Molten Salt Reactor Analysis with SCALE

Benjamin Betzler
Donny Hartanto
Research & Test Reactor Physics Group
Nuclear Energy & Fuel Cycle Division

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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

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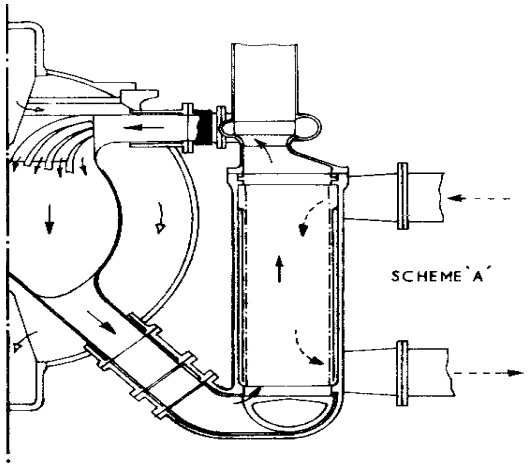
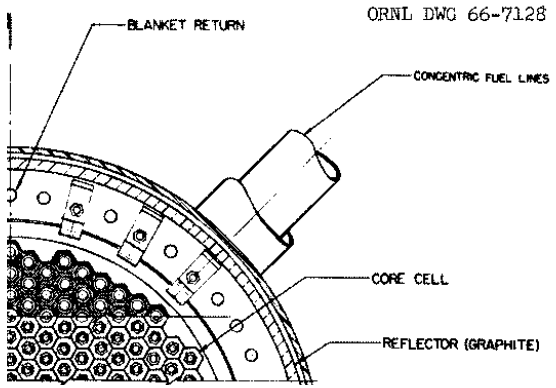
Liquid-fueled molten salt reactors are any reactor technology that dissolves fuel within a carrier salt

- 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



½-core fast spectrum design.[1]



¼-core thermal spectrum design.[2]

[1] "An Assessment of a 2500MWe Molten Chloride Salt Fast Reactor" (1974).
[2] "Design Studies of 1000-MW(e) Molten-Salt Breeder Reactors" (1966).

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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**

