Developments and Application of SCALE/TRITON for Molten Salt Reactor Analysis

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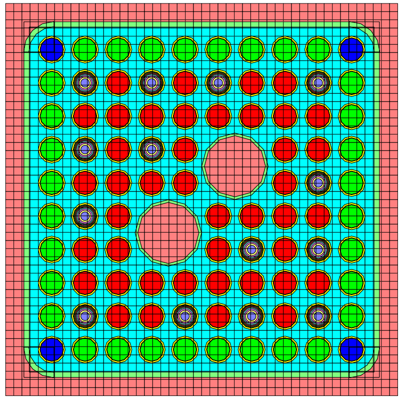
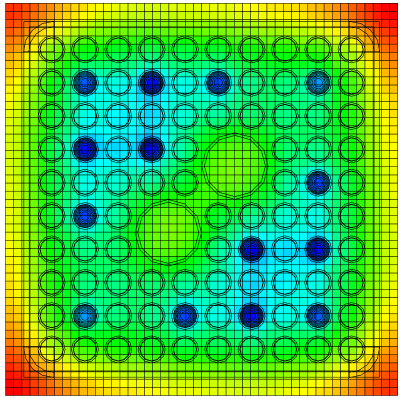
Liquid-Fueled Molten Salt Reactors

Extend SCALE methods developed for solid fuel reactors

- Solid fuel reactor characteristics
  - Fission products and actinides remain with the fuel until reprocessing (if applicable)
  - Excess reactivity control occurs with soluble boron/burnable absorbers



SCALE/TRITON calculation



Burnup-dependent constants

Core simulator (e.g., PARCS)

- Liquid fuel reactor differentiating characteristics
  - Delayed neutron precursor drift
  - Continuous and/or batch processing methods
  - Leverage existing tools for modeling isotopic changes during operation

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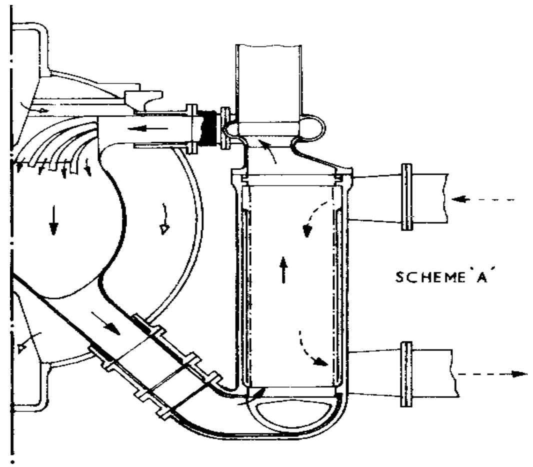
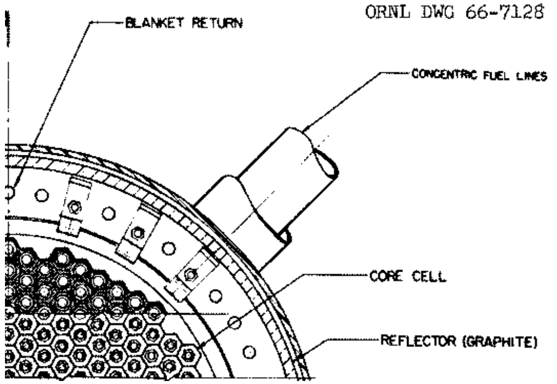
Liquid-Fueled Molten Salt Reactors
Core designs using molten fuel salt

- Fast spectrum molten salt reactor (MSR) cores are usually large volumes of salt
- Thermal spectrum 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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Reactor Physics Characteristics
Neutronic modeling and simulation

- Delayed neutron precursor drift occurs in flowing fuel
  - Delayed neutron precursors are radioactive fission products that release neutrons upon decaying
  - In solid fuel systems, the movement of these delayed neutron precursors is negligible
  - In liquid fuel systems, the precursors move away from their birth location and may decay outside the core, *changing the neutron source distribution within the core*
- Fission source calculated by standard lattice physics codes is biased
  - Prompt neutrons and some delayed neutrons are emitted in the liquid fuel while it is still inside the core
  - Some delayed neutrons are emitted after the liquid fuel leaves the core (coolant loop, chemical processing, etc.)
  - Effect on *k* eigenvalue is on the order of a few hundred pcm

Reactor Physics Characteristics

Effect of precursor drift on transport equations

- Additional term in the neutron transport and precursor equations accounts for the precursor movement

$$\frac{1}{v}\frac{\partial \psi}{\partial t} + \hat{\mathbf{\Omega}} \cdot \nabla \psi + \Sigma \psi(\mathbf{r}, E, \hat{\mathbf{\Omega}}, t) = \iint \Sigma_s(E', \hat{\mathbf{\Omega}}' \rightarrow E, \hat{\mathbf{\Omega}}) \psi' dE' d\mathbf{\Omega}' + \\ + \sum_{j}^{J} \frac{\chi_j}{4\pi} \lambda_j C_j + \iint \frac{\chi_p}{4\pi} (1-\beta) \bar{\nu} \Sigma_f \psi' dE' d\mathbf{\Omega}' + \frac{S}{4\pi}$$

$$\frac{\partial C_j}{\partial t} + \nabla \cdot \mathbf{u} C_j(\mathbf{r}, t) + \lambda_j C_j = \iint \beta_j \bar{\nu} \Sigma_f \psi' dE' d\mathbf{\Omega}', \quad \text{for} \quad j = 1, \ \ldots, \ J,$$

