

Implementation of Molten Salt Reactor Tools in SCALE

Benjamin R. Betzler
Jeffrey J. Powers
Nicholas R. Brown
Bradley T. Rearden

SCALE Workshop – Oak Ridge, TN
27 September 2017



SCALE Code System

Analysis enabling nuclear technology advancements

SCALE 6.2 – SCALE 7.0

2016 – present:

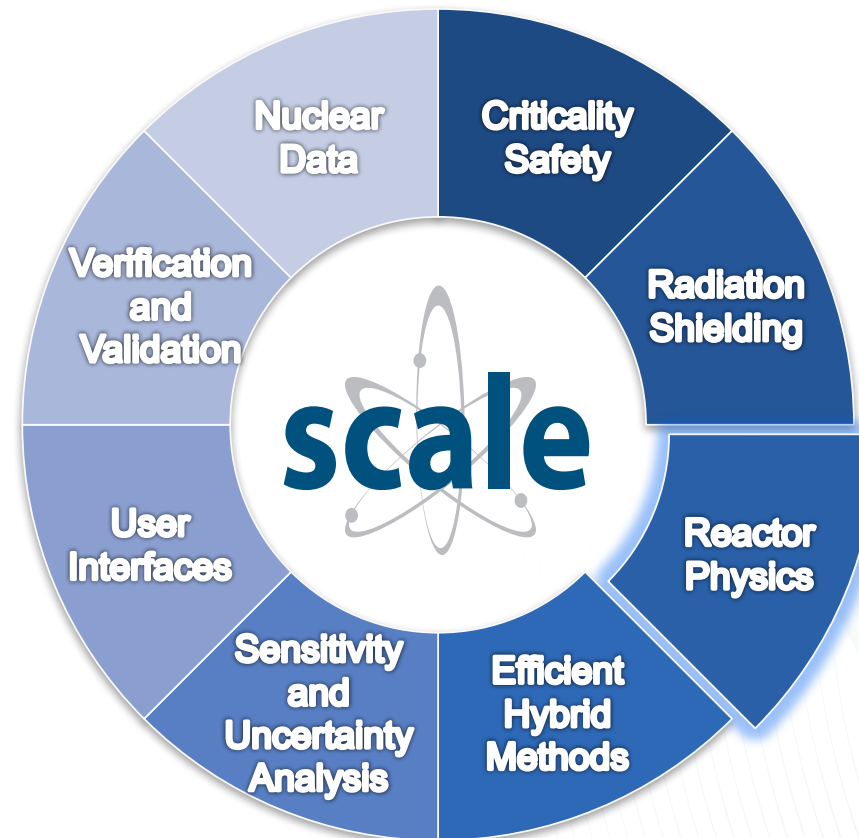
**Increased Fidelity,
Infrastructure Modernization,
Parallelization, Quality
Assurance**

Solutions for extremely complex systems

High-fidelity shielding, depletion and sensitivity analysis in continuous energy

Modern, modular software design

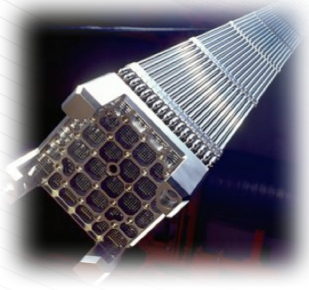
Scalable from laptops to massively parallel machines



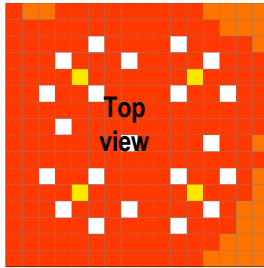
- Transport
 - Monte Carlo
 - Deterministic
- Point depletion

SCALE Code System

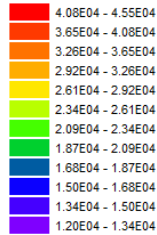
Reactor physics and used fuel characterization



