Molten Salt Reactor Analysis with SCALE

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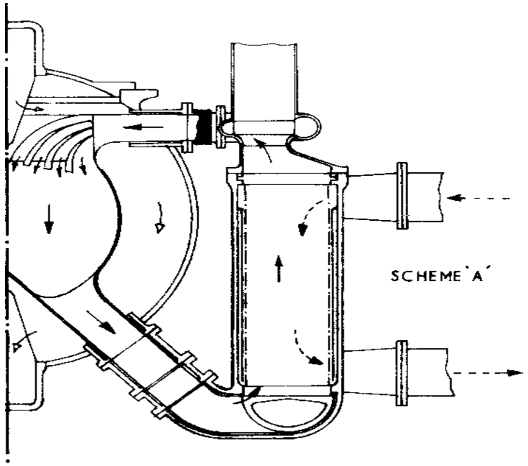
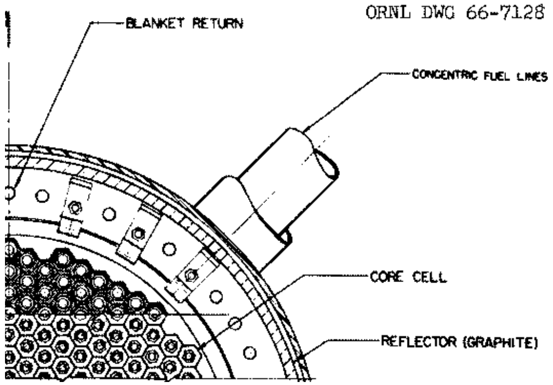
SCALE Users' Group Workshop
Oak Ridge National Laboratory
April 26–28, 2023

Introduction

- **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]

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[1] “An Assessment of a 2500MWe Molten Chloride Salt Fast Reactor” (1974).

[2] “Design Studies of 1000-MW(e) Molten-Salt Breeder Reactors” (1966).

Introduction

Key differences of Molten Salt Reactors (MSRs) to LWRs for Mod&Sim:

- Continuous circulation of the fuel
- Consideration of both core and loop
- Nuclide removal from the fuel (fission product removal)
- Nuclide feed to the fuel (refueling)

Results of interest:

- System-average fuel salt composition as a function of time
- Location-dependent fuel salt inventory in the system
- Neutronic characteristics (reactivity, power distribution, etc.) at specific point in time

SCALE features of interest:

- TRITON-KENO/Shift using flow block
- ORIGEN using removal feature

Tutorials Goals

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

- Focus is on new mixture flow definitions with the TRITON module introduced in SCALE 6.3:
  - Learn how to set up removal rate in FLOW block input.
  - Learn how to read isotopic inventory using FULCRUM and OBIWAN.
  - Learn how to set up feed rate in FLOW block input.