- Often, delayed and prompt fission is effectively lumped
- Effect on fuel cycle simulations is negligible

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Reactor Physics Characteristics
Material feeds and removals

- Solid fueled-reactors typically exhibit a reactivity swing during operation
  - Starting with excess positive reactivity compensates for the loss of fissile material over the course of a cycle of operation
  - Excess reactivity is mitigated via specific fuel loading, soluble boron in the coolant (PWR), burnable absorbers (LWR), and/or control rods, which are gradually removed and/or depleted
  - Neutrons are effectively lost in absorbers and control rods
- Liquid-fueled MSRs have potential for low excess reactivity
  - Continuous or batch feed of fissile and fertile material during operation
  - Continuous removal of fission products reduces neutron absorption
  - Better neutron economy leads to greater fuel utilization

Reactor Physics Characteristics

Challenges in depletion modeling and simulation

- Depletion with continuous and batch feeds and removals
  - Continuous processes in liquid fuel systems remove fission gases and potentially other elements during operation
  - In addition to continuous processes, material may be added to and removed from the liquid in batches at specific times
- Point depletion equation describing the rate of change of nuclide *i*

$$\frac{dN_i}{dt} = \sum_{j=1}^{m} l_{ij}\lambda_j N_j + \bar{\Phi}\sum_{k=1}^{m} f_{ik}\sigma_k N_k - (\lambda_i + \bar{\Phi}\sigma_i + \cancelto{0}{r_i})N_i$$

Decay rate of nuclide *j* into nuclide *i*

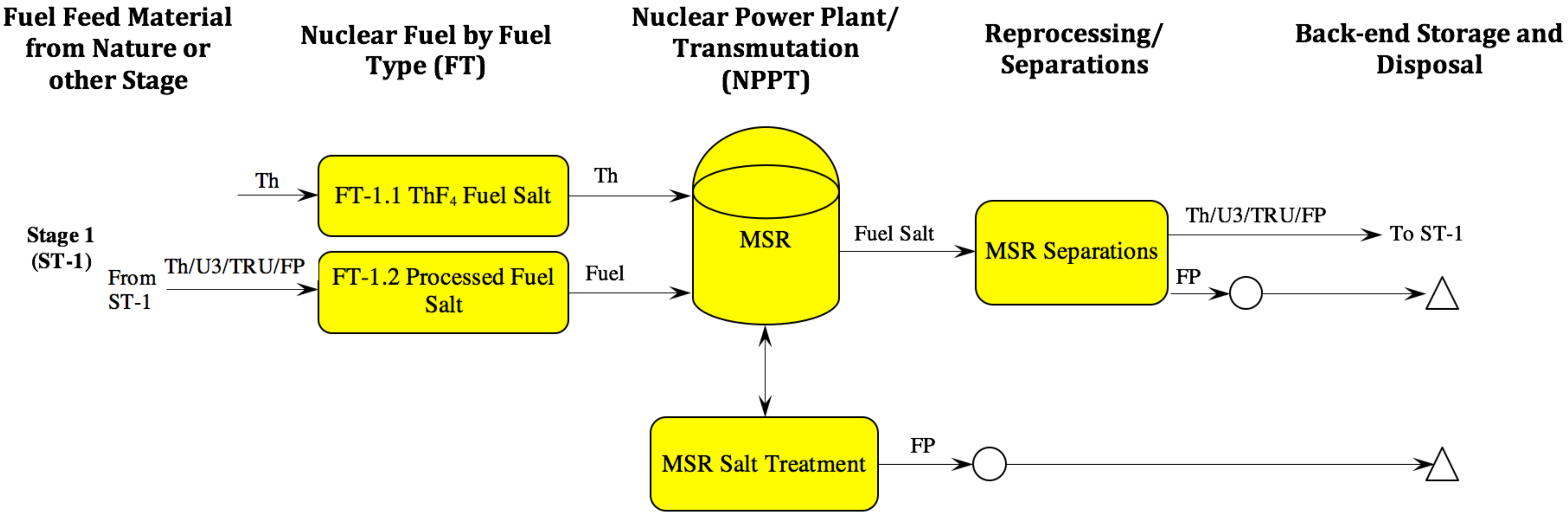
Production rate of nuclide *i* from irradiation

Loss rate of nuclide *i* due to decay, irradiation, or other means

Reactor Physics Characteristics

Fuel cycle and reactor physics calculations are more similar

- Continuous recycle of ^{233}U/Th with new Th fuel in thermal critical reactors



Note: Only primary material flows are shown. Material flows from imperfect separations (losses), low-level waste, and other secondary streams that will be produced in performing various fuel cycle functions are not shown.