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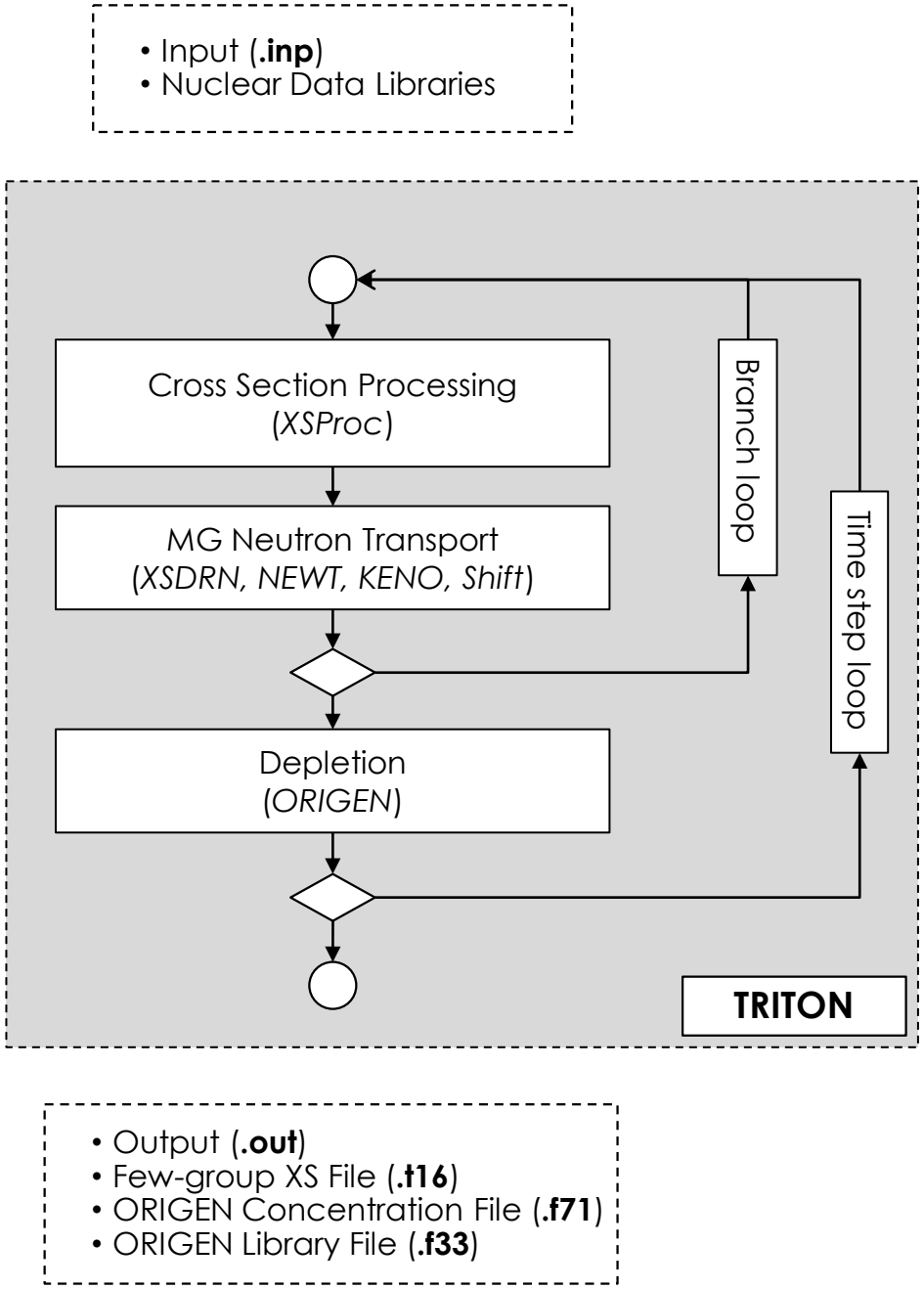
The **Multi-Group** Control Sequence

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



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The depletion equation, as solved by ORIGEN

Rate of Change in Nuclide Concentration = Production Rate of Nuclide − Loss Rate of Nuclide

Rate of Change in Nuclide Concentration = Decay into Nuclide by other Nuclides + Production of Nuclide from Irradiation − Loss of Nuclide through Decay, Irradiation, or Other Means

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

$$\frac{d\bar{N}(\mathbf{x},t)}{dt} = \bar{\bar{A}}(\mathbf{x},t)\,\bar{N}(\mathbf{x},t)$$

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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 → length coordinates)
  - Requires knowledge of core neutron spectrum → cannot easily take into account changes in inventory that greatly affect spectrum

