SCALE Lattice Physics Applications to 3D Nodal Diffusion Simulations with NESTLE

Dr. G. Ivan Maldonado, Professor
UT Department of Nuclear Engineering
UT/ORNL Joint Faculty in Reactor Physics

SCALE USERS' GROUP WORKSHOP
SEPTEMBER 26-28, 2017

Overview of Presentation

- Overview of UTK NESTLE/SCALE Contributors
- Overview and Update on NESTLE
- Selected SCALE to NESTLE Project Illustrations
  - VVER 1000 Modeling and Simulation
  - SMR Modeling

Overview of UTK NESTLE and SCALE Contributors

NESTLE/SCALE PhD Projects

- **Luciano, Nicholas** (PhD, December 2016). Sensitivity of VVER-1000 Spent Fuel Pin Nuclide Inventory to Operational Parameters.
- **Gentry, Cole** (PhD, January 2016). Topic: Development of a Reactor Physics Analysis for the Plank-Based and Liquid Salt-Cooled Advanced High Temperature Reactor.
- **George, Nathan** (Ph.D., March 2015). Topic: Assessment of Reactivity Equivalence for Enhanced Accident Tolerant Fuels in Light Water Reactors.
- **Hart, Shane** (Ph.D., December 2014). Topic: On-the-fly Doppler Broadening Methods for the Scale Transport Code.
- **Ottinger, Keith** (Ph.D., July 2014). Topic: “Multi-Cycle Boiling Water Reactor Fuel Cycle Optimization.”
- **Hernandez, Hermilo** (Ph.D., August 2010). Thesis: "Robust Parallel Algorithms for Minor Actinide Transmutation Rate Maximization in combined Within-Lattice and Within-Core Environments.”
- **Galloway, Jack** (Ph.D., July 2010). Thesis: "Boiling Water Reactor Core Simulation with Generalized Isotopic Inventory Tracking for Actinide Management.”

