Dynamic Material Flow Simulation of an Integrated Pyroprocessing

22 Oct 2014
Department of Nuclear Fuel Cycle System Development
Hyo Jik LEE
**Introduction**

**M&S characteristics**

- M&S live at the intersection between experiment & theory.
- A model is an expression of theory and running the simulation and the collection of the results is virtual experiment.
- Provide insights that are often impractical or impossible to discover through real-world experimental and theoretical analysis alone.

---

Three Pillars for Scientific Understanding

- Experiment
- Modeling & Simulation
- Theory
Regarding pyroprocessing M&S, a three-tiered modeling architecture was proposed a few years ago for the development of a pyroprocessing plant-level simulator at KAERI.

The architecture is becoming a solid foundation to study the modeling and simulation for pyroprocessing since it covers various time and spatial scales using two different systems such as a discrete event and continuous system.
Architecture for Pyroprocessing Simulator

1st tier
- Unit process model
  - Chemical and physical process model
  - Time driven dynamics

2nd tier
- Operation model
  - DES model
  - Event driven dynamics

3rd tier
- Plant model
  - An integrated material flow framework
  - Analysis modules & visualization modules

Analysis modules & visualization modules

3rd tier
• An integrated material flow framework
• Analysis modules & visualization modules

2nd tier
• DES model
• Event driven dynamics

1st tier
• Chemical and physical process model
• Time driven dynamics
A pyroprocessing simulator has three tiered modeling architecture; process, operation and plant level models at the 1st, 2nd and 3rd tiered model, respectively.

- **Process model** dealing with electro-chemistry needs cumulating of SNF experimental data and it is difficult to obtain reliable one.
- **Operation model** dealing with mechanical operation between processes needs discrete event based model, which is more or less easy to implement.
- **Plant model** has a material flow framework to track mass via every stream and also include various analysis modules.

To rapidly build integrated material flow without waiting for all process model accomplishment, an approach to the 2nd tiered operation model based development is more appropriate.

We have pyroprocessing flowsheet providing integral mass balance not dynamic.

However, it can be changed into dynamic mass balance if we have some additional information on unit process such as process time, batch capacity, and operation sequence.

In such a way, we could accomplish dynamic material flow.
Flow Diagram of Pyroprocessing

- Decladding/Voloxidation/Pelletization
  - Semi-volatile FPs
  - O₂/Ar
  - Hull
  - LLW

- Off-gas Treatment

- Salt Treatment
  - Used Salt
  - Clean Salt
  - (U + TRU + FP) Oxide

- Oxide Reduction
  - (U + TRU + FP) Metal
  - Clean Salt

- Electro-Refining
  - U recovery
  - SFR

- Final Waste Form

- Electro-Winning
  - SFR Fuel

- Storage
  - U Ingot

- Reuse

- SFR Fuel Fabrication

TRU : Transuranic elements
NM : Noble metal elements
FP : Fission products
Oxide Reduction Process

- Fresh Salt (LiCl, Li₂O)
- Offgas (O₂)
- Reduced metal
- Recovered Salt (1st campaign)
- Regenerated Salt (from 3rd campaign)
- Concentrated Salt
- Recovered Salt (from 2nd campaign)

Flowchart:
- Input Port
- Output Port

Steps:
1. Oxide SNF → P2-1 Electrolytic Reduction → Reduced metal with salt
2. P2-2 Cathode Processing
   - Recovered Salt (1st campaign)
   - Recovered Salt (from 2nd campaign)
3. W4-1 LiCl Purification
   - Concentrated Salt
Pyroprocessing is a batch type process. It means that process does not proceed seamlessly because pre-and post-operations retard flow advance.

In pyroprocessing material flow, it is critical to embody complex operation sequence and to manage numerous chemical elements.

Electrolytic reduction receives oxide spent fuel and three types of LiCl salt as inputs whereas it sends reduced metal and oxygen as two outputs.
Implementation

- **Section of Developing Tool**
  - Used SW: ExtendSim

- **Gathering information** from process developers
  - operation sequence, operation time, batch capacity and flowsheet information

- **Modeling of operation sequence** associated with event
  - events: receipt of feed material, departure of product, etc.

