Molten Salt Reactor Modeling and Simulation

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Presentation Outline

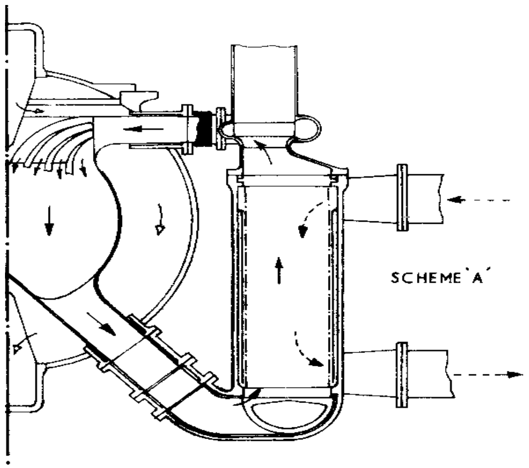
Understanding challenges with simulation molten salt reactors

- Introduction and background
- Reactor physics analysis challenges
  - Neutronics
  - Depletion
- Impacts on fuel cycle analysis
- Example cases
- Summary and future work

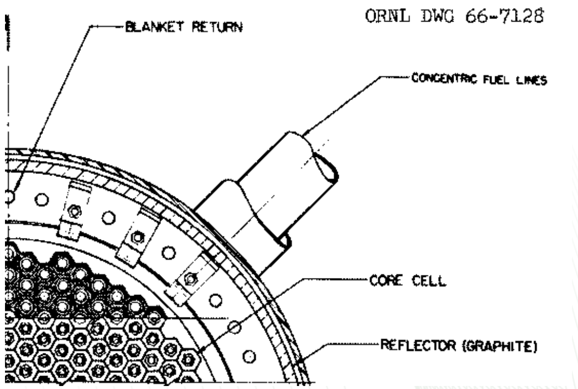
Liquid-Fueled Molten Salt Reactors

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]

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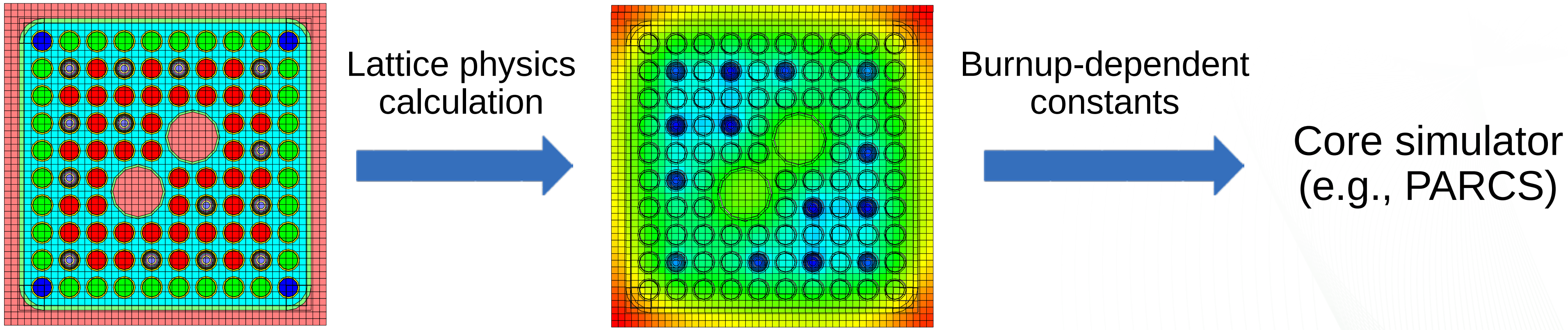
[1] "An Assessment of a 2500MWe Molten Chloride Salt Fast Reactor" (1974).