NESTLE/SCALE MS Projects

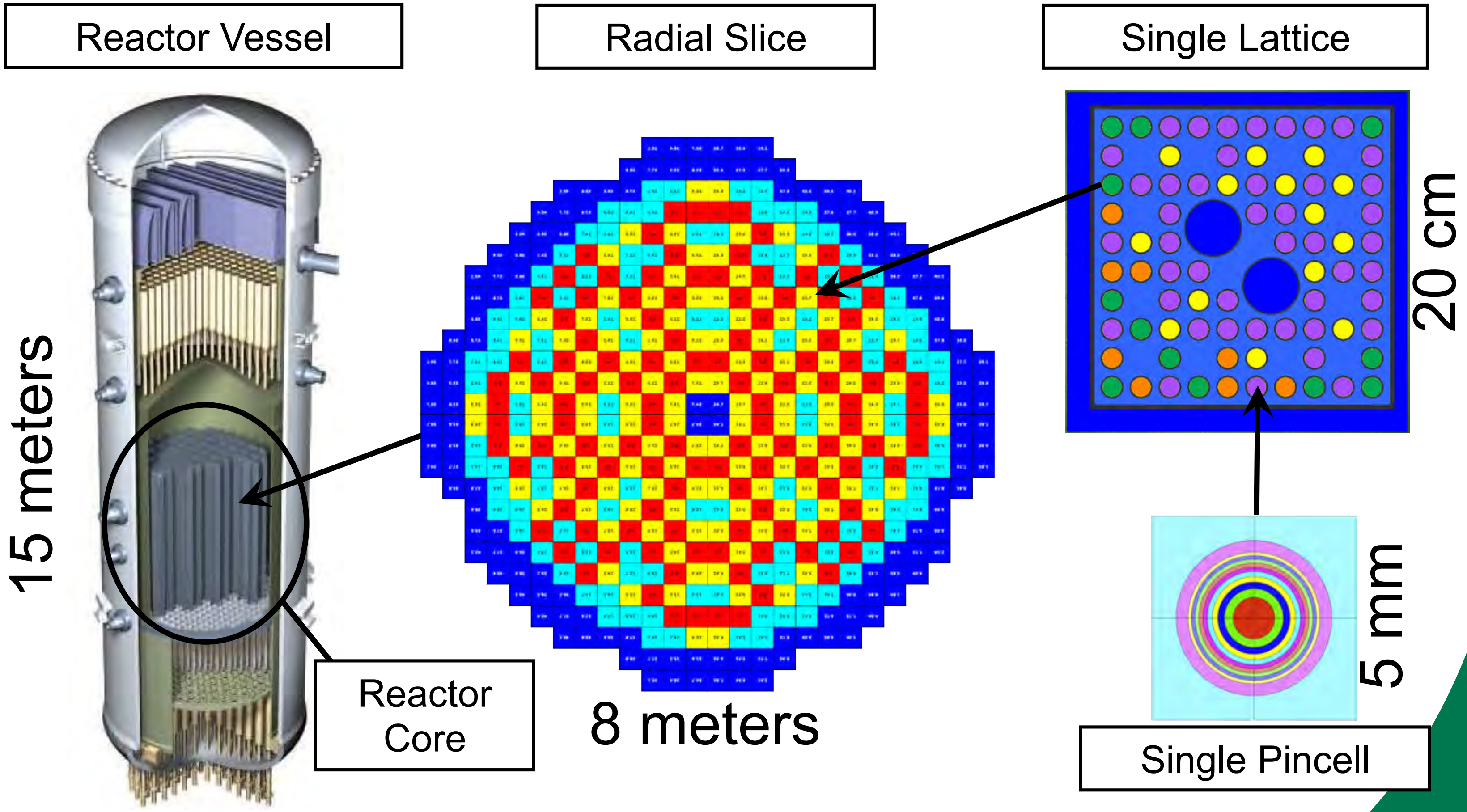
- **Mervin, Brenden** (MS, May 2010). “Development of SCALE-based Educational Modules to Innovate Reactor Physics and Criticality Safety Curricula.”
- **Hart, Shane** (MS, May 2010). Project: “CANDU Core Modeling and Refueling Simulations using SCALE and NESTLE.”
- **Murphy, James E.** (MS, December 2011). Project #1: “PWR Lattice Physics Benchmark of TRITON against CASMO.” Project #2: “PWR Core and Spent Fuel Pool Analysis using SCALE and NESTLE.”
- **Morris, Sam** (MS, December 2011). Project #1: “Validation of KENO V.a. Computer Code by Modeling Benchmark Critical Experiments.” Project #2: “Analysis of Small-Sample Reactivity Experiments in the MINERVE Reactor.”
- **Lastres, Oscar** (MS, December 2011). Project #1: “Studies of Plutonium-238 Production at the High Flux Isotope Reactor.” Project #2: “Validation of Heavy Element Processing Campaigns 51-59 Data using the TCOMP and SCALE Code.”
- **George, Nathan** (MS, December 2011). “Uranium-Based Fully Ceramic Micro-Encapsulated Fuel in Light Water Reactors.”
- **Gentry, Cole** (MS, May 2012), Thesis: “An Investigation of the use of Ceramic Microencapsulated Fuel for Transuranic Waste Recycling in PWRs.”
- **Collins, Eric P.** (MS, May 2014). Topic: “Advances in Modeling Control Rod Depletion.”
- **Jones, Elizabeth** (MS, May 2015). Thesis: “User Perspective and Analysis of the Continuous-Energy Sensitivity Methods in SCALE 6.2 using TSUNAMI-3D.”
- **Eckleberry, Troy** (MS, November 2016). Project #1: “Validation of KENO Thermal Moderator Doppler Broadening Method in SCALE 6.2 Beta5 Using Continuous-Energy B-VII.1 Library.” Project #2: “Reactivity Impact of Accident Tolerant Claddings in and Equilibrium PWR Core.”

A few members of the M-team

David Dixon (UTK), Cole Gentry*, Ondrej Chvala (UTK), Eric Collins (Westinghouse),
Elizabeth Jones, Ivan Maldonado, AJ Pawel (UTK)
Nathan George (DNFSB), Nick Luciano*, Shane Hart*, Kelly Kenner (TVA).
(*) Currently employed at Oak Ridge National Laboratory

Overview and Update on NESTLE

Today’s Commercial Modeling and Simulation: Lattice Physics to 3D Nodal Diffusion



Reactor Vessel

Radial Slice

Single Lattice

15 meters

20 cm

Reactor Core

8 meters

5 mm

Single Pincell

Commercial Lattice to Nodal Simulators

- CASMO/SIMULATE (Studsvik/Scandpower)
- TGBLA/PANACEA (GE)
- PHOENIX/POLCA (Westinghouse BWR)
- PARAGON/ANC (Westinghouse PWR)
- CASMO/MICROBURN/NEMO (AREVA)
- … many more

Some Background on NESTLE

- Few-Group Multi-Dimensional Nodal Core Simulator
- Employs the Nodal Expansion Method (NEM)
- Solves Eigenvalue, Adjoint, Fixed-Source, Steady-State, Transient problems in Cartesian and Hexagonal geometry
- Developed originally at NC State University by Prof. Paul J. Turinsky and students (1980-2000's)
  - Old version available through RSICC
  - No lattice physics integration
  - No BWR Capabilities, mostly a PWR code
  - No generalized isotope tracking
  - Limited to 2 or 4 energy groups
- New Developments and Upgrades adopted by UTK since around 2008, initially with ORNL

What’s New with NESTLE-UTK?

