Fuel Cycle Performance of Fast Spectrum Molten Salt Reactor Designs

Andrei Rykhlevskii¹, Benjamin R. Betzler², Andrew Worrall², Kathryn Huff¹
Advanced Reactors and Fuel Cycles Group

¹University of Illinois at Urbana-Champaign
²Oak Ridge National Laboratory

Aug 26, 2019

ILLINOIS
Motivation

- Fuel cycle performance analysis for four Fast Molten Salt Reactor (MSR) concepts requires a depletion simulation over the system lifetime (60 years).
- Full-core 3D 60-year depletion calculations for MSRs using Monte Carlo code (Serpent/Shift) are computationally prohibitive (16 mln neutron histories per state point to obtain uncertainty $\pm 7\,pcm$).
- We want to reduce the cost by performing depletion simulations for representative simplified unit cells using deterministic code (TRITON).

Depletion calculations of MSR with continuous fuel reprocessing

1. Develop high-fidelity 3D models of four different Fast Spectrum MSRs using Monte Carlo code Serpent 2 [1].
3. Perform depletion simulation with on-line continuous feeds and removals to estimate fuel cycle performance of selected designs.
MSR (Molten Salt Reactor) types

### Stationary Fuel

1. Graphite block with TRISO fuel, clean salt works as coolant (Fluoride-Salt-Cooled High-Temperature Reactor (FHR))

2. Plate Fuel: hexagonal fuel assembly is similar in shape to a typical sodium-cooled reactor

3. Fuel Inside Radial Moderator (FIRM)

4. Liquid fuel salt inside fuel rods cooled by clean salt (Moltex Stable Salt Reactor)

### Mobile Fuel

1. Mobile solid fuel elements (pebbles) cooled by clean salt (PB-FHR)

2. **Circulating molten fuel salt** which also works as coolant (Molten Salt Breeder Reactor (MSBR), Molten Salt Fast Reactor (MSFR))
Stationary and Mobile Solid fuel

Figure 1: TRISO fuel particle (top) and FHR fuel designs (bottom). Source [3].
Mobile, Circulating, Liquid Fuel

Figure 2: EVOL MSFR is an example of reactor design with liquid, mobile, circulating fluoride salt fuel (Image courtesy of Elsa Merle-Lucotte, 2015).
Why Molten Salt Reactors with circulating fuel?

Liquid-fueled MSR designs have following **potential** advantages:

1. High coolant temperature (600-750°C) ⇒ potentially high thermal efficiency, process heat for chemical industry
2. Fuel diversity (\(^{235}\text{U},\) \(^{233}\text{U},\) Thorium, U/Pu)
3. Strong negative temperature feedback of liquid fuel
4. Passive safety ⇒ fuel drains into tanks in emergency
5. High fuel utilization ⇒ less nuclear waste generated
6. On-line (continuous) fuel reprocessing and refueling
7. Can produce more fissile material than it consumes (breeder)
8. Nuclear Spent Fuel Transmuter
9. Unmoderated ⇒ no replacement of an irradiated moderator needed
Why Molten Salt Reactors with circulating fuel?

Liquid-fueled *Fast Spectrum* MSR designs have following potential advantages:

1. High coolant temperature (600-750°C) ⇒ potentially high thermal efficiency, process heat for chemical industry
2. Fuel diversity ($^{235}$U, $^{233}$U, Thorium, U/Pu)
3. Strong negative temperature feedback of liquid fuel
4. Passive safety ⇒ fuel drains into tanks in emergency
5. High fuel utilization ⇒ less nuclear waste generated
6. On-line (continuous) fuel reprocessing and refueling
7. Can produce more fissile material than it consumes (breeder)
8. Nuclear Spent Fuel Transmuter
9. Unmoderated ⇒ no replacement of an irradiated moderator needed
1 Introduction
   Motivation
   Fast Molten Salt Reactors