Legend:

NU = Natural Uranium	DF = Discharged Fuel	PWR = Pressurized Water Reactor	△ = Nuclear Waste Disposal
DU = Depleted Uranium	FP = Fission Products	SFR = Sodium Fast Reactor	○ = Nuclear Material Storage
LEU = Low-enriched Uranium	TRU = Transuranics	UOX = Uranium Oxide	→ = Nuclear Material Transport
U3 = U produced by Th fuel	MA = Minor Actinides	MOX = Mixed Oxide	/ = Co-separated products
	MSR = Molten Salt Reactor	ThF_4 = Thorium Tetrafluoride	

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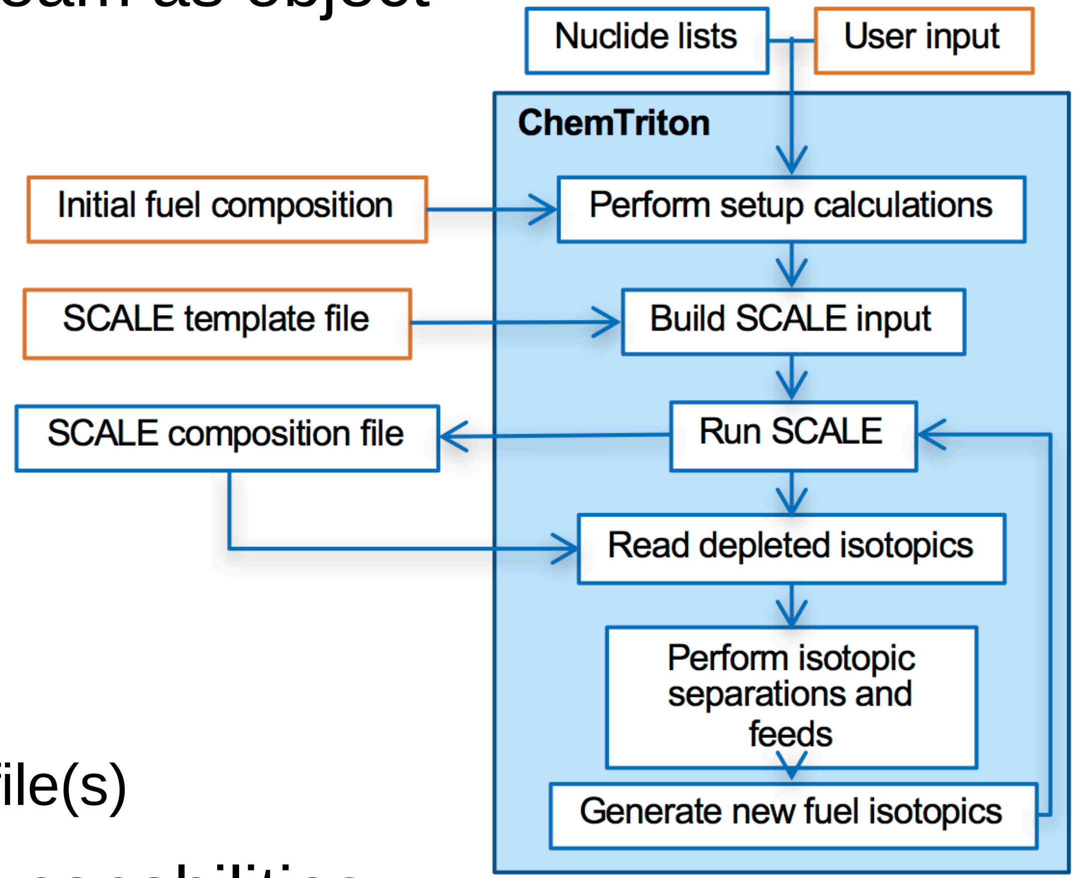
Molten Salt Reactor Tools in SCALE

Implement MSR modeling and simulation capabilities

- Account for the flowing fuel materials in a liquid-fueled system
  - Model precursor drift and its effect on neutronics and depletion
  - Remove isotopes with specific rates or portions of the fuel salt
- Draw on reactor physics tools within the SCALE code system
  - Neutron transport and depletion
  - Strong quality assurance program
- Provide ORNL modeling and simulation tools applicable to liquid-fueled reactor problems
  - Assessment of MSR impact on fuel cycle outcomes
  - Fuel cycle and core optimization and design

Molten Salt Reactor Fuel Cycle Analysis
Computational methods and models (ChemTriton)

- Object-oriented Python script: material stream as object
- Tracks characteristics of each stream
  - Volume, isotopic composition, and mass, etc.
- Available actions for each stream
  - Read and write stream isotopic information in SCALE standard composition format
  - Separate out specific isotopes from stream
  - Feed in specific isotopes to stream
  - Combine and split streams
  - Run SCALE using an external input template file(s)
- Variable feed/removal rate and multi-zone capabilities

