Neutron Kinetics in Liquid-Fueled Nuclear Reactors
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Outline

1 Introduction
   ARFC Research Group
   Molten Salt Reactors

2 Point Kinetics & TH Coupling
   Point and Multi-point Kinetics

3 Spatial Kinetics & TH Coupling with Precursor Advection
Advanced Reactors and Fuel Cycles group (PI: Kathryn Huff)

Figure: Current undergraduate and graduate students.
Figure: Past ARFC Group members who contributed to this work.
Insights at Disparate Scales

High-Fidelity Reactor Modeling and Simulation

Global-Scale Nuclear Fuel Cycle Analysis

System-level impacts of design choices

Dominant physics of promising technologies
Types of Molten Salt Reactors

Stationary Fuel
- Prismatic graphite block with TRISO fuel and coolant channels (e.g. FHR DR, TMSR-SF1). Clean salt coolant.
- Stationary TRISO pebble matrix (e.g. TMSR-SF)

Mobile Fuel
- Mobile solid fuel elements, such as pebbles. Clean salt coolant. (e.g. PB-FHR/Kairos)
- Non-circulating fuel salt, “can-type”. (e.g. Terrapower MCFR)
- Circulating fuel salt “pool-type”. (e.g. MSRE, MSBR, MSFR, Terrestrial MSR, TAP MSR, etc.)
Figure: The AHTR [4] is an example of a fluoride salt cooled reactor design fueled by a stationary, solid prismatic graphite TRISO compacts, and cooled by clean fluoride salt. Image source [5].
Mobile Solid Fuel

Figure: The PB-FHR is an example reactor design fueled by solid, mobile graphite pebbles, with TRISO particles embedded in them. Image source [1].
Mobile, Non-Circulating, Liquid Fuel

Figure: The MCFR from TerraPower is an example reactor design with liquid, mobile, non-circulating chloride salt fuel. Image source [12, 2].
Figure: The MSBR [8] is an example reactor design with liquid, mobile, circulating fluoride salt fuel, including breeding behavior due to varying channel shapes and sizes. Image source [9].
Why Molten Salt Reactors?

Main advantages of liquid-fueled Molten Salt Reactors (MSRs) [3]

1. High coolant temperature (600-750°C).
2. Various fuels can be used (\(^{235}\text{U},^{233}\text{U},\) Thorium, U/Pu).
3. Increased inherent safety.
4. High fuel utilization \(\Rightarrow\) less nuclear waste generated.
5. Online reprocessing and refueling.

Main advantages of MSBR [8]

1. Produces more fissile material than it consumes (breeding ratio 1.06).
2. Thorium cycle limits plutonium and minor actinides.
Challenges in Liquid-Fueled Reactor Simulation

1. Contemporary burnup codes cannot treat fuel movement.
2. Neutron precursor locations drift before neutron emission.
3. Operational and safety parameters change during reactor operation.
4. Neutronics and thermal hydraulics are tightly interdependent.

Figure: Challenges in simulating MSRs (Image courtesy of Manuele Aufiero, 2012).
Approaches

**Point Reactor Kinetics [6]**

Only appropriate for stationary or nearly stationary fuels.

**Simulation of online reprocessing and depletion (SaltProc) [10, 11]**

1. Create high-fidelity full-core neutronics model of the core neutronics can be necessary for reducing compounding error.
3. Enables day-to-day resolution of neutronics and reprocessing modeling over many decades of depletion and fuel cycle performance.

**Multiphysics simulation of MSR (Moltres) [7]**

1. Steady-state and transient coupling of neutron fluxes, precursor drift, and thermal-hydraulics.
2. Incorporates advective movement of delayed neutron precursors.
3. 2D axisymmetric and 3D geometries supported.
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PyRK: Python for Reactor Kinetics

Figure: Special purpose reactor kinetics python tool (https://github.com/pyrk/pyrk) [6]. Research software for simple PRKE: *caveat emptor.*

