Module 5: Reactor Physics

George Flanagan PhD

Nuclear Energy and Fuel Cycles Division

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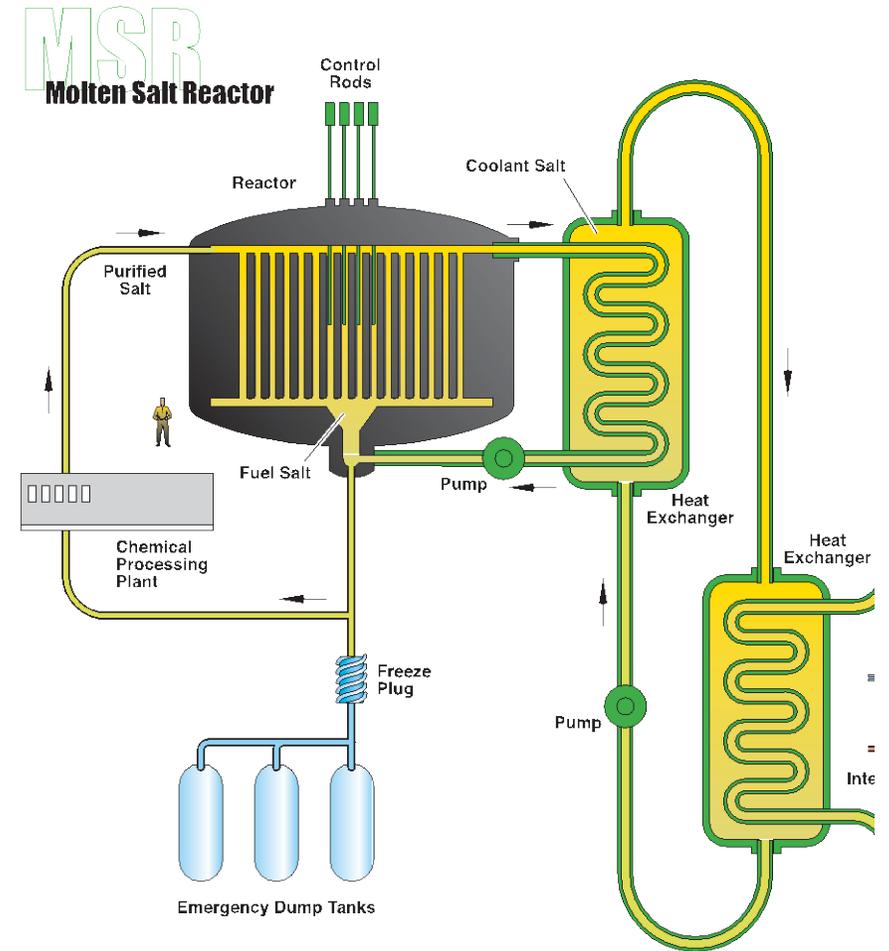
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Overview

- Applications and advantages of MSRs

- Neutron flux spectrum characteristics

- Neutronic aspects of liquid fueled reactors that are different from solid fueled reactors

  - Delayed neutron precursor motion

  - Fission product removal

  - Fission gas bubble flow

- Reactivity feedback effects in MSRs

- Challenges

  - Nuclear data availability and uncertainty

  - Modeling tools, group structures, etc.

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Liquid-fueled Molten Salt Reactors:
Unique Reactor Physics Characteristics

- Liquid fuel reactor as a chemical plant
  - Simplifying the handling and reprocessing of fuel
  - Fuel (and delayed neutrons) flows around primary loop
  - Continuous production of gaseous fission and transmutation products in the salt

- Complex chemical processes
  - Online removal of fission products (e.g., sparging)
  - Online or batch feed of fissile material
  - Batch discard of fuel material

- Thermal spectrum and fast spectrum MSRs are possible
  - Fluoride and chloride salts
  - FLiBe salt and graphite moderator are "classic" thermal MSR configuration

Source: *A Technology Roadmap for Generation IV Nuclear Energy Systems.* GIF-002-00.

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Why Liquid Fuel Molten Salts?

- Enables high temperature at low pressure

- Online chemistry adjustment
  - Can include fuel processing

- Potential for inherent safety depending on design options
  - Fuel salt thermal expansion provides negative reactivity insertion
  - Fuel draining under thermal excursions
  - Low excess reactivity – fuel normally in most reactive configuration

- Potential to substantially reduce actinide waste production
  - Eliminates requirement for precision fuel fabrication

- MSRs can be refueled as "infinite batch" reactors
  - Results in maximum possible burnup

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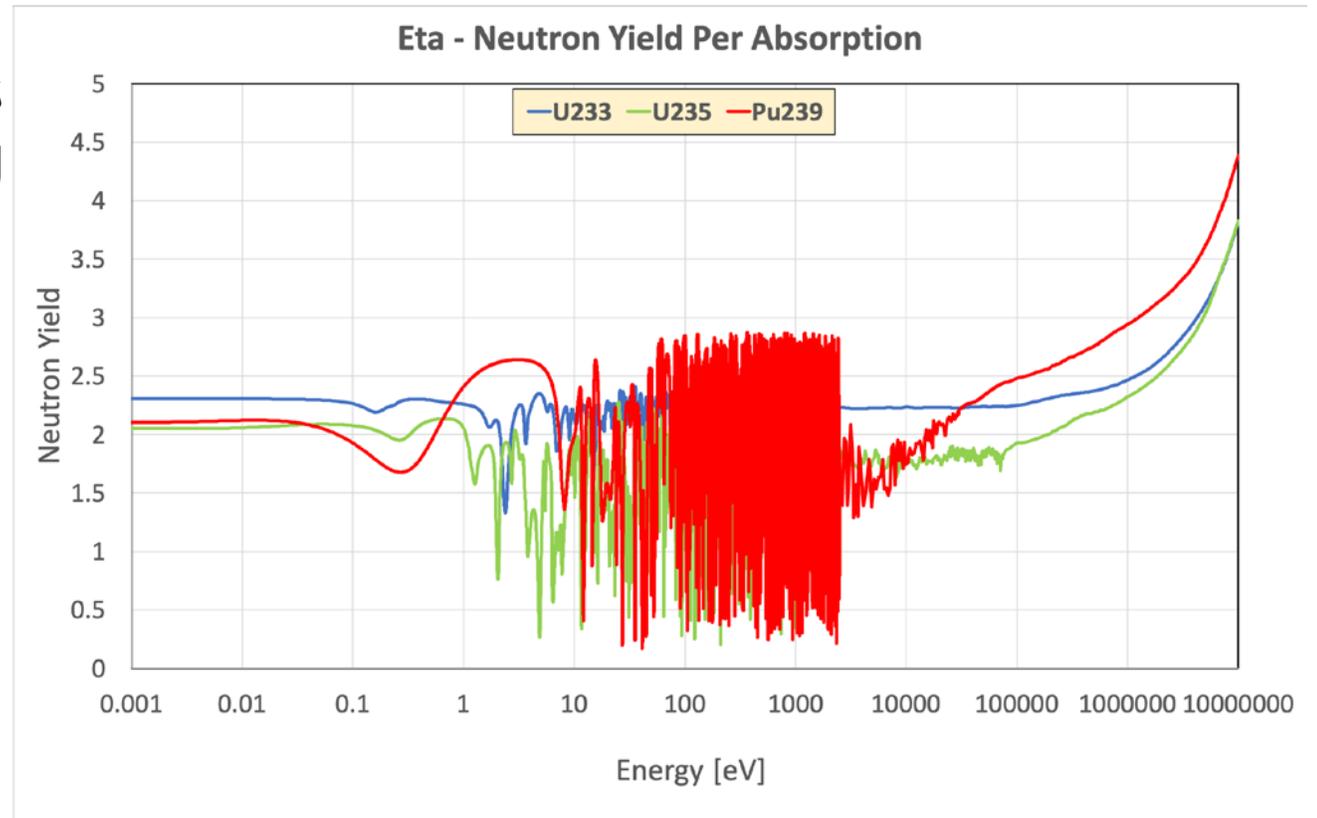
Neutronics Advantages of MSRs