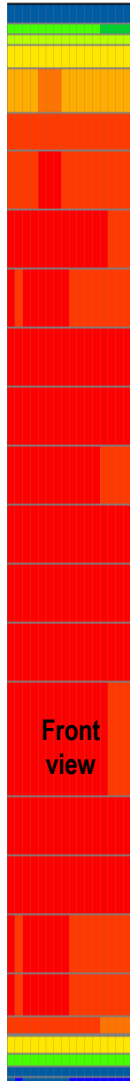
Pin-by-pin burnup and radioactive source terms



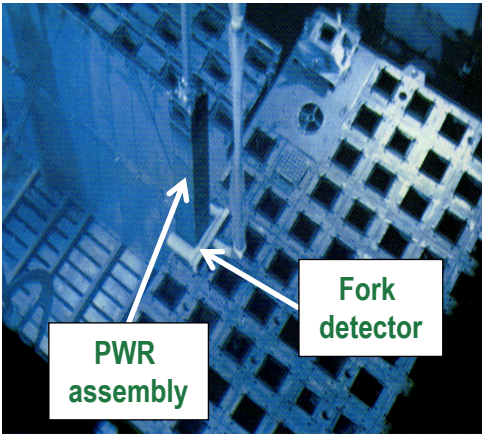
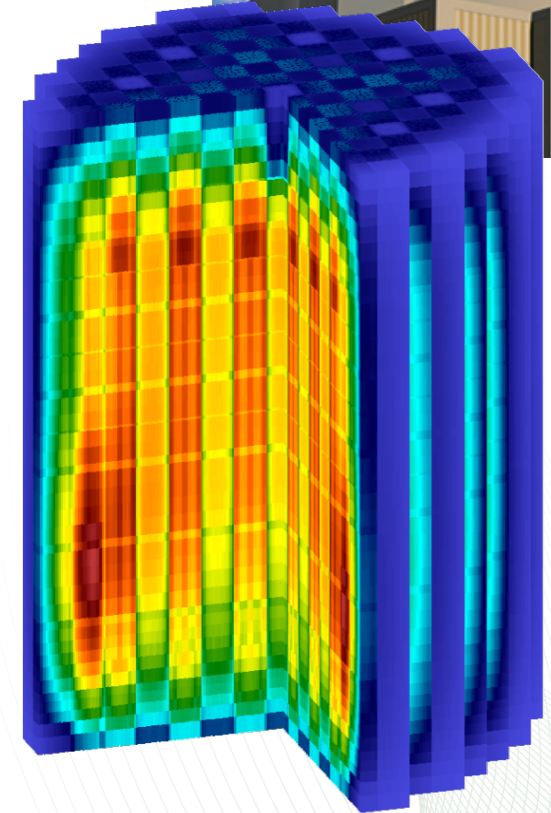
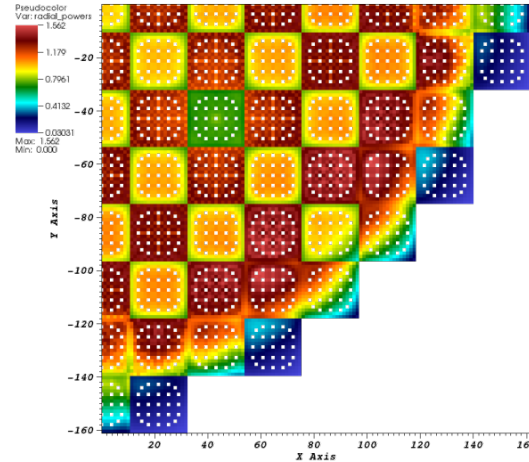
Burnup (MWd/MTU)



Front view



Power distribution for AP-1000 reactor



ORCA: Automator

Reactor type grid layout table

Column grid labels	Row grid labels	Assemblies per row
1 R	1	7
2 P	2	11
3 N	3	13
4 M	4	13
5 L	5	15
6 K	6	15
7 J	7	15
8 H	8	15
9 G	9	15
10 F	10	15
11 E	11	15
12 D	12	13
13 C	13	13
14 B	14	11
15 A	15	7

