Molten Salt Reactor Analysis with SCALE

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Demonstrate capabilities for reactor physics and fuel cycle analyses of liquid-fueled systems

- Primary concern is modeling material moving in and out of fuel mixtures during irradiation
- Focus is on new mixture flow definitions with the TRITON module
  - Development of a computational model
  - Verification activities for material flow scenario
  - Postprocessing to perform fuel cycle analysis
- ORIGEN for comparative simplified analysis
- ORIGEN for resolving short-time phenomena

Introductions of the tutorial participants with desired application space
Liquid-fueled molten salt reactors are any reactor technology that dissolves fuel within a carrier salt

- Fast spectrum molten salt reactor (MSR) cores usually have large volumes of salt
- Thermal spectrum MSR cores incorporate fixed moderator material
- Multiple fuel stream designs include
  - Different salt compositions
  - Fissile and fertile salt compositions
- Multiple spectrum zones include
  - Different fuel-to-moderator ratios
  - Driver and blanket zones for breeding

SCALE Reactor Physics
Computational Tools
SCALE Reactor Physics Calculations

The Physics

3 fundamental parts:

Cross section processing in case of multigroup calculations
- Cross Section Library
- Material Concentrations
- Geometry
- Temperature

Cross Section Processing
- MG Cross sections

Multigroup (MG) or continuous-energy (CE) neutron transport
- MG or CE Cross sections
- Material Concentrations
- Geometry

MG or CE Transport
- k-effective
- Flux-dependent QOIs

Depletion
- Material Concentrations
- Material Transition Matrices
- Power level
- Time step

Depletion/Decay
- New Material Concentrations

Automatic execution of these parts through SCALE’s control sequence **TRITON**
The Multi-Group Control Sequence

TRITON sequence functions include:

- Cross section processing with XSProc
- Neutron transport:
  - 1D (XSDRN), 2D (NEWT), or 3D (KENO)
- Transport-to-depletion coupling
  - Normalizes power/flux levels
  - Prepares transition matrices for ORIGEN
  - Manages time-stepping (predictor-corrector)
- Branch calculations for 2-D lattice physics analysis
- Model updates
  - From depletion: concentration changes
  - From user input: Geometry, temperature, concentration changes

• Output (.out)
• Few-group XS File (.t16)
• ORIGEN Concentration File (.f71)
• ORIGEN Library File (.f33)
The depletion equation, as solved by ORIGEN

\[
\frac{dN_i}{dt} = \sum_{j=1}^{m} l_{ij} \lambda_j N_j + \bar{\Phi} \sum_{k=1}^{m} f_{ik} \sigma_k N_k - (\lambda_i + \bar{\Phi} \sigma_i + r_i)N_i
\]

\[
\frac{d\bar{N}(x, t)}{dt} = \bar{A}(x, t) \bar{N}(x, t)
\]
Molten Salt Reactor
Physics Tools
SCALE approaches for MSR

• TRITON-MSR (new in SCALE 6.3 currently in beta)
  – Ability to account for flowing fuel materials in a liquid-fueled system
    • Material feeds and removal with specific rates to and from depleted materials
    • Tracking of removed materials that are not irradiated
  – Draws on reactor physics tools within the SCALE code system
    • Neutron transport and depletion
    • Strong quality assurance program

• ORIGEN standalone (available in any SCALE version)
  – Investigate inventory throughout system following “slugs” of fuel
  – Uses standard ORIGEN input (with transformation from time \rightarrow length coordinates)
  – Requires knowledge of core neutron spectrum \rightarrow cannot easily take into account changes in inventory that greatly affect spectrum
Workflow to generate time-dependent power distributions and material compositions for MELCOR

\[ P_d(z,t) \]

\[ P_f(r,z,t) \]

\[ N_i(z) \]

\[ \phi_n(z) \]

Core Slice (axial. refl.)

.f33, .f71 files

SCALE

TRITON-KENO

Full Core

System Loop

ORIGEN

TRITON-KENO ORIGEN

\( P_P(d,\theta) (z,t) \)
There is a role for simulations of multiple levels of fidelity within a reactor analyst’s toolbox

- Well-stirred pot assumption with the scaled flux approximation is appropriate and ideal for long-term fuel cycle simulations
- Simplified flow characterizations can help identify key phenomena or impacts of material movement
- High-fidelity simulations can provide more meaningful results

<table>
<thead>
<tr>
<th>Scaled flux</th>
<th>Advection depletion</th>
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<tbody>
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<td>• Fuel cycle simulation</td>
<td>• Spatial composition distribution</td>
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<td>• Long time composition</td>
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</table>
The TRITON-MSR flow block defines material movement

• TRITON offers a FLOW block that allows users to specify fractional removal and continuous feed from/to mixture.

\[
\frac{dN_i}{dt} = \sum_{j \neq i} (l_{ij}\lambda_j + f_{ij}\sigma_i\phi)N_j(t) - \left(\lambda_i + \sum_k \lambda_{rem,ik} + \sigma_i\phi\right)N_i(t) + S_i(t)
\]