- Online refueling and reprocessing

- Excellent neutron economy

- Low absorption materials and no cladding

- Online criticality maintenance
  - High availability

- Flexible fuel composition
  - Without blending and fabrication
  - Enables actinide recycling

- Excess neutrons
  - Thorium breeding and/or actinide burning
  - Fixed fuel cost

- Fuel presence in salt
  - Negative thermal feedback coefficient

- Low source term
  - Low radiotoxic risk

- Low fuel load
  - Low excess reactivity

Safety, Economics, Sustainability

Source: J. Křepel et al. 2014. "Fuel cycle advantages and dynamics features of liquid fueled MSR," *Annals of Nuclear Energy* 64: 380-397.

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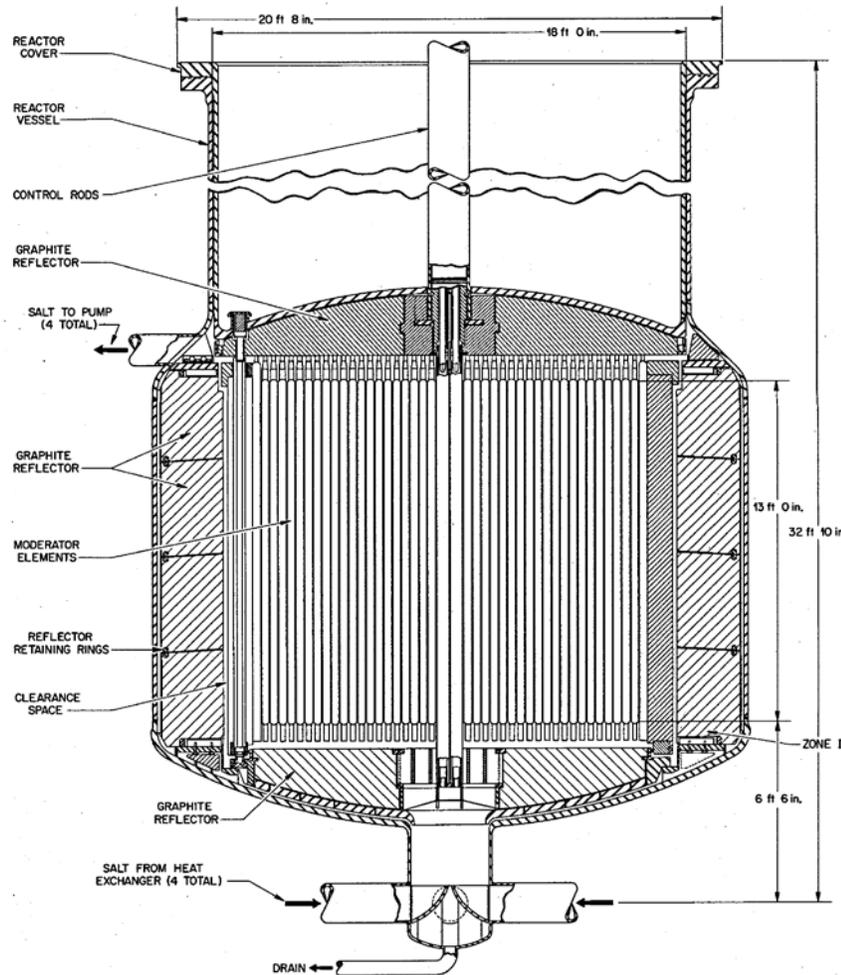# MSRs Are Flexible Fuel Cycle Machines

- MSRs may be operated with a variety of fissile feed materials, as burner, breeder, or self-sustaining reactors

- LEU, Th/^{233}U, U/Pu, U/TRU, etc.

- MSRs can breed ^{233}U from ^{232}Th in any spectrum: thermal, intermediate or fast

Eta - Neutron Yield Per Absorption

ENDF/B-VIII.0

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Two-zone MSBR Geometry Design Example

Fissile fuel is "bred" in the blanket channels

Source: J.J. Powers et al. "An Inventory Analysis of Thermal-Spectrum Thorium-Fueled Molten Salt Reactor Concepts." *PHYSOR 2014*