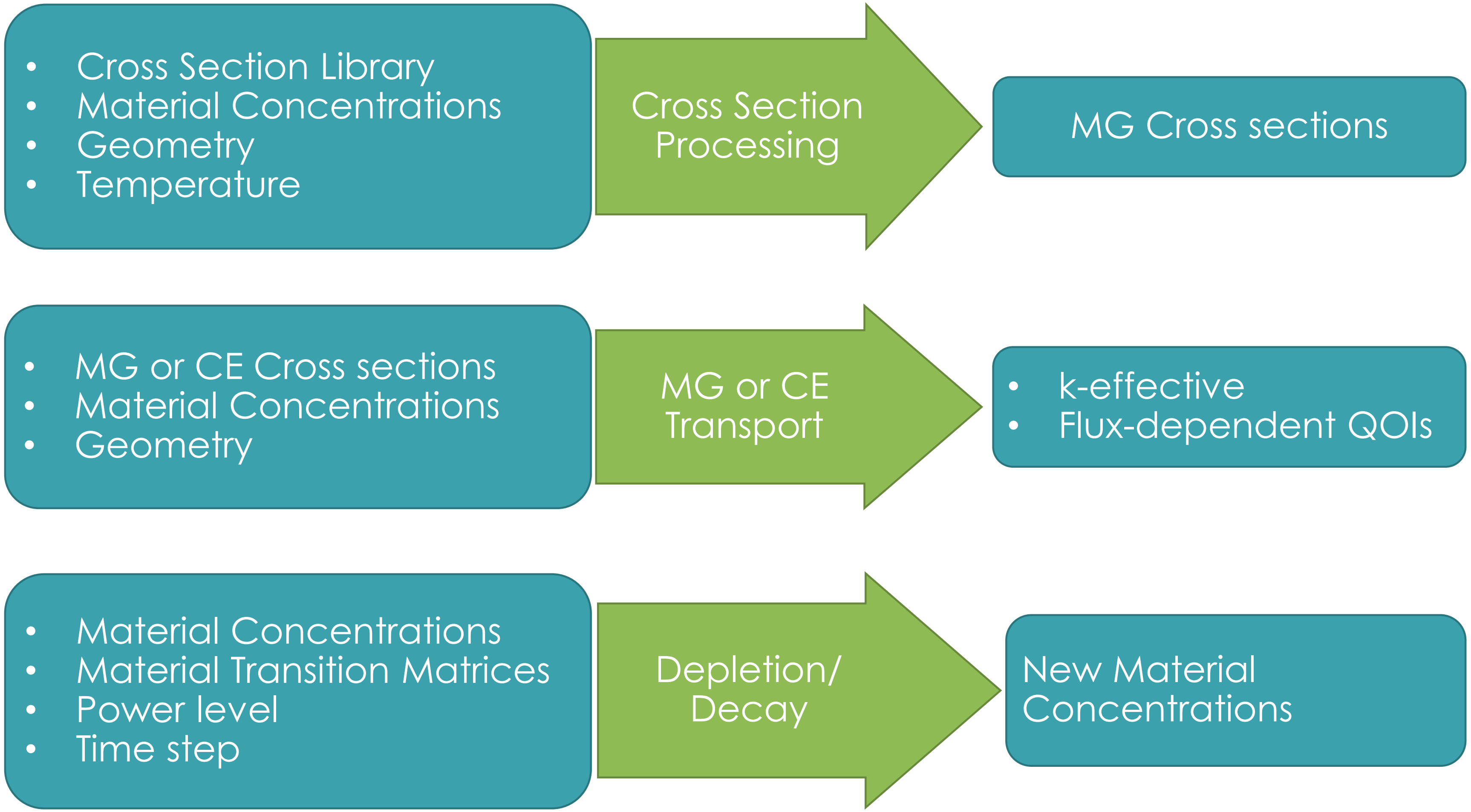
- Additional demonstration using ORIGEN with removal feature for comparative simplified analysis.