- **Write Database** for in-out stream mass flow
  - Record in-out mass flow at corresponding event.
Integrated Pyroprocessing Model
Oxide Reduction Model

LiCl / Li2O addition

P2-1 Electrolytic Reduction

P2-2 Cathode Processing

W3-1 Offgas O

W4-1 LiCl Purification

W4-2 LiCl Waste Form Fab
### Basic Operation Input Parameters

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrolytic reduction</td>
<td>50</td>
<td>96 for 1st batch of every campaign 2 for others</td>
<td>20</td>
<td>96 for last batch of every campaign 2 for others</td>
</tr>
<tr>
<td>Cathode Processing</td>
<td>100</td>
<td>2</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>LiCl salt purification</td>
<td>50 (kgSalt/batch)</td>
<td>0</td>
<td>164</td>
<td>1</td>
</tr>
</tbody>
</table>

- A batch capacity is generally different from those of other unit processes.
- The operation times in specific batch sequence are different from those in normal operations.
Basic Operation Input Parameters (cont.)

- **P2-1: Electrolytic Reduction**

<table>
<thead>
<tr>
<th>Reduction ratio (%)</th>
<th>Dissolution ratio (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Actinide (U, Pu, ...)</td>
<td>99.5%</td>
</tr>
<tr>
<td>Rare earth (La, Ce, ..)</td>
<td>30%</td>
</tr>
<tr>
<td>Cs, Sr and Ba</td>
<td>100%</td>
</tr>
</tbody>
</table>

  The ratio of salt to reduced metal: 20%

- **P2-2: Cathode Processing**

  Salt Recovery Ratio: 99%

- **W4-1: LiCl purification**

  Salt Regeneration Ratio: 90%
P2-1: Electrolytic Reduction

Material Balance in terms of SNF & Salt

- **Input Port**
- **Output Port**

**P2-1: Electrolytic Reduction**

- **Oxide Spent Nuclear Fuel**
- **Fresh Salt (LiCl, Li₂O)**
- **Reduced metal with salt**
- **Recovered Salt (1<sup>st</sup> campaign)**
- **Recovered Salt (from 2<sup>nd</sup> campaign)**
- **Regenerated Salt (from 3<sup>rd</sup> campaign)**
- **Concentrated Salt**

**P2-2: Cathode Processing**

- **Reduced metal**
- **Recovered Salt**

**W4-1: LiCl Purification**

- **Concentrated Salt**

**M<sub>x</sub>O<sub>y</sub>**

**Oxide → Metal (M<sub>x</sub>O<sub>y</sub> → xM)**

- **Cs, Sr and Ba**
- **LiCl bath**

**Offgas (O<sub>2</sub>)**
# Integral Mass Balance: Electrolytic Reduction (equiv. 200 batch operations)

## Integral Mass Balance in terms of SNF and Salt

<table>
<thead>
<tr>
<th>Material via stream</th>
<th>type</th>
<th>SNF mass (kg)</th>
<th>Salt (LiCl, Li₂O)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxide spent nuclear fuel</td>
<td>feed</td>
<td>11,331</td>
<td>-</td>
</tr>
<tr>
<td>Recovered salt</td>
<td>feed</td>
<td>5</td>
<td>350</td>
</tr>
<tr>
<td>Regenerated salt</td>
<td>feed</td>
<td>6</td>
<td>1,146</td>
</tr>
<tr>
<td>Fresh salt</td>
<td>feed</td>
<td>-</td>
<td>824</td>
</tr>
<tr>
<td><strong>Sum of inputs</strong></td>
<td></td>
<td>11,341</td>
<td>2,320</td>
</tr>
<tr>
<td>Cathode product</td>
<td>product</td>
<td>9,997</td>
<td>1,935</td>
</tr>
<tr>
<td>O₂</td>
<td>product</td>
<td>1,331</td>
<td>-</td>
</tr>
<tr>
<td><strong>Sum of outputs</strong></td>
<td></td>
<td>11,328</td>
<td>1,935</td>
</tr>
<tr>
<td>remaining salt</td>
<td>hold-up</td>
<td>13</td>
<td>385</td>
</tr>
<tr>
<td><strong>Hold-up change</strong></td>
<td></td>
<td>13</td>
<td>385</td>
</tr>
</tbody>
</table>