MSBR Zone I

MSBR Zone II
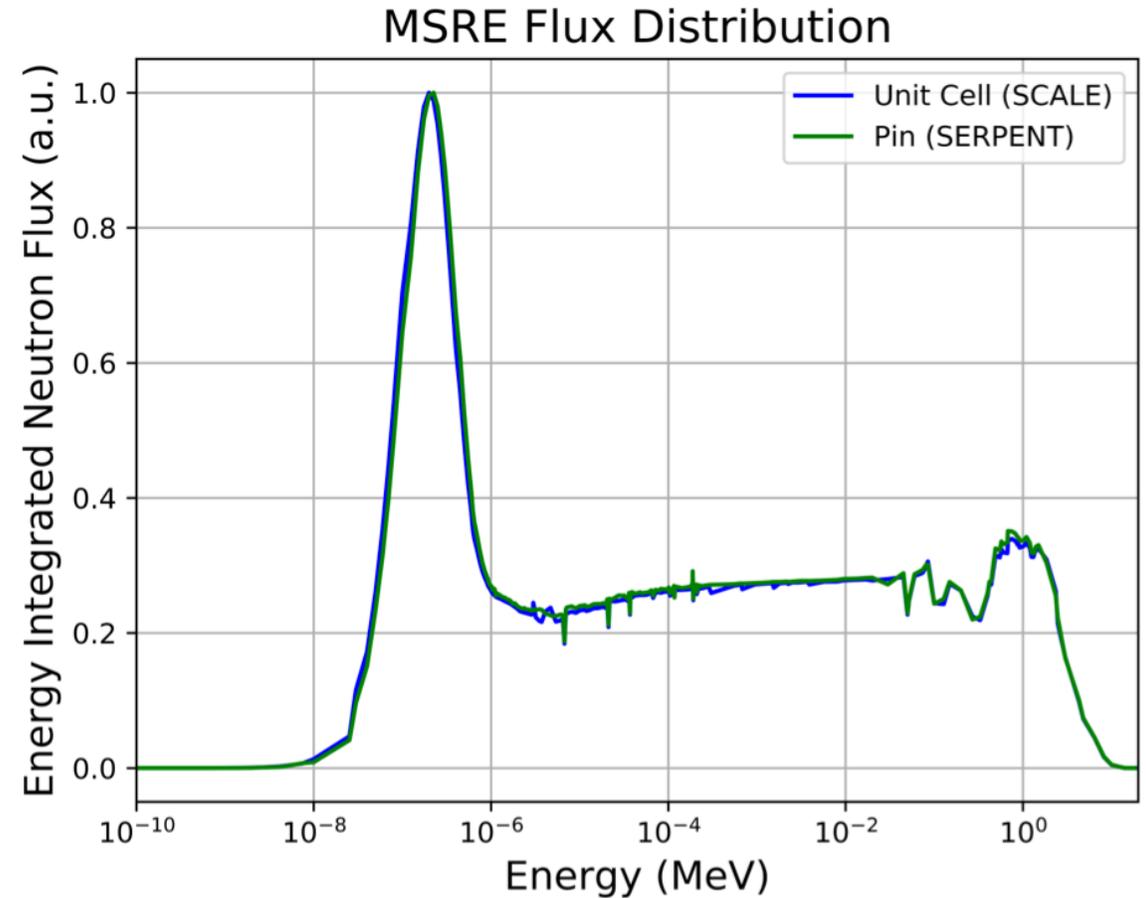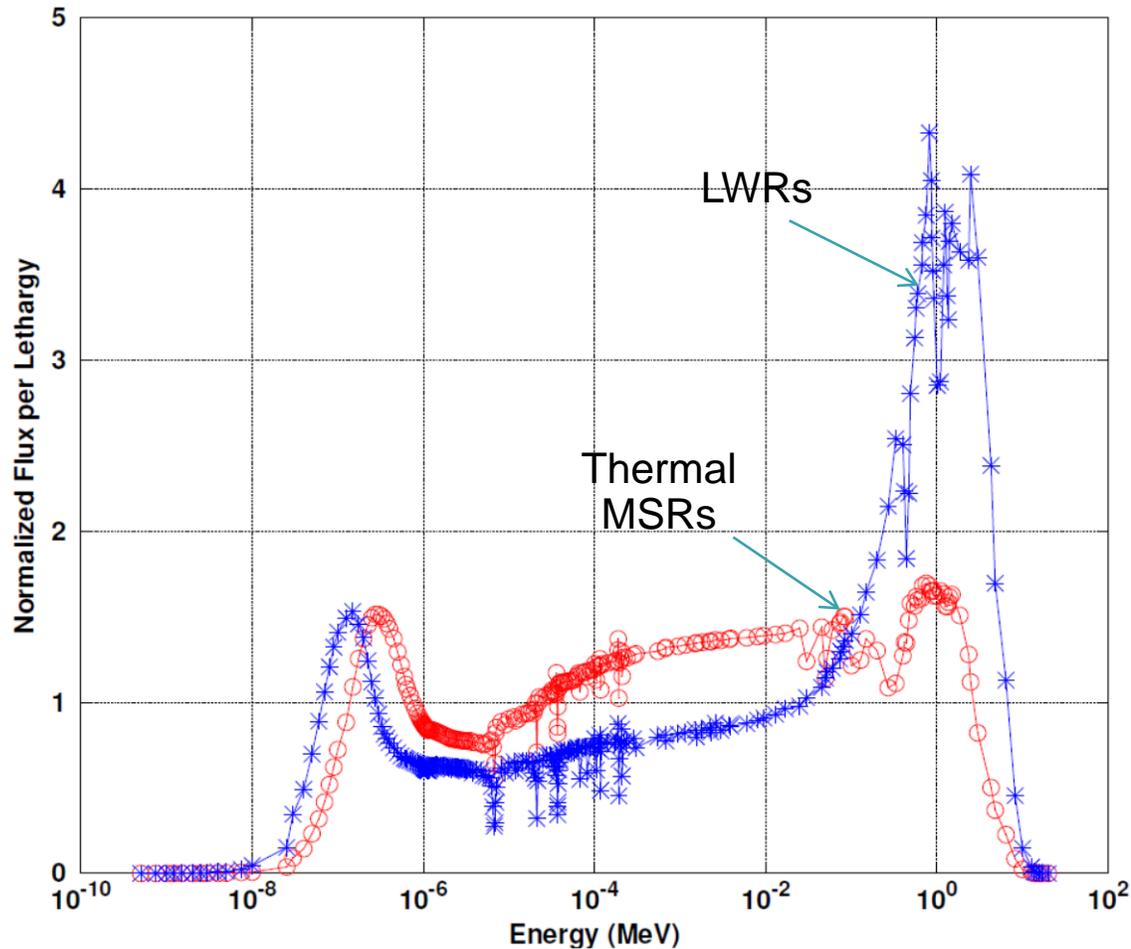
Blanket zone

Driver zone

Source: R. C. Robertson. 1971. *Conceptual Design Study of a Single-Fluid Molten-Salt Breeder Reactor.* ORNL-4541

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Key Differences in LWR and MSR Flux Spectrum

- Typical LWR diffusion length (6 cm) vs. typical fluoride salt MSR diffusion length (16 cm)
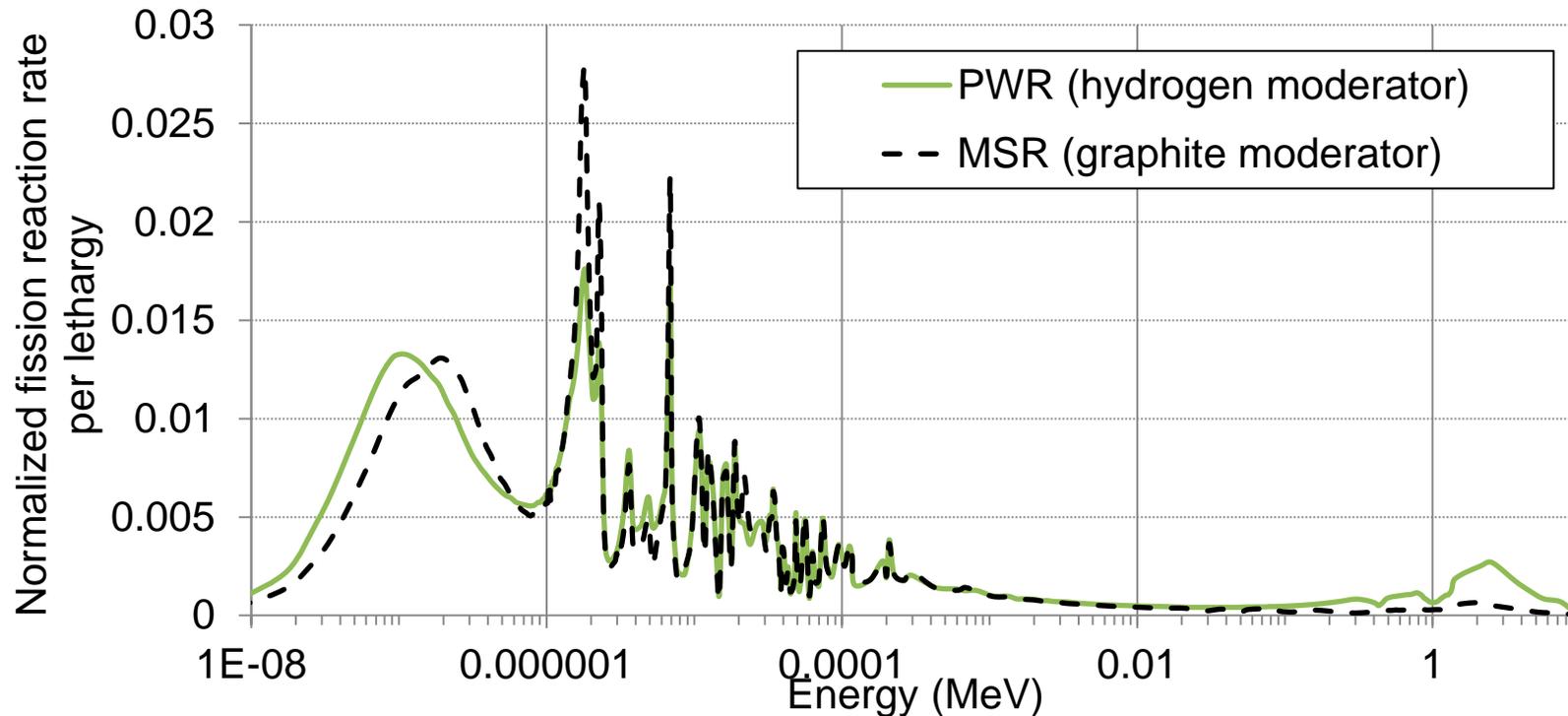

C.A. Gentry. 2016. *Development of a Reactor Physics Analysis Procedure for the Plank-Based and Liquid Salt-Cooled Advanced High Temperature Reactor.* Dissertation, University of Tennessee Knoxville.