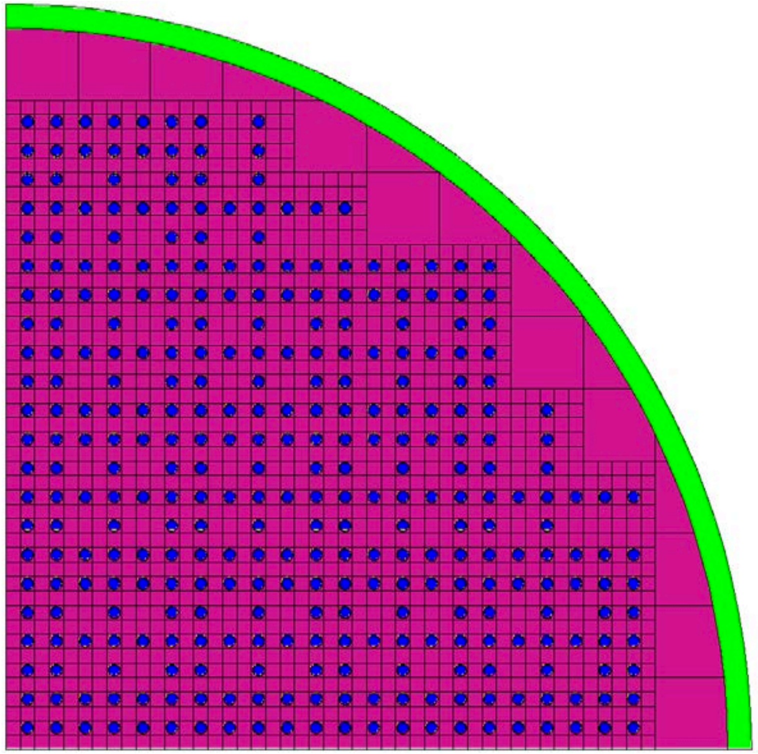


B. R. Betzler, J. J. Powers, and A. Worrall, “Molten Salt Reactor and Fuel Cycle Modeling and Simulation with SCALE,” Annals of Nuclear Energy, 101, pp. 489–503 (2017).

Transatomic Power Corporation ChemTriton Analysis

Reactor characteristics, geometry, and mission

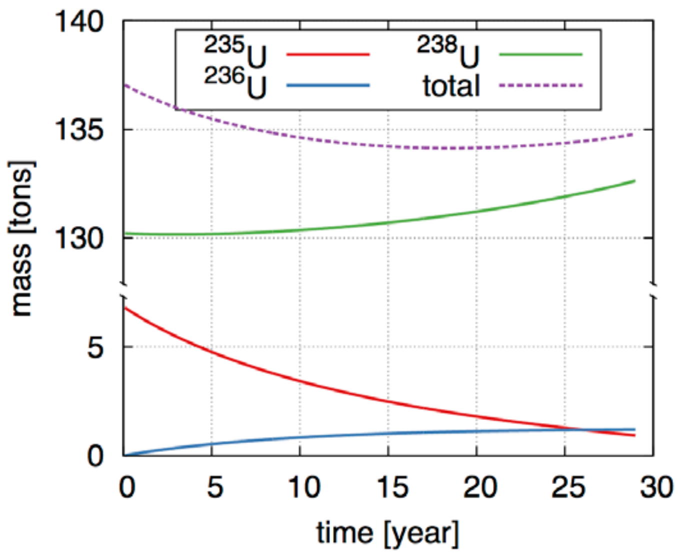
- 1250 MW MSR with an LiF-based uranium fuel salt
  - Active core measures 3 m by 3 m
  - Low-enriched uranium (LEU) in UF_4 at 27.5 mol%
  - Spectrum shifts from intermediate (initial) to thermal
  - Zirconium hydride metal rods clad in silicon carbide in configurable moderator rod assemblies (3-cm pitch)
- Designed to operate for ~30 years
  - At fixed intervals, moderator rod assemblies are reconfigured to decrease the salt volume fraction (SVF) during operation
  - Higher SVFs during early years of operation drive generation of fissile plutonium, which enables reaching higher burnup
  - Online removal of fission products: volatile gases, noble metals, volatile fluorides, and rare earth elements
  - LEU fuel feed rate at 480 kg/year

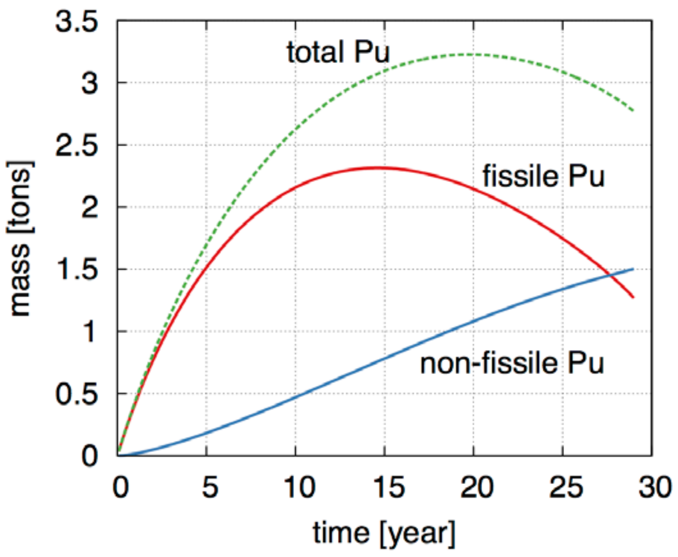


Transatomic Power Corporation ChemTriton Analysis

Evolution of core parameters during operation

- Total heavy metal concentration is held constant during operation to limit changes to thermophysical properties of the salt
  - Most of the initial loaded fissile material is depleted by core end of life
  - Plutonium is bred during the first several years of operation
  - Fuel cycle comparisons to typical light-water reactors