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

Liquid-Fueled Molten Salt Reactors

Methods have built-in assumptions for solid fuel reactors

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



Lattice physics calculation

Burnup-dependent constants

Core simulator (e.g., PARCS)

- Liquid fuel reactor characteristics
  - Fuel flows with carrier material (delayed neutron precursor drift)
  - Includes continuous and batch chemical processing and fueling

Reactor Physics Analysis

Challenges in 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 Analysis

Effect of precursor drift on transport equations

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

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

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

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

Reactor Physics Analysis

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*

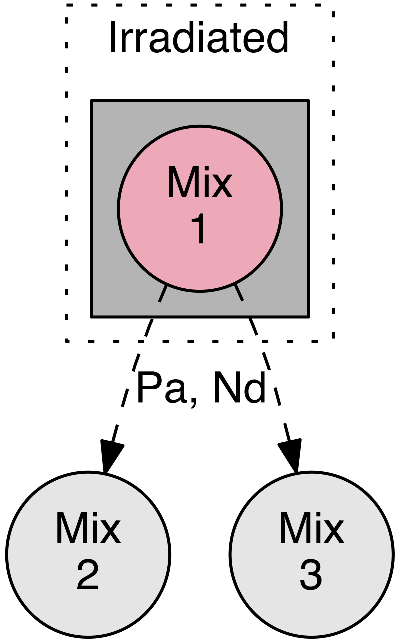
Production rate of nuclide *i* from irradiation

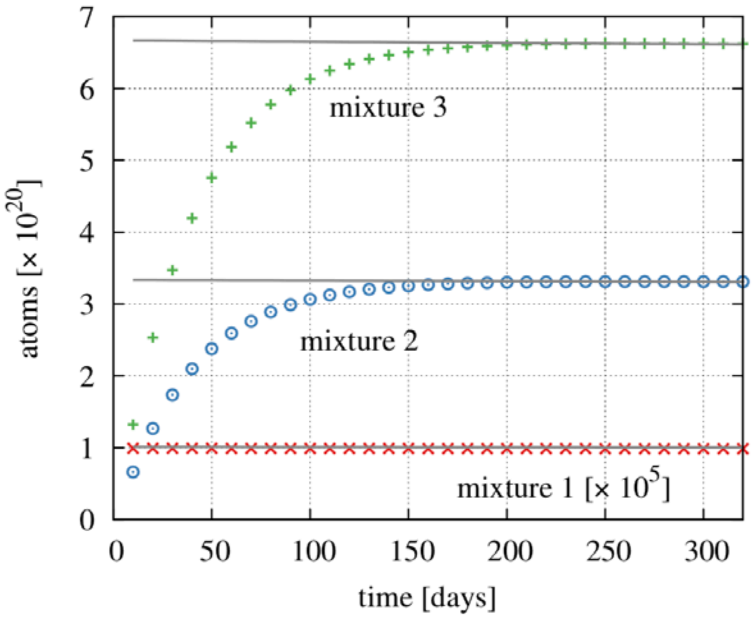
Loss rate of nuclide *i* due to decay, irradiation, or other means

