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ANS Winter 2024 Slides: MCCAFE: The Monte Carlo Constructor for ATR Fuel Elements

November 2024

Changing the World's Energy Future

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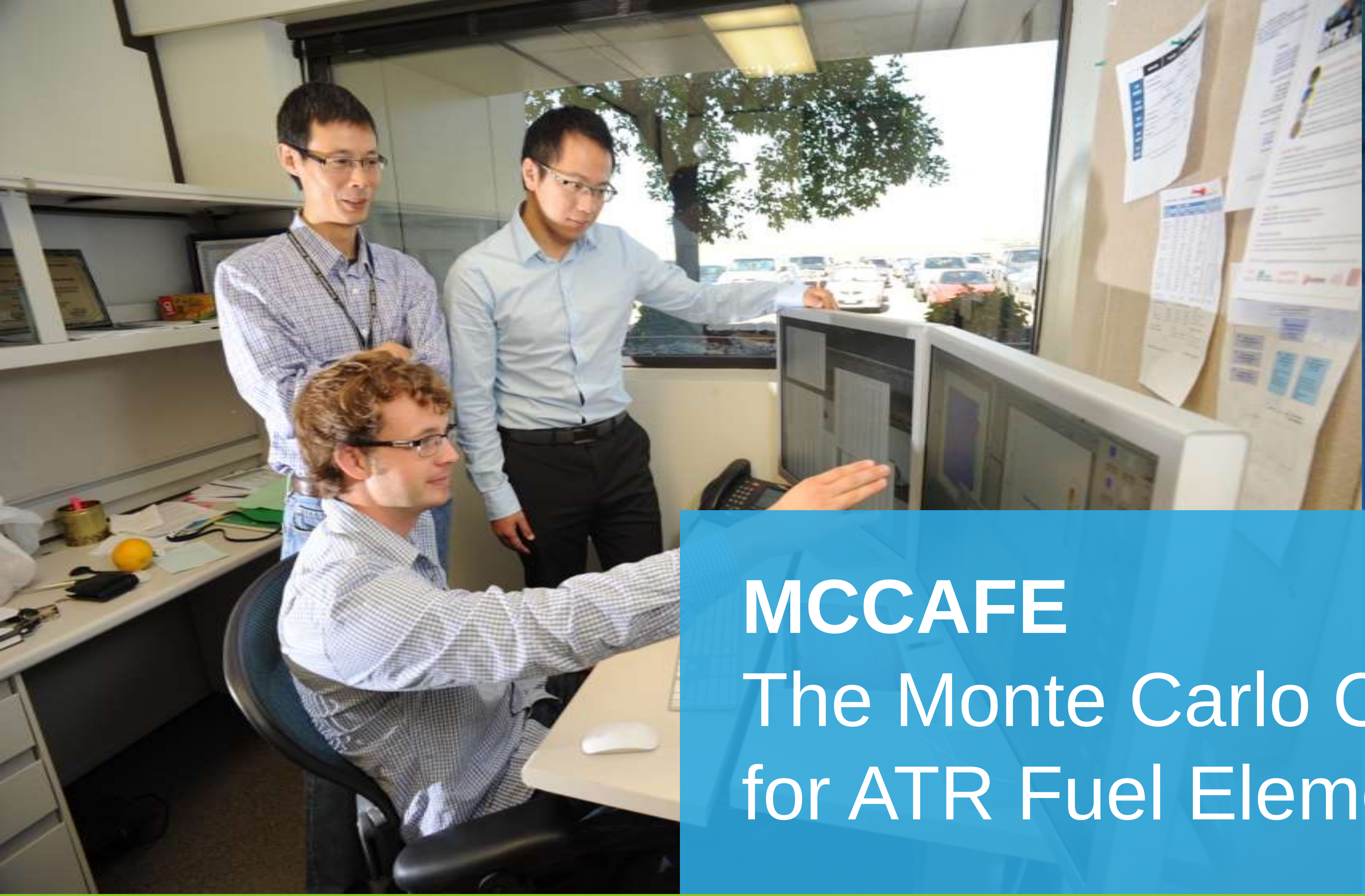