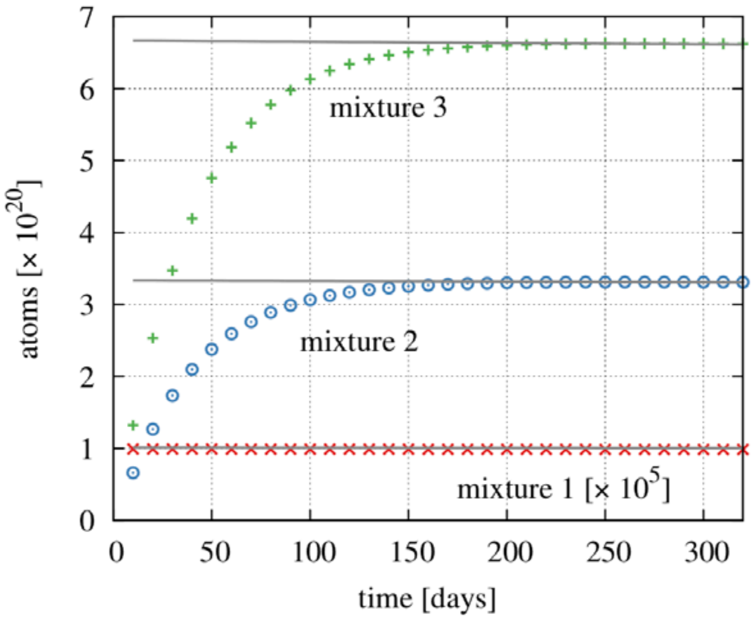


Parameter	LWR	Transatomic Power
Loaded fuel (MT/GWt-year)	7.31	4.16
Waste (MT/GWt-year)	6.92	3.77
Resource utilization (%)	~0.6	~1.0

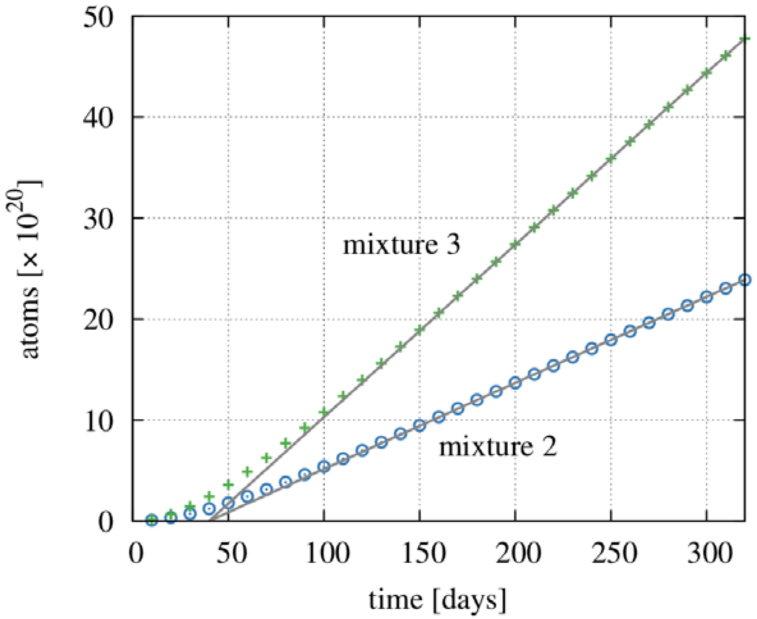
ORIGEN Continuous Removals Internal Capability

Three-mixture test problem

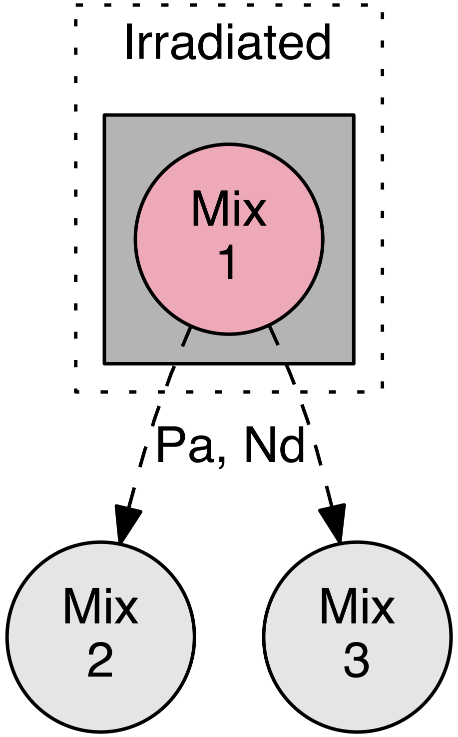
- Mixture 1 is irradiated ^{233}U and ^{232}Th; mixture 2 and 3 are initially empty
  - Analytic solutions (in gray below) for material quantities exist
  - Simulates removal of protactinium in a Th-fueled MSR