CODE
- Complete overhaul to modern Fortran and modularized
- Many bug fixes, documentation, removal of dead code
- Simplified user input syntax, assembly defined inputs
- Restart files now available for each depletion step
- Improved options for output formatting. Plotting of 2D slices, 3D distributions and limit violations w GNU Plot.

MODELING
- Haling depletion
- Multi-dimensional Cross Section Interpolation
- Variable N-group capability for energy treatment
- Lattice Physics Integration and Couplings to:
    - SCALE (Triton/Polaris)
    - Serpent2
    - CASMO4
- Applied to PWR, BWR, SMR, VVER, FHR

New Software Engineering

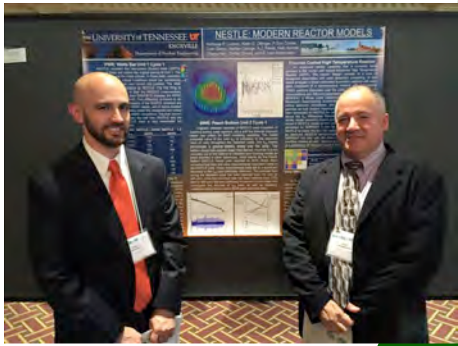
- NESTLE wiki provides documentation for developers and users.
- In-source documentation of new and legacy components.
- Distributed software repository can allow developers from anywhere to work separately and as a team.
- Nightly testing of the code to ensure new features comply with existing use.
- We have built NESTLE for Linux, Windows, or Mac OSX platforms

Summary of Activities

- Workshop Provided at PHYSOR 2014 in Kyoto
- Workshop Provided at MC2015 in Nashville
- Workshop Planned for PHYSOR 2018 in Cancun
  - Release to RSICC and/or Open Access projected 2017/18

Active Models Available:

- PWR (Watts Bar) – AJ Pawel
- BWR (Peach Bottom 2, Laguna Verde) – J. Galloway, Nathan George
- SMR (mPower inspired UTK model) – Kelly Kenner, Keith Ottinger
- VVER (Temelin and other benchmarks) – Nick Luciano
- LSCR (Liquid Salt Cooled Reactor w GA Tech) – Cole Gentry



Special Topics Include:

- Multicycle Fuel Optimization – Keith Ottinger
  - BWR/PWR Optimization (ATF NEUP project, aggressive operation, load follow)
  - SMR Development of 48-month cycle with control rod patterns
  - VVER Fuel Optimization (Czech Visiting Students)
- Pin-Wise Microscopic Depletion (VVER focus) – Nick Luciano
- Nuclear Security Applications (various, Nick Luciano)

Selected SCALE to NESTLE Project Illustrations

VVER-1000 Modeling

Nick Luciano

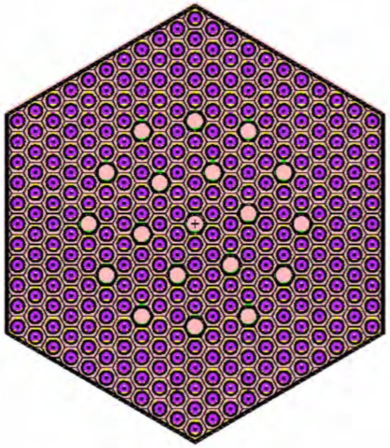
AER VVER-1000 Benchmark Khmelnitsky Unit 2 (Nick Luciano)

- Netishin, Ukraine
- 2 units, 2 planned
- 950 MWe
- VVER 1000 v320
- Startup: 2005