- Multiple precursor groups ($j$ groups)
- Multiple decay heat groups ($k$ groups)
- Lumped Parameter thermal hydraulics model
- Optional 1-D conduction in pebble fuel compacts
- Object-oriented, geometry and material agnostic framework
Point Reactor Kinetics

\[ p = \text{reactor power} \]  \hspace{1cm} (1)

\[ \rho(t, T_{\text{fuel}}, T_{\text{cool}}, T_{\text{mod}}, T_{\text{refl}}) = \text{reactivity} \]  \hspace{1cm} (2)

\[ \beta = \text{fraction of neutrons that are delayed} \]  \hspace{1cm} (3)

\[ \beta_j = \text{fraction of delayed neutrons from precursor group } j \]  \hspace{1cm} (4)

\[ \zeta_j = \text{concentration of precursors of group } j \]  \hspace{1cm} (5)

\[ \lambda_{d,j} = \text{decay constant of precursor group } j \]  \hspace{1cm} (6)

\[ \Lambda = \text{mean generation time} \]  \hspace{1cm} (7)

\[ \omega_k = \text{decay heat from FP group } k \]  \hspace{1cm} (8)

\[ \kappa_k = \text{heat per fission for decay FP group } k \]  \hspace{1cm} (9)

\[ \lambda_{FP,k} = \text{decay constant for decay FP group } k \]  \hspace{1cm} (10)

\[ T_i = \text{temperature of component } i \]  \hspace{1cm} (11)
Point Reactor Kinetics

\[
\frac{d}{dt} \begin{bmatrix}
  p \\
  \zeta_1 \\
  \vdots \\
  \zeta_J \\
  \omega_1 \\
  \vdots \\
  \omega_K \\
  T_i \\
  \vdots \\
  T_I
\end{bmatrix} = \begin{bmatrix}
  \rho(t, T_i, \cdots) - \beta \frac{p}{\Lambda} \\
  \frac{\beta_1}{\Lambda} p - \lambda_{d,1} \zeta_1 \\
  \vdots \\
  \frac{\beta_j}{\Lambda} p - \lambda_{d,j} \zeta_j \\
  \frac{\beta_J}{\Lambda} p - \lambda_{d,J} \zeta_J \\
  \kappa_{1} p - \lambda_{FP,1} \omega_1 \\
  \vdots \\
  \kappa_{k} p - \lambda_{FP,k} \omega_k \\
  \kappa_{kp} p - \lambda_{FP,k} \omega_k \\
  f_i(p, C_{p,i}, T_i, \cdots) \\
  \vdots \\
  f_I(p, C_{p,I}, T_I, \cdots)
\end{bmatrix}
\]

(12)
The heat flow out of body $i$ is the sum of surface heat flow by conduction, convection, radiation, and other mechanisms to each adjacent body, $j$:

$$Q = Q_i + \sum_j Q_{ij}$$

$$= Q_i + \sum_j \frac{T_i - T_j}{R_{th,ij}}$$

$$\dot{Q} = \text{total heat flow out of body } i \ [J \cdot s^{-1}]$$

$$Q_i = \text{other heat transfer, a constant } [J \cdot s^{-1}]$$

$$T_i = \text{temperature of body } i \ [K]$$

$$T_j = \text{temperature of body } j \ [K]$$

$$j = \text{adjacent bodies } [-]$$

$$R_{th} = \text{thermal resistance of the component } \ [K \cdot s \cdot J^{-1}]$$.
**Figure:** The pebble fuel can be assumed approximately stationary, as their movement is not comparable to the longest precursor decay times.
Point Reactor Kinetics

Figure: Total reactivity during ramped reactivity insertion as a function of inserted reactivity [13].
PB-FHR Example

Figure: Average fuel temperature (left) and average normalized core power (right) during a ramp reactivity insertion in the PB-FHR [13].
Figure: Fuel temperature rise following 1$ ramp reactivity insertion, calculated with multipoint and single point kinetics in PyRK [13].
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Full-core SERPENT model of MSBR

Figure: Plan (left) and elevation (right) view of MSBR model.
Figure: Detailed plan view of graphite reflector and moderator elements.
Moderator element geometry (Zone I)

**Figure:** Molten Salt Breeder Reactor Zone I unit cell geometry from the reference [8] (left) and SERPENT 2 (right).
Online reprocessing method

SaltProc capabilities

- Remove specific isotopes from the core with specific parameters (reprocessing interval, mass rate, removal efficiency)
- Add specific isotopes into the core
- Maintain constant number density of specific isotope in the core
- Store stream vectors in an HDF5 database for further analysis or plots
- Generic geometry: an infinite medium, a unit cell, a multi-zone simplified assembly, or a full-core

Figure: Flow chart for the SaltProc.
Online reprocessing method

- Continuously removes all poisons, noble metals, and gases.
- $^{233}\text{Pa}$ is continuously removed from the fuel salt into a decay tank.