^{233}Pa



^{233}U



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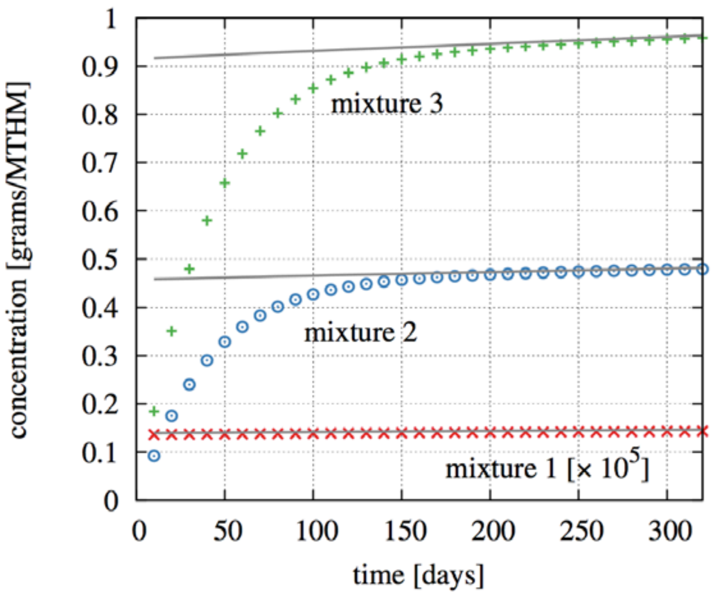
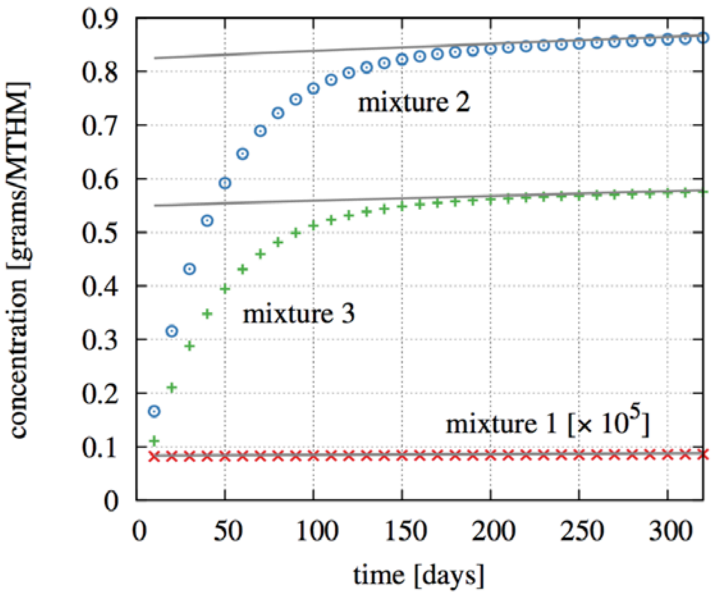
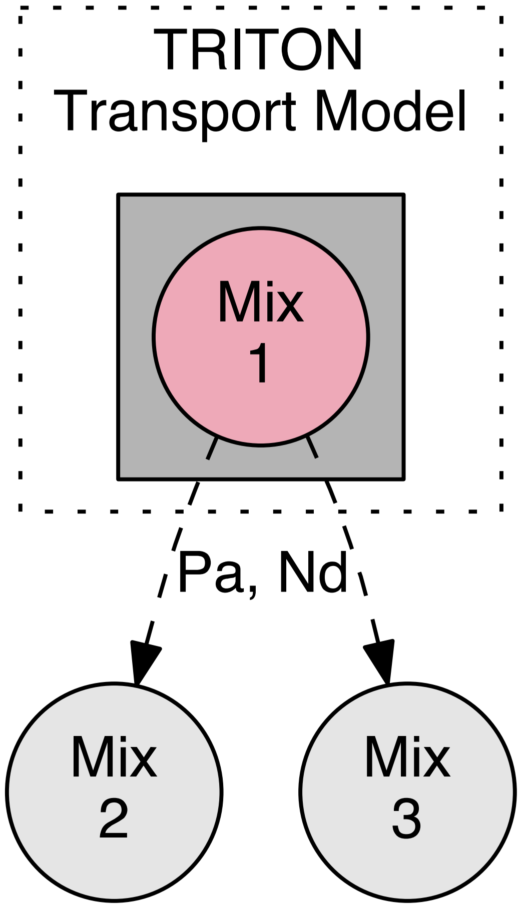
TRITON Continuous Removals Capability
Three-mixture test problem

- Incorporating ChemTriton-like tools in SCALE, performing continuous removals and feeds in ORIGEN through SCALE/TRITON
- Th-based MSR unit cell model