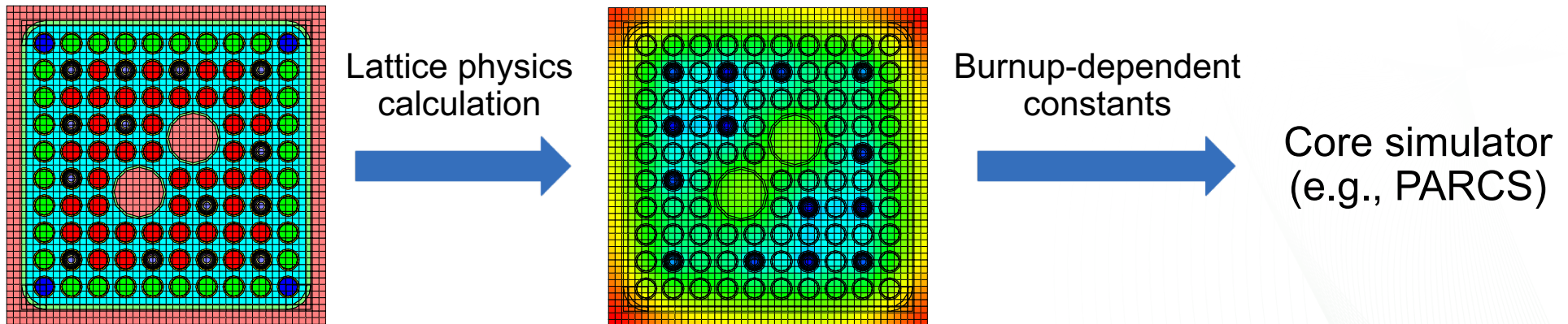
Total assemblies: 193

User interface for facility-wide source term characterization

Liquid-Fueled Molten Salt Reactors

Extending methods 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

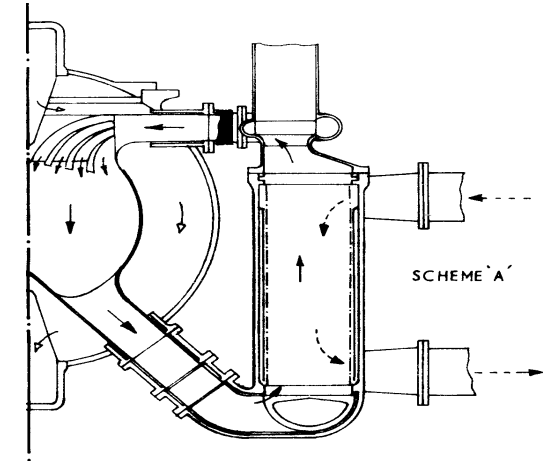


- Liquid fuel reactor characteristics
 - Fuel flows with carrier material (delayed neutron precursor drift)
 - Includes continuous and batch chemical processes

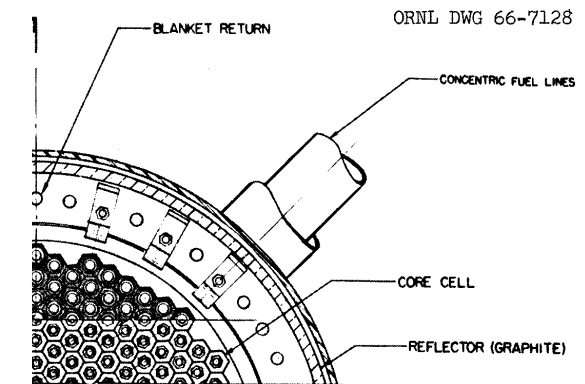
Liquid-Fueled Molten Salt Reactors

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



1/2-core fast spectrum design.¹



1/4-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).