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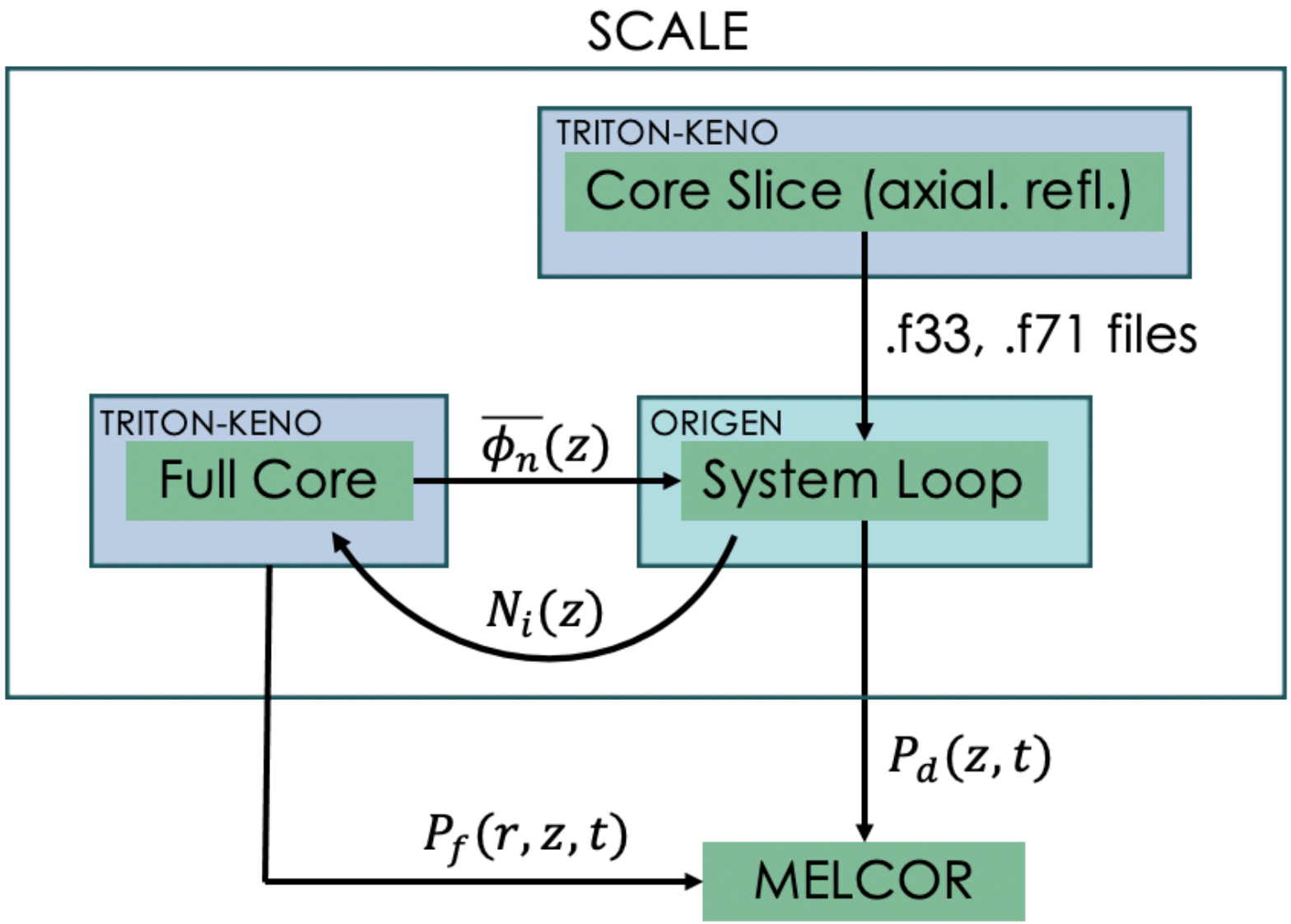
Workflow to generate time-dependent power distributions and material compositions for MELCOR



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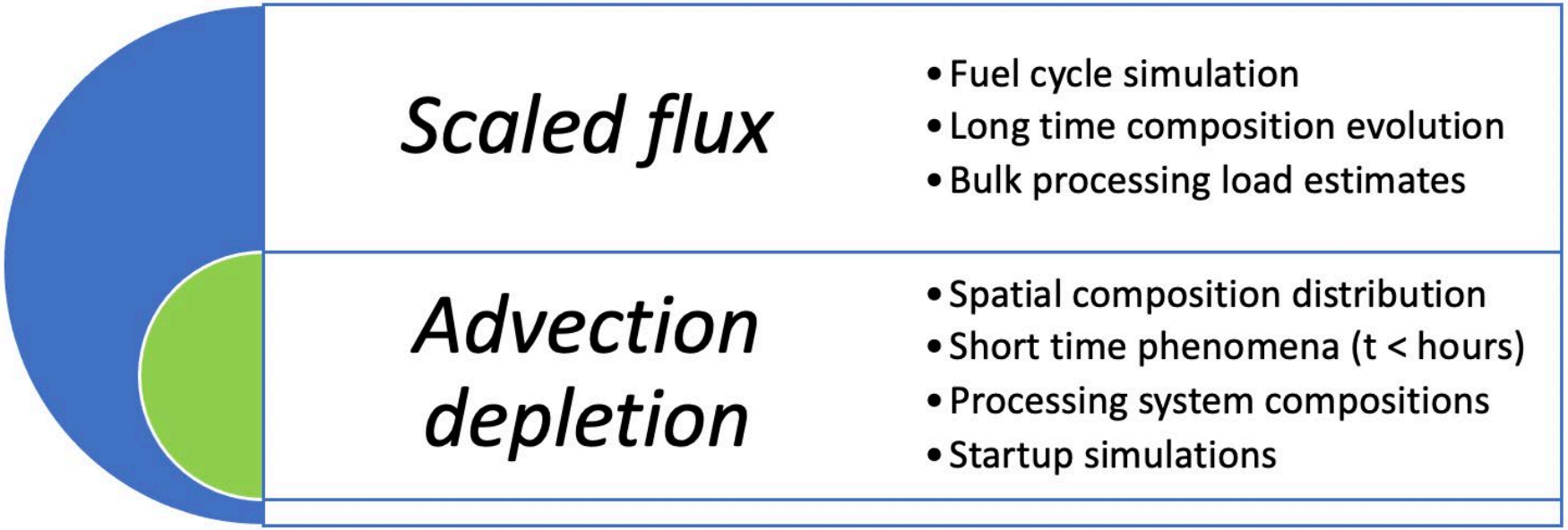
There is a role for simulations of multiple levels of fidelity within a reactor analyst's toolbox