^{233}Pa



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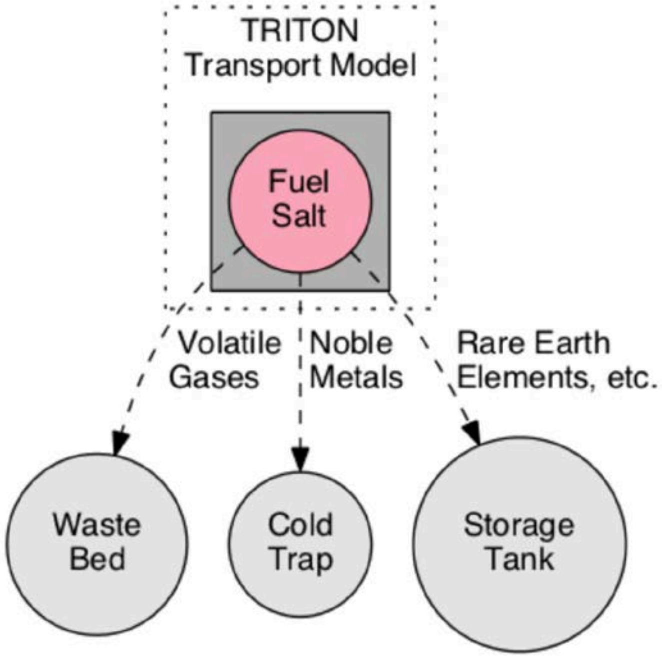
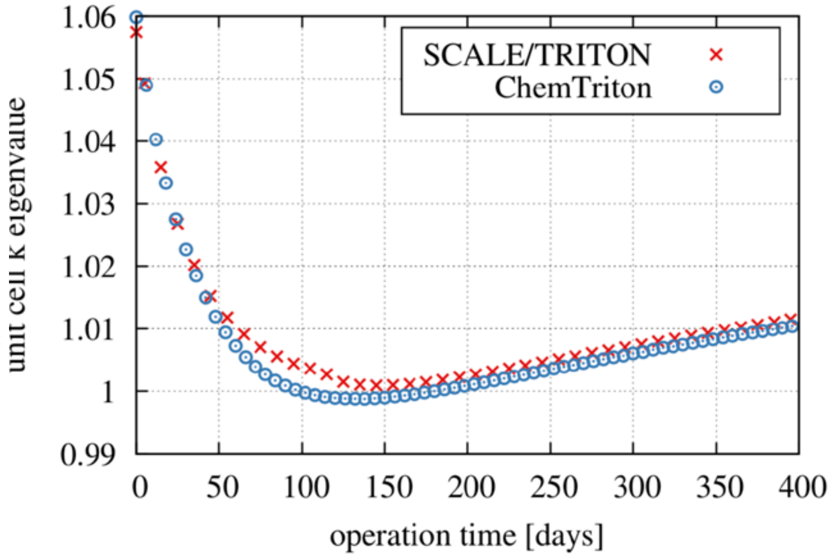
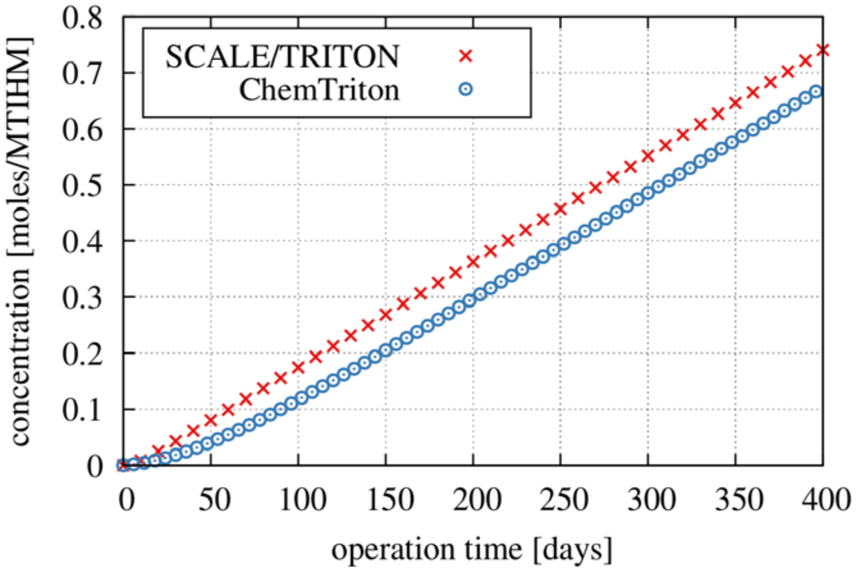
TRITON Continuous Removals Capability
Use case without feedback

- Comparisons to ChemTriton show some differences due to semi-continuous removal methodology
  - Small differences in isotopic concentrations from including rates in the depletion solve