2 Methodology

3 Results

4 Conclusions

5 Acknowledgements
Fast Spectrum MSR depletion simulation

Depletion simulations were performed using SCALE/TRITON 6.2.4 Alpha [4]:

- Truly continuous (online) salt reprocessing (removals and feeds)
- Supports only constant or piecewise feed and removal rates
- Depletion over the system lifetime (60 years)
- Simplified geometry (unit cell), a $16 \times 16$ spatial mesh
- 238-group ENDF-B/VII.0 cross-section library

Four different fast MSR designs:

1. European MSFR [5]
2. Molten Chloride Salt Fast Reactor (MCSFR) [6]
3. REBUS-3700 [7]
4. Molten Salt Actinide Recycler and Transmuter (MOSART) [8]
Selected Fast Spectrum MSR designs

Table 1: Principal data of selected fast spectrum MSR designs.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>MSFR</th>
<th>MCSFR</th>
<th>REBUS-3700</th>
<th>MOSART</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P \ [\text{MW}_{th}]$</td>
<td>3,000</td>
<td>6,000</td>
<td>3,700</td>
<td>2,400</td>
</tr>
<tr>
<td>$V_{fuel} \ [\text{m}^3]$</td>
<td>18</td>
<td>38</td>
<td>55.6</td>
<td>49.05</td>
</tr>
<tr>
<td>$V_{fertile} \ [\text{m}^3]$</td>
<td>7.3</td>
<td>75</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Fuel salt</td>
<td>LiF-ThF$_4$-$^{233}$UF$_4$</td>
<td>NaCl-UCl$_3$-$^{239}$PuCl$_3$</td>
<td>NaCl-TRUCI$_3$</td>
<td>LiF-BeF$_2$-ThF$_4$-TRUF$_3$</td>
</tr>
<tr>
<td>Fertile salt</td>
<td>LiF-ThF$_4$</td>
<td>NaCl-UCl$_3$</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Fuel cycle</td>
<td>Th/$^{233}$U</td>
<td>U/Pu</td>
<td>U/TRU</td>
<td>Th/$^{233}$U</td>
</tr>
<tr>
<td>$m_{init \ fissile} \ [\text{t}]$</td>
<td>7.726</td>
<td>9.400</td>
<td>18.061</td>
<td>9.637</td>
</tr>
</tbody>
</table>
Geometry approximation

Figure 3: Full-core 3D models of MSFR (upper left), MCSFR (lower left), REBUS-3700 (upper right), and MOSART (lower right) and 2D representative unit cell model (center) showing fuel salt (red), fertile salt (green), and structural material (blue).
Unit cell model construction

Simplified unit cell geometry for each MSR concept was selected as follows:

1. Fuel-to-fertile salt ratio for unit cell was consistent with full-core model:
   \[
   \frac{V^f_{core}}{V^f_{blanket}} = \frac{A^u_{core}}{A^u_{blanket}}
   \]

2. Size of unit cell was adjusted to obtain \( k^u_{\infty} \) as close to \( k^f_{\text{eff}} \) as possible.

3. Structural material volume for unit cell was varied to get neutron energy spectrum shape close to full-core spectrum.
The geometry and size for unit cell are optimized using specific rules:

1. Multiplication factor has less than 300pcm difference between approximated and full-core geometry

2. Pearson correlation coefficient $r$ for neutron spectrum:

$$r = \frac{\sum_{i=1}^{N} (\Phi_i^f - \bar{\Phi}_i^f)(\Phi_i^u - \bar{\Phi}_i^u)}{\sqrt{\sum_{i=1}^{N} (\Phi_i^f - \bar{\Phi}_i^f)^2 \sum_{i=1}^{N} (\Phi_i^u - \bar{\Phi}_i^u)^2}} > 0.995$$

3. Approximation error $\delta$ in total neutron flux:

$$\delta = \left| \frac{\sum_{i=1}^{N} (\Phi_i^f - \Phi_i^u)}{\sum_{i=1}^{N} \Phi_i^f} \right| \times 100\% < 3\%$$
Fuel Cycle Performance Evaluation Metrics