- 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



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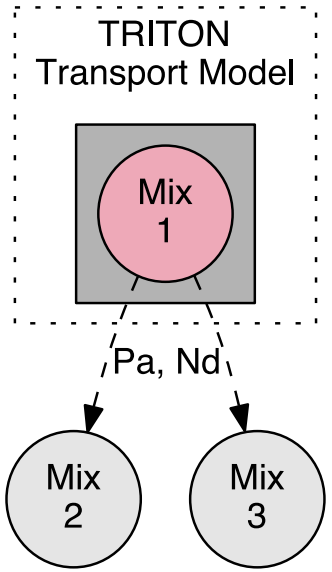
TRITON-MSR

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.

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

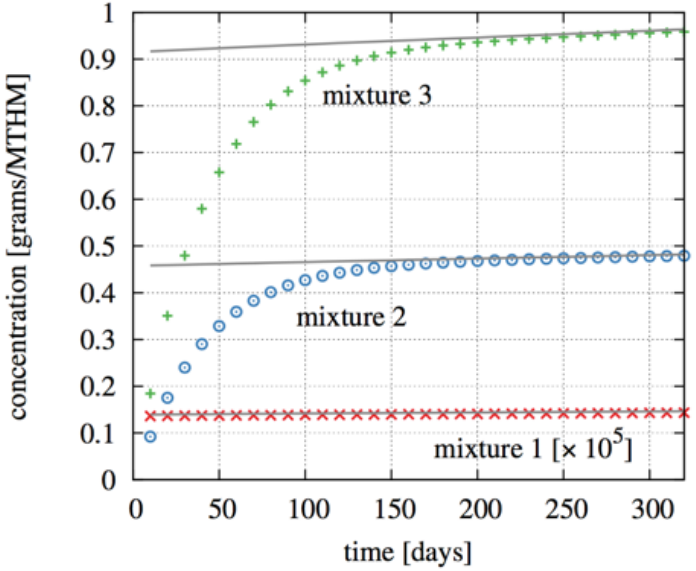


- Example: Th-based MSR unit cell model.
  - Removal of Pa and Nd from irradiated mixture into initially empty mixtures 2 and 3:

$$\lambda_{rem,mix1 \rightarrow mix2}$$

  - 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).
[2] "Modeling Molten Salt Fission Product Removal with SCALE" (2020).