Photo: www.energoatom.kiev.ua

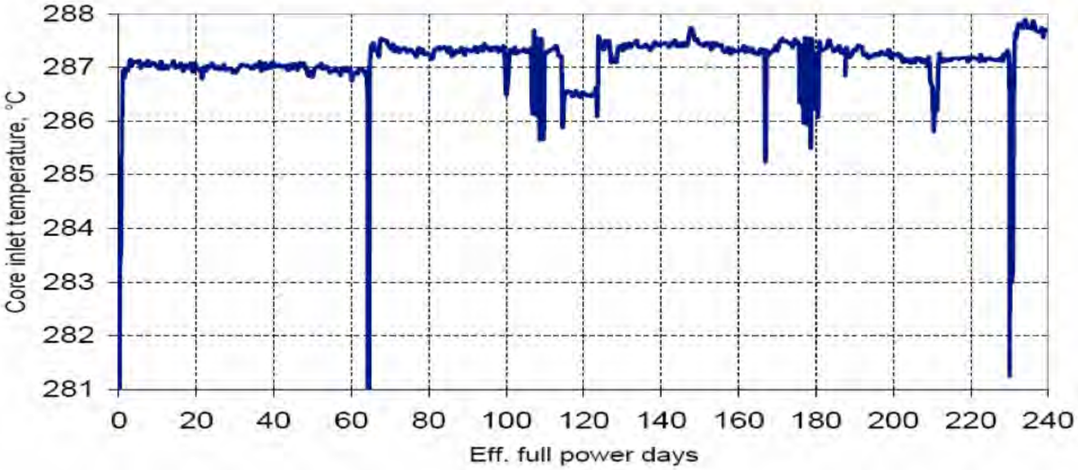
Benchmark was proposed "for validating and verifying the whole package of codes and data libraries for reactor physics calculations including FA modeling, FA data preparation and reactor core modeling."

Khmelnitsky-2 Benchmark Data

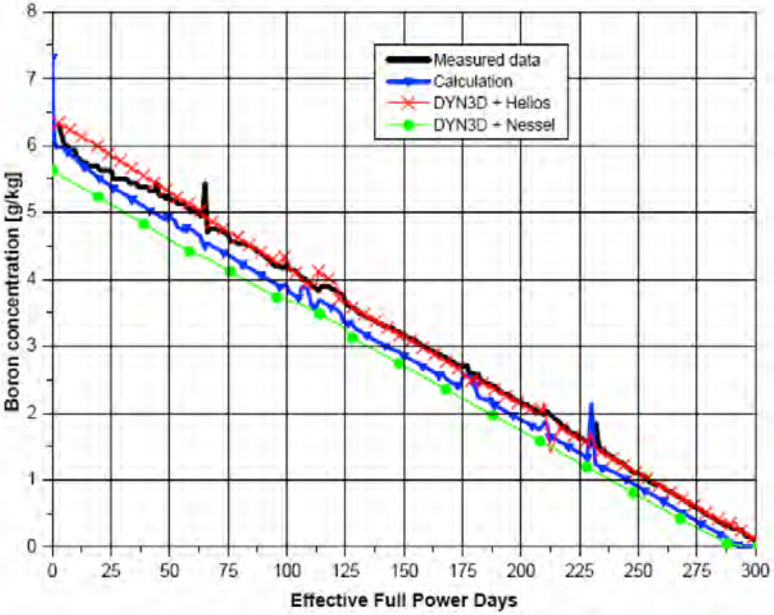


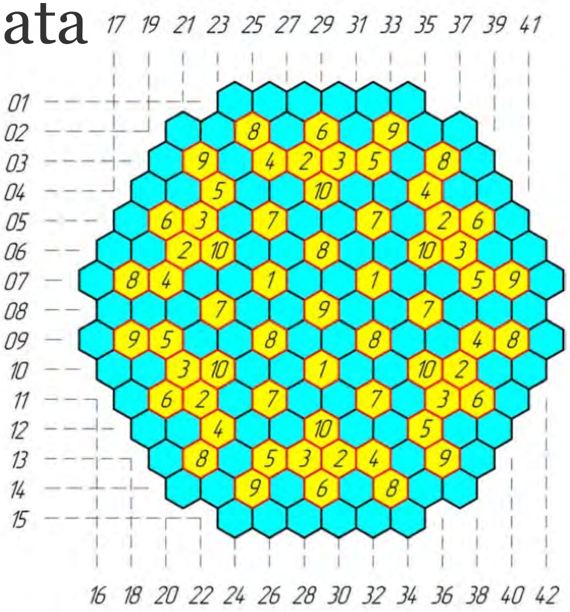
◉ fuel pin with enrichment 1.3% (2.2%) ^{235}U