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**

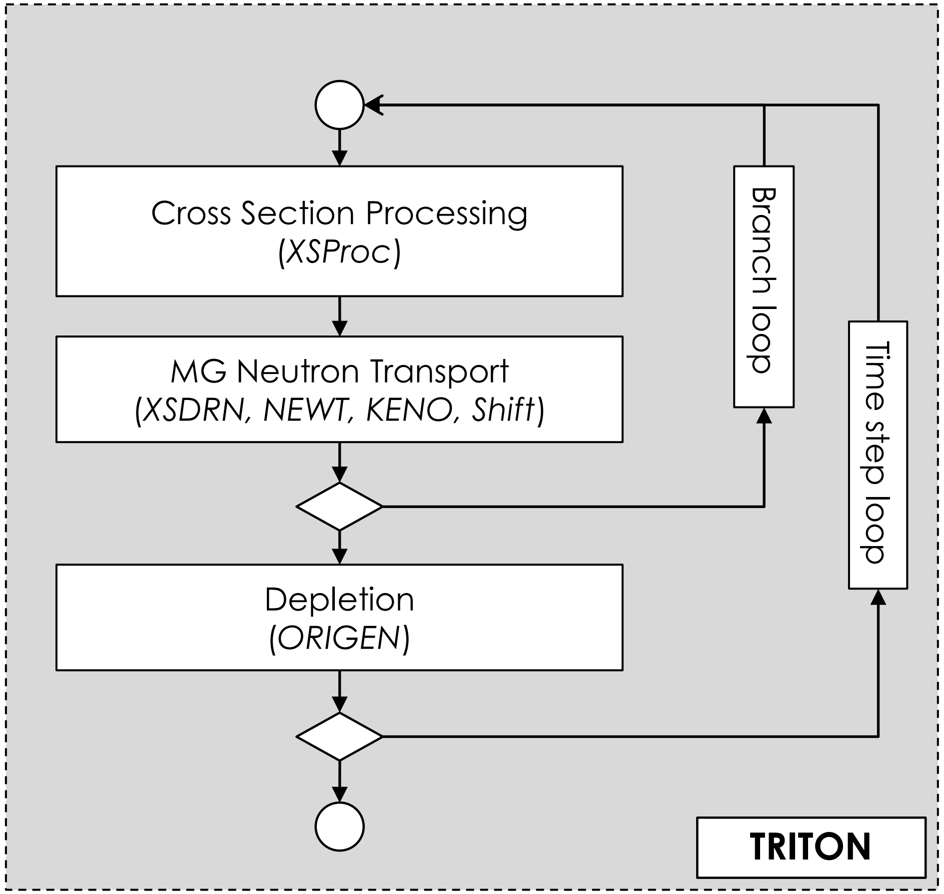
The **Multi-Group** Control Sequence

- Input (**.inp**)
- Nuclear Data Libraries

TRITON sequence functions include:

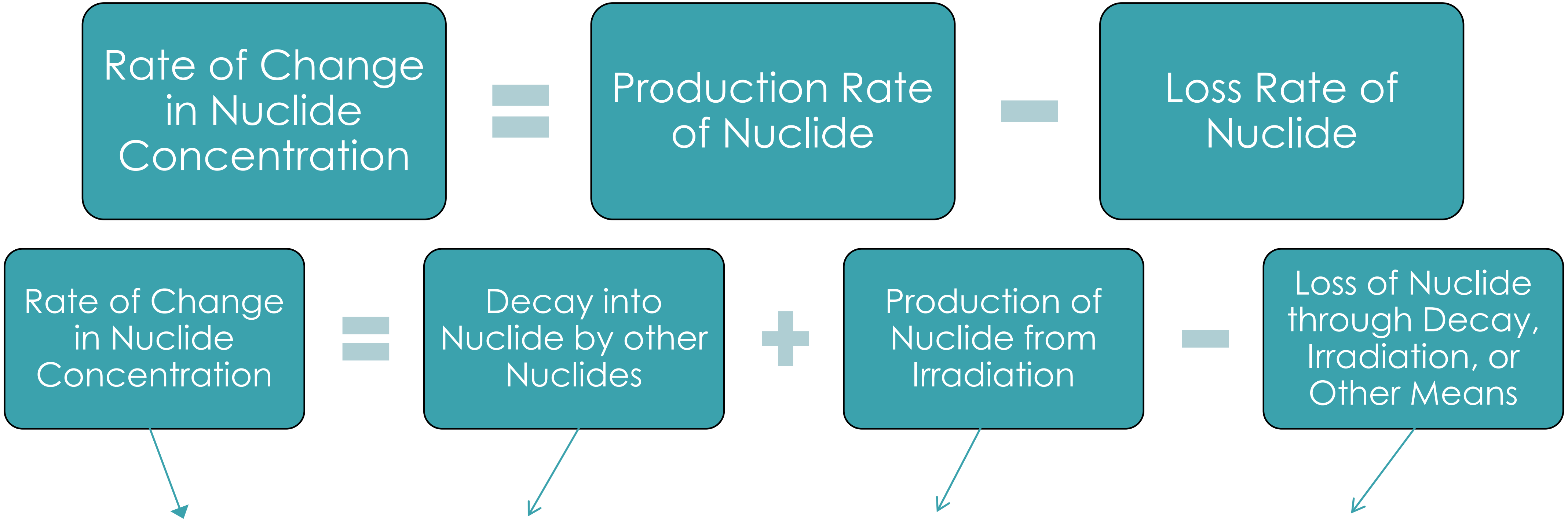
- Cross section processing with XSProc
- Neutron transport:

  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



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

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

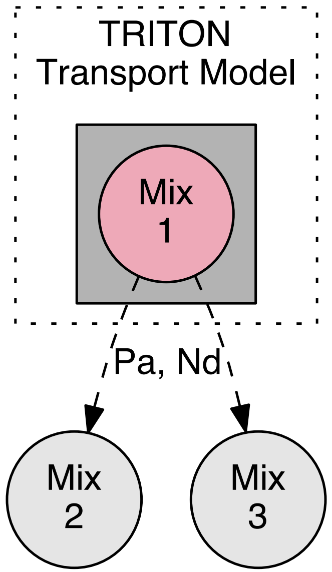
$$\frac{d\bar{\mathbf{N}}(\mathbf{x},t)}{dt} = \bar{\bar{\mathbf{A}}}(\mathbf{x},t)\,\bar{\mathbf{N}}(\mathbf{x},t)$$