November 19, 2024

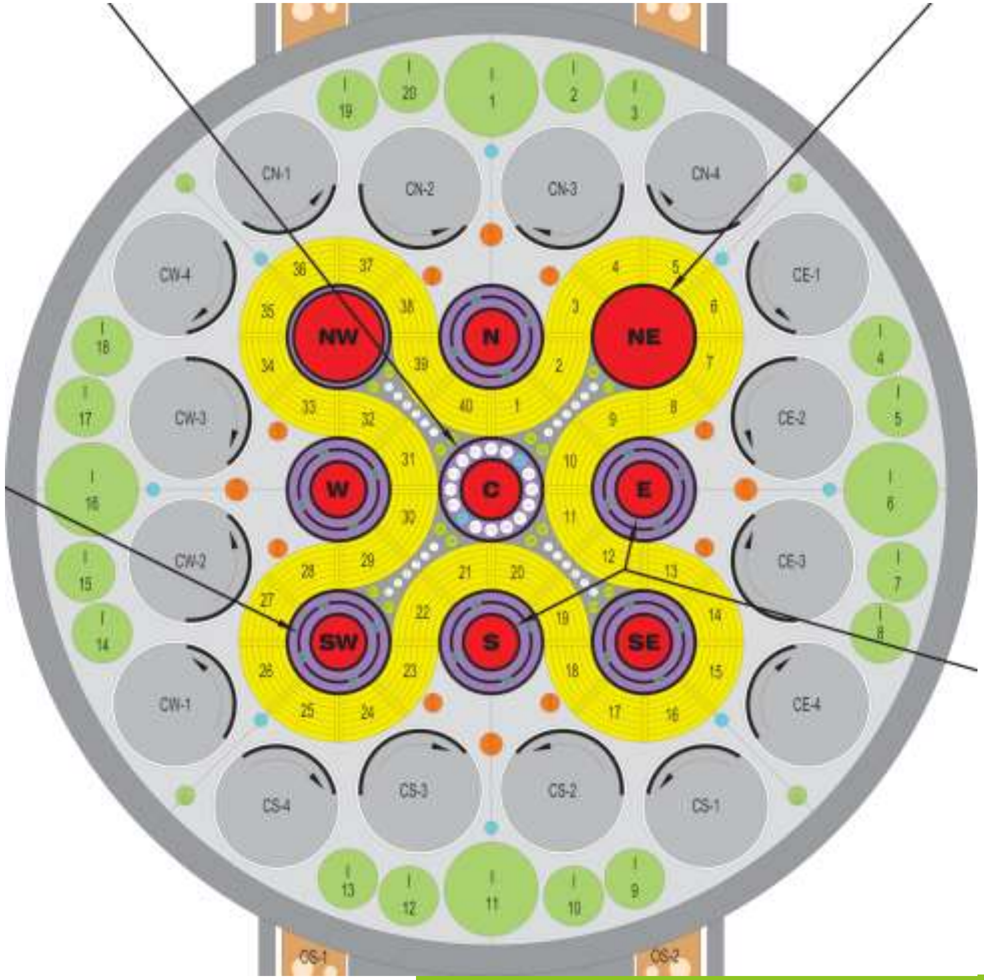
Travis J. Labossiere-Hickman

MCCAFE
The Monte Carlo Constructor for ATR Fuel Elements

Background

Introduction to Irradiation Experimentation in the Advanced Test Reactor

- The Advanced Test Reactor (ATR) at Idaho National Laboratory (INL) is the world's premier test reactor.
- The ATR is heavily used for irradiation experimentation across the public and private sectors.
- This unique reactor core is usually simulated using Monte Carlo methods.
- Modeling an irradiation experiment accurately involves capturing the core's effects on the experiment.
- Some simplifications are made to keep experiment cycle depletion calculations computationally practical.



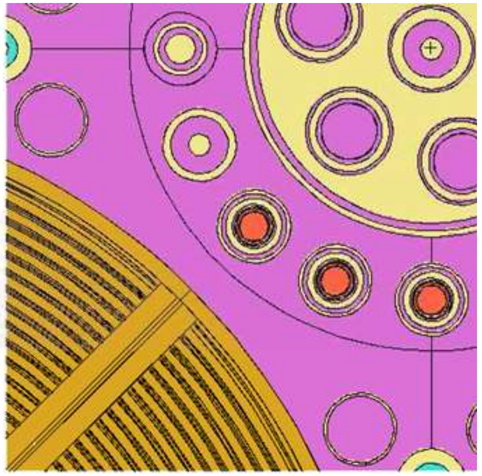
ATR Neutronics at Two Scales

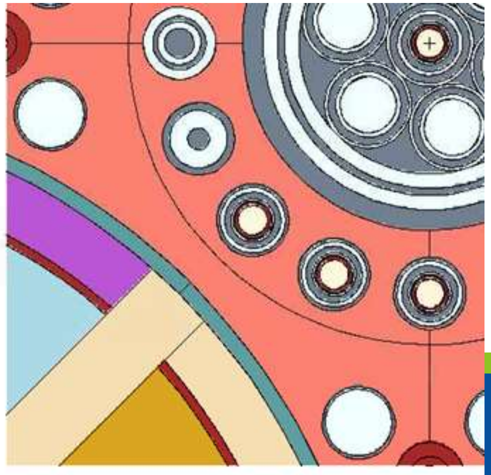
Reactor & Safety Engineering

- High-fidelity core model
- Eigenvalue solution
- Approximated experiments
- Driver fuel depletion

Neutronics Analysis

- Simplified three-region core model
- Fixed-source solution
- Approximated driver fuel
- Experiment depletion

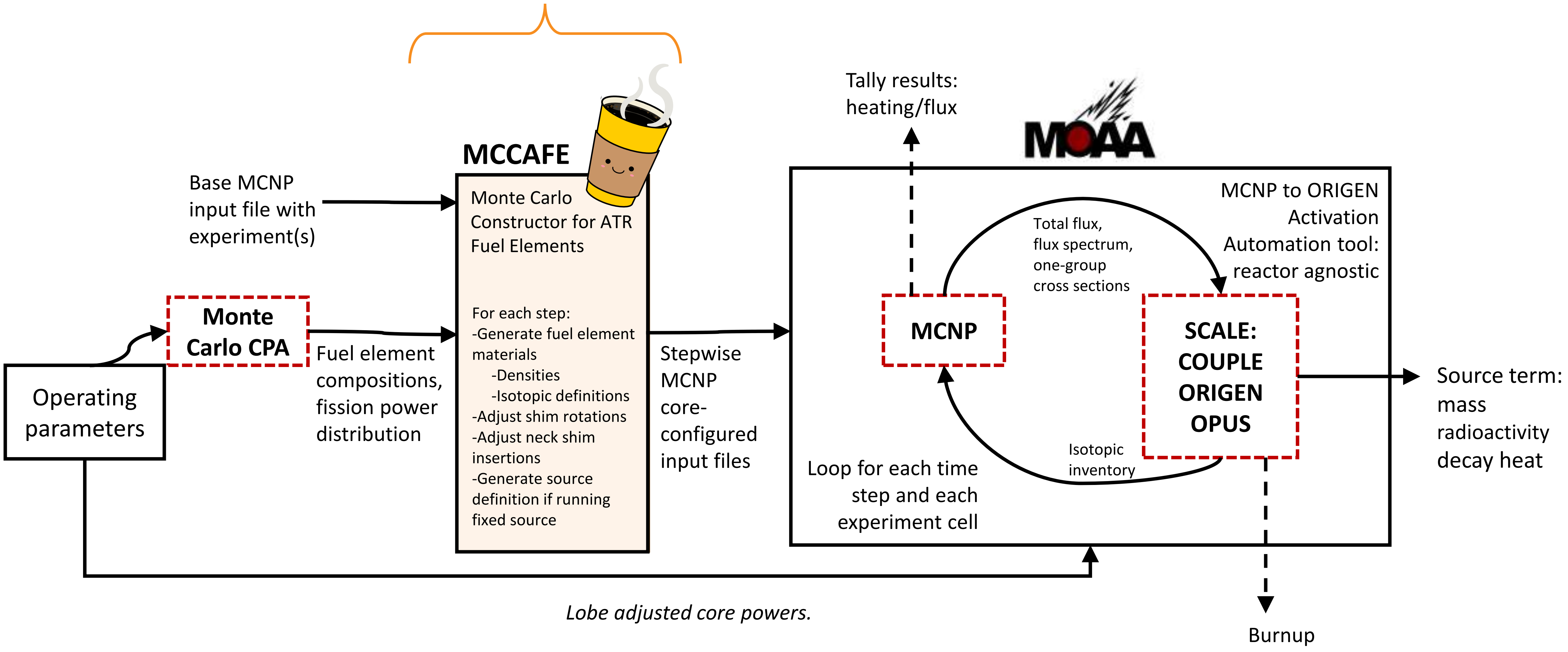




About the Three-Region Model

- Simplified, fixed-source model
- Real geometry: 40 fuel elements × 19 fuel plates
- Fuel element simplification:
  - Homogenized into 3 radial regions
  - Discretized 7 axial zones
- 3 regions × 7 zones × 40 elements = 840 driver fuel cells
- Each cell has a unique isotopic composition and source probability