Nd in Cold Trap

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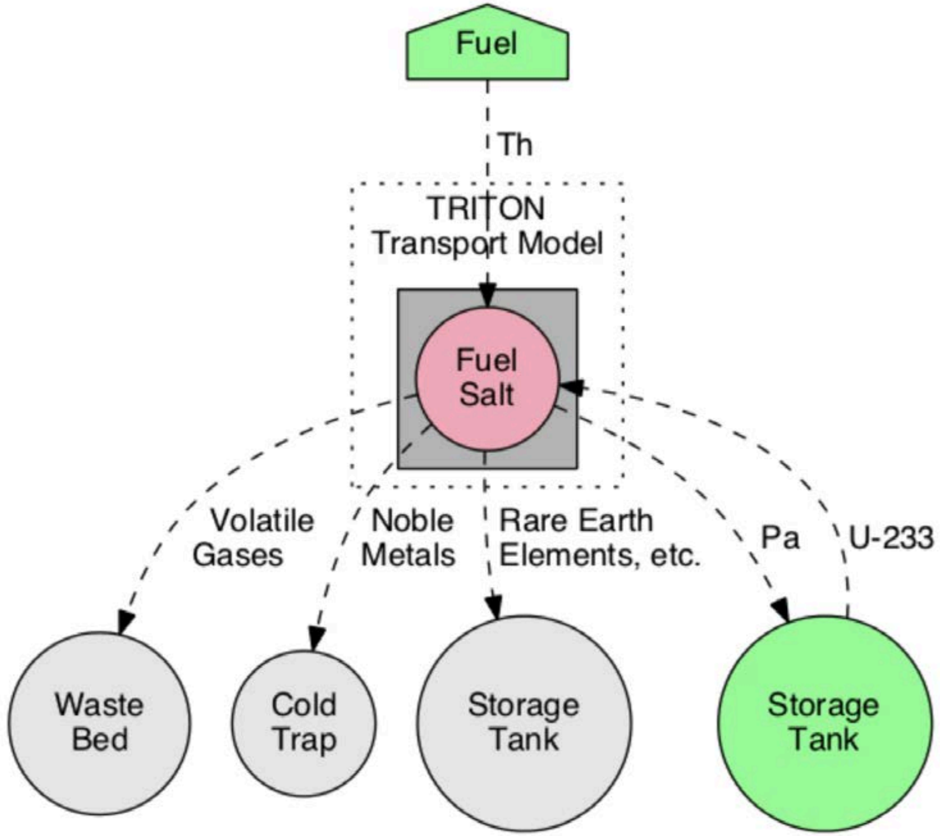
TRITON Continuous Removals Capability

Multiple mixture problem

- Application to more complex use cases with several removal mixtures and storage and recycling tanks
- Implementation of a feedback (circular movement of material) is non-trivial
  - Requires iteration scheme
  - Converge on material feed rates



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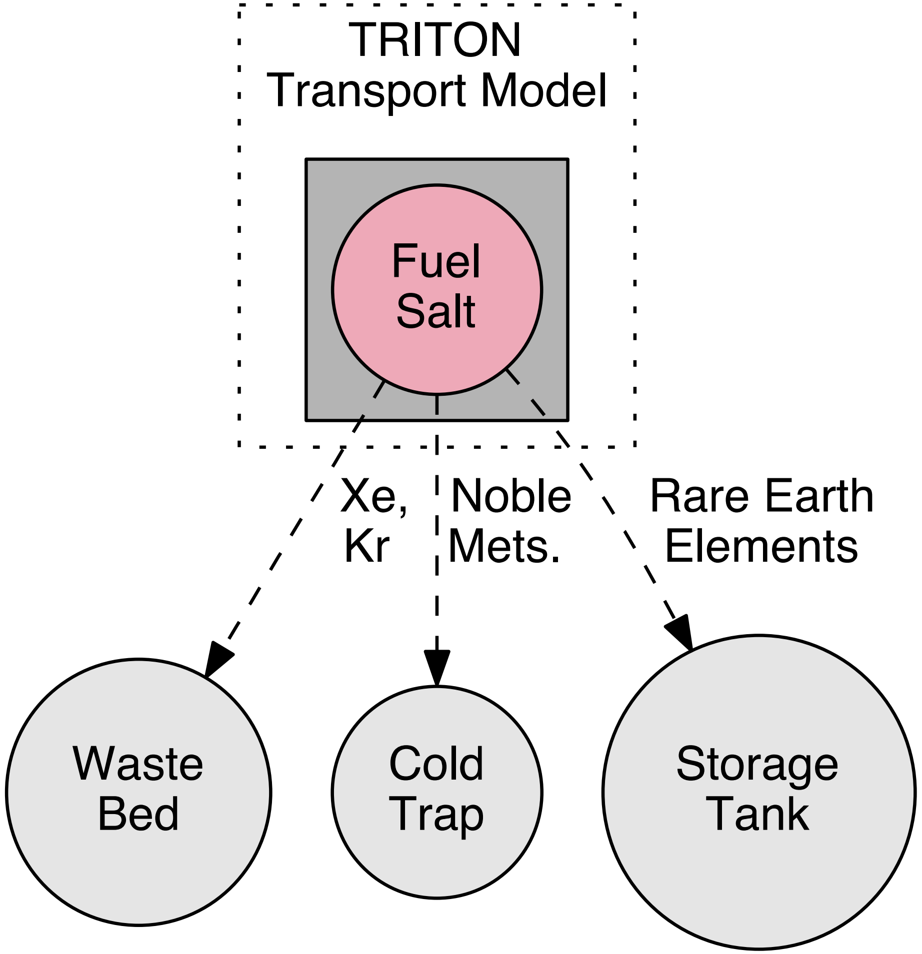
Ongoing Efforts

Molten salt reactor tools implementations

- Finalize testing in SCALE/TRITON
- Finalize input implementation
- Finalize TM on these tools
  - Recommendations for parameterizing chemical processes
  - Pertinent example problems



Questions

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