SCALE Molten Salt Reactor Physics Tools

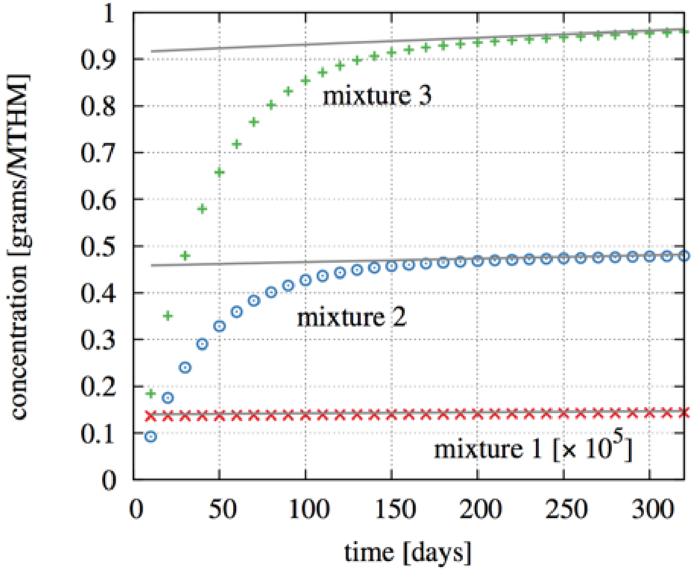
TRITON FLOW Block

- 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:
    $$S(t) \approx \lambda_{rem,mix1\rightarrow mix2}N(t)$$



TRITON FLOW Block

- TRITON's **FLOW** block was introduced
- Subblock of the **TIMETABLE** block that determines time-dependent nuclide feed or removal
- Input parameters:
  - I = mixture ID
  - **from** (**to**) = identifier from which mixture nuclides are removed (from I1) and to which mixture they are added (to I2)
  - **type** = type of addition or removal of nuclides from/to mixture:
    - **fractional_removal** requires from and to
    - **continuous_feed** requires to and does not permit from
  - **units** = unit of the flow rate constant used:
    - removal: **pers** (1/second)
    - feed: **gpers** (grams/second), **kgpers** (kg/second), **molpers** (moles/second)
  - M = number of **nuclides** to which change is applied
  - N_i = nuclide ID for the ith nuclide in the list, i = 1 to M
  - R_i = **rates** for the ith nuclide in the list, i = 1 to M
  - t_j = **time** (days) in calculation where multiplier f_j is set, i = 1 to C
  - f_j = **multiplier** to vary specified flow rate at time t_j, i = 1 to C
  - C = number of time steps.

```
read timetable
 flow
  from I1 to I2
  type fractional_removal
  units       [pers]
  nuclides    [N1 N2 ... NM]   end
  rates       [R1 R2 ... RM]   end
  time        [t1 t2 ... tC]   end
  multiplier [f1 f2 ... fC]   end
 end flow
end timetable
```

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

TRITON FLOW Block – Nuclide-specific rates

- In case of overlapping specifications in the nuclide block, the assigned rates are processed in the order: all > element > nuclide
- Example:

```
nuclides u     all   u-235  end
rates    1e-3  1e-4  1e-5   end
```

- The above block is processed in the following order:
  - assign rate **1e-4** to **all**
  - assign rate **1e-3** to **u**
  - assign rate **1e-5** to **u-235**
- In other words:
  - a rate of 1e-5 is assigned to U-235
  - a rate of 1e-3 is assigned to all uranium isotopes besides U-235
  - a rate of 1e-4 is assigned to all nuclides besides all uranium isotopes
- The order in which ”all”, elements, and nuclides are specified is irrelevant

TRITON FLOW Block – Decay of mixtures outside the system

- TRITON now permits mixtures outside of the system, not experiencing flux, but considering nuclide decay
  - Example: Nuclides in off-gas system, waste storage, etc