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Example TRITON-MSR flow definitions for feeds and removal & tracking

FLOW block for continuous feed of nuclides into a mixture:

```
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:

```
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
```


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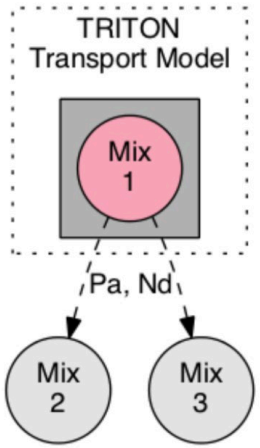
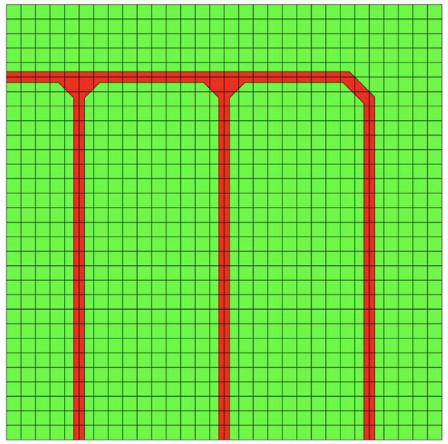
Technical workflow for the use of TRITON-MSR tools

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.





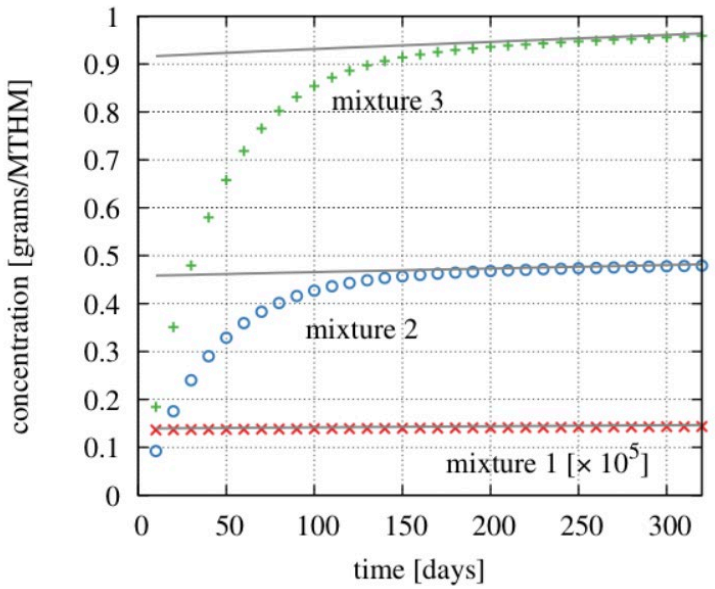
Output

- 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.