\[ \Sigma \text{Input} = \Delta \text{Hold-up} + \Sigma \text{Outputs} \]
<table>
<thead>
<tr>
<th>Batch #</th>
<th>Inputs (kg)</th>
<th>Hold-up (kg)</th>
<th>Outputs (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Oxide SNF</td>
<td>SNF in recovered salt</td>
<td>SNF in regenerated salt</td>
</tr>
<tr>
<td>1</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>56.59</td>
<td>0.02</td>
<td>-</td>
</tr>
<tr>
<td>4</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>5</td>
<td>56.59</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>6</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>7</td>
<td>56.59</td>
<td>0.05</td>
<td>-</td>
</tr>
<tr>
<td>8</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>9</td>
<td>56.59</td>
<td>0.08</td>
<td>-</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>41</td>
<td>56.59</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>42</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>43</td>
<td>56.59</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>44</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>45</td>
<td>56.59</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>46</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>47</td>
<td>56.59</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>81</td>
<td>56.59</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>82</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>83</td>
<td>56.59</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>84</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>85</td>
<td>56.59</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>86</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>87</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>194</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>195</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>196</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>197</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>198</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>199</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>200</td>
<td>56.67</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Total</td>
<td>11,331.06</td>
<td>4.55</td>
<td>5.66</td>
</tr>
</tbody>
</table>

ΣInputs = ΔHold-up + ΣOutputs
## Dynamic Mass Balance: Salt (LiCl, Li2O)

<table>
<thead>
<tr>
<th>Batch #</th>
<th>Inputs (kg)</th>
<th>Hold-up</th>
<th>Outputs</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Fresh salt</td>
<td>recovered salt</td>
<td>regenerated salt</td>
</tr>
<tr>
<td>1</td>
<td>404.00</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>-</td>
<td>19.67</td>
<td>-</td>
</tr>
<tr>
<td>4</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>5</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>6</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>7</td>
<td>-</td>
<td>19.64</td>
<td>-</td>
</tr>
<tr>
<td>8</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>9</td>
<td>-</td>
<td>19.61</td>
<td>-</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>41</td>
<td>42.26</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>42</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>43</td>
<td>19.38</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>44</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>45</td>
<td>19.37</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>46</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>47</td>
<td>19.37</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>81</td>
<td>0.17</td>
<td>-</td>
<td>19.17</td>
</tr>
<tr>
<td>82</td>
<td>-</td>
<td>-</td>
<td>19.17</td>
</tr>
<tr>
<td>83</td>
<td>0.17</td>
<td>-</td>
<td>19.17</td>
</tr>
<tr>
<td>84</td>
<td>-</td>
<td>-</td>
<td>19.16</td>
</tr>
<tr>
<td>85</td>
<td>0.17</td>
<td>-</td>
<td>19.16</td>
</tr>
<tr>
<td>86</td>
<td>-</td>
<td>-</td>
<td>19.16</td>
</tr>
<tr>
<td>87</td>
<td>0.17</td>
<td>-</td>
<td>19.16</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>194</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>195</td>
<td>0.17</td>
<td>-</td>
<td>19.06</td>
</tr>
<tr>
<td>196</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>197</td>
<td>0.17</td>
<td>-</td>
<td>19.06</td>
</tr>
<tr>
<td>198</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>199</td>
<td>0.17</td>
<td>-</td>
<td>19.06</td>
</tr>
<tr>
<td>200</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Total</td>
<td>824.24</td>
<td>349.83</td>
<td>1,146.07</td>
</tr>
</tbody>
</table>

\[ \sum \text{Inputs} = \Delta \text{Hold-up} + \sum \text{Outputs} \]
Dynamic Mass Balance of SNF

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)

SNF total (kg)
Accumulated Mass Balance of SNF

SNF total (kg)

hold-up, cumulative recovered salt & regenerated salt

SNF total (kg)

batch#
Dynamic Mass Balance: Salt (LiCl)

**Fresh Salt Addition**

- **Recovered salt**
- **Regenerated salt**

**Recycling Salt Addition**

- **Recovered salt**
- **Regenerated salt**

**Hold-up Change**

- **Salt Entrained with Cathode Product**
Accumulated Mass Balance of Salt (LiCl)

Accumulated Fresh Salt

Accumulated Recycling Salt

Hold-Up Salt

Accumulated Salt Entrained with Cathode Product
Conclusions

- **DES based modeling** was applied to build a pyroprocessing operation model, specifically, oxide reduction model.

- DES modeling could **embody complex operation sequence**.

- A database associated with events enabled the model to **manage (write & read) numerous chemical elements**.

- **A dynamic material flow** was accomplished through ExtendSim’s internal database and item blocks.

- It is a meaningful step to **build a framework of material flow** for pyroprocessing.

- Based on the developed material flow framework, **an integrated pyroprocessing simulator** will continue to be in progress for the purpose of assessing technical feasibility, identifying operation research issues, and supporting facility design.
email: hyojik@kaeri.re.kr