the one from Murray’s Law give lower entropy production
  – Channel width has the biggest influence on entropy production
  – Peclet number analysis gives range of current densities to use
PEM fuel cell

• PEM = Proton exchange membrane or polymer electrolyte membrane
• Core element: ion exchange membrane (mostly Nafion)
• Fuel: H₂ & O₂
• Exhaust: H₂O + excess gases

Anode: \[ \text{H}_2(g) \rightarrow 2\text{H}^+(aq) + 2e^- \]
Cathode: \[ \frac{1}{2}\text{O}_2(g) + 2\text{H}^+(aq) + 2e^- \rightarrow \text{H}_2\text{O}(l) \]
Overall: \[ \text{H}_2(g) + \frac{1}{2}\text{O}_2(g) + t_w \text{H}_2\text{O} (l) \rightarrow (t_w+1) \text{H}_2\text{O}(l) \]
• 1 – Current collector
• 2 – Flow field plate
• 3 – Gas diffusion layer (GDL)
• 4 – Anode
• 5 – Membrane
• 6 – Cathode
Introduction

• Tree-shaped patterns proven to increase performance of PEMFCs compared to serpentine patterns [1]
• Uniform outlet flow rate to achieve uniform fuel distribution
• Murray’s Law for scaling should deliver minimum EP [2]
• One of the goal is to have Pe<1 at the outlet

Questions

• Questions:
  – Is Murray’s law the most efficient scaling for FCs?
  – How does the width influence the entropy production?
  – How can you estimate the exact pressure drop in the most accurate way?
  – Can we define a design criterion based on the Peclet number?
1D tree-shaped flow field pattern

\[ l_{j,i} = \frac{1}{2 \frac{j}{k}} l_0 \]

\[ w_{j,i} = a^j w_0 \]

\[ Q_{j,i} = \frac{1}{2j} Q_0 \]

\[ \left( \frac{dS_{irr}}{dt} \right)_{j,i} = -Q_{j,i} \frac{\Delta p_{j,i}}{T} \]

\[ \frac{dS_{irr, spec.}}{dt} = \frac{dS_{irr}}{dt} w_{j,i}^{-1} \]

- Rectangular channels
- Constant depth
1D tree-shaped flow field pattern

$k=2$

$k=3$
1D tree-shaped flow field pattern

• If lengths are scaled:
  – Rectangular area
  – Can have crossovers

• Therefore → no length scaling

• Space filling (25cm$^2$):
  – Gen. 0: $l=24$mm
  – Gen. 1: $l=12$mm
  – Gen. 2: $l=12$mm
  – Gen. 3: $l=6$mm
  – Gen. 4: $l=6$mm
1D – Pressure drop

\[ \Delta p_{i,j} = -\frac{128\mu l_{i,j}}{\pi d_{i,j}^3} Q_{i,j} \]

- 3 different cases investigated
  - Hydraulic diameter \((d_{j,i}=D_{j,i})\)
    \[ D_{j,i} = \frac{2w_{j,i}h_{j,i}}{w_{j,i} + h_{j,i}} \]
  - Equivalent area
    \[ d_{j,i} = \sqrt{\frac{4}{\pi}} w_{j,i} h_{j,i} \]
  - Analytic solution of HP-flow for rectangular channels
    \[ \Delta p_{j,i} = -Q_{j,i} \frac{12\mu l_{j,i}}{h_{j,i}^3 w_{j,i}^3} \left[ 1 - \sum_{n=0}^{\infty} \frac{192}{(2n+1)^5 \pi^5} \frac{h_{j,i}}{w_{j,i}} \tanh \left( \frac{2n+1}{2} \frac{\pi w_{j,i}}{h_{j,i}} \right) \right]^{-1} \]


30.08.2019
<table>
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<th>Study</th>
<th>Investigation</th>
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<th>Method</th>
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<td>1</td>
<td>Flow rate &amp; $\Delta p$ calc. method dependency on TEP &amp; TSEP</td>
<td>Flow rate, $\Delta p$ calculation method, $w_0$</td>
<td>1D</td>
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<tr>
<td>2</td>
<td>Murray’s Law and entropy production</td>
<td>$a$, $w_0$</td>
<td>1D</td>
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<tr>
<td>3</td>
<td>1D $\Delta p$</td>
<td>$a$, $\Delta p$ calculation method</td>
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<td>4</td>
<td>Flow rate distribution</td>
<td>$a$, $w_0$</td>
<td>3D</td>
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<td>5</td>
<td>3D TEP &amp; TSEP</td>
<td>$a$, $w_0$, flow rate</td>
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<td>6</td>
<td>Comparison 1D &amp; 3D $\Delta p$</td>
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<td>3D, 1D</td>
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<td>7</td>
<td>Peclet number</td>
<td>characteristic length, $w_0$, $a$, flow rate</td>
<td>1D</td>
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</table>
1D – Total entropy production results