```
read timetable
'gaseous fission product removal
  flow
    from 1 to 7
    type continuous
    units pers
    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 gpers
    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
```

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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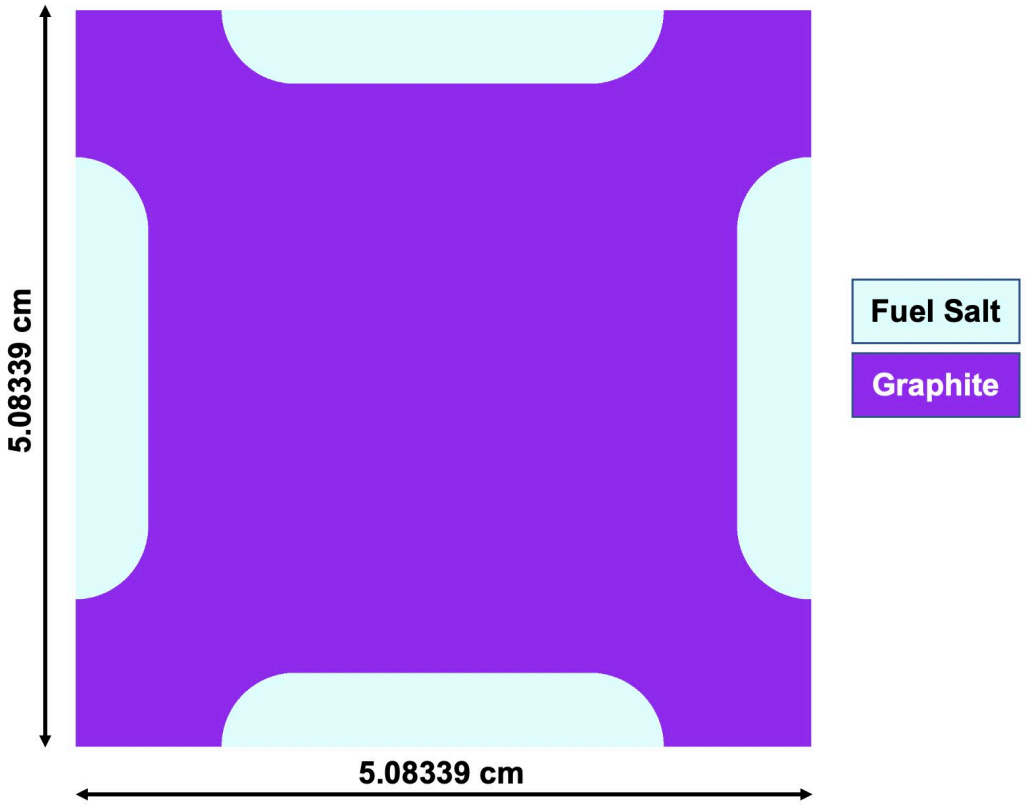
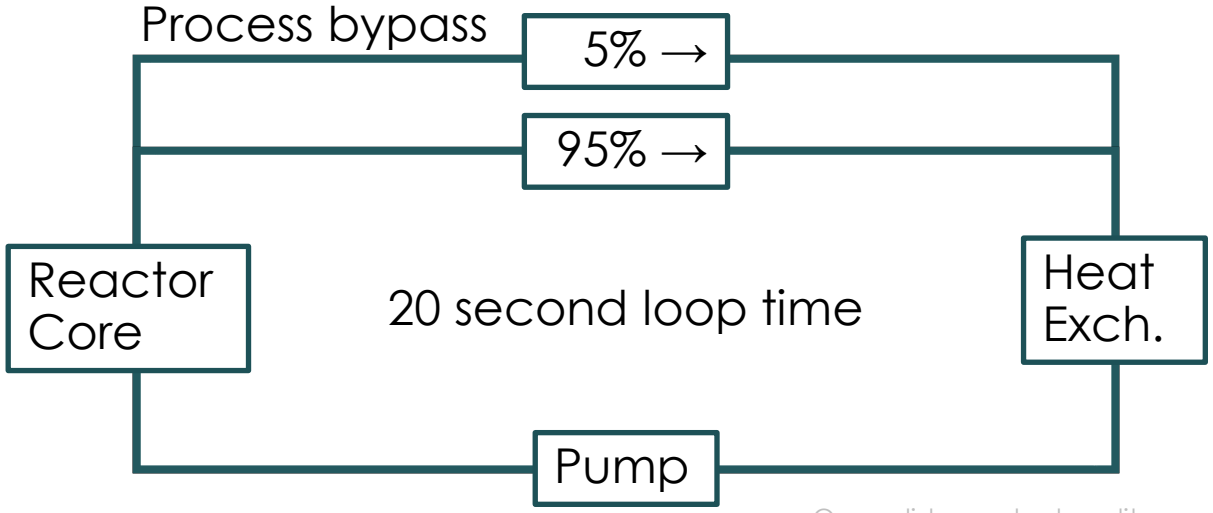
TRITON-MSR Tutorial Problem 1a

- 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





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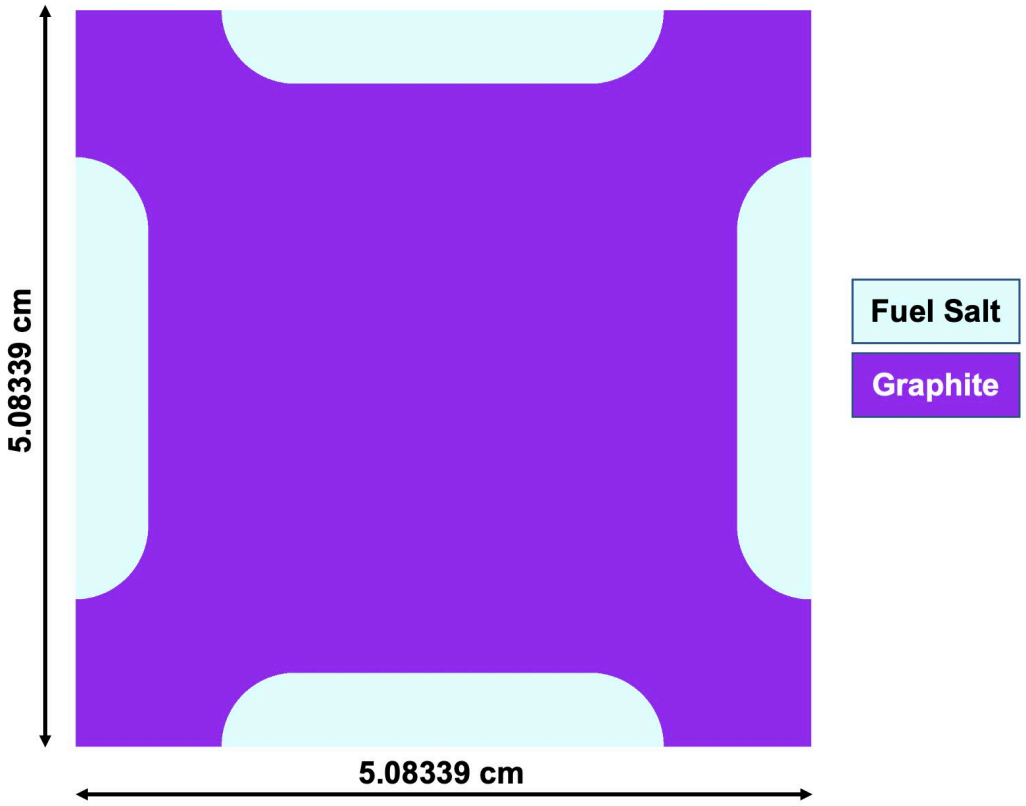
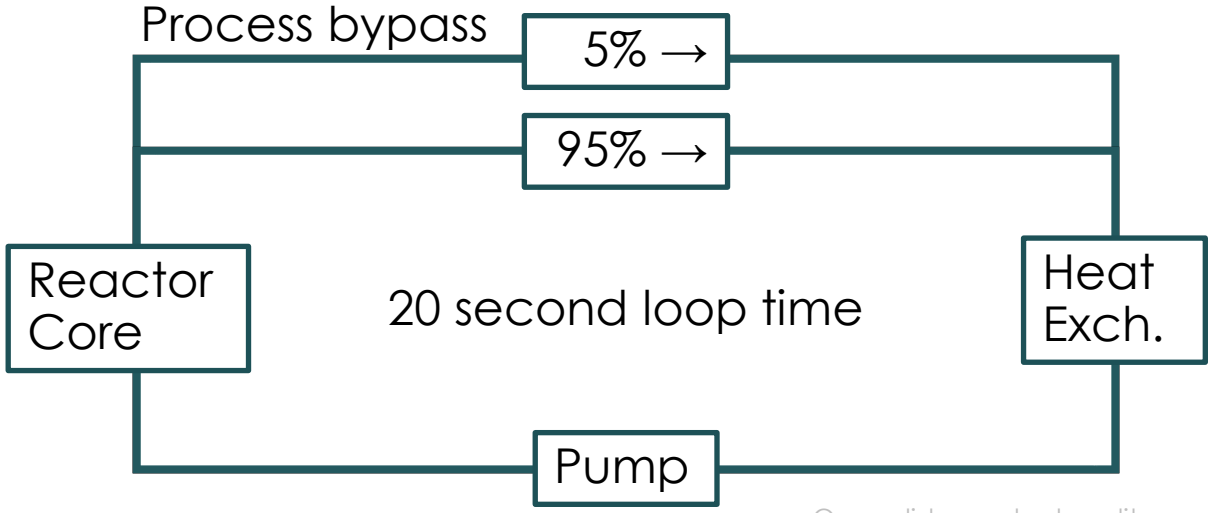
TRITON-MSR Tutorial Problem 1b

