Numerical Simulation of Flow Electrolysers: Effect of Various Geometric Parameters

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Outline

• Electrolysis and its Industrial applications
• Objective of this work
• Governing equations and boundary conditions
• Validation of the computational approach
• Effect of inlet channel length
• Effect of offset between anode and cathode
• Effect of size of anode
• Conclusion
Electrolysis and its Industrial Applications

- Electroplating
- Electrolytic etching of metal surface
- Cleaning and preservation of old artifacts
- Production of aluminium, lithium, sodium, potassium, magnesium
- Production of electrolytic copper as a cathode, from refined copper of lower purity as an anode
- Caustic soda production

Schematic diagram of an electrolyser
Objective of this Work

- To study the effect of various geometrical parameters on performance of electrolyser
- Reduction in power consumption by Potential minimization
- Calculation of excessive power required for special cases
- Inlet channel length
- Offset between anode and cathode
- Length of anode

How We Proceed

- Applicable governing equations and boundary conditions.
- Validation of computational approach.
- Effect of geometrical parameters (inlet channel length, offset, anode length) on potential.
- Conclusions.
Governing Equations and Boundary Cond.

Navier-Stokes Equations
\[ \nabla \cdot \mathbf{u} = 0 \quad \rho \mathbf{u} \cdot \nabla \mathbf{u} = \mu \nabla^2 \mathbf{u} - \nabla p + \rho \mathbf{g} \]

Nernst-Planck equations
\[ \nabla \cdot \mathbf{N}_i = 0 \]

Possible boundary conditions for NP equations

<table>
<thead>
<tr>
<th>Current/potential BC</th>
<th>Concentration BC</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n_i = 0 ) (Electrical insulation)</td>
<td>( c = c_0 ) (Constant concentration)</td>
</tr>
<tr>
<td>( i = i_0 ) (Constant inward current density)</td>
<td>( -\mathbf{n} \cdot \mathbf{N}_i = i_o / F ) (Constant flux)</td>
</tr>
<tr>
<td>( i = -i_0 ) (Constant outward current density)</td>
<td>( -\mathbf{n} \cdot \mathbf{N}_i = 0 ) (Zero flux)</td>
</tr>
<tr>
<td>( v = v_o ) (Constant potential)</td>
<td>( -\mathbf{n} \cdot \left( -D_i \nabla c_i - \frac{z_i F}{RT} D_i c_i \nabla \phi \right) = 0 ) (Convective flux)</td>
</tr>
<tr>
<td>Wall</td>
<td>Current potential boundary cond.</td>
</tr>
<tr>
<td>-------</td>
<td>----------------------------------</td>
</tr>
<tr>
<td>1</td>
<td>Insulation</td>
</tr>
<tr>
<td>2</td>
<td>Insulation</td>
</tr>
<tr>
<td>3</td>
<td>Insulation</td>
</tr>
<tr>
<td>4</td>
<td>Current density</td>
</tr>
<tr>
<td>5</td>
<td>Voltage</td>
</tr>
<tr>
<td>6</td>
<td>Insulation</td>
</tr>
</tbody>
</table>

**Equations:**

- **Boundary Conditions:**
  - Insulation: \( \mathbf{n} \cdot \mathbf{i} = 0 \)
  - Concentration: \( c_2 = c_o \)
  - Zero flux: \( -\mathbf{n} \cdot \mathbf{N}_2 = 0 \)
  - Faraday’s law: \( -\mathbf{n} \cdot \mathbf{N}_2 = \pm \frac{i_0}{F} \)
  - Convective flux: \( -\mathbf{n} \cdot (D_c \mathbf{c} - z F \mathbf{v} \times \mathbf{c}) = 0 \)

- **Governing Equations:**
  - Flux continuity: \( \nabla \cdot \mathbf{j} = 0 \)
  - Faraday’s law: \( \mathbf{j} = \sigma \mathbf{E} + \mathbf{N} \times \mathbf{B} \)
  - Conservation of mass: \( \nabla \cdot \mathbf{c} = 0 \)
  - Reaction rate: \( \mathbf{N} = f_c \mathbf{c} \)
  - Convective flux: \( \mathbf{f}_c = D \nabla \mathbf{c} \nabla \cdot (D \mathbf{c} \nabla V) = 0 \)
  - Convective term: \( \nabla \cdot (\mathbf{v} \mathbf{c}) = \mathbf{N} \cdot \nabla \mathbf{c} + \mathbf{c} \nabla \cdot \mathbf{v} \)
Validation of the Computational Approach