$w_0=1\text{mm}$

<table>
<thead>
<tr>
<th>Current density [A/m²]</th>
<th>Flow rate [m³/s]</th>
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<tbody>
<tr>
<td>10000</td>
<td>$5.7104 \times 10^{-6}$</td>
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<tr>
<td>5000</td>
<td>$2.8552 \times 10^{-6}$</td>
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<tr>
<td>1000</td>
<td>$5.7104 \times 10^{-7}$</td>
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<td>$5.7104 \times 10^{-8}$</td>
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<tr>
<td>10</td>
<td>$5.7104 \times 10^{-9}$</td>
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</table>

**Total Entropy Production [J/Ks]**

![Graph showing total entropy production vs. channel width for different current densities and flow rates. The graph includes lines for different geometries and current densities.](image-url)
1D – Entropy production

\( w_0 = 1 \text{mm} \)

![Graph showing total entropy production vs. channel width for different values of TEP and TSEP parameters. The x-axis represents channel width (mm), and the y-axis represents total entropy production (J/Ks). The graph includes lines for different values of the parameters.]
a. $w_0=1\text{mm}$ $a=0.70$

b. $w_0=1\text{mm}$ $a=0.79$

c. $w_0=1\text{mm}$ $a=0.90$
• Flow rate shifts entropy production to higher or lower values
• Murray’s law does not give lowest entropy production values
• Strong dependency on width from 0.5 to 2mm
• Form of pressure curve changes with $a$
• Reason for Murray’s Law not being the optimum
3D – Simulation setup

- Channel depth constant 1mm, channel width 1, 1.5, 2, 2.5 & 5mm
- $\alpha$ varied between 0.79, 0.9 and 1
- 4 generation levels
- Hexahedral mesh
- Incompressible, isothermal, laminar
- OpenFoam 4.1, simpleFoam
3D – Velocity & flow rate

- 1mm $a=0.79$
- 10000 A/m$^2$
3D – Velocity & flow rate

Difference in outlet flow rates 1mm a=0.79 1000 mA/cm²

<table>
<thead>
<tr>
<th>w₀ = 1mm, a = 0.79</th>
<th>10000 A/m²</th>
<th>5000 A/m²</th>
<th>1000 A/m²</th>
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<td>8.53</td>
<td>8.62</td>
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</table>
3D – Specific entropy production

\[
\left( \frac{dS_{\text{irr,specific}}}{dt} \right)_{j,i} = \left( \int_{V_{j,i}} -\frac{1}{T} \Pi : \nabla v dV \right) \frac{1}{w_{j,i}}
\]


| TEP | | | | | |
|-----|----------|----------|
| 10000 | 10000 | 100 | 100 |
| A/m² | A/m² | A/m² | A/m² |
| 0.79 | 0.79 | 0.90 | 0.90 |
| 1.00 | 1.00 | 1.00 | 1.00 |

| TSEP | | | | | |
|-----|----------|----------|
| 10000 | 10000 | 100 | 100 |
| A/m² | A/m² | A/m² | A/m² |
| 0.79 | 0.79 | 0.90 | 0.90 |
| 1.00 | 1.00 | 1.00 | 1.00 |
3D – Summary

• Uniform flow distribution (beside $w_0=5\text{mm}$ cases)

• Results give same conclusions than for the 1D calculations
  – Murray’s Law does not deliver the lowest entropy production
  – Increase in width $\rightarrow$ decrease in entropy production

• Most exact pressure drop calculation method depends on channel shape
Peclet number

\[ P_e = \frac{L_u}{D} \]
Due to uniform flow distribution, PEMFC can be subdivided

Allows for approximation with 1D model

Advantages of this pattern:
- Easy to change space filling properties
- Increase in generation levels does not increase pressure drop significantly (a>0.79)
- This is due to the scaling

Compared to serpentine:
- Lower pressure drops achieveable (1 order of magnitude) [6]
- Uniform fuel distribution

Not only applicable for PEMFCs, but also other fuel cells

Conclusions

- Tree-shaped pattern provides uniform velocity/flow rate at end of last branches
- The higher the $a$, the lower the entropy production
- Scaling parameter $a$ acc. to Murray’s Law not optimal
- To use the hydraulic diameter approximation, overestimates the pressure drop and EP.
- The best way depends on the channel shape
- The Peclet number analysis gives a range of current densities where $Pe<1$ can be achieved
Thank you for your attention!

Any questions?

Acknowledgements:
We gratefully acknowledge the support from NTNU in Trondheim and the Research Council of Norway through its Centre of Excellence funding scheme with Project No. 262644 (PoreLab) and UNINETT Sigma2 - the National Infrastructure for High Performance Computing and Data Storage in Norway