ORNL/TM-2019/1418 Modeling Molten Salt Reactor Fission Product Removal with SCALE Pedro jr. Vincente Valdez, Benjamin R. Betzler, William A. Wieselquist, and Massimilano Fratoni

Fission Reaction Rate Spectrum of MSR vs Typical PWR

- Graphite moderator results in a harder fission reaction spectrum without substantial volume increase
  - Neutron migration length in carbon over 60 cm versus under 6 cm in water

- Radiation damage impacts on graphite lifetime is an important consideration in thermal spectrum MSRs

Source: N. R. Brown et al. 2015. "Sustainable thorium nuclear fuel cycles: A comparison of intermediate and fast neutron spectrum systems." *Nuclear Engineering and Design* 289: 252-265.

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Neutron Flux Spectrum of MSRs

- The neutron flux spectrum of MSRs can vary significantly as a function of energy, even for the same design

- Example is the startup of a thorium fuel cycle using U/Pu from spent nuclear fuel
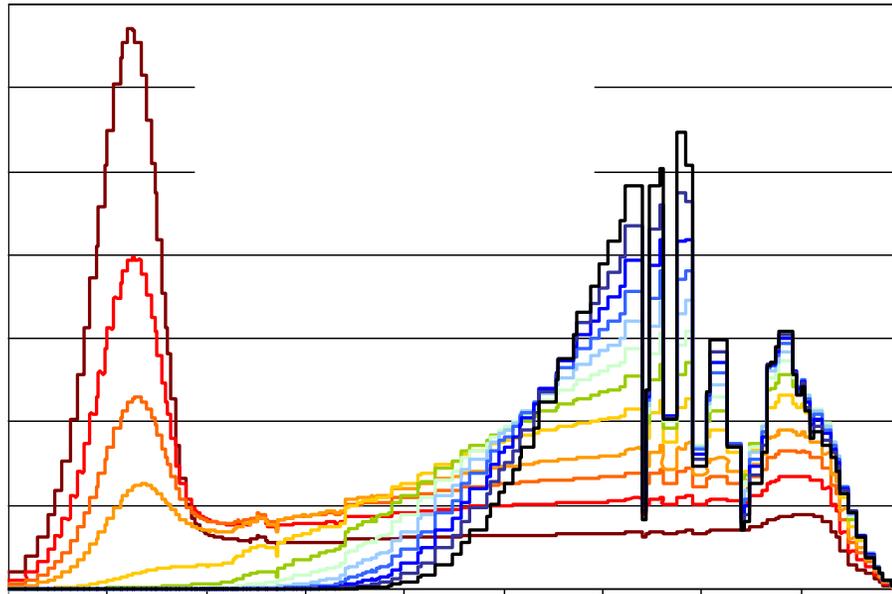

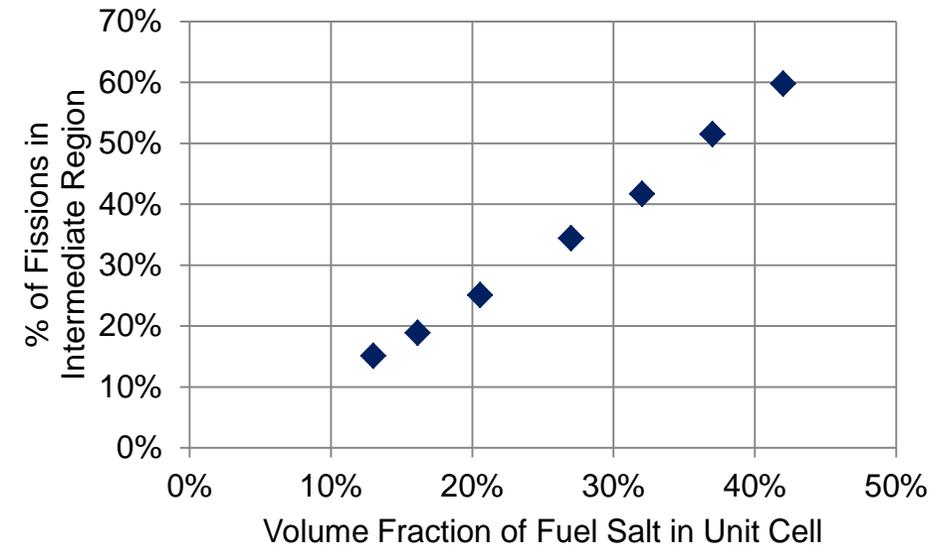Spectrum softens during transition from U/Pu to Th/^{233}U fuel

Source: B. Betzler et al. 2016. "Modeling and Simulation of the Start-up of a Thorium-Based Molten Salt Reactor," in *Proceedings of PHYSOR 2016*

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Fuel Salt versus Moderator Ratio

- Neutron flux spectrum shifts as fuel salt is added to the system and moderator is removed

- Enrichment is adjusted to maintain criticality in these examples

Source: J. Křepel et al. 2014. "Fuel cycle advantages and dynamics features of liquid fueled MSR," *Annals of Nuclear Energy* 64: 380-397. (Used with permission from Elsevier)
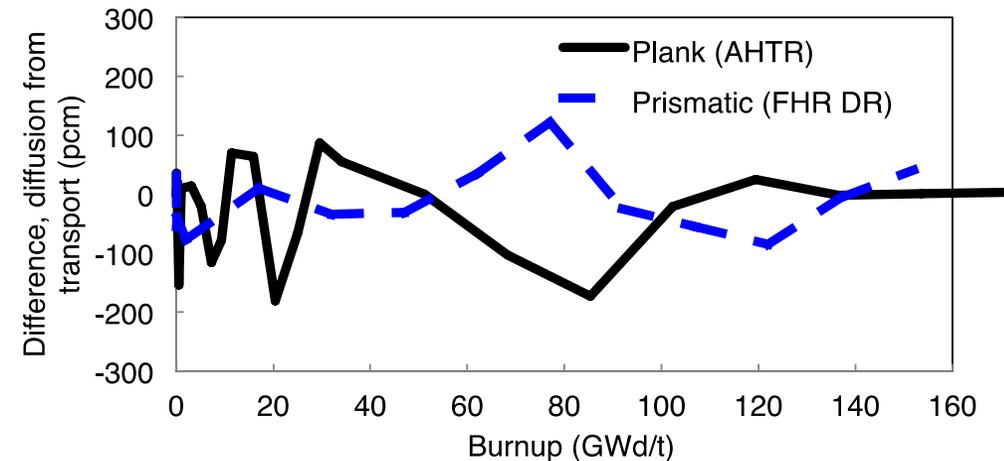

Source: N. R. Brown et al. 2015. "Sustainable thorium nuclear fuel cycles: A comparison of intermediate and fast neutron spectrum systems." *Nuclear Engineering and Design* 289: 252-265.