- Decay in mixtures is enabled via keyword **decayonly** in the DEPLETION block

- These decayonly mixtures are only existing on the ORIGEN side, but not in the neutron transport model

- Their volume is by default set to 1 cm^3 and their mass is set according to the specified density for this volume (see data on ORIGEN concentration file)

- TRITON’s mass normalization is not affecting the volumes or masses of these mixtures.

```
read depletion
 -1 decayonly 2
end depletion

read timetable
 flow from 1 to 2
  type fractional_removal
  units pers
  nuclides     xe  end
  rates      2e-2  end
  time       0.0   end
  multiplier 1.0   end
 end flow
end timetable
```

TRITON FLOW Block – Nuclide removal and feed interaction

- In removal mode, users might observe slight inconsistencies in the removed compared to the fed nuclide amounts after a TRITON depletion/decay step
- In the absence of any other nuclide production or removal mechanism, the nuclide density in the source material is:

$$\frac{\mathrm{d}N_i}{\mathrm{d}t} = -\lambda_{i,rem} N_i(t)$$

- In order to connect the removal from source material to the feed rate into the target material, the removal is integrated numerically over a substep and recast as a nuclide feed for this specific substep **s**:

$$S_{i,s} = \int_{t_{s-1}}^{t_s} \lambda_{i,rem}\, N_i(t)\mathrm{d}t$$

- The approximation for N_i over a substep uses a weighted essentially non-oscillatory (WENO)–like scheme that takes the nuclide amounts at the beginning and end of a substep and determines a combination of logarithmic and linear interpolation.
- **If there are particularly strong removals, then it may be necessary to introduce additional small time steps** (i.e., additional depletion/decay steps in the BURNDATA block) to better handle the numerical integration on the substeps.

TRITON FLOW Block – Removal and feed rate

Removal Rate

- Commonly, the removal of fission products is specified in cycle time T_c [unit of time], defined as the time to process the whole salt at a specific rate.

$$T_c = \frac{V_{tot}}{\dot{v}}$$

- Considering the isotope removal efficiency ϵ_i, the isotope removal rate then can be calculated as:

$$\lambda_{r,i} = \frac{\epsilon_i}{T_c}[1/s]$$

Feed Rate

- Constraint:
  - Keep the amount of all nuclides, only actinides, or actinides and fission products constant.
  - The amount kept constant can be the number of atoms or the mass.
- Procedure:
  - Perform a TRITON calculation that includes only the fractional removal block.
  - Get the amount (e.g., of U-235) that was removed from the fuel salt through depletion
  - Calculate the feed rate $[\text{unit of mass}/s]$ from the amount removed.

Hombourger, B., Křepel, J., & Pautz, A. (2020). The EQL0D fuel cycle procedure and its application to the transition to equilibrium of selected molten salt reactor designs. Annals of Nuclear Energy, 144. doi:10.1016/j.anucene.2020.107504

TRITON FLOW Block – Notes

- Removal or feed rates are provided for each nuclide
- Multipliers are used to modify a specified rate over time if desired
- t1 in the time array must be 0.0
- The multiplier is interpreted based on the initial flow rate
- The feed rate is adjusted with TRITON’s mass normalization factor to correctly consider feed to normalized mixture mass
- Just as for temperature and density changes, **TRITON applies linear interpolation between the data provided at specific times.** To hold a rate/multiplier pair constant over a time interval, that rate/multiplier pair should be specified at the same value at both the beginning and the end of this time interval.

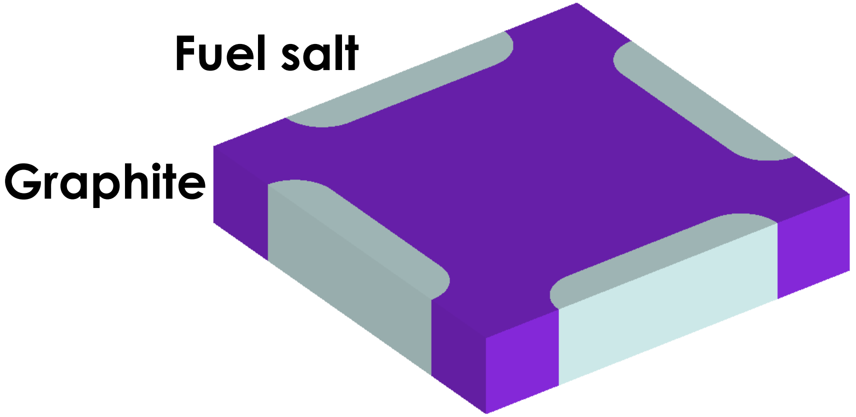
Warning: The unit for continuous feed is not correctly converted in SCALE 6.3.0. This issue is fixed in SCALE 6.3.1. **Workaround for SCALE 6.3.0:** The desired target rate R in gram/second can be requested by specifying instead R x avogadro_constant x 1e-24 / molar_mass. Then, an additional multiplication with the mass normalization factor must be performed.