• Example: Th-based MSR unit cell model.
  - Removal of Pa and Nd from irradiated mixture into initially empty mixtures 2 and 3:
    \[\lambda_{rem,mix1\rightarrow mix2}\]
  - Pa and Nd concentrations in waste mixtures 2 and 3 reach equilibrium based on the removal rate from mixture 1 and their decay rates.
  - TRITON determines the equivalent source for mix 2:
    \[S(t) \approx \lambda_{rem,mix1\rightarrow mix2}N(t)\]

1 "Molten Salt Reactor Fuel Depletion Tools in SCALE" (2019).
Example TRITON-MSR flow definitions for feeds and removal & tracking

**FLOW block for continuous feed of nuclides into a mixture:**

```plaintext
read timetable
  flow
    to I2
    type continuous_feed
    units [pers or gpers]
    nuclides [N1 N2 ... NM] end
    rates [R1 R2 ... RM] end
    time [t1 t2 ... tC] end
    multiplier [f1 f2 ... fC] end
  end flow
end timetable
```

**FLOW block for fractional removal of nuclides from one mixture to another:**

```plaintext
read timetable
  flow
    from I1 to I2
    type fractional_removal
    units [pers or gpers]
    nuclides [N1 N2 ... NM] end
    rates [R1 R2 ... RM] end
    time [t1 t2 ... tC] end
    multiplier [f1 f2 ... fC] end
  end flow
end timetable
```
Technical workflow for the use of TRITON-MSR tools

**Input**

- Define TRITON-NEWT 2D model.
- Define flow/removal rates between mixtures.
- New decay-only mixtures can be defined to represent an out-of-core inventory, e.g., tanks.
- Must scale down power to adjust for out-of-core salt in the main loop.

**Output**

- Inventory of every mixture is produced as a function of time.
- ORIGEN 1-group cross sections libraries for each mixture is also generated.
- Use OPUS or convert the isotopic data to generate isotopic composition in time.

**Analysis**

- Outputs must be normalized to provide the total amount in the system or relevant densities
- Relate these trends in terms of burnup or masses

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**Example Code**

```plaintext
read timetable
'gaseous fission product removal
flow
from 1 to 7
  type continuous
  units perm
  nuclides Xe  Kr end
  rates  4.067e-5  4.067e-5 end
  time  0.0 end
  multiplier 1.0 end
end flow
'thorium feed
flow
  to 1
  type continuous
  units gpero
  nuclides u-238 u-235 end
  rates  0.65  0.35 end
  time  0.0 end
  factor 3.63256e-04 end
end flow
end timetable
```
TRITON-MSR Tutorial Problem 1a

- Run the provided starter problem
- Read the .f71 file to determine the depletion rate of fissile and/or fertile material
- Save as a new file and define a feed rate to compensate for the depletion of the material
- Rerun, and examine the .f71 file
- Make time-dependent plots
TRITON-MSR Tutorial Problem 1b

- Save as a new file and define removals to two additional waste mixtures using the composition definition and decay only option
  1. Pump bowl: 99% efficient removal of noble gases Xe and Kr
  2. Process bypass: 50% efficient removal of noble metals Se, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Sb, and Te
- Rerun, and examine the .f71 file
- Make time-dependent plots

Diagram:
- Reactor Core
- Heat Exch.
- Pump
- Process bypass
- 5% → 95% → 20 second loop time
TRITON-MSR Tutorial Problem 2

• Replicate tutorial problem 1 with ORIGEN
ORIGEN-MSR
To characterize physical flow processes, consider additional terms describing the flow behavior

- The reaction-advection-diffusion equation takes on a general form

\[ \frac{d\tilde{N}}{dt} = A(\tilde{x}, t)\tilde{N}(\tilde{x}, t) - \nabla \cdot [u(\tilde{x}, t)\tilde{N}(\tilde{x}, t) - D(\tilde{x}, t)\nabla \tilde{N}(\tilde{x}, t)] + \dot{S}(\tilde{x}, t) \]

- Ignoring diffusion yields the reaction-advection equation

\[ \frac{d\tilde{N}}{dt} = A(\tilde{x}, t)\tilde{N}(\tilde{x}, t) - \nabla \cdot [u(\tilde{x}, t)\tilde{N}(\tilde{x}, t)] + \dot{S}(\tilde{x}, t) \]

- Lagrangian flow specification can eliminate the spatial dependence in the reaction-advection equation

- For a simplified one-dimensional problem, this specification essentially becomes a slug (or plug) flow model
Pursue near term functionalities to solve the reaction-advection equation for a simple MSR primary loop

• Leverage a standard SCALE simulation to yield an estimate of the spatial distribution of all radioisotopes within a simplified molten salt reactor loop

• Relies on recasting the equation

\[
\frac{d\bar{N}(x, t)}{dt} = \bar{A}(x, t) \bar{N}(x, t) - \nabla \cdot (\mathbf{u}(x, t) \bar{N}(x, t)) + \bar{S}(x, t)
\]

and assume a slug flow model (no mixing in the direction of flow)

An approximation of the radioisotope distribution (\(^{138}\)Xe shown above) within the primary loop of the Molten Salt Reactor Experiment showing the generation of the gas within the core (from fission) and its removal within the pump.
TRITON-MSR Tutorial Problem 3

• Generate short-time phenomena with ORIGEN