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MSR Spectrum: Challenges

- Although diffusion calculations have been shown to work well for MSRs, fine energy group and few energy group structures are not well defined

- These group structures would need to be developed for each MSR type

- For thermal spectrum (graphite moderated, fluoride salt) MSRs with LEU fuel, 4-group structure developed for FHRs may be a good starting point

Group #	Upper Bound	Lower Bound
1	2.0000E+01	9.1188E-03
2	9.1188E-03	2.9023E-05
3	2.9023E-05	7.3000E-07
4	7.3000E-07	1.0000E-12

Source: C. Gentry, G. I. Maldonado, and K. S. Kim. 2016. *"Development of a Two-Step Reactor Physics Analysis Procedure for Advanced High Temperature Reactors,"* in *Proceedings of PHYSOR 2016: Unifying Theory and Experiments in the 21st Century.*

Source: N.R. Brown et al. 2016. "Preconceptual design of a fluoride high temperature salt-cooled engineering demonstration reactor: core design and safety analysis." *Annals of Nuclear Energy* 103: 49-59.

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Delayed Neutron Precursor Drift

- Because the fuel is flowing, approximately 50% of delayed neutrons are generated outside of the core region

- This impacts the value of β and the controllability of the reactor

Source: B. Ade, B. Betzler, et. al., *MSR Modeling Tools: Past, Present and Future*, presented at the Advanced Reactor Working Group Modeling & Simulation Workshop, EPRI, Charlotte, NC, January 24-25, 2017.
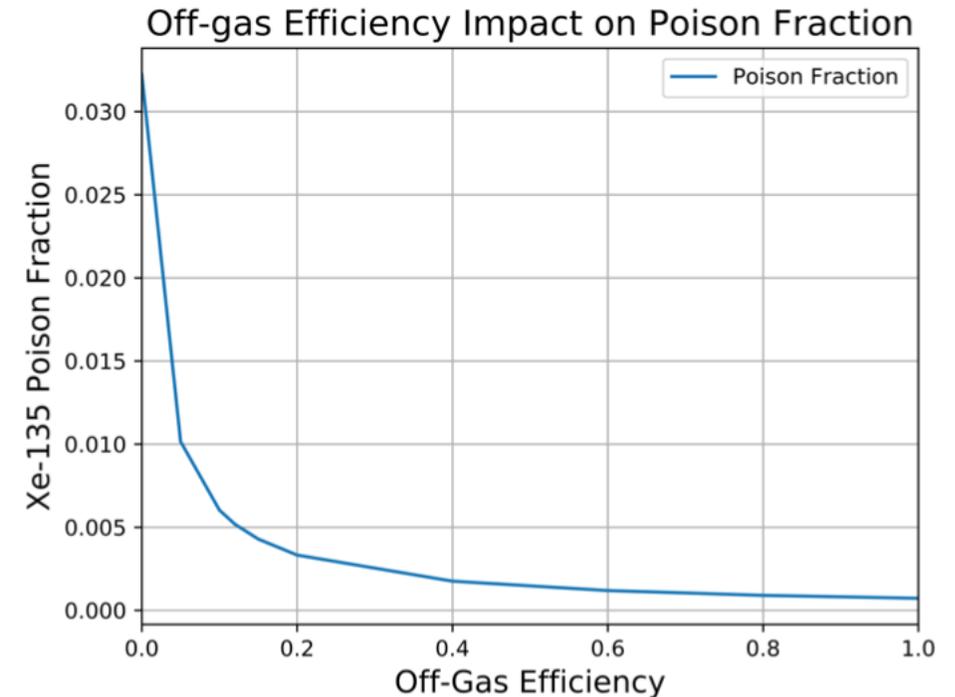
Consequences of Moving Fuel in MSRs

- Fuel carries delayed neutron precursors out of the core
  - Solid fuel reactors are critical due to delayed neutrons emitted from precursor decay (fundamental α eigenvalue is limited by the precursor decay constants and is on the order of s^{-1})
  - Without delayed neutron precursors, the reactor is uncontrollable (prompt α eigenvalues are much greater in magnitude than precursor decay constants)

- 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 in the core
  - Some delayed neutrons are emitted after the liquid fuel leaves the core (coolant loop, chemical processing, etc.)
  - Neutronics tools need delayed neutron convection term to model fission source for MSRs

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Fission Product Removal

- Some MSR designs are intended to actively separate fission and/or transmutation products

- Even if there is no active separation, there will be passive separation, e.g., noble gas fission products

- Fission product gas bubbles may impact reactor stability
  – Although MSRE was shown to be stable during operation

MSRE ^{135}Xe poison fraction as a function of stripping efficiency

Off-gas Efficiency Impact on Poison Fraction

ORNL/TM-2019/1418

Modeling and Simulation of MSRs:
Depletion (Bateman) Equations

- ORIGEN solves a set of depletion equations using fluxes provided from a transport calculation

- These equations describe the rate of change of the nuclides in the problem

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

| 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 |

- For a solid fuel reactor, the fuel is stationary; there is no additional removal or feed term

Source: B. Betzler et al. 2016. "Modeling and Simulation of the Start-up of a Thorium-Based Molten Salt Reactor," in *Proceedings of PHYSOR 2016*.

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Modeling and Simulation of MSRs:
Depletion (Bateman) Equations

- **For a liquid fuel reactor, the additional removal/feed term is likely nonzero**
  - Represents removal of fission products, addition of fertile and fissile material, etc.
  - Must be expressed in terms of a decay constant
  - An accurate removal/feed rate must take into account liquid fuel flow rates and reactor design

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

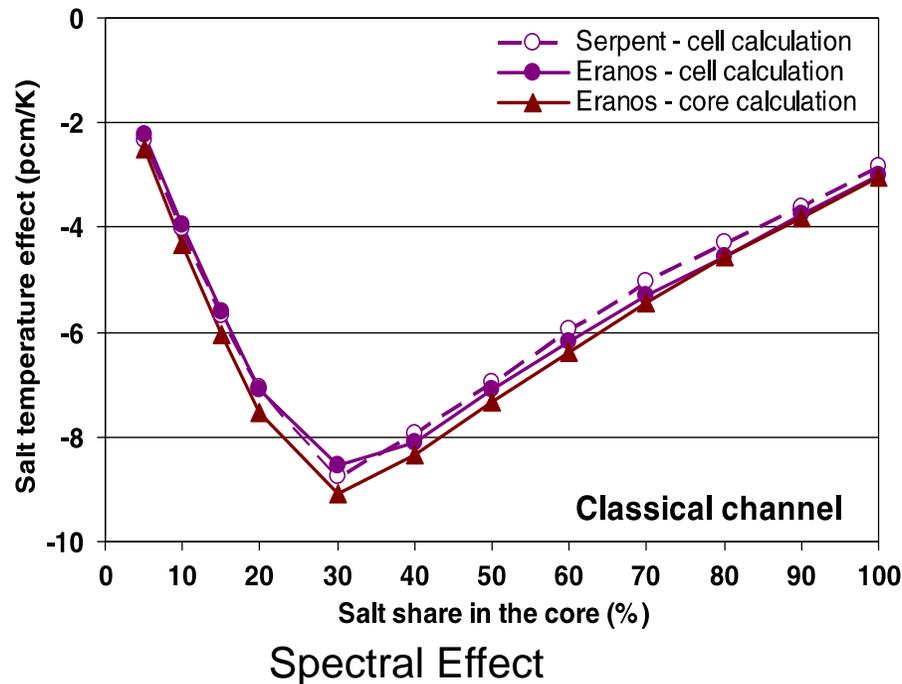- **For a solid fuel reactor, the fuel is stationary; there is no additional removal or feed term**