Figure: Protactinium isolation with uranium removal by fluorination [8].

$^{232}\text{Th} + \frac{1}{0}\text{n} \rightarrow ^{233}\text{Th} \xrightarrow{\beta^-} ^{233}\text{Pa} \xrightarrow{\beta^-} ^{233}\text{U}$
Strong absorbers \(^{233}\text{Th},^{234}\text{U}\) accumulating in the core

Fissile materials other than \(^{233}\text{U}\) are bred into the core \((^{235}\text{U},^{239}\text{Pu})\)

The multiplication factor stabilizes after approximately 6 years

**Figure:** \(k_{\text{eff}}\) during a 20 years depletion simulation.
Introduction

Point Kinetics & TH Coupling

Spatial Kinetics & TH Coupling with Precursor Advection

Power and breeding distribution

Figure: Normalized power density

Figure: $^{232}\text{Th}$ neutron capture reaction rate normalized by total flux
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Point Kinetics & TH Coupling
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$^{232}$Th refill rate

- Fluctuation due to batch-wise removal of strong absorbers
- Feed rate varies due to neutron energy spectrum evolution
- $^{232}$Th consumption is 100 g/GWh$_e$

Figure: $^{232}$Th feed rate over 20 years of MSBR operation
MOOSE Framework

- Fully-coupled, fully-implicit multiphysics solver
- MOOSE interfaces with libMesh to discretize simulation volume into finite elements
- Residuals and Jacobians handed off to PetSc which handles solution of resulting non-linear system of algebraic equations
- Automatically parallel (largest runs >100,000 CPU cores!)
- Built-in mesh adaptivity
- Intuitive parallel multiscale solves

Figure: Multi-physics Object-Oriented Simulation Environment (MOOSE).
Moltres (Coupling in MOOSE)

- **Moltres**: Describes MSR governing equations with residual functions.
- **MOOSE & LibMesh**: Discretize physics via FEM, couple PDEs & system of equations.
- **PetSc**: Solve algebraic system of equations using Newton methods.
Inro to Moltres

- Fluid-fuelled, molten salt reactors
- Multi-group diffusion (arbitrary groups)
- Advective movement of delayed neutron precursors
- Navier-Stokes thermal hydraulics
- 3D unstructured
- 2D axisymmetric
- 3D structured
Acquiring Moltres

```bash
git clone https://github.com/arfc/moltres
cd moltres
git submodule init
git submodule update
```
**Diffusion in Moltres**

\[
\frac{1}{v_g} \frac{\partial \phi_g}{\partial t} - \nabla \cdot D_g \nabla \phi_g + \Sigma^r_g \phi_g = \sum_{g \neq g'}^G \Sigma_{g' \to g}^s \phi_{g'} + \chi_g^p \sum_{g'=1}^G (1 - \beta) \nu \Sigma_{g' \to g}^f \phi_{g'} + \chi_g^d \sum_{i=1}^I \lambda_i C_i
\]  

(21)

\( v_g \) = speed of neutrons in group \( g \)  
\( \phi_g \) = flux of neutrons in group \( g \)  
\( t \) = time  
\( D_g \) = Diffusion coefficient for neutrons in group \( g \)  
\( \Sigma^r_g \) = macroscopic cross-section for removal of neutrons from group \( g \)  
\( \Sigma_{g' \to g}^s \) = macroscopic cross-section of scattering from \( g' \) to \( g \)  
\( \chi_g^p \) = prompt fission spectrum, neutrons in group \( g \)  
\( G \) = number of discrete groups, \( g \)  
\( \nu \) = number of neutrons produced per fission  
\( \Sigma_{g}^f \) = macroscopic cross section for fission due to neutrons in group \( g \)  
\( \chi_g^d \) = delayed fission spectrum, neutrons in group \( g \)  
\( I \) = number of delayed neutron precursor groups  
\( \beta \) = delayed neutron fraction
Moltres Delayed Neutrons

\[ \frac{\partial C_i}{\partial t} = \sum_{g'=1}^{G} \beta_i \nu \sum_{g' \neq f} \phi_{g'} - \lambda_i C_i - \frac{\partial}{\partial z} uC_i \] (38)
Moltres Fuel Temperature

\[
\rho_f c_{p,f} \frac{\partial T_f}{\partial t} + \nabla \cdot (\rho_f c_{p,f} \vec{u} \cdot T_f - k_f \nabla T_f) = Q_f
\]  