Neutronics As-Run Analysis Workflow



Purpose of MCCAFE

- A new piece of the ATR cycle analysis puzzle
- Two stages of neutronics Monte Carlo solutions:
  1. ATR core physics analysis (CPA)
     - Experiment reactivities, axial power perturbation, etc. restricted by Safety Analysis Report: SAR-153
  2. Neutronics analysis of experiment
     - Informed by cycle-specific CPA results*
- Connect precalculated reactor data to stepwise experiment calculations
  - Driver fuel isotopics
  - Fixed-source spatial distribution
- Include measured (or projected) neck shim insertions and outer shim control cylinder (OSCC) rotations
- **Put it all together into a series of MCNP input files**

About the Software

- Custom-developed under INL's nuclear quality assurance (NQA-1) program
- Highly configurable
- Written in Python
- Multithreaded
- Online documentation
- User interfaces:
  - YAML input file
  - Python API
- In production use as of ATR Cycle 171A

Monte
Carlo
Constructor of
ATR
Fuel
Elements

Functions

Operating Parameters

Nuclear Data Management and Analysis System (NDMAS)

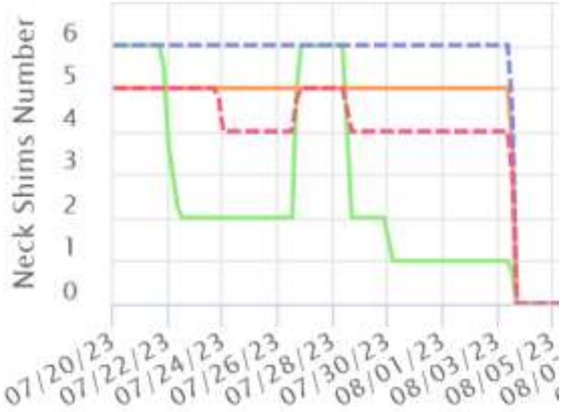
The purpose of NDMAS is to import, qualify, graph, analyze, store, and deliver data collected as part of nuclear fuel and materials research programs conducted at the INL Advanced Test Reactor. [1]

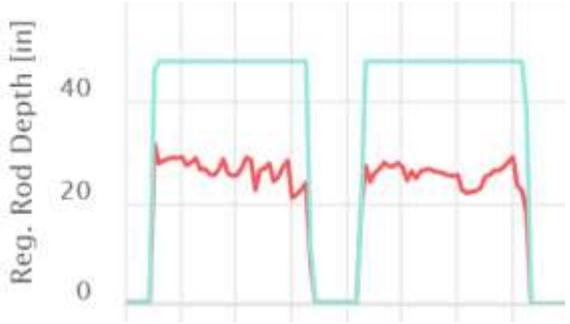
- Quality-assured, hourly data concerning ATR instrumentation and controls
  - "[I]ncluding lobe, quadrant, and total powers (MW), outer shim control cylinder positions (degrees), neck shim positions (in or out), and control rod positions (in)" [1]
- Can be paired with CPA solution or used directly by MCCAFE

[1] https://ndmashome.inl.gov/atrops/SitePages/Home.aspx
(Restricted to collaborators)

Neck Shim Insertions

- ATR neck shims are essentially control rods
- Hafnium poison at insertion; zircaloy follower at withdrawal
- ATR has four sets of six neck shims: NE, SE, SW, NW
- Twenty-two of the shims are either completely inserted or completely withdrawn
- Shims NW4 and SW4 are the regulating rods: continuously variable withdrawal
- For more details, see benchmark evaluation: HEU-MET-THERM-022 § 1.2.3