Motivation

Develop MSR modeling and simulation capabilities in SCALE

- 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

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

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

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

- Often, delayed and prompt fission is effectively lumped

Reactor Physics Analysis

Notation

- Total, prompt, and delayed nuubar (average neutrons released per fission)

$$\bar{\nu}(\mathbf{r}, E) = \bar{\nu}_p(\mathbf{r}, E) + \bar{\nu}_d(\mathbf{r}, E)$$

- Total, prompt, and delayed χ (neutron emission) spectra (J precursor groups)

$$\chi = \chi_p(1 - \beta) + \sum_{j=1}^J \chi_j \beta_j$$

- β (delayed neutron fraction)

$$\beta = \frac{\bar{\nu}_d}{\bar{\nu}}$$

- α (group normalized neutron fraction)

$$\beta_j = \alpha_j \beta$$

Delayed Neutron Precursor Drift Models

Molten Salt Reactor Experiment Zero-Dimensional (0D) Model

- Molten Salt Reactor Experiment (MSRE) 0D model
- Consideration of in-core (τ_c) and out-of-core (τ_e) times to correct for the delayed neutron precursors that exit the core before decaying

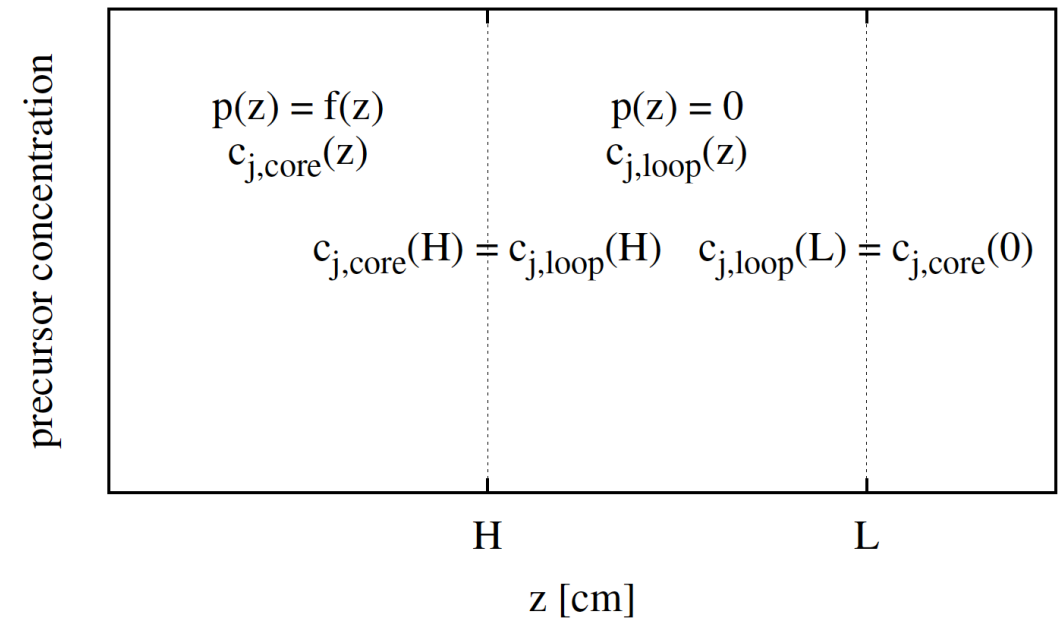
$$\frac{dc_j(t)}{dt} = -\lambda_j c_j(t) + \frac{\bar{\beta}_j(t)}{\Lambda(t)} p(t) - \frac{c_j(t)}{\tau_c} + \frac{c_j(t - \tau_e) e^{-\lambda_j \tau_e}}{\tau_c}$$

Delayed Neutron Precursor Drift Models

One-dimensional (1D) model

- A 1D precursor drift model has been implemented into SCALE
 - Considers a 1D velocity and power profile
 - Accounts for recirculating precursors

$$v(z) \frac{dc_j(z)}{dz} = -\lambda_j c_j(z) + \frac{\bar{\beta}_j}{\Lambda} p(z)$$



1D precursor drift problem showing boundary conditions.