Reactor Physics Analysis

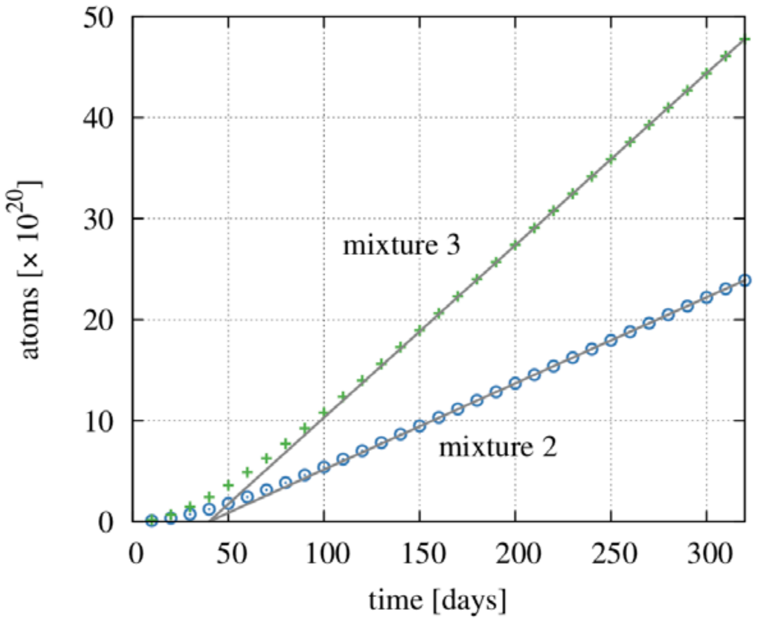
Two mixture problem example

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





^{233}Pa



^{233}U

Reactor Physics Analysis

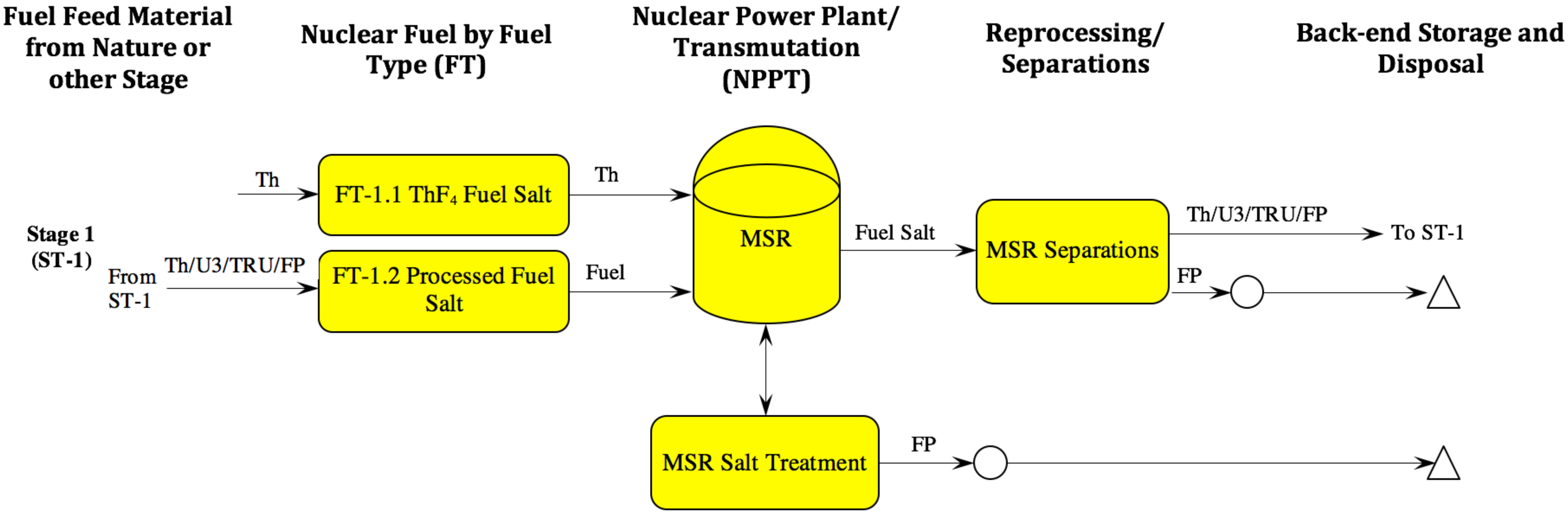
Approaches for molten salt reactor modeling and simulation

- Historically, many conceptual designs used a neutron balance table to demonstrate the neutron behavior at equilibrium
- Simulating the changing isotopic composition of the irradiated fuel salt
  - Modeling removal as a continuous process
  - Approximating continuous removal as a semi-continuous process via batching
  - Continuous process model with tracking of waste and alternate irradiated materials
- Calculating the out-of-core delayed neutron source
  - Zero-dimensional model
  - One-dimensional model
  - Multi-dimensional model with or without coupled TH calculations

Reactor Physics Analysis

Integrates more tightly with fuel cycle analysis

- Reactor physics performance of a molten salt reactor is not well understood without simulating material additions and removals



Fuel Feed Material from Nature or other Stage

Nuclear Fuel by Fuel Type (FT)

Nuclear Power Plant/ Transmutation (NPPT)

Reprocessing/ Separations

Back-end Storage and Disposal

Stage 1 (ST-1)