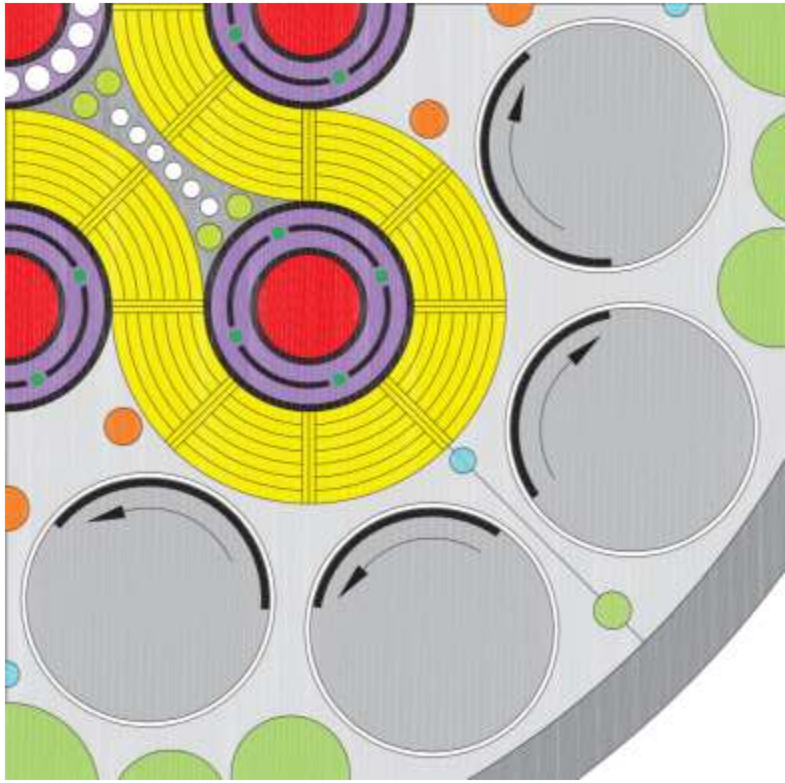




OSCC Rotations

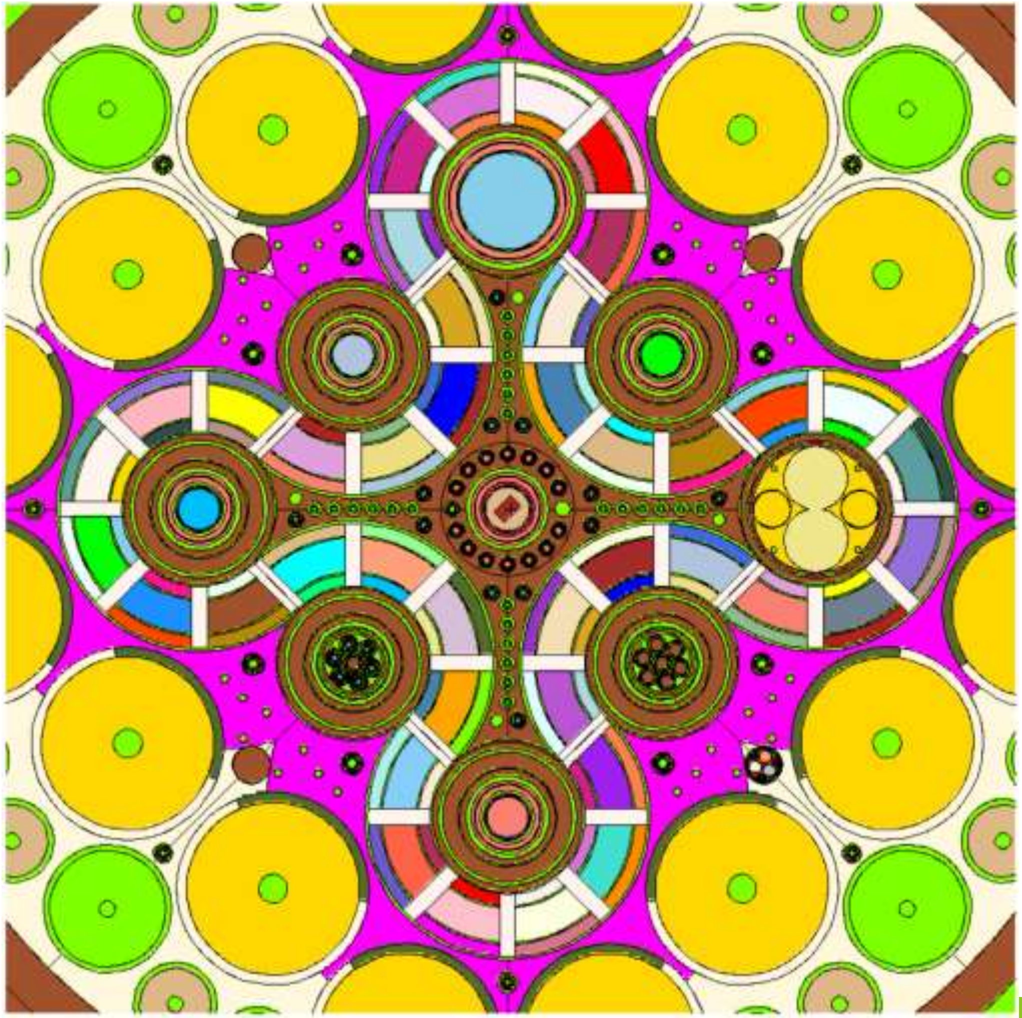
- ATR OSCCs are essentially control drums
- Hafnium poison arc and beryllium reflector arc
- ATR has four sets of four ganged OSCCs
  - Two clockwise, two counterclockwise

When the outer shim control cylinders are set to 0 degrees, the straight line extending from the center of the OSCC to the center of the neighboring flux trap bisects the hafnium absorber of each of the eight No. 1 and No. 4 cylinders. The bisectors of No. 2 and No. 3 OSCCs are 35 degrees away from the lines connecting centers of the corresponding OSCCs to the neighboring flux trap centers. [1]

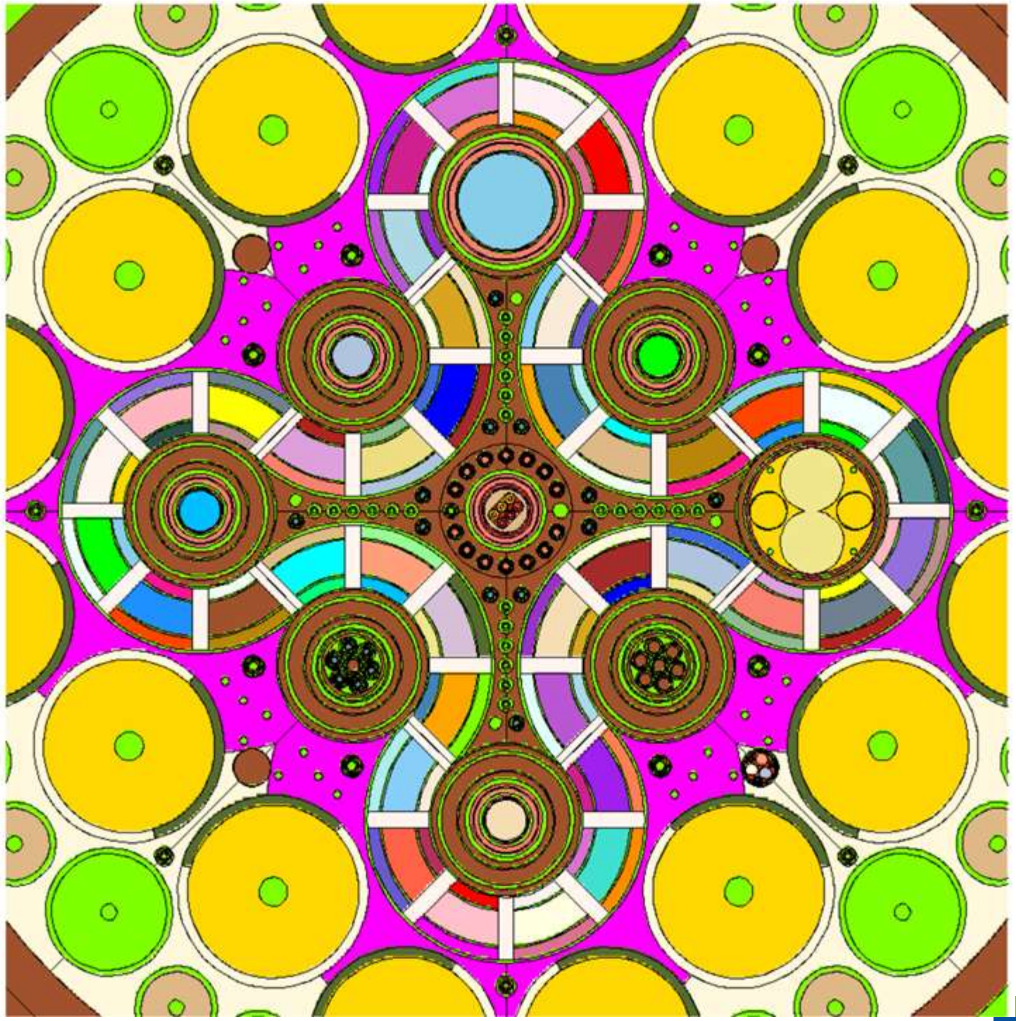


[1] HEU-MET-THERM-022 § 1.2.5

OSCC Rotations (continued)



OSCC Rotations (continued)