Delayed Neutron Precursor Drift Models

Applying correction factors to account for drift

- Objective is to obtain flow-adjusted parameters (χ and $\bar{\nu}$)

$$\chi^f = \chi_p(1 - \beta^f) + \sum_{j=1}^J \chi_j \beta_j^f \quad \bar{\nu}^f = \bar{\nu}_p + \bar{\nu}_d^f$$

- Use correction factors from the precursor solutions

- Axially dependent correction factor: $F_j(z) = \frac{C_{j,\text{drift}}(z)}{C_{j,\nu=0}(z)}$

- Integrated correction factor: $F_j = \frac{\int_{z_1}^{z_2} C_{j,\text{drift}}(z) dz}{\int_{z_1}^{z_2} C_{j,\nu=0}(z) dz}$

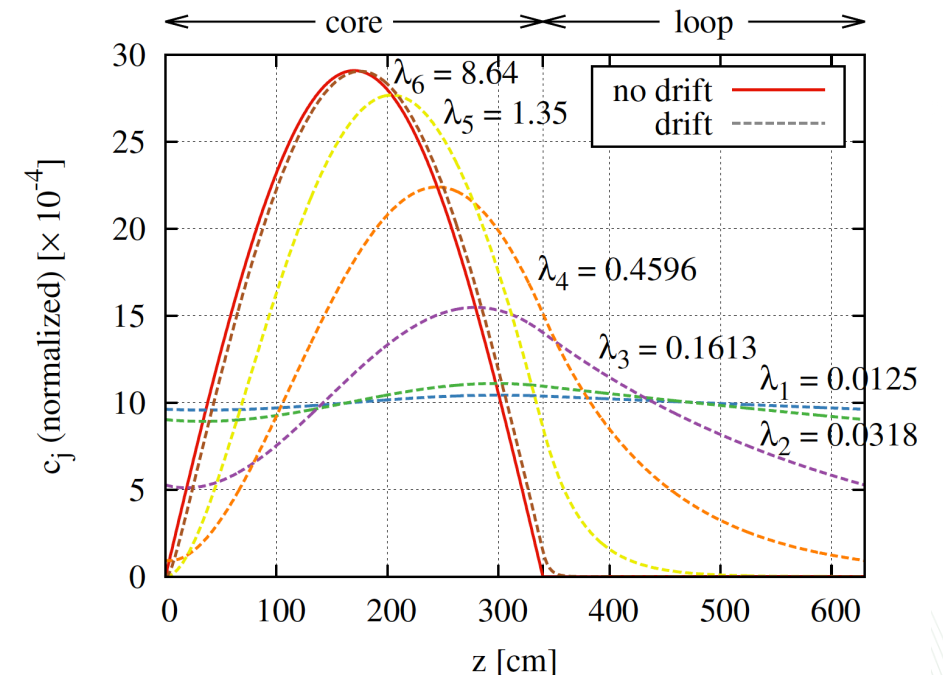
Delayed Neutron Precursor Drift Solutions

Analytical solutions for precursor drift

- To provide solutions for testing precursor drift modules
- 0D model is unable to account for effects from power shapes

Analytic Correction Factors (F) Using Different Models

j	0-D	Core-averaged 1-D	
		$p(z) = C$	$p(z) \sim \sin(z)$
1	0.5493	0.5403	0.5403
2	0.5635	0.5417	0.5421
3	0.6480	0.5788	0.5885
4	0.7772	0.7236	0.7660
5	0.9059	0.8961	0.9518
6	0.9840	0.9838	0.9987
total	0.7405	0.6994	0.7287

