A Role for Theoretical Chemistry in Nuclear Engineering!

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Role for Theoretical Chemistry

1. **Liquid core**
   
   Despite the design being inherently simple, the testing, verification and existing database does not readily apply.

2. **Thorium**
   
   The fuel is Uranium 233 which is not naturally found but must be obtained from the “fertile” element thorium. Since this was not the best solution for weapons, the process is not well known.

3. **Chemical Processing**
   
   Without CONTINUOUS chemical processing, the full advantage of thorium for a power reactor is not realized. One must sequester the intermediate product from the reactor core and that is a unique industrial chemical process - NOT a nuclear technology.
Role for Theoretical Chemistry

$\text{Th}^{4+}$ in $\text{Li}^+$, $\text{Be}^{++}$ and $\text{F}^-$

Thermodynamic Activities

Transport properties

Electrokinetic phenomena

Fluoride “solvent” $T \sim 1000K$
$3\text{LiF} : \text{BeF}_2$

$\text{LiF} : \text{BeF}_2$
Viscosity of LiF:BeF$_2$ mixtures

![Graph showing viscosity of LiF:BeF$_2$ mixtures at different temperatures (873K and 1200K). The graph compares experimental data and simulation results.](image-url)
### Transport Coefficients

<table>
<thead>
<tr>
<th>system</th>
<th>$\kappa$</th>
<th>$\eta \times 10^4$</th>
<th>$D_+ \times 10^4$</th>
<th>$D_- \times 10^4$</th>
<th>$\lambda$</th>
</tr>
</thead>
<tbody>
<tr>
<td>LiCl (1200K)</td>
<td>6.03(7.13)</td>
<td>7.78(7.37)</td>
<td>1.62(2.03)</td>
<td>0.936(0.951)</td>
<td>0.643(0.534)</td>
</tr>
<tr>
<td>NaCl (1300K)</td>
<td>3.71(4.10)</td>
<td>7.21(6.81)</td>
<td>1.28(1.32)</td>
<td>1.03(1.07)</td>
<td>0.509(0.478)</td>
</tr>
<tr>
<td>KCl (1300K)</td>
<td>2.65(2.73)</td>
<td>5.75(6.26)</td>
<td>1.23(1.25)</td>
<td>1.16(1.14)</td>
<td>0.343(0.345)</td>
</tr>
</tbody>
</table>

**TABLE I**: Simulation results compared with experiment values, in brackets:

- $\kappa$ – the electrical conductivity (in $\Omega^{-1} \text{cm}^{-1}$)
- $\eta$ – the shear viscosity (in $\text{Pa s}^{-1}$)
- $D_+$ and $D_-$ – the diffusion coefficients of cation and anion (in $\text{cm}^2 \text{s}^{-1}$)
- $\lambda$ – the thermal conductivity $\text{Wm}^{-1} \text{K}^{-1}$.
Increase cell voltage -> deposition of $M^{3+}$

Separability of fission products

Activity coefficients

$$\eta = 1 - \frac{x_{M^{3+}}^{\text{final}}}{x_{M^{3+}}^{\text{initial}}} = 1 - \frac{\gamma_{N^{3+}}}{\gamma_{M^{3+}}} \exp \left[ - \frac{3F(E_{M^{3+}}^0/M - E_{N^{3+}}^0/N)}{RT} \right]$$
Transmutation by changing the interaction potential $U(\lambda)$.

\[
\Delta G_{tot} = -RT \ln \left( \frac{\gamma_{\text{MCl}_3}}{\gamma_{\text{NCl}_3}} \right)
\]

\[
\Delta G_1^{res} = \int_0^1 \left\langle \frac{\partial U(\lambda)}{\partial \lambda} \right\rangle d\lambda.
\]
99.9% separability requires $\Delta E = 0.149$ V

<table>
<thead>
<tr>
<th>Redox couple</th>
<th>$E^0$ (V)</th>
<th>$\frac{RT}{3F} \ln \left( \frac{\gamma_{M^{3+}}}{\gamma_{La^{3+}}} \right)$ (V)</th>
<th>$E'_{\text{calc}}$ (V)</th>
<th>$E'_{\text{exp}}$ (V)</th>
</tr>
</thead>
<tbody>
<tr>
<td>U</td>
<td>0.65</td>
<td>0.00 ± 0.03</td>
<td>0.65 ± 0.03</td>
<td>0.63$^a$, 0.60$^c$, 0.65$^{d,e}$</td>
</tr>
<tr>
<td>Sc</td>
<td>0.38</td>
<td>-0.14 ± 0.06</td>
<td>0.24 ± 0.06</td>
<td>0.295$^a$</td>
</tr>
<tr>
<td>Tb</td>
<td>0.26</td>
<td>-0.08 ± 0.03</td>
<td>0.18 ± 0.03</td>
<td>0.17$^b$</td>
</tr>
<tr>
<td>Y</td>
<td>0.22</td>
<td>-0.10 ± 0.03</td>
<td>0.12 ± 0.03</td>
<td>0.02$^a$, 0.02$^d$</td>
</tr>
<tr>
<td>La</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>