Th

FT-1.1 ThF_4 Fuel Salt

Th

From ST-1

Th/U3/TRU/FP

FT-1.2 Processed Fuel Salt

Fuel

MSR

Fuel Salt

MSR Separations

Th/U3/TRU/FP

To ST-1

FP

MSR Salt Treatment

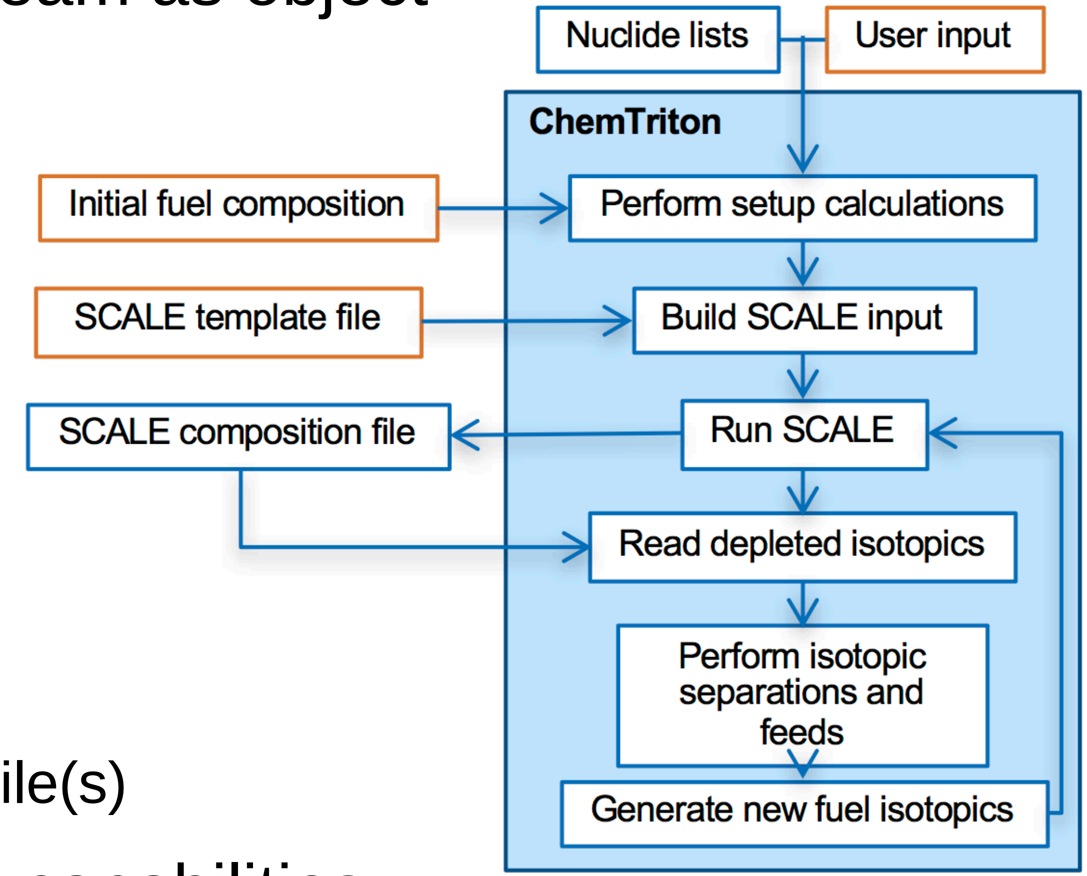
FP

EG26: Continuous recycle of ^{233}U/Th with new Th fuel in thermal critical reactors

Molten Salt Reactor Modeling and Simulation Tools

ChemTriton material tracking script

- 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

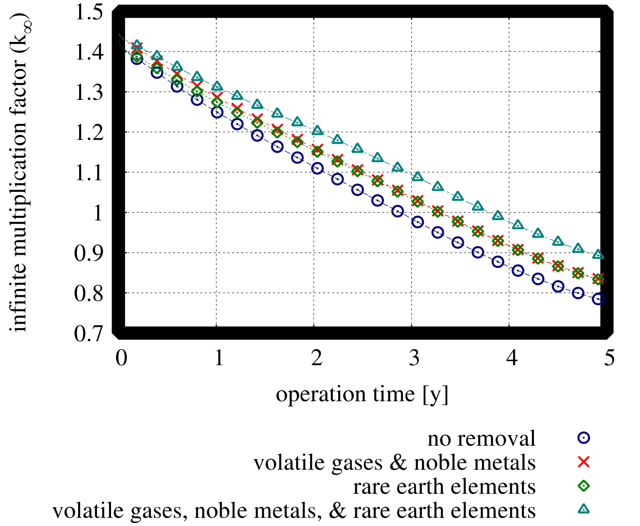


B. R. Betzler, J. J. Powers, and A. Worrall, “Molten Salt Reactor and Fuel Cycle Modeling and Simulation with SCALE,” Annals of Nuclear Energy, 101, pp. 489–503 (2017).

Thermal Spectrum Reactor Performance

Effect of different material removal rates

- Some elements have strong effect on reactivity and reactor operation
  - Cycle times depend on the processing technology
    - Defined as the time it takes to completely remove a given element
  - Continuous removal of highly absorptive elements has largest impact



Calculated k-infinity of a unit cell with different removal groupings.