Source: B. Betzler et al. 2016. "Modeling and Simulation of the Start-up of a Thorium-Based Molten Salt Reactor," in *Proceedings of PHYSOR 2016.*

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Example MSR Separation Processes

Single-Fluid Molten-Salt Breeder Reactor. ORNL-4541

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Reactivity Feedback Effects

- Fuel salt temperature (spectral) and density
  - Net negative (density component may be positive or negative)

- Moderator temperature
  - May be negative or positive

- Moderator thermal expansion
  - Negative, but longer time scale

- Changes in flow rate
  - Stable, depending on design

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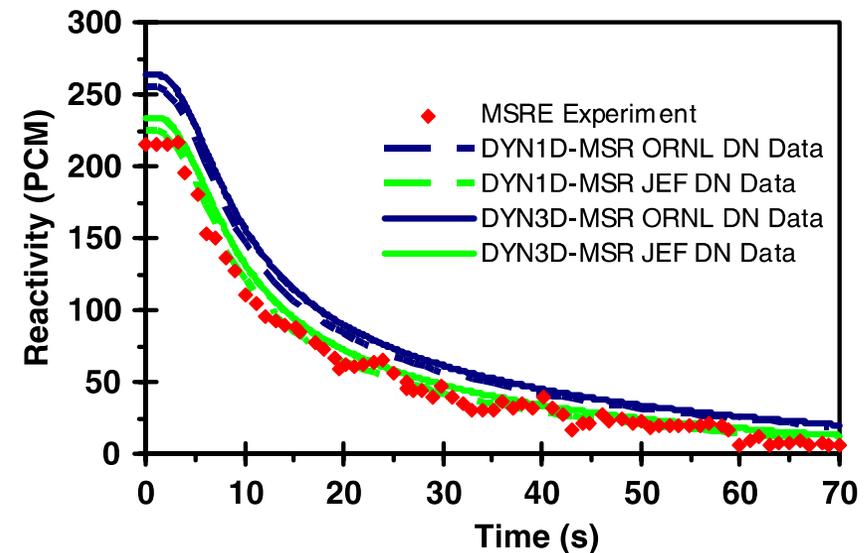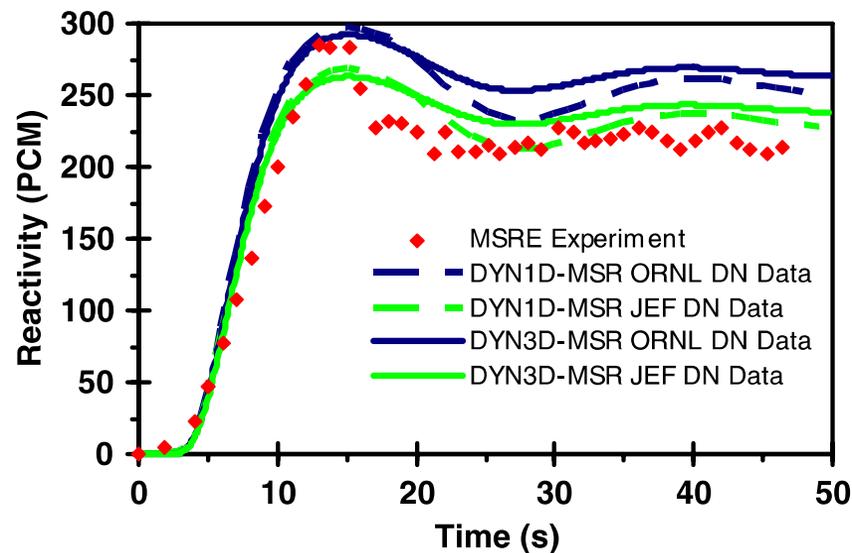# Example Fuel Salt Temperature and Density Reactivity Feedback Effects

- Net effect is negative, driven by strongly negative fuel temperature spectral effect

- Density component can sometimes be positive

Spectral Effect

Density Effect

Source: J. Křepel et al. 2014. "Fuel cycle advantages and dynamics features of liquid fueled MSR," *Annals of Nuclear Energy* 64: 380-397. (Used with permission)

Reactivity Effects of Delayed Neutron Precursor Drift (1/2)

- Experimental observations from MSRE and model predictions for fuel pump start-up and coast-down transients

- Results from DYN3D German nodal kinetics code in two groups, similar to US NRC code PARCS

- US NRC code PARCS needs modification for delayed neutron precursor motion

Source: J. Křepel et al. 2007. "DYN3D-MSR spatial dynamics code for molten salt reactors." *Annals of Nuclear Energy* 34: 449-462.

Reactivity Effects of Delayed Neutron Precursor Drift (2/2)

- Experimental observations from MSRE and model predictions for natural circulation transient

- This example shows that neutronics codes (DYN3D) with the fidelity of the US NRC code PARCS can accurately predict passive safety performance of MSRs (if modified for precursor drift)