Functions

Source Distribution

Fixed-Source Model

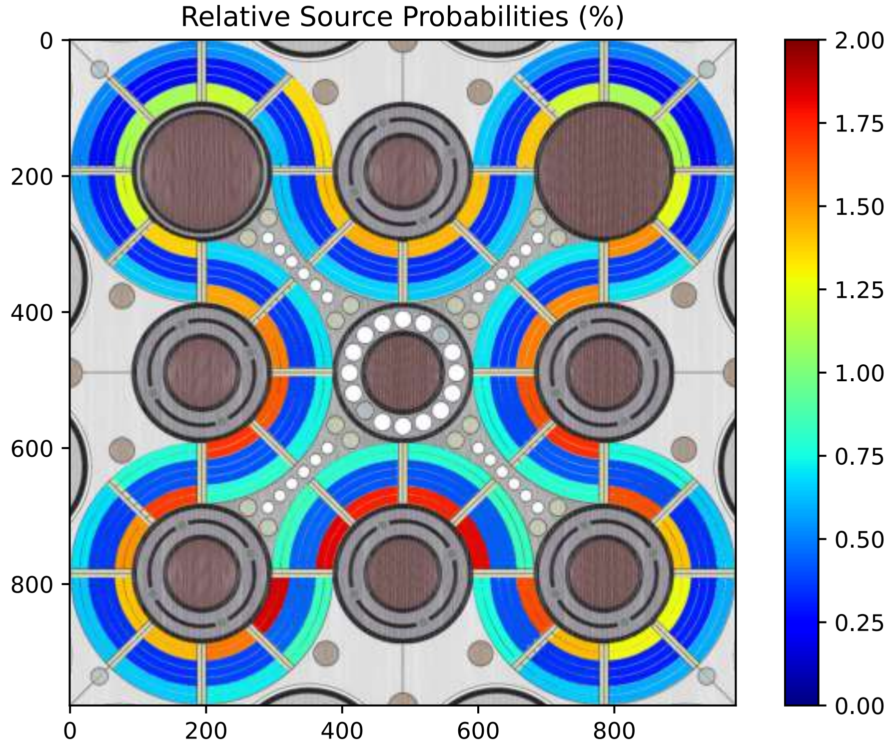
- The energy distribution is assumed to be the Watt fission spectrum.
- Each of the 840 fuel cell regions has an associated spatial probability.
- MCCAFE generates the fixed source spatial distribution for each time step.
- Several methods are implemented:
    1. Lookup table (legacy method)
    2. Lookup table (volume-weighted)
    3. Direct source probabilities.
- The spatial probability distribution **is paired to the ATR controls and driver fuel composition** at any given time step.

Methods 1–2: Lookup Table

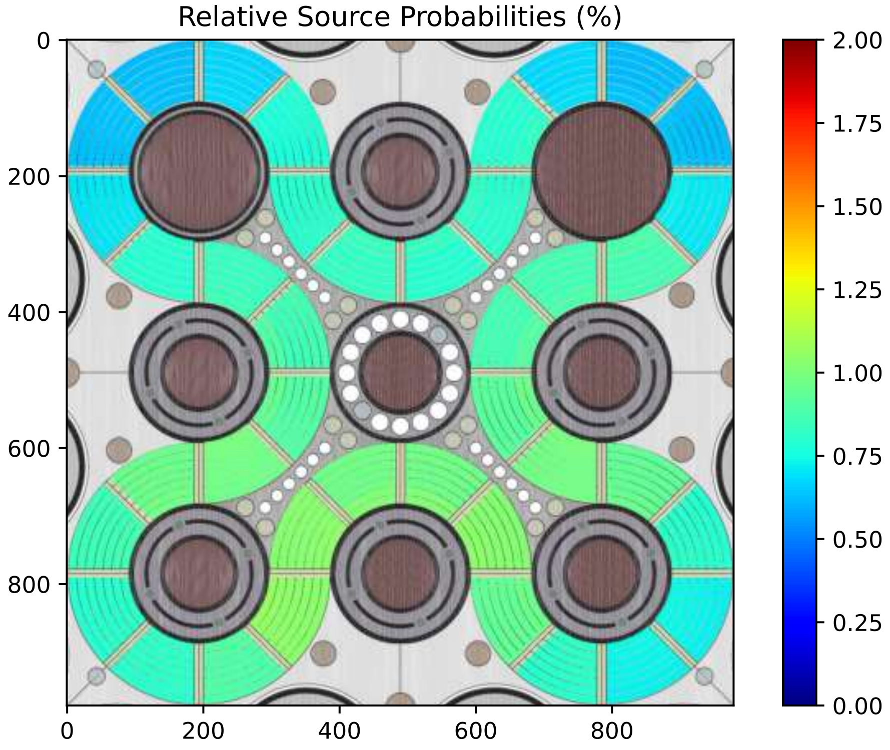
- Based on historical PDQ and HELIOS core results
- Chang and colleagues at INL developed internal correlation: complicated mathematics
- Spatial probabilities are based on fuel element power and ^{235}U mass
- More recently, the method was improved by volume-weighting radial regions

Methods 1–2: Lookup Table (continued)