Effect of processing group removals on core lifetime for a thermal MSR.

Removals	Core lifetime	
	time [y]	additional [+%]
None	2.73	-
Volatile gases	2.93	7.5
Noble metals	2.92	7.1
Seminoble metals	2.74	0.3
Volatile fluorides	2.74	0.4
Rare earth elements	3.12	14.4
Discard	2.73	0.2
Gases and noble metals	3.14	15.1
Gases, noble metals, and rare earth elements	3.63	32.9

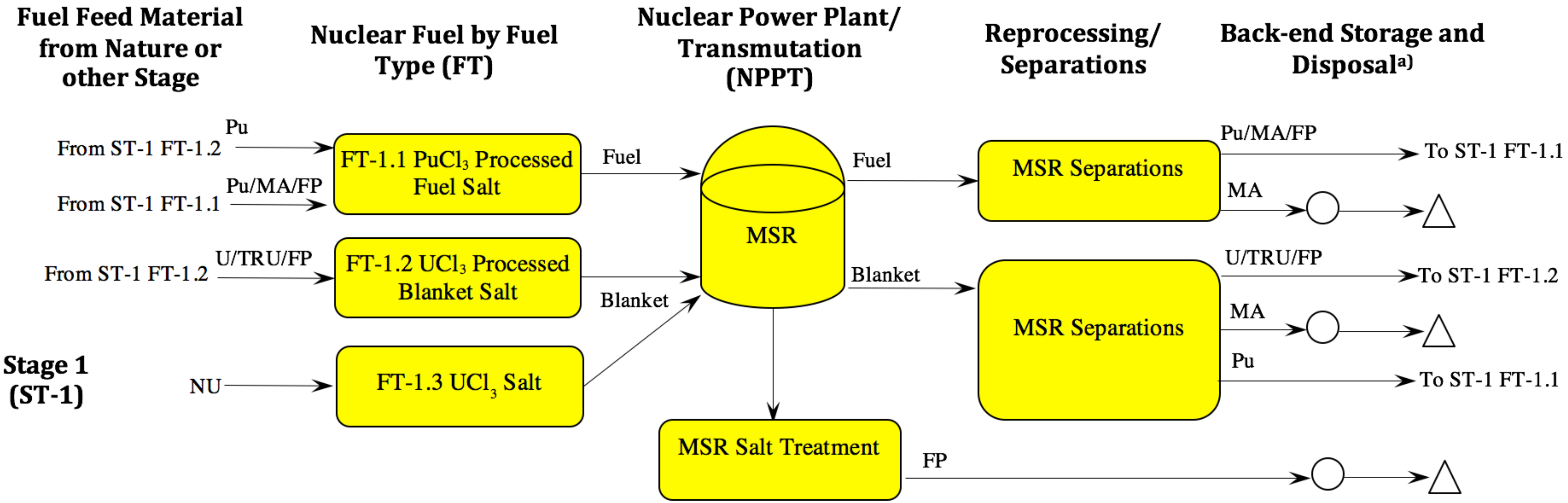
Removal rates of different processing groups.

Processing Group	Elements	Cycle time
Volatile gases	Xe, Kr	20 s
Noble metals	Se, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Sb, Te	20 s
Seminoble metals	Zr, Cd, In, Sn	200 d
Volatile fluorides	Br, I	60 d
Rare earth elements	Y, La, Ce, Pr, Nd, Pm, Sm, Gd	50 d
	Eu	500 d
Discard	Rb, Sr, Cs, Ba	3435 d

DOE-NE Fuel Cycle Evaluation and Screening Study

Evaluation groups selected for assessment of MSR impact

- EG23: Continuous recycle of U/Pu with new natural-U fuel in fast critical reactors



Fuel Feed Material from Nature or other Stage

Nuclear Fuel by Fuel Type (FT)

Nuclear Power Plant/ Transmutation (NPPT)

Reprocessing/ Separations

Back-end Storage and Disposal[a)]

From ST-1 FT-1.2 → Pu

From ST-1 FT-1.1 → Pu/MA/FP

FT-1.1 PuCl$_3$ Processed Fuel Salt

From ST-1 FT-1.2 → U/TRU/FP

FT-1.2 UCl$_3$ Processed Blanket Salt

NU → FT-1.3 UCl$_3$ Salt

Stage 1 (ST-1)