(39)

- \( \rho_f \) = density of fuel salt  
- \( c_{p,f} \) = specific heat capacity of fuel salt  
- \( T_f \) = temperature of fuel salt  
- \( \vec{u} \) = velocity of fuel salt  
- \( k_f \) = thermal conductivity of fuel salt  
- \( Q_f \) = source term = \( \sum_{g=1}^{G} \epsilon_{f,g} \sum_{f,g} \phi_g \)  

(40)  
(41)  
(42)  
(43)  
(44)  
(45)
\( \rho_g c_{p,g} \frac{\partial T_g}{\partial t} + \nabla \cdot (-k_g \nabla T_g) = Q_g \)  

(46)

\( \rho_g = \text{density of graphite moderator} \)  

(48)

\( c_{p,g} = \text{specific heat capacity of graphite moderator} \)  

(49)

\( T_g = \text{temperature of graphite moderator} \)  

(50)

\( k_g = \text{thermal conductivity of graphite moderator} \)  

(51)

\( Q_g = \text{source term in graphite moderator} \)  

(52)
Fig. 6. MSRE Reactor Vessel.
Table 2
Simulation input parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet temp.</td>
<td>922</td>
<td>$K$</td>
<td>MSRE nominal (Robertson, 1965)</td>
</tr>
<tr>
<td>Wall temp.</td>
<td>922</td>
<td>$K$</td>
<td>MSRE nominal (Robertson, 1965)</td>
</tr>
<tr>
<td>Neutron groups</td>
<td>2</td>
<td>1</td>
<td>User</td>
</tr>
<tr>
<td>Precursor groups</td>
<td>6</td>
<td>1</td>
<td>User</td>
</tr>
<tr>
<td>Reactor radius</td>
<td>72.5</td>
<td>cm</td>
<td>≈MSRE radius (70.2 cm) (Robertson, 1965)</td>
</tr>
<tr>
<td>Reactor height</td>
<td>151.75</td>
<td>cm</td>
<td>User</td>
</tr>
<tr>
<td>$k_f$</td>
<td>0.0553</td>
<td>W cm$^{-1}$ K$^{-1}$</td>
<td>User</td>
</tr>
<tr>
<td>$c_{p_f}$</td>
<td>1967</td>
<td>J K$^{-1}$ kg$^{-1}$</td>
<td>Robertson (1965)</td>
</tr>
<tr>
<td>$\rho_f$</td>
<td>2.146 $\cdot 10^{-3}$ e$^{-\eta(T_f - 922)}$</td>
<td>kg cm$^{-3}$</td>
<td>Robertson (1965)</td>
</tr>
<tr>
<td>$\gamma_f$</td>
<td>2.12 $\cdot 10^{-4}$</td>
<td>K$^{-1}$</td>
<td>Robertson (1965)</td>
</tr>
<tr>
<td>$k_d$</td>
<td>.312</td>
<td>W cm$^{-1}$ K$^{-1}$</td>
<td>Haubenreich and Engel (1970)</td>
</tr>
<tr>
<td>$c_{p_d}$</td>
<td>1760</td>
<td>J K$^{-1}$ kg$^{-1}$</td>
<td>Cammi et al. (2011)</td>
</tr>
<tr>
<td>$\rho_d$</td>
<td>1.86 $\cdot 10^{-3}$ e$^{-\eta(T_d - 922)}$</td>
<td>kg m$^{-3}$</td>
<td>Cammi et al. (2011)</td>
</tr>
<tr>
<td>$\zeta_d$</td>
<td>1.8 $\cdot 10^{-5}$</td>
<td>K$^{-1}$</td>
<td>Robertson (1965)</td>
</tr>
</tbody>
</table>

Figure: Data used in [7].
Table 1
Fuel salt composition is the BOL enriched uranium composition in the MSRE design (Robertson, 1965).