Original Method



Volume-Corrected

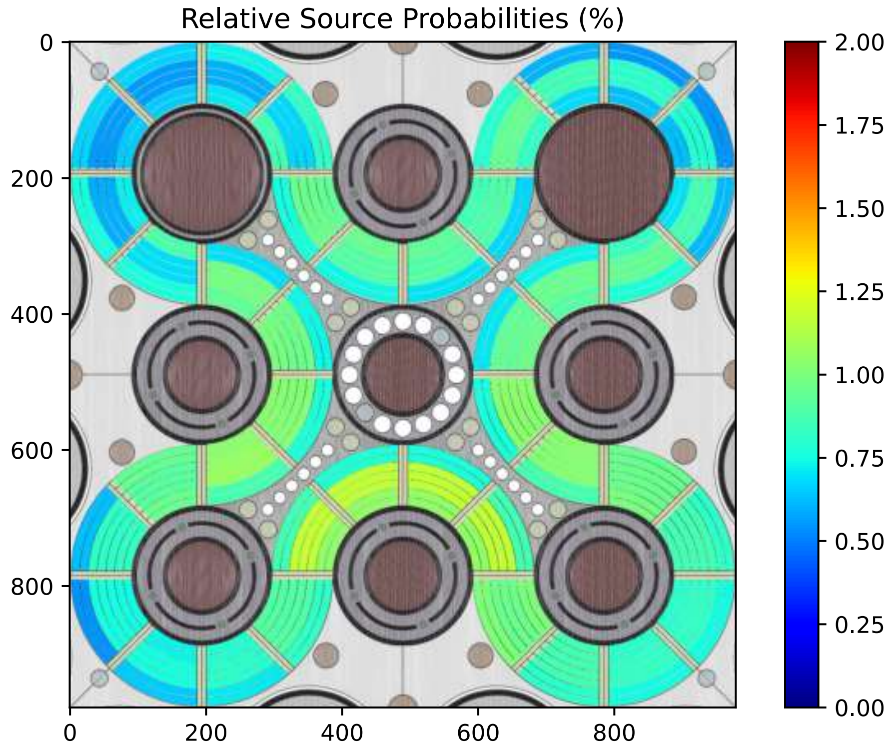


Method 3: Neutron Production Rates

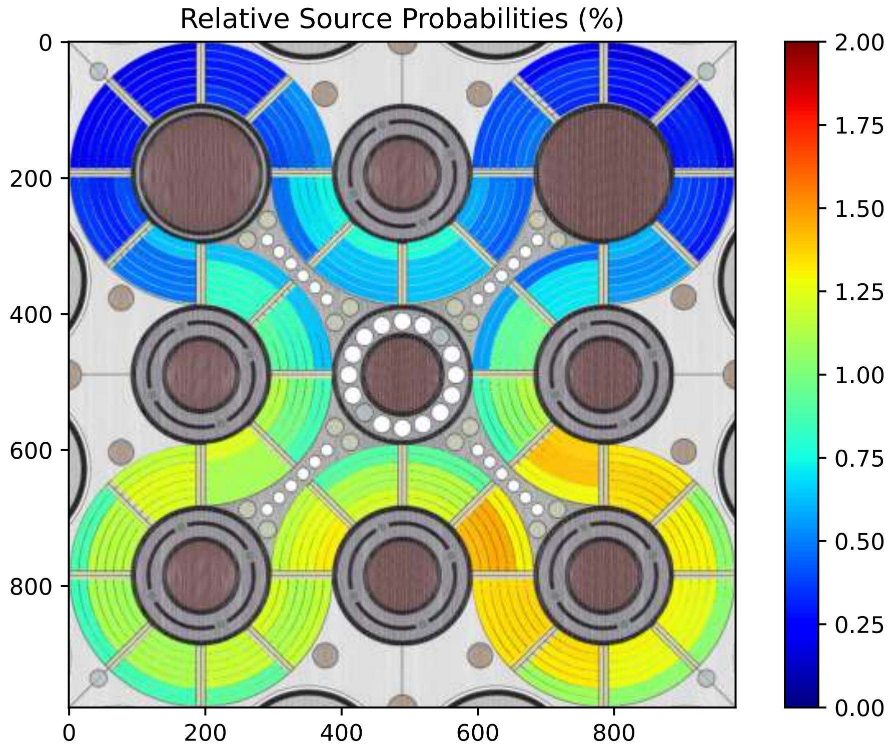
- Based on high-fidelity Monte Carlo core solutions over 840 fuel cells
- Spatial probabilities are proportional to tallied neutron production rates from CPA
- Significantly more data bookkeeping than the lookup table methods and more difficult to prepare for a projection calculation
- Truer to actual core behavior

Method 3: Neutron Production Rates (continued)

Steady-State Cycle



PALM* Cycle



* PALM: powered axial locator mechanism

Functions

Fuel Composition

Fuel Composition Model

- Each of the 840 fuel cells homogenizes fuel meat, cladding, and coolant over that volume of the geometry.
- Two fuel composition models are implemented:
  1. Lookup table
  2. Direct atom densities.
- Several methods to approximate materials are implemented:
  - MCCAFE always models uranium, borated coolant, cladding materials, and some fission product poisons.
  - Isotopics are **downstream** of CPA: approximations only impact experiment depletions, not core depletion.

Method 1: Lookup Table

- Similar to source probability:
  - Based on historical core results
  - Chang and colleagues at INL developed internal tables
- Fixed structural nuclides
- ^{235}U and ^{10}B masses per fuel element provided directly by user
- ^{135}Xe and ^{149}Sm based on correlation with ^{235}U mass

Method 2: Atom Densities

- Atom densities from the CPA depletions are homogenized over each region and used directly
- Significantly more data bookkeeping than the lookup table methods:
  - More difficult to prepare
  - MCNP simulation slowdown becomes a real issue

Nuclide Reduction Methods

- White-listed nuclides
  - Nuclides corresponding to the original lookup table method are always exempt from removal from the driver fuel materials
- Numeric threshold
  - 10^{-24} at/b-cm by default
  - Ignorant of physics, other than the white-listed nuclides
- Depletion chain simplification
  - Remove nuclides based on their contribution to macroscopic 1GXS
  - Developed by Olin Calvin (INL, University of Idaho)
  - Check out our paper to be presented at M&C 2025

Conclusion

Adoption of MCCAFE

- MCCAFE accelerates ATR model generation using measured parameters and precalculated ATR isotopics.
- Through automation, MCCAFE standardizes work, reduces human error, simplifies technical checking, and accelerates analysis.
- The faster, more accurate work will enhance advanced fuels and claddings research and help reduce modeling uncertainties.
- The software was first used in a production as-run analysis for Cycle 171A.

Future Work

- Quantify effects of driver fuel nuclide reduction methods
  - See you at M&C 2025
- Perform full-cycle depletions using each source and fuel method for a set of experiments with different neutronic characteristics
- Evaluate surface source (`RSSA`) method as alternative to full-core fixed-source
- Implement options to update isotopes for 19-plate eigenvalue models

Acknowledgments

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- This research made use of the resources of the High Performance Computing Center at Idaho National Laboratory, which is supported by the Office of Nuclear Energy of the U.S. Department of Energy and the Nuclear Science User Facilities under Contract No. DE-AC07-05ID14517.
- This work was supported through the U.S. Department of Energy under DOE Idaho Operations Office Contract DE-AC07-05ID14517. Accordingly, the U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, world-wide license to publish or reproduce the published form of this manuscript, or allow others to do so, for U.S. Government purposes.

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Questions?