Source: J. Křepel et al. 2007. "DYN3D-MSR spatial dynamics code for molten salt reactors." *Annals of Nuclear Energy* 34: 449-462. (Used with permission)
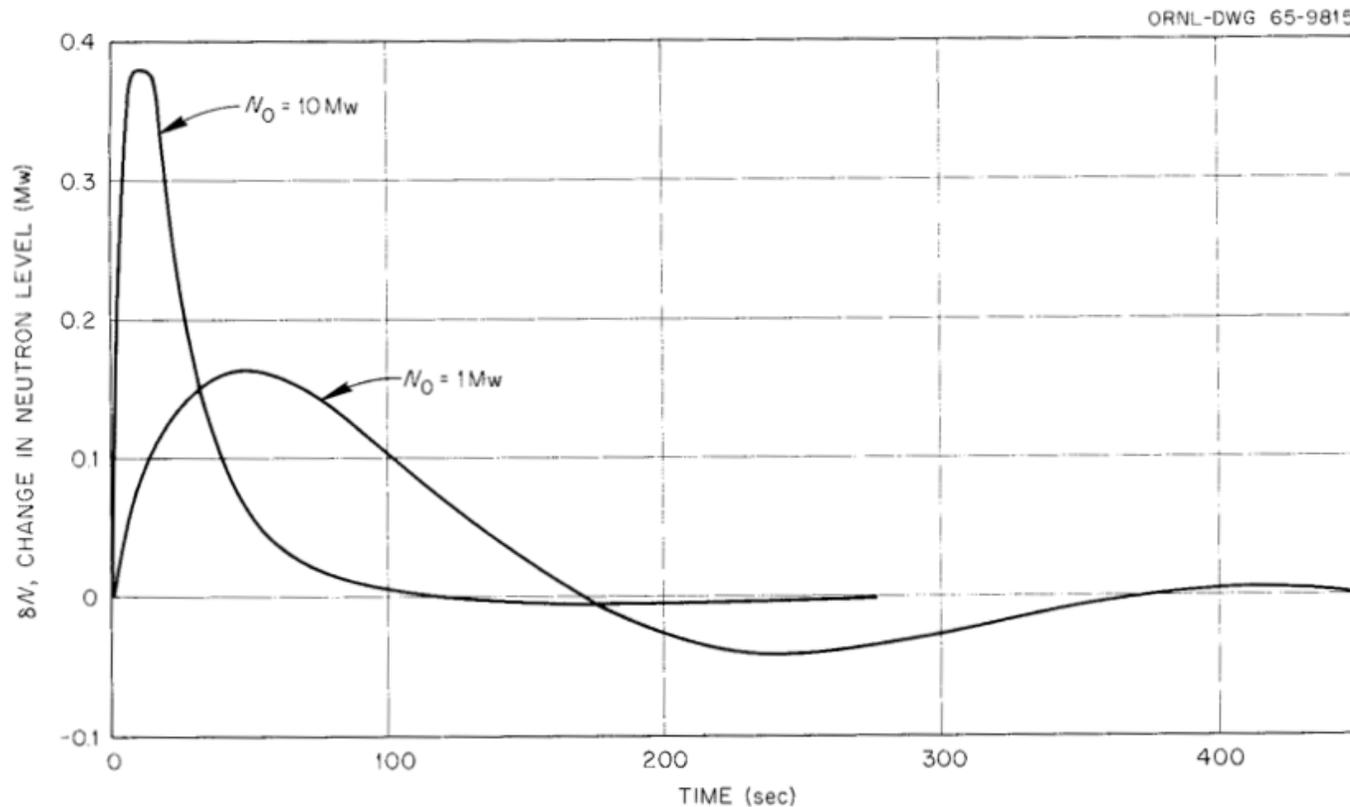
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Stability of MSRE and Reactivity Feedback

- MSRE was determined analytically to be inherently stable

- Predictions were confirmed experimentally

- Example: reactivity insertion behavior

ORNL-DWG 65-9815

MSRE transient response to +0.01% δk step reactivity input when operating at 1 and 10 MW

ORNL/TM-1070

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Nuclear Data Availability and Uncertainty

- Nuclear data uncertainties impact the ability to predict MSR neutronics

  - Absorption reactions

    - in lithium are important for thermal spectrum fluoride salt MSRs

    - in chlorine are important for fast spectrum chloride salt MSRs

  - Thermal neutron scattering

    - $S(\alpha,\beta)$ libraries are needed, especially for Li and Be in FLiBe

- Some examples follow for thermal spectrum and fast spectrum MSRs
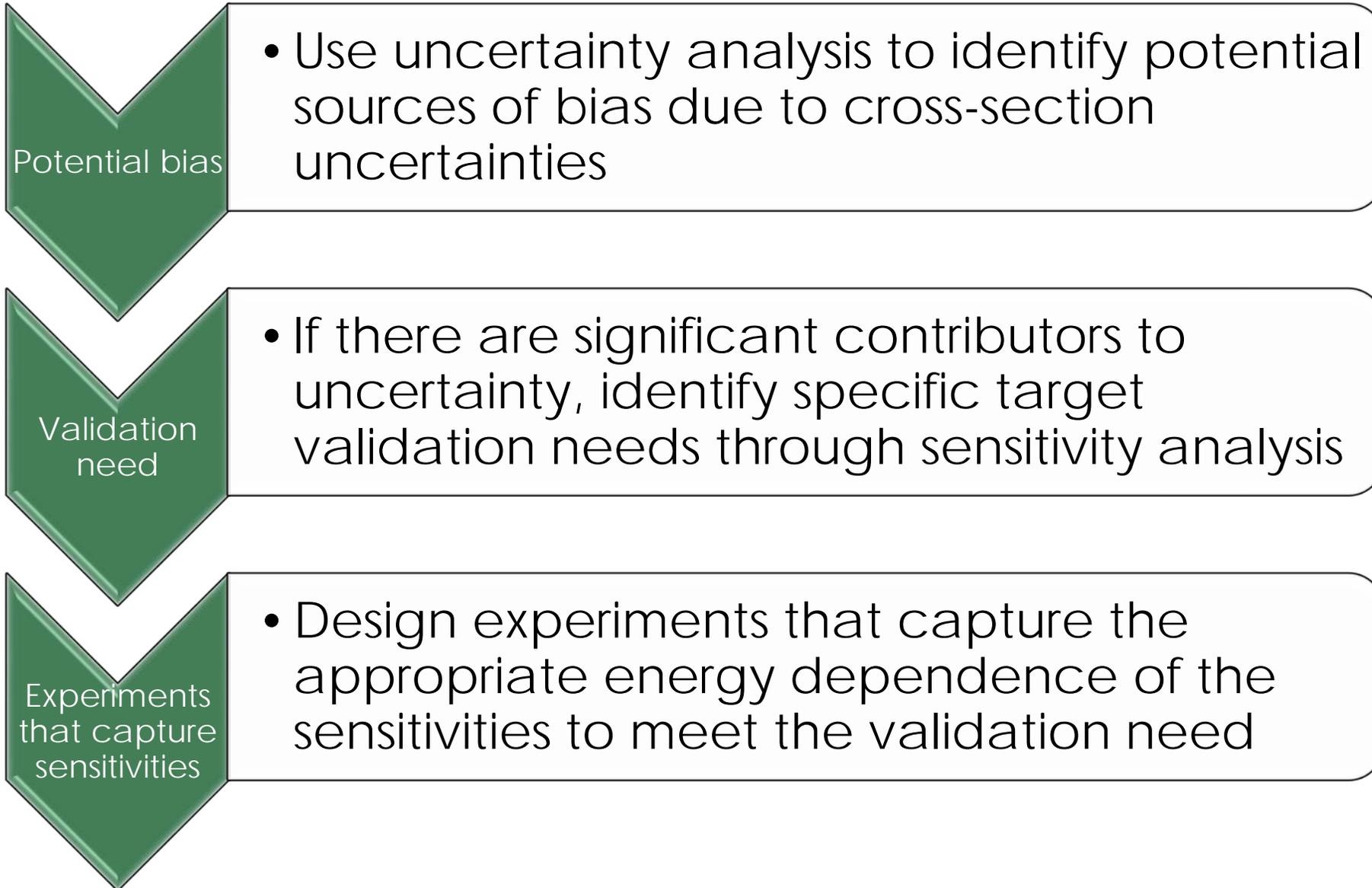
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Example: Sensitivity and Uncertainty (S/U) Analysis

- Identify potential sources of bias due to neutron cross-sections through uncertainty analysis

- Use sensitivity profiles as a function of energy as a tool to design informed experiments that can address those potential sources of bias

$$S_{k,\Sigma} = \frac{\delta k / k}{\delta \Sigma / \Sigma}$$

- At the high level, the goal of S/U analysis is to:
  - Have high quality critical experiments for validation of reactor physics calculations for fluoride salt reactor concepts: operations and design
  - Assess adequacy of ENDF cross-sections

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Source: ORNL/TM-2016/729

S/U Analysis

Potential bias
- Use uncertainty analysis to identify potential sources of bias due to cross-section uncertainties