Fuel

Blanket

MSR

Fuel

Blanket

MSR Salt Treatment

FP

MSR Separations

Pu/MA/FP → To ST-1 FT-1.1

MA

MSR Separations

U/TRU/FP → To ST-1 FT-1.2

MA

Pu → To ST-1 FT-1.1

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	MA = Minor Actinides	MSR = Molten Salt Reactor	△ = Nuclear Waste Disposal
TRU = Transuranics	FP = Fission Products	/ = Co-separated products	○ = Nuclear Material Storage
			→ = Nuclear Material Transport

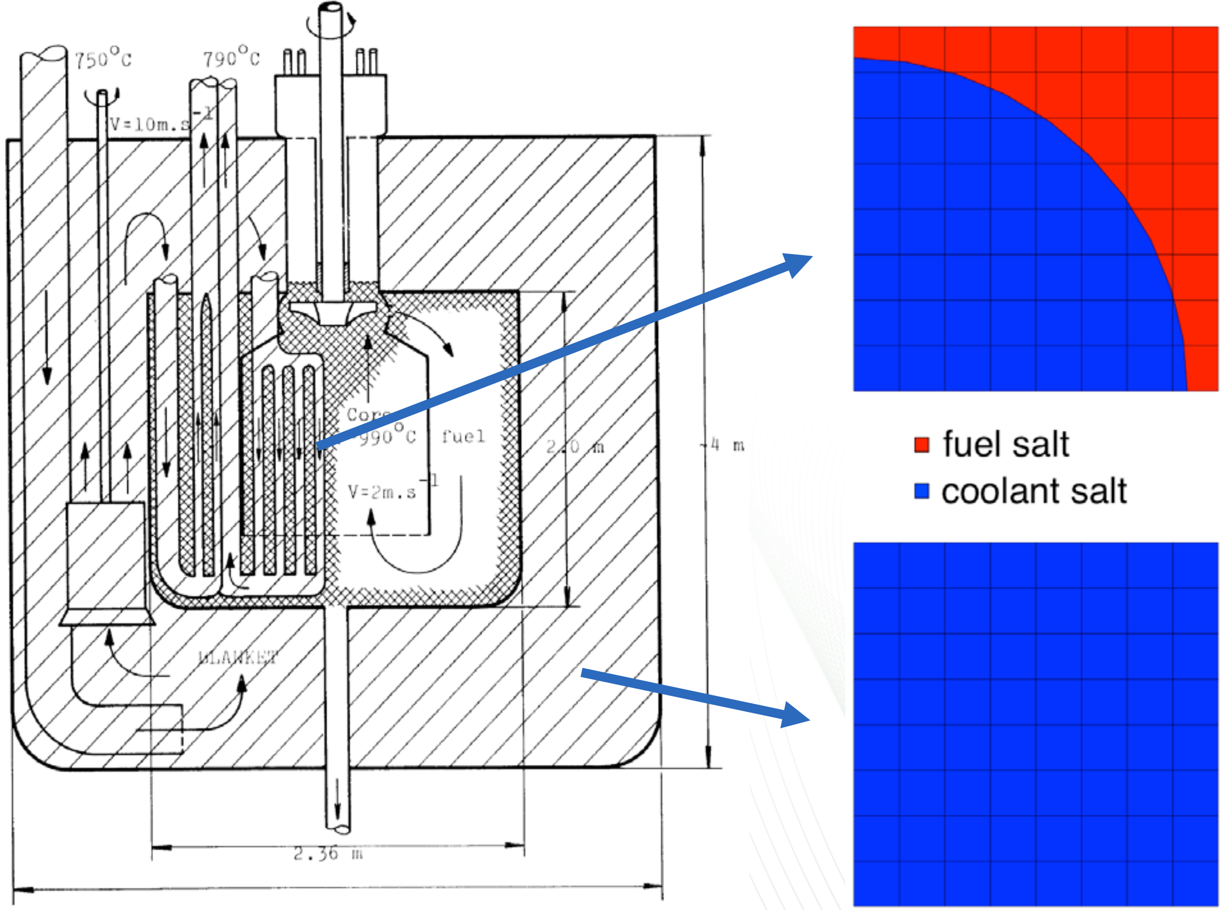
a) To account for realistic fuel separation processes that are unable to completely separate all MAs, a fraction of MAs in the fuel sent back through the reactor.