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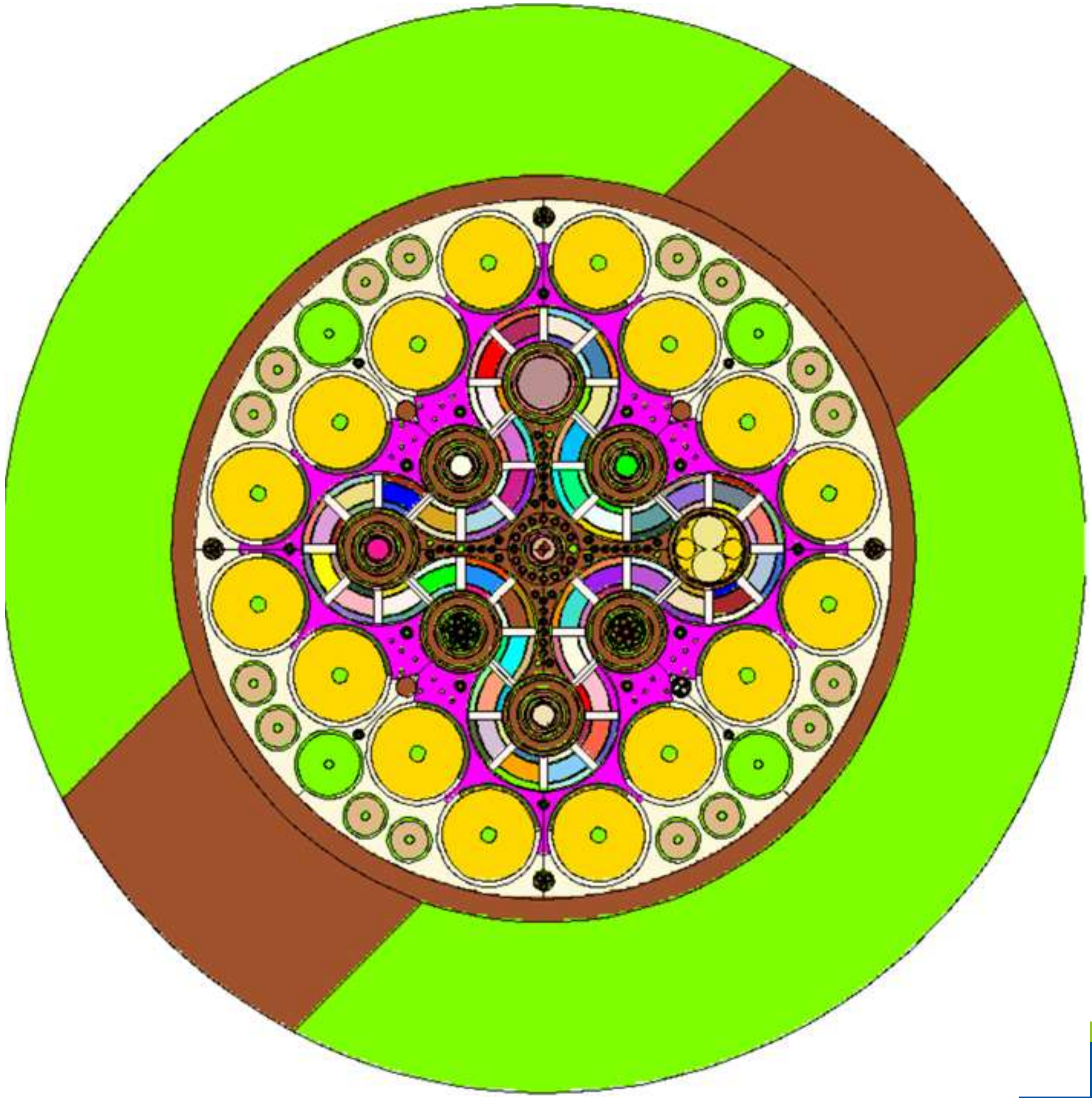
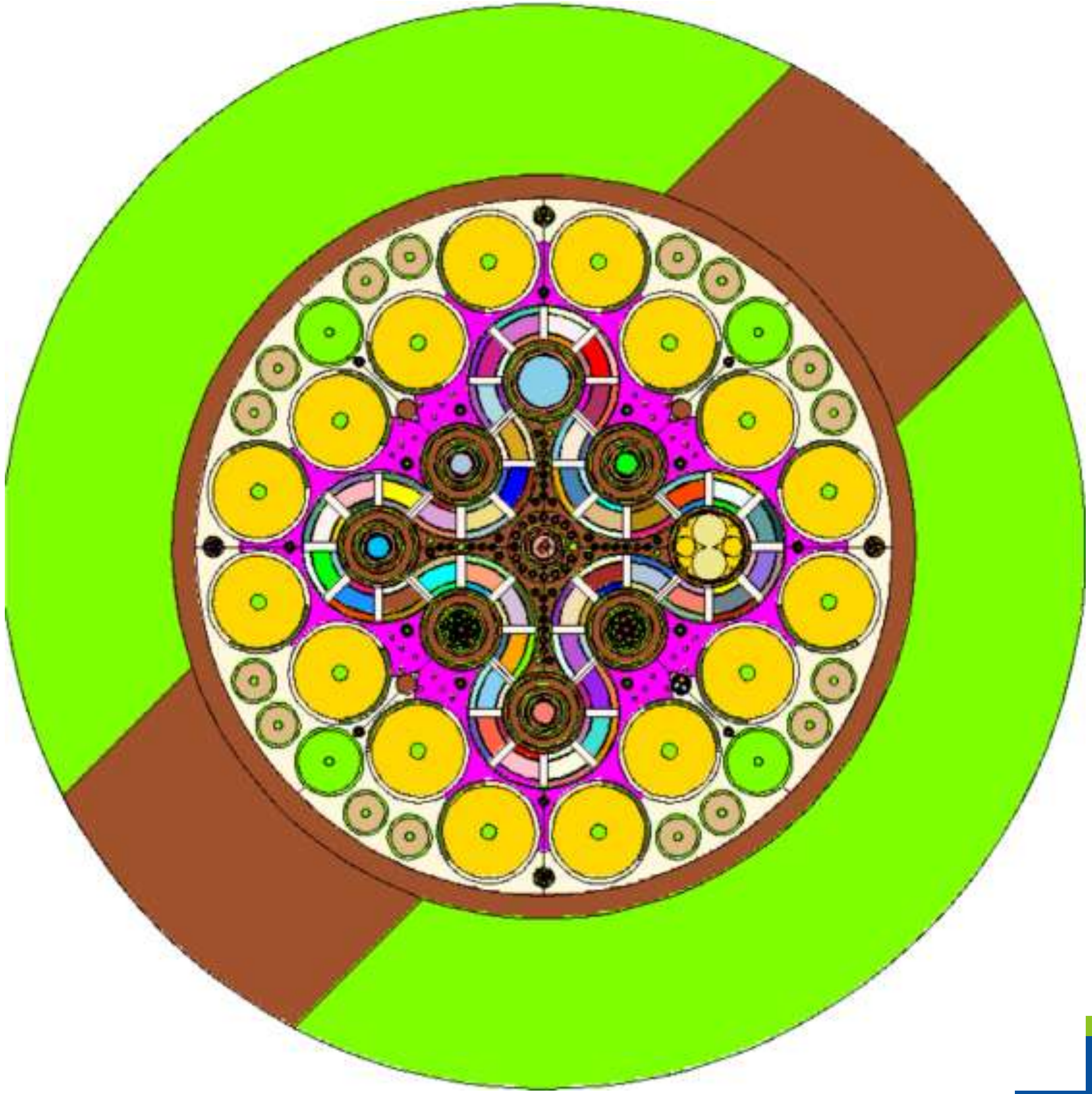
Backup Slides