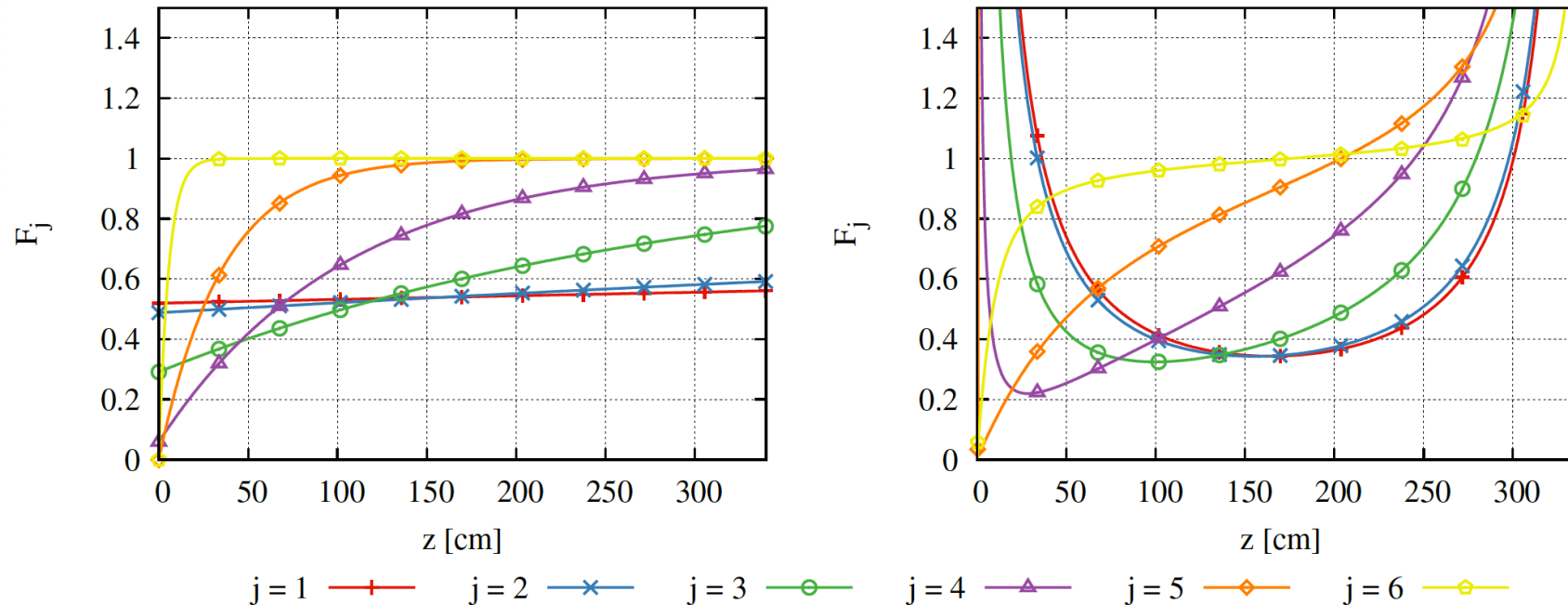


Delayed neutron precursor concentrations in the primary loop of a liquid-fueled MSR.

Delayed Neutron Precursor Drift Solutions

Effect of power shape on correction factors

- Power shape greatly affects the in-core distribution of precursors
- Sinusoidal power profiles result in large factors near core boundaries

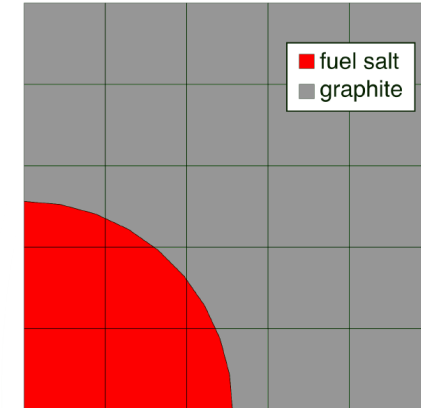


Comparison of axially dependent group correction factors from SCALE and analytical solutions with constant (left) and sinusoidal (right) power profiles. Analytical solutions are plotted as a line; SCALE solutions are plotted as points.

Delayed Neutron Precursor Drift Applications

Simple Molten Salt Breeder Reactor (MSBR) unit cell model

- Two-dimensional (2D) transport model of an MSBR unit cell
 - ^{233}U and thorium tetrafluorides dissolved in a FLiBe carrier salt
 - Graphite moderator blocks
- 1D precursor drift model
 - 340 cm core height
 - 630 cm primary length
 - 48 cm/s velocity
- 2D model used to generate group constants for a 15 cm region before the outlet of the core