Note: Fulcrum of SCALE 6.3.0 shows some validation errors although the FLOW block might be valid. The calculation will still run. This issue is fixed in SCALE 6.3.1.

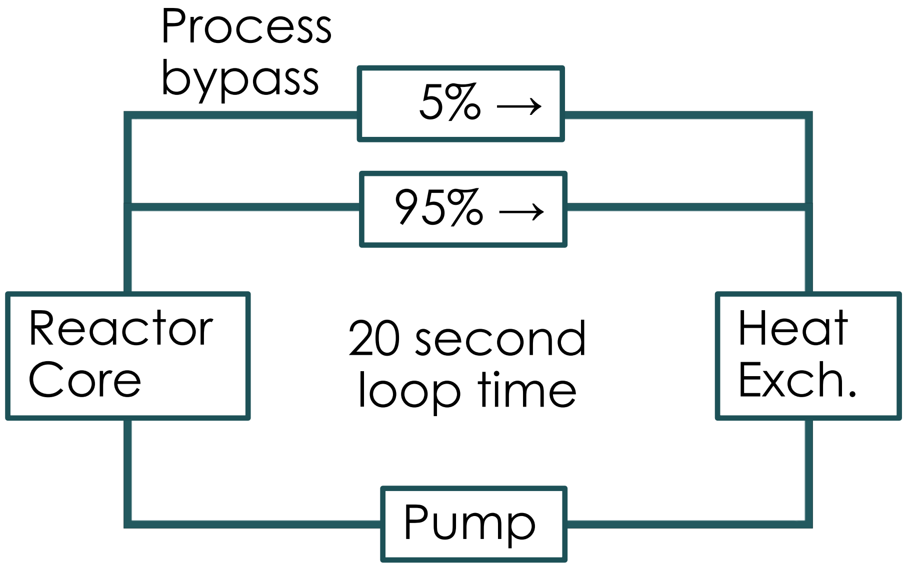
Workshop

Tutorial Problem 1a

- Open "*msre_stringer_starter.inp*" and save as "*msre_stringer_removal.inp*"
- Create two mixtures, mix 11 and 12, to collect removed nuclides
  - Initialize both mixtures with He-4 at 1e-20 atoms/barn-cm at 300K
- Create **FLOW** blocks for two removal mechanisms:
  - Pump bowl: 99% efficient removal of noble gases Xe and Kr
  - Process bypass: 50% efficient removal of noble metals Se, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Sb, and Te
- Add **DEPLETION** block:
  - Deplete fuel, and decay mixtures 11 and 12



MSRE graphite stringer cell



Process bypass

5% →

95% →

Reactor Core

20 second loop time

Heat Exch.