**Nuclear Fuel Cycle Evaluation and Screening**

- The DOE-NE funded a study to conduct an evaluation and screening of nuclear fuel cycle options
- The study formulated sixteen Evaluation Metrics (EM)

**Evaluation metrics calculated based on continuous reprocessing depletion herein:**

1. Natural uranium per energy generated (for MCSFR, REBUS-3700)
2. Natural thorium per energy generated (for MSFR, MOSART)
3. Mass of spent nuclear fuel (SNF) + high level waste (HLW) disposed per energy generated
4. Mass of depleted uranium (DU) + recovered uranium (RU) + recovered thorium (RTh) disposed per energy generated
Figure 4: Neutron flux energy spectrum for full-core and unit cell models for two-fluid MSFR (top) and MCSFR (bottom). The neutron population per cycle and the number of active/inactive cycles for Serpent simulations were chosen to obtain a balance between reasonable uncertainty for a transport problem ($\pm 10\,\text{pcm}$ for multiplication factor).
Figure 5: Neutron flux energy spectrum for full-core and unit cell models for single-fluid REBUS-3700 (left) and MOSART (right). Uncertainty for multiplication factor is ±10 pcm.
Approximation accuracy for depletion calculations

Figure 6: Discrepancy in mass of important isotopes in REBUS-3700 for full-core and unit cell depletion calculations using SERPENT2 without reprocessing.
Figure 7: Infinite multiplication factor for four reactor designs during 60 years of operation.
Evolution of heavy metal inventory: MSFR and MCSFR

Figure 8: MSFR (left) and MCSFR (right) heavy metal isotopic salt content during operation calculated with the unit cell model (238-group transport).
Evolution of heavy metal inventory: MOSART and REBUS-3700

Figure 9: MOSART (left) and REBUS-3700 (right) heavy metal isotopic salt content.
### Table 2: The E&S evaluation metrics of selected fast spectrum MSR designs

<table>
<thead>
<tr>
<th>Parameter</th>
<th>MSFR</th>
<th>MCSFR</th>
<th>REBUS</th>
<th>MOSART</th>
</tr>
</thead>
<tbody>
<tr>
<td>Evaluation Group</td>
<td>EG28</td>
<td>EG23</td>
<td>EG24</td>
<td>EG28</td>
</tr>
<tr>
<td>Natural U or Th Utilization [t/GWe-yr]</td>
<td>0.663(Th)</td>
<td>0.973(U)</td>
<td>0.834(U)</td>
<td>0.402(Th)</td>
</tr>
<tr>
<td>Mass of SNF+HLW disposed [t/GWe-yr]</td>
<td>0.866</td>
<td>0.894</td>
<td>0.813</td>
<td>0.820</td>
</tr>
<tr>
<td>Mass of DU+RU+RTh disposed [t/GWe-yr]</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Products from Reprocessing/Separation technology [t]:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RU</td>
<td>8.7</td>
<td>83.2</td>
<td>92.6</td>
<td>3.9</td>
</tr>
<tr>
<td>RTh</td>
<td>41.9</td>
<td>0.0</td>
<td>0</td>
<td>12.9</td>
</tr>
<tr>
<td>Transuranic elements (TRU)</td>
<td>0.36</td>
<td>32.8</td>
<td>18.9</td>
<td>12.9</td>
</tr>
<tr>
<td>Fission products (FP)</td>
<td>69.51</td>
<td>140.3</td>
<td>79.6</td>
<td>54.1</td>
</tr>
</tbody>
</table>
Outline

1 Introduction
   Motivation
   Fast Molten Salt Reactors

2 Methodology

3 Results

4 Conclusions

5 Acknowledgements
Conclusions

FS-MSR design depletion with simplified unit cell vs full-core geometry

- Relative error in one-group neutron flux < 3.15%
- Correlation coefficient > 0.9956
- Depleted mass relative error for major isotopes < 1% (for REBUS)
- 20× speedup