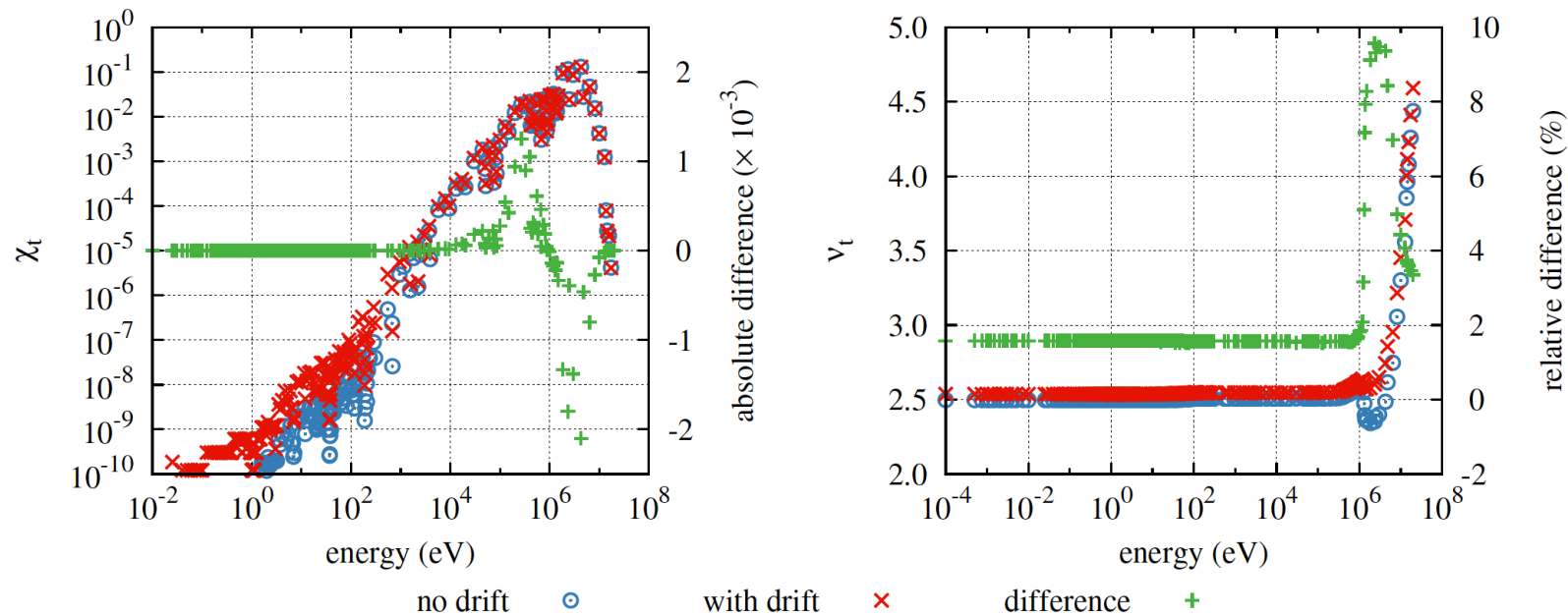


SCALE 2D transport
MSBR unit cell.

Delayed Neutron Precursor Drift Applications

Effect on fission emission spectrum and nubar

- Large effect on the number of neutrons emitted per fission
- Over six times the amount of delayed precursors located in the region with respect to the solution without precursor drift



Flow-adjusted χ (left) and nubar (right) using the correction factors.

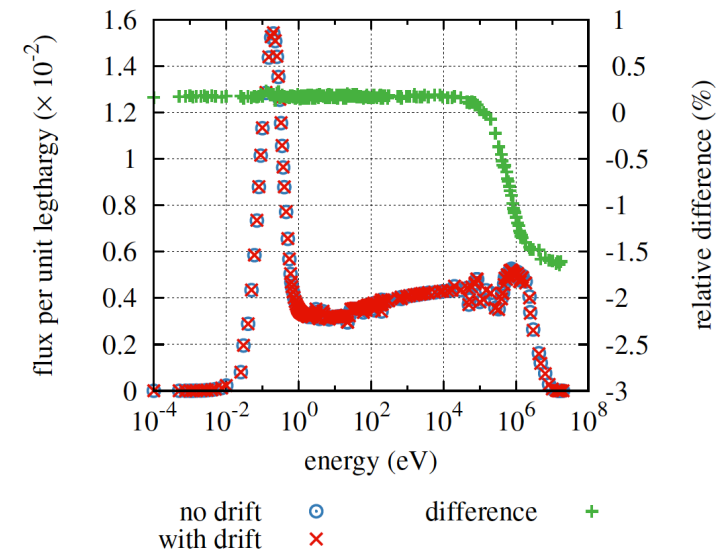
Delayed Neutron Precursor Drift Applications