- 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





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TRITON-MSR Tutorial Problem 2

- Replicate tutorial problem 1 with ORIGEN

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ORIGEN-MSR

To characterize physical flow processes, consider additional terms describing the flow behavior

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

$$\frac{d\vec{N}}{dt} = \boldsymbol{A}(\vec{x},t)\vec{N}(\vec{x},t) - \nabla \cdot \left[\mathbf{u}(\vec{x},t)\vec{N}(\vec{x},t) - \boldsymbol{D}(\vec{x},t)\nabla\vec{N}(\vec{x},t)\right] + \vec{S}(\vec{x},t)$$

- Ignoring diffusion yields the reaction-advection equation

$$\frac{d\vec{N}}{dt} = \boldsymbol{A}(\vec{x},t)\vec{N}(\vec{x},t) - \nabla \cdot \left[\mathbf{u}(\vec{x},t)\vec{N}(\vec{x},t)\right] + \vec{S}(\vec{x},t)$$

- 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

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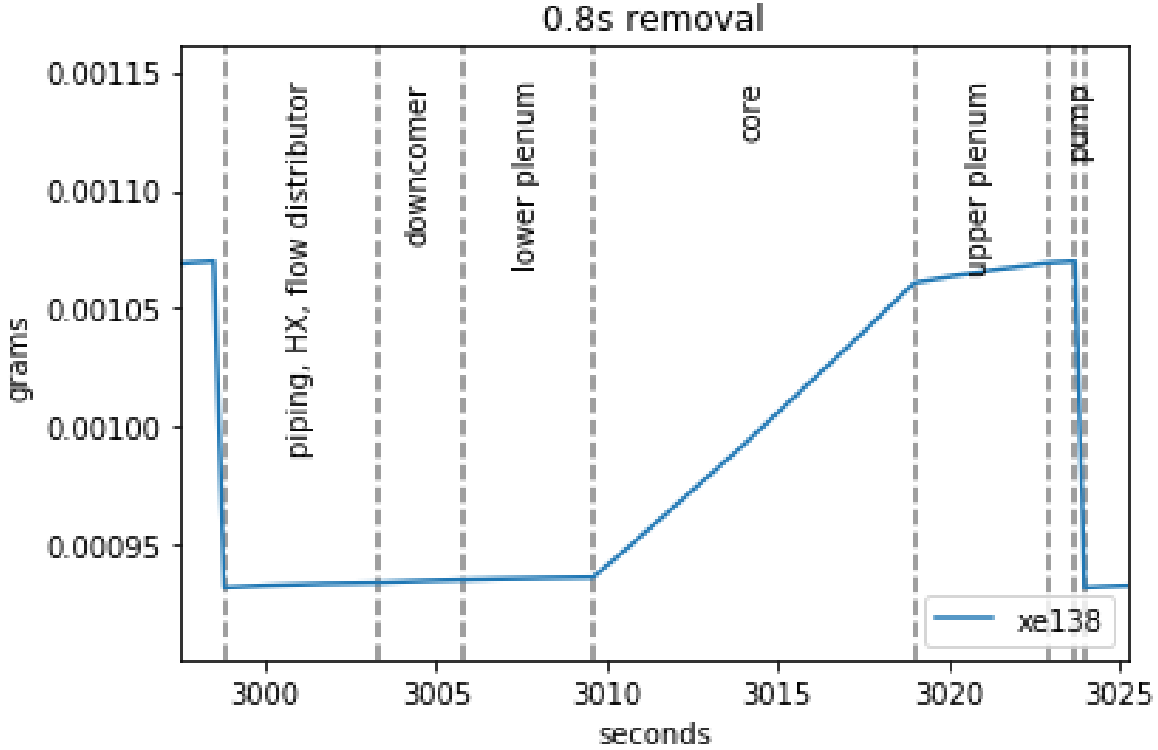
Pursue near term functionalities to solve the reaction-advection equation for a simple MSR primary loop

- 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

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

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.

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TRITON-MSR Tutorial Problem 3

- Generate short-time phenomena with ORIGEN

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