Continuous reprocessing depletion simulations for four FS-MSR concepts

- All four selected designs are able to maintain criticality while the salt inventory is kept constant during lifetime
- Fuel utilization varies from 0.402 tTh/GWe-yr for MOSART to 0.973 MTU/GWe-yr for MCSFR (Metric Bin A, < 3.8 t/GWe-yr)
- SNF+HLW generation for all four designs is consistent with fast spectrum fuel cycle technologies (Metric Bin A, < 1.65 t/GWe-yr)
- No DU+RU+RTh disposed, assuming we recover all U/Th from the salt
- Fuel Cycle Performance of these fast MSRs is consistent with other fast reactor technologies
**Future work**

**Future research effort**

1. Code-to-code validation of SCALE/TRITON Alpha against another continuous reprocessing code (e.g., SERPENT2) and batch-wise Python package SaltProc [9]

2. MSFR simulation with additional protactinium isolation system which enhance $^{233}$U breeding

3. MSFR simulation with another startup composition (transuranic (TRU)) to evaluate its performance as a waste burner

4. MCSFR might be optimized to operate with enriched uranium as startup composition instead of $^{239}$Pu

5. Accident safety analysis using coupled neutronics/thermal-hydraulics code, such as Moltres [10]
This research was supported by the DOE-NE Systems Analysis and Integration Campaign and by an appointment to the Oak Ridge National Laboratory Nuclear Engineering Science Laboratory Synthesis (NESLS) Program, sponsored by US Department of Energy and administered by the Oak Ridge Institute for Science and Education.

Kathryn D. Huff is supported by the Nuclear Regulatory Commission Faculty Development Program, the National Center for Supercomputing Applications, the NNSA Office of Defense Nuclear Nonproliferation R&D through the Consortium for Verification Technologies and the Consortium for Nonproliferation Enabling Capabilities, the International Institute for Carbon Neutral Energy Research (WPI-I2CNER), sponsored by the Japanese Ministry of Education, Culture, Sports, Science and Technology, and DOE ARPA-E MEITNER program award DE-AR0000983.


Final report 249696, EURATOM, France, 2015.


arfc/saltproc: Code for online reprocessing simulation of molten salt reactor with external 
depletion solver SERPENT. 
Zenodo, March 2018.

Introduction to Moltres: An application for simulation of Molten Salt Reactors. 
Table 3: Principal data of selected fast spectrum MSR designs.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>MSFR</th>
<th>MCSFR</th>
<th>REBUS-3700</th>
<th>MOSART</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal power, MW</td>
<td>3,000</td>
<td>6,000</td>
<td>3,700</td>
<td>2,400</td>
</tr>
<tr>
<td>Fuel salt volume, m³</td>
<td>18</td>
<td>38</td>
<td>55.6</td>
<td>49.05</td>
</tr>
<tr>
<td>Fertile salt volume, m³</td>
<td>7.3</td>
<td>75</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Fuel and fertile salt initial composition, mol%</td>
<td>LiF-ThF$_4$-2$^{233}$UF$_4$ (77.5-19.9-2.6)</td>
<td>NaCl-UCl$_3$-2$^{239}$PuCl$_3$ (60-36-4)</td>
<td>55mol%NaCl+(16.7at.%TRU)Cl$_3$</td>
<td>LiF-BeF$_2$-ThF$_4$-TRUF$_3$ (69.7-27-1.3)</td>
</tr>
<tr>
<td>Fuel cycle</td>
<td>Th/$^{233}$U</td>
<td>U/Pu</td>
<td>U/TRU</td>
<td>Th/$^{233}$U</td>
</tr>
<tr>
<td>Initial fissile inventory, t</td>
<td>7.726</td>
<td>9.400</td>
<td>18.061</td>
<td>9.637</td>
</tr>
<tr>
<td>Fissile/fertile salt</td>
<td>973/973</td>
<td>1008/923</td>
<td>900</td>
<td>933</td>
</tr>
</tbody>
</table>