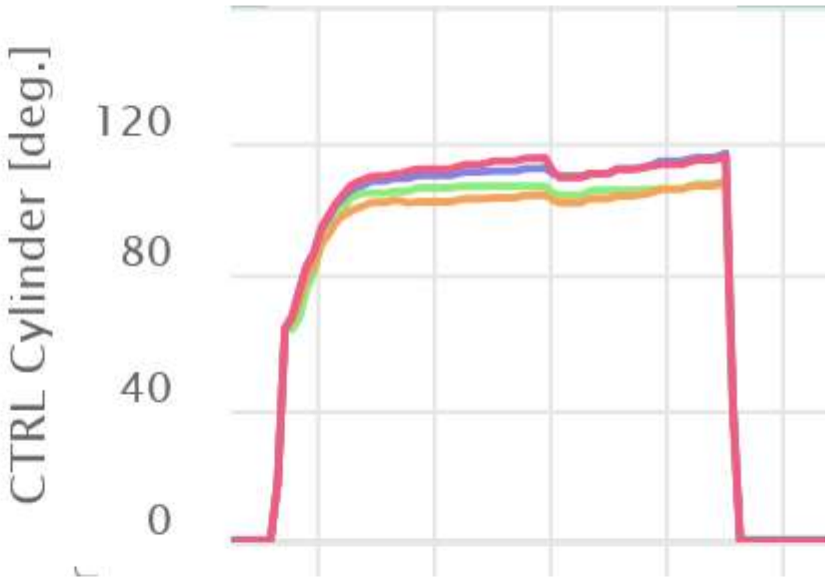
OSCCs at Shutdown



OSCCs at +90 Degrees

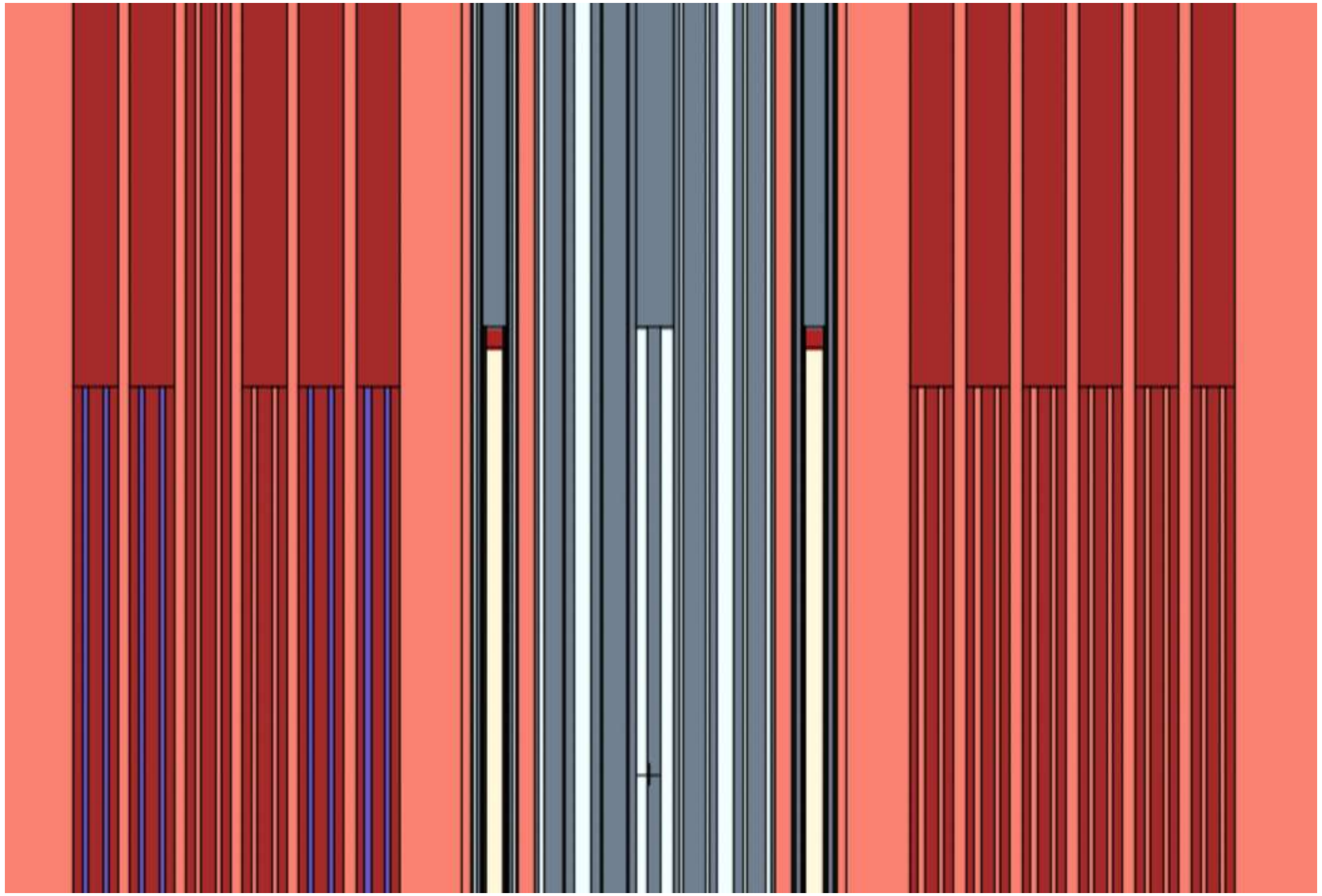


OSCC History for Short Cycle



Neck Shim Withdrawal

Left: SE | Right: NW



Source Distribution Card Examples

```
sp1    d
       0.0658  0.1066  0.1362  0.2908  0.1311  0.0970  0.0424
       0.0653  0.1111  0.1434  0.3115  0.1359  0.0994  0.0485
       0.0624  0.1082  0.1362  0.2961  0.1306  0.0970  0.0496
```

```
sp1    d
       0.0259  0.0433  0.0568  0.1233  0.0538  0.0389  0.0168
       0.1013  0.1769  0.2328  0.5124  0.2197  0.1577  0.0778
       0.0461  0.0827  0.1061  0.2345  0.1010  0.0731  0.0367
```

Verification

- MCCAFE has been extensively tested on real and fictional models.
- Continuous integration testing ensures that software requirements remain met.
- *Pictured:* fictional model with completely different geometry than the ATR core.