<table>
<thead>
<tr>
<th>Component</th>
<th>Mass fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li-7</td>
<td>.1090</td>
</tr>
<tr>
<td>Li-6</td>
<td>$5 \times 10^{-6}$</td>
</tr>
<tr>
<td>F-19</td>
<td>.6680</td>
</tr>
<tr>
<td>Be-9</td>
<td>.0627</td>
</tr>
<tr>
<td>U-235</td>
<td>.0167</td>
</tr>
<tr>
<td>U-238</td>
<td>.0344</td>
</tr>
</tbody>
</table>

Figure: Data used in [7].
Moltres (coupling in MOOSE)
Moltres Precursor Drift

The image contains several graphs with contour plots showing variations in concentration ($C$, in units of $cm^{-3}$) as a function of radial distance ($r$, in cm) and axial distance ($z$, in cm). Each graph represents different scenarios, labeled $C_1$, $C_2$, $C_3$, $C_4$, $C_5$, and $C_6$, with concentrations ranging from $10^{-4}$ to $10^{-5}$. The graphs illustrate how the concentration changes across different layers within a reactor or system, potentially depicting the spatial distribution of precursors under various conditions.

From the graphs, it appears that the concentration decreases with increasing axial distance ($z$) and is consistent across different radial distances ($r$), indicating a uniform distribution along the radial axis but a decrease along the axial direction. This could be indicative of a precursor reaction or diffusion process that is more active at the beginning of the reactor and diminishes as the reaction progresses or as the precursor is consumed.
Moltres MSRE Comparison

Fig. 11. Moltres and MSRE design (Briggs, 1964, p. 99) predicted axial temperature profiles in hottest channel and adjacent graphite.
Fig. 12. The thermal and fast flux profiles at the core mid-plane \((z = H/2)\) for the Moltres 2-D cylindrical axisymmetric model and the MSRE design model (Briggs, 1964, p. 92) \((r = 0\) is radial center of core).
**Fig. 13.** Moltres axial flux profiles along the core center line and MSRE design axial flux profiles 21.336 cm (8.4 inches) from the core center line (Briggs, 1964, p. 91).
Figure: Cuboidal MSR steady-state temperature and fast neutron flux tests by Gavin Ridley.
Ordinary tools cannot capture kinetics in mobile fuels or long term fuel cycle performance of liquid-fuelled reactors.

**SaltProc**
- New tool **SaltProc** was developed to simulate fuel depletion in MSRs.
- **SaltProc** was tested for the MSBR conceptual design, equilibrium fuel salt composition was found and verified against recent studies.

**Moltres**
- New tool **Moltres** was developed for modeling coupled physics in novel molten salt reactors.
- 2D-axisymmetric and 3D multiphysics models are presented.
- **Moltres** demonstrated strong parallel scaling (up to 384 physical cores) but further optimization required.
- Over 55,000 node-hours were consumed on **Blue Waters** to perform this research.
Future research

Future Directions

1. Improved TH capabilities in Moltres will enable more realistic precursor drift.
2. Equilibrium state search for Transatomic MSR (>30,000 node-hours).
3. Fuel cycle performance analysis for load-following regime (>40,000 node-hours).
4. Light Water Reactor (LWR) fuel transmutation in MSR viability (>30,000 node-hours).
5. Start exploring transients in Moltres, e.g. explore responses to reactivity insertion or gaseuous poison removal (>70,000 node-hours).
Acknowledgements

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- Alex Lindsay (Idaho National Laboratory), Gavin Ridley (University of Tennessee-Knoxville).
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Processing options for MSR fuels

- Elements that escape from fuel salt
- Elements that can be removed without processing
- Elements that can be removed only by chemical processing of fuel salt
Introduction
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BBBLE GENERATOR AND GAS SEPARATOR for MSBR
Chemical processing facility for MSBR
Introduction

Point Kinetics & TH Coupling

Spatial Kinetics & TH Coupling with Precursor Advection

Multiplication factor dynamics during Rb, Sr, Cs, Ba removal (3435 days)
MSBR neutron energy spectrum for different regions
Fissile isotopes in the MSBR core

![Graphs showing the normalized number density of various fissile isotopes over time.]

- U232
- Pu238
- Pu241
- Am241
- Am242
- Cm244
- Cm243
- Cm243
- Cf249
- Cf251

Time step [days]

Normalized number density
MSBR plain view