Effect on criticality and spectrum

- Effect on criticality align with theoretical expectations
- Small observed effect on the neutron spectrum (consider this for use in cross section processing)

SCALE-calculated k using flow-corrected constants
(core-averaged constants included).

Condition	Core-averaged		Last 15 cm	
	NEWT k	Δk [pcm]	NEWT k	Δk [pcm]
no drift	1.06984	—	1.06984	—
with $\bar{\nu}_t^f$	1.06867	-117	1.08738	1754
with $\bar{\chi}_t^f$	1.06984	0	1.06997	13
with $\bar{\nu}_t^f, \bar{\chi}_t^f$	1.06867	-117	1.08749	1765
est. $\Delta k^{(a)}$	—	-116	—	1710



Normalized neutron flux in the two-dimensional unit cell with and without precursor drift.

Delayed Neutron Precursor Drift Applications

Effect on group constant generation

- Two-group constants perform fairly well for this thermal system
- Largest effect is due to the flow-adjusted nu_{bar}

SCALE-calculated two-group cross sections using flow-corrected constants (core-averaged constants included).

Constant	No drift	Middle 15 cm ^(a)	Last 15 cm ^(a)
$k_{\text{eff}}^{(b)}$	1.06984	1.06820 (0.15)	1.08749 (1.62)
$k_{\infty}^{(c)}$	1.07034	1.06868 (0.16)	1.08796 (1.62)
$\Sigma_{\text{tr},1}$	0.32781	0.32776 (0.02)	0.32839 (0.18)
$\Sigma_{\text{tr},2}$	0.40862	0.40862 (0.00)	0.40862 (0.00)
$\Sigma_{\text{a},1} \times 10^{-3}$	1.66403	1.66370 (0.02)	1.66771 (0.22)
$\Sigma_{\text{a},2} \times 10^{-3}$	5.63859	5.63859 (0.00)	5.63859 (0.00)
$(\bar{\nu}\Sigma_{\text{f}})_1 \times 10^{-3}$	1.24340	1.24108 (0.19)	1.26791 (1.93)
$(\bar{\nu}\Sigma_{\text{f}})_2 \times 10^{-3}$	7.13632	7.12545 (0.15)	7.25026 (1.57)
$\Sigma_{1,2} \times 10^{-3}$	3.73485	3.73403 (0.02)	3.74442 (0.26)

^(a) Absolute difference (%) in parenthesis.

^(b) From NEWT transport.

^(c) Using two-group cross sections.

Ongoing Efforts

Molten Salt Reactor Tools

- Determine the effect of flow-adjusted constants on self-shielding calculations
- Implement into Monte Carlo transport
- Integrate material-accounting capabilities with the transport and depletion modules within SCALE
 - Provide the SCALE transport and depletion tool with access to continuous removal capabilities
 - Develop a method to include the removed states
- Develop inputs to interact with these tools, with intentional generic implementation to provide a broader application space

Adapting SCALE Methods for MSR Analysis

Key points

- Detailed a simple 1D model for calculating precursor distribution
- Used correction factors to generate flow-adjusted parameters to implement during neutron transport calculations
- Demonstrated in applications to analytic and MSR problems
 - Analytic problems verify performance of the 1D model in SCALE
 - Application to a simple unit cell problem aligns with theoretical expectations
- Defined continuing scope of the implementation of MSR tools into SCALE

Acknowledgements

- This work is supported by the US Department of Energy, Office of Technology Transitions, Technology Commercialization Fund. The authors would also like to thank M. A. Jessee, R. A. Lefebvre, and S. W. Hart for their help with the SCALE implementation and quality assurance process.