Validation need
- If there are significant contributors to uncertainty, identify specific target validation needs through sensitivity analysis

Experiments that capture sensitivities
- Design experiments that capture the appropriate energy dependence of the sensitivities to meet the validation need
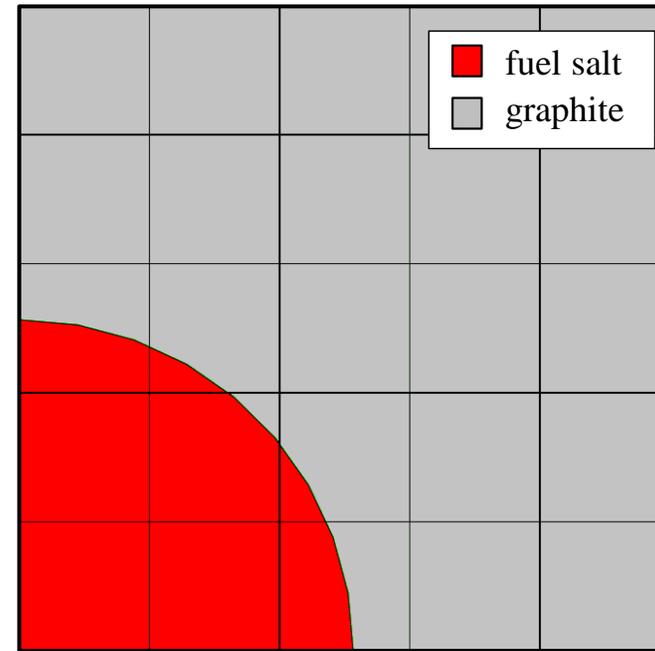
Source: ORNL/TM-2016/729

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Sensitivity and Uncertainty (S/U) Analysis of MSR Application Models

- Model of a typical liquid fueled MSR unit cell geometry were adapted for S/U analysis

- Scoping S/U analysis was completed for MSR models
  - Both Th/^{233}U and LEU fueled MSR

S/U analysis of MSR LEU model shows uncertainty contributions from ^{7}Li, C, ^{19}F

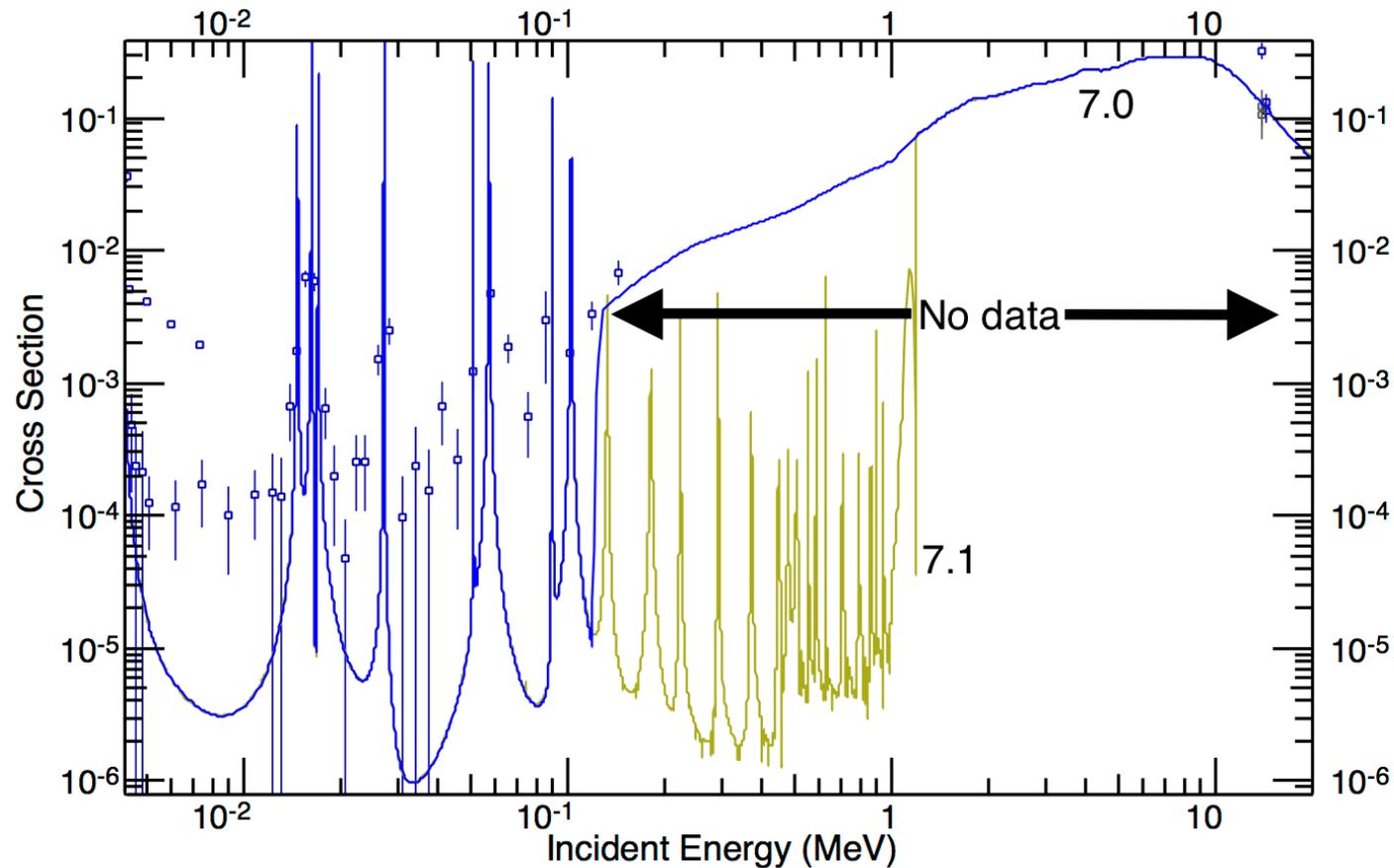| | fuel salt |
| | graphite |

MSR Model

Source: J. J. Powers, T. J. Harrison, and J. C. Gehin. 2013. "A New Approach for Modeling and Analysis of Molten Salt Reactors Using Scale." *Proceedings of the 2013 International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2013).*

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Observation from S/U Analysis

- For liquid fueled thermal spectrum fluoride salt reactors ^{7}Li seems to be the most significant contributor to potential bias in the FLiBe salt
  - For the range of ^{7}Li enrichments considered and the limited set of application models

- Unlike LWRs, SFRs, and HTGRs, there is an almost total lack of available benchmarks for MSRs
  - Integral critical experiments would support salt reactor development

Source: ORNL/TM-2016/729

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Example: ^{35}Cl (n,p) for Chloride Salt Reactors

- Discrepancies in libraries (e.g., ENDF/B VII.0 vs. ENDF/B VII.1) and lack of data in the fast energy range significantly impacts criticality predictions (1000s of pcm)

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Conclusions

- MSRs present potential neutronics advantages
  - "Infinite batch" refueling (low excess reactivity)
  - Possibility for online removal of fission products
  - Strong potential for inherent safety and stability

- MSRs are very different from traditional solid fueled systems due to fuel cycle flexibility and delayed neutron precursor drift

- There is a wide variety of different MSR concepts with many different salts, potential missions, and neutronic characteristics

- US NRC tools such as PARCS need modification to account for reactor physics of MSRs

- Very strong need for benchmark experiments and validation data to benchmark simulation tools

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