Reactions:

\[ 2\text{Cl}^- \rightarrow \text{Cl}_2 \uparrow +2e \text{ (at the anode)} \]
\[ 2\text{H}_2\text{O} + 2e \rightarrow 2\text{OH}^- + \text{H}_2 \uparrow \text{ (at the cathode)} \]

\( \text{Na}^+ \) (species 1, \( C_1 \)), \( \text{Cl}^- \) (species 2, \( C_2 \)) and \( \text{OH}^- \) (species 3, \( C_3 \)) are the ions carrying currents.

Size of the domain:

- Electrode length: 0.1m
- Gap between electrodes: 0.03m
- Main channel length: 0.08m

Concentration profile of species 1 at the outlet for \( i_o = 10000 \text{A/m}^2 \), \( \text{u}_o = 0.01 \text{m/s} \), \( \text{c}_o = 600 \text{mol/m}^3 \)


Validation of the Computational Approach

Concentration profile of species 1 at the outlet for $u_o = 0.05$ m/s, $i_o = 10000$ A/m$^2$, $c_o = 600$ mol/m$^3$

Potential profile at the outlet for $u_o = 0.01$ m/s, $i_o = 10000$ A/m$^2$, $c_o = 600$ mol/m$^3$
Effect of Inlet Channel Length

Comparison of geometries with and without inlet channels

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Current density for constant applied voltage</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>J (A/m²)</td>
</tr>
<tr>
<td>G-1</td>
<td>6729.16</td>
</tr>
<tr>
<td>G-2</td>
<td>7067.30</td>
</tr>
</tbody>
</table>

Effect of Inlet Channel Length

Range of parameters:
- Two charged species- (Na+ and Cl)
- Current density- (2000 - 10,000A/m²)
- Base case- No inlet channel.
- Inlet length- (20% to 100% of electrode length)
- Inlet flow velocity -0.03 m/s
- Initial electrolyte concentration -600 mol/m³

2Cl⁻ → Cl₂↑ +2e⁻ (Anodic reaction)
Na⁺ + e⁻ → Na (Cathodic reaction)
Effect of Inlet Channel Length

Potential Vs Inlet length Plots

2,000 A/m²

4,000 A/m²
Effect of Inlet Channel Length

Potential Vs Inlet length Plots

6,000 A/m²

10,000 A/m²

8,000 A/m²
Effect of providing offset between the location of anode and cathode at current density 10,000 A/m²

As expected, as the offset increases, the potential difference across the electrode increases for a given current density.

It is therefore better to design an electrolyser in which anode and cathode are of different length such that the offset between the anode and cathode is kept minimum.

anode length 20 cm and cathode length 50 cm.

No inlet channel
Effect of Size of Anode

Constant total current 2000A.

The offset between the anode and cathode is zero for these simulations.

As the length of anode reduces, the potential difference between the electrode increases.

Effect of varying anode length on potential difference at current at current 2000 A
Effect of Size of Anode

Surface normalized potential and current density vector plots for anode of 50 cm lengths at current 2000 A

Surface normalized potential and current density vector plots for anode of 10 cm lengths at current 2000 A
Conclusions

The simulations reported in this work provide useful insights into how the performance of a flow electrolyser is affected when certain geometric parameters namely inlet channel length, offset between anode and cathode and the length of anode are changed.

The results also show that providing an inlet channel having length about 20-30% of electrode length improves the performance of electroneutral bulk.

Results show that providing offset, increases the potential drop for same applied current and hence leads to inefficient electroneutral bulk.

Simulations also show that as length of one of the electrode reduces, keeping the current same, performance of electroneutral bulk degrades.

These multiphysics simulations also highlight that it is important to consider both Nernst-Planck and Navier Stokes equations while simulating electroneutral bulk of a flow electrolyser.
THANKS FOR YOUR ATTENTION!

QUESTIONS, COMMENTS?