Current Density in the Mark IV with Cadmium Pool

Jun Li, David McNelis
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Advanced Fuel Cycle
Electro-Refiner Models

- ANL (PYRO, GPEC, Engineering model of Mk-V)
- INDIA (Numerical simulation)
- JAPAN (TRAIL, DEVON)
- INL/UI: 1D and 2D Model
- KAERI/SEOUL: RFIN + 3D Hydro-dynamic
Mark-IV Direct Deposit Mode

\[ U \leftrightarrow U^{3+} + 3e^- \]
Mass Transfer Process

Butler-Volmer Boundary

Diffusion Layer

Butler-Volmer Boundary

Anode

Molten Salt Bulk

Cathode

$U^3+ \text{ Transfer in the salt}$

$U$ (Bulk movement +diffusion+ Electric Field)

$U \leftrightarrow U^3+ + 3e^-$
Overview of CFD Model

- 3D Simulation of the Mark-IV Electro-Refiner
- Comprehensive modeling of the effect of fluid dynamic, electric field, electro-chemical reaction
- Reactions assumed to happen at the interface of molten salt and electrode/Cd pool
- ANSYS-CFX coupled with in-house Fortran Program
Model Highlights

- Molten Salt is modeled as incompressible viscous fluid mixed with uranium and the rest of the compositions
- Mass transfer rate of each species at the electrode surface:
  \[ N_j = \frac{i_j}{z_j F} \]
- Electro-chemical reaction rate described by Butler-Volmer equation:
  \[ i_j = i_{0,j} \left[ \exp \left( \frac{z_j \beta F}{RT} \eta \right) - \exp \left( - \frac{z_j (1 - \beta) F}{RT} \eta \right) \right] \]
- Cell Potential:
  \[ E_{cell} = \eta_a + \Phi_{ohm} + \eta_c \]
# Model Parameters

<table>
<thead>
<tr>
<th>Species</th>
<th>U</th>
<th>Pu</th>
<th>Nd</th>
<th>Zr</th>
</tr>
</thead>
<tbody>
<tr>
<td>Charge Number</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>4</td>
</tr>
<tr>
<td>Standard Electrode Potential (V vs. 1 wt% Ag/AgCl)</td>
<td>-1.249</td>
<td>-1.833</td>
<td>-2.358</td>
<td>-0.838</td>
</tr>
<tr>
<td>Diffusion Coefficient in Molten Salt (m²/s)</td>
<td>9.92E-10</td>
<td>1.08E-09</td>
<td>1.50E-09*</td>
<td>1.13E-09</td>
</tr>
<tr>
<td>Diffusion Coefficient in Cd (m²/s) *</td>
<td>1.50E-09</td>
<td>1.50E-09</td>
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<td></td>
</tr>
<tr>
<td>Activity Coefficient in Molten Salt</td>
<td>5.79E-03</td>
<td>6.62E-03</td>
<td>3.50E-03</td>
<td>4.48E-03</td>
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<tr>
<td>Activity Coefficient in Cd</td>
<td>7.50E+01</td>
<td>1.38E-04</td>
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<tr>
<td>Exchange Current Density (A/m²)**</td>
<td>18</td>
<td>18</td>
<td>18</td>
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<tr>
<td>Transfer Coefficient*</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
</tr>
</tbody>
</table>

* assumed value  
** calculated value, assumed to be the same for all interfaces and species

The electric conductivity of the molten salt is 205 mho/m
Current Density and Electric Potential (1)

Contour plot = Electric Potential Distribution
Vector plot = Current Density Distribution
Current Density and Electric Potential (2)

Contour plot = Electric Potential Distribution
Vector plot = Current Density Distribution
Current Density and Electric Potential (3)

Contour plot = Electric Potential Distribution
Vector plot = Current Density Distribution
U Concentration at Top of the Cd Pool
Pu Concentration at Top of the Cd Pool
Pu Mass Fraction Gradient at Top of the Cd Pool
Mass Flow Rate at Anode (1)

Mass Flow Rate at Right Anode Surface

- **U**
- **Pu**
- **Nd**
- **Zr**
- **Current (A)**

Time (min)

Applied Current (A)

Mass Flow Rate (kg/m²/s)
Mass Flow Rate at Right Anode Surface

Mass Flow Rate (kg/m²/s)

Applied Current (A)

Time (min)

Zr

Current (A)
Mass Flow Rate at Anode (3)
Mass Flow Rate at Cathode (1)
Mass Flow Rate at Cathode (2)

Mass Flow Rate at Cathode Surface

- Pu
- Nd
- Zr

Applied Current (A)

Time (min)

 Mass Flow Rate (kg/m²/s)
Cell Potentials

Cell Potential (vs. the vessel wall)

- Left Anode Potential (V)
- Right Anode Potential (V)
- Cathode Potential (V)
- Current (A)

Time (min) vs. Applied Current (A) and Potential (V)
Observations

- Electric field distribution affects the electric-chemical reaction rate
- Zr is dissolving slowly during the direct deposit mode even when anode voltage is low
- Cd pool is serving as a “passing tunnel” for U
- Region in Cd pool closer to the anodes has higher concentration of U and Pu
Discussion

- Experimental data is needed to validate the model:
  - Model error
  - Parameter error

- Application of the model:
  - Determine parameters
  - Parameter sensitivity study – guide the experiments
  - Mass tracking/material accountability/safeguard