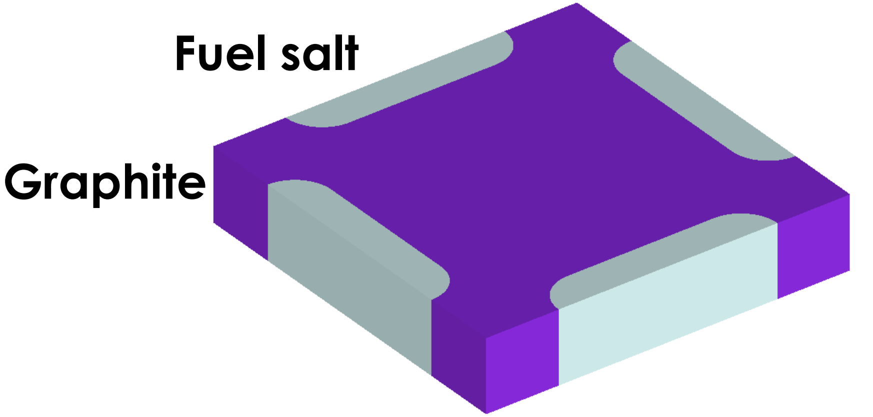
Pump

Tutorial Problem 1a

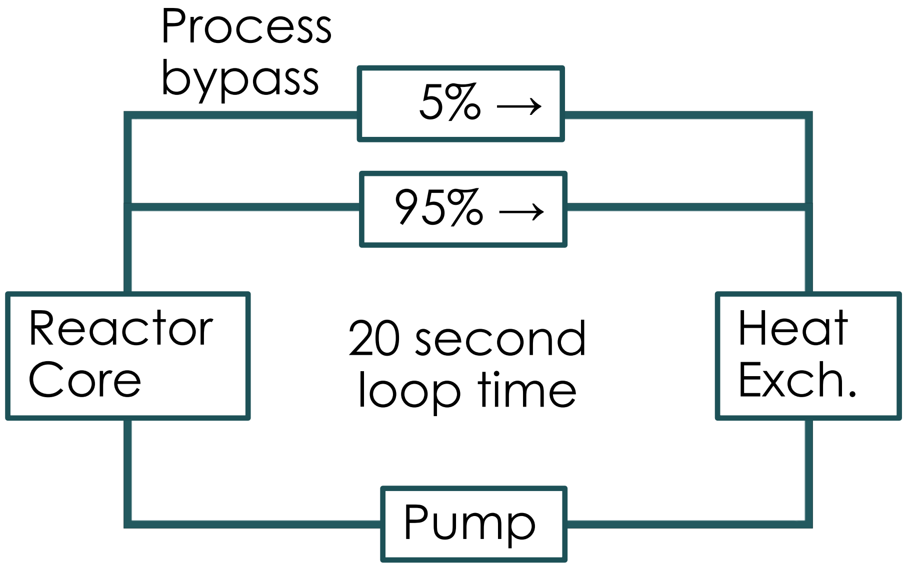
- Add **BURNDATA** block:
  - Calculate specific power from full core power of 8 MWth and the system fuel mass
  - Deplete for 375 days in 5 steps

System part	Fuel mass [MTU]
Core	0.1707
Loop (pipes, OGS, HX, pump, etc.)	0.0473

- Run calculation and interrogate output:
  - Track k_{inf} as a function of time
  - Load the F71 file into Fulcrum and study the fission product and noble metal concentrations in the fuel mixture and in mixtures 11 and 12
- Discussion:
  - What difference in terms of k_{inf} do you expect without the removal blocks?