DOE-NE Fuel Cycle Evaluation and Screening Study

Evaluation groups selected for assessment of MSR impact

- Unit cell models of the molten chloride fast breeder reactor (MCFBR)
  - Simulation of approach to equilibrium
  - Zone power ratios taken from literature

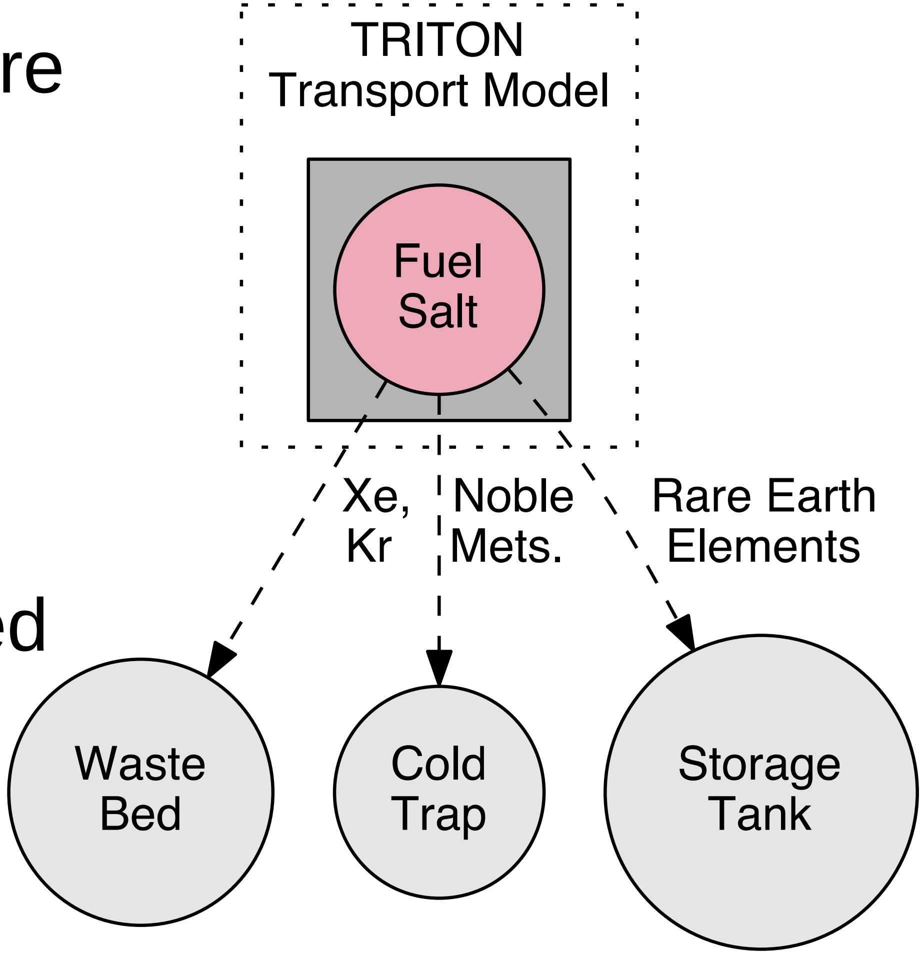
Parameter	Value
Power	2000 MWt (800 MWe)
Fuel salt composition	$PuCl_3$-NaCl
Coolant salt composition	UCl_3-NaCl
Fuel salt temperature	1260 K
Coolant temperature	1066 K
Fuel salt volume	3.37 m^3
Coolant salt volume in tubes	4.85 m^3
Coolant salt volume in blanket	41.1 m^3
Coolant tube pitch	1.38 cm
Coolant tube outer diameter	1.26 cm
Core total volume fraction	16.7% (8.23 m^3)
Blanket total volume fraction	83.3% (41.1 m^3)



Summary and Future Work

Improving molten salt reactor analysis tools

- Two main challenges with modeling MSRs are due to delayed neutron precursor drift and continuous processing of the liquid fuel
- Motivated by growing interest in MSRs and analysis needs, tools were developed to perform fuel cycle analysis of MSRs
- Capabilities of these tools are being improved
  - Delayed neutron precursor drift model
  - Continuous processing capabilities
  - User interface to interact with these tools



Questions