MSRE graphite stringer cell

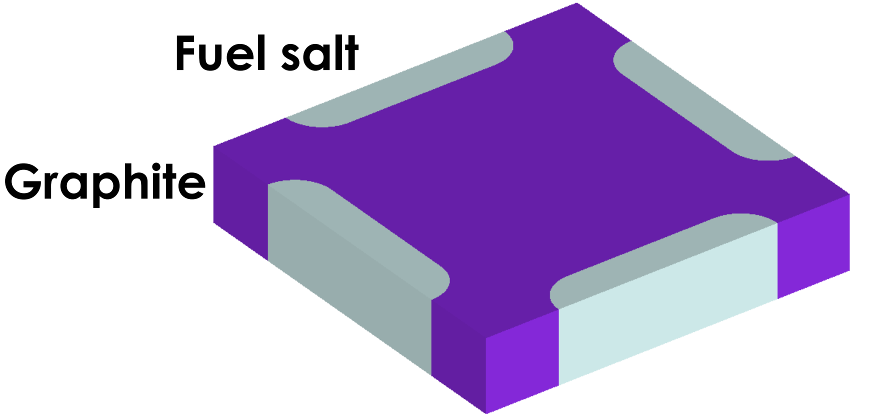


Tutorial Problem 1b

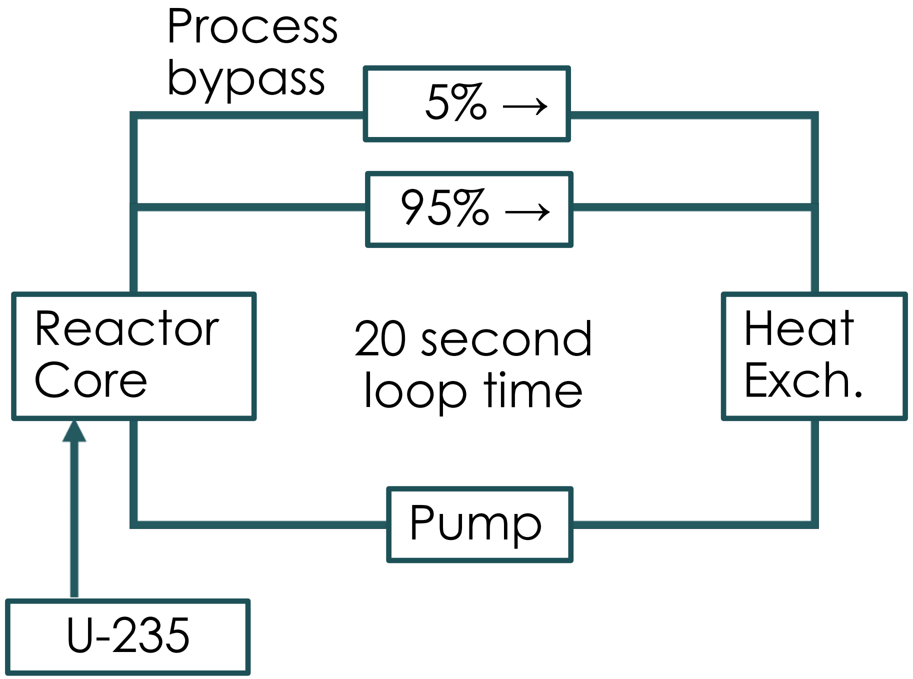
- Copy "*msre_stringer_removal.inp*" and save as "*msre_stringer_feed_and_removal.inp*"

- Add a **FLOW** block to feed U-235:
  - Calculate the total mass of U-235 removed in the removal-only depletion calculation
  - From this, determine the U-235 feed rate in unit grams/second.
  - Multiply this with 2.5626E-03 to address unit conversion issue (Sorry ☹)

- Run calculation and interrogate output:
  - Track k_{inf} as a function of time: How does it compare to the removal-only k_{inf} development?
  - Why is k_{inf} not constant although U-235 was fed to compensate for the removal through fission?
  - Load the F71 into Fulcrum to study the U-235 concentration in the fuel mixture, and compare to the removal-only result.



MSRE graphite stringer cell

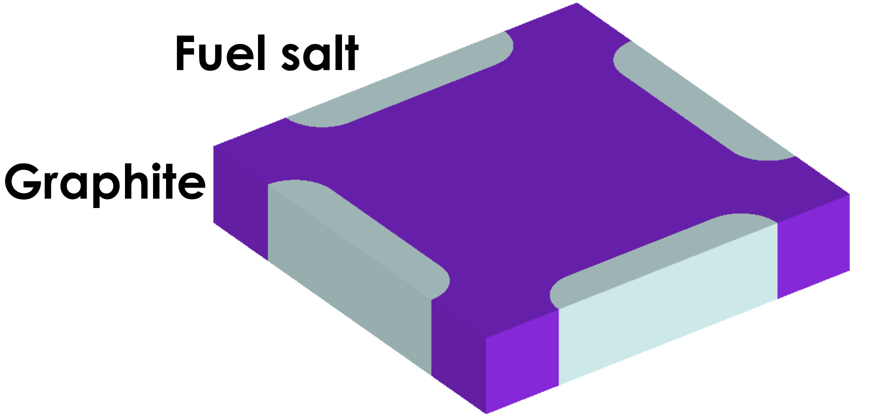


Tutorial Problem 2

- Replicate tutorial problem 1a with ORIGEN.

- Copy “*msre_origen_starter.inp*” and save as “*msre_origen.inp*”
  - Use the F33 file for fuel salt from TRITON
  - Define the irradiation time and power
  - Define the fuel mixture. To be consistent with TRITON, the fuel mixture is normalized to 1 MTIHM
  - Add the processing rate for fission products.

- Run calculation and interrogate output:
  - Load the F71 file into Fulcrum to study the Xe and Kr concentration in the fuel mixture, and compare to the TRITON result.



MSRE graphite stringer cell