○ guide tube / central guide tube



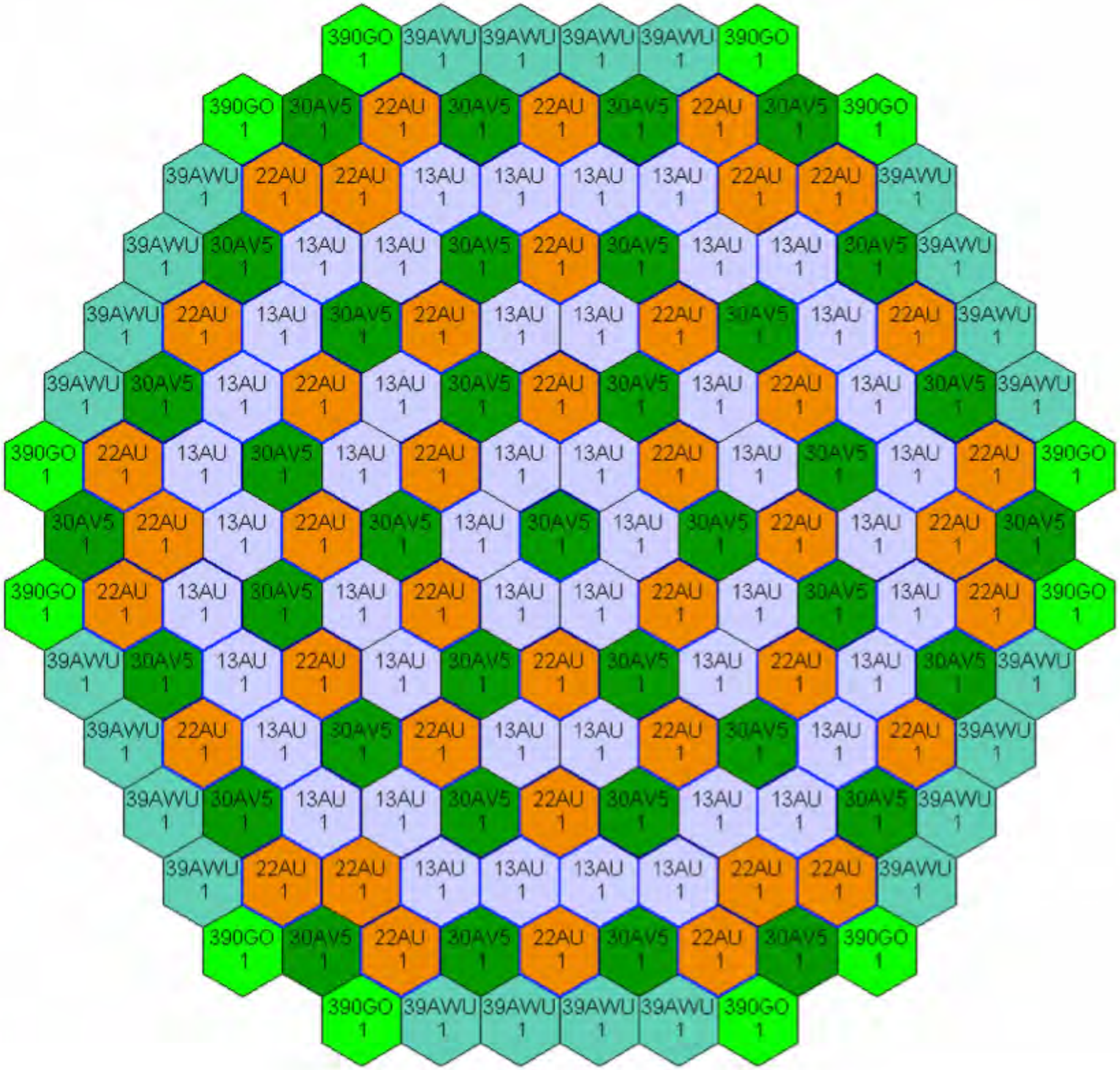
4 Cycles of Plant Data





Positions of the Control Rod Groups in the reactor core

Core Map



390GO 39AWU 39AWU 39AWU 39AWU 390GO
1 1 1 1 1 1

390GO 30AV5 22AU 30AV5 22AU 30AV5 22AU 30AV5 390GO
1 1 1 1 1 1 1 1 1

39AWU 22AU 22AU 13AU 13AU 13AU 13AU 22AU 22AU 39AWU
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39AWU 30AV5 13AU 13AU 30AV5 22AU 30AV5 13AU 13AU 30AV5 39AWU
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39AWU 22AU 13AU 30AV5 22AU 13AU 13AU 22AU 30AV5 13AU 22AU 39AWU
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30AV5 22AU 13AU 22AU 30AV5 13AU 30AV5 13AU 30AV5 22AU 13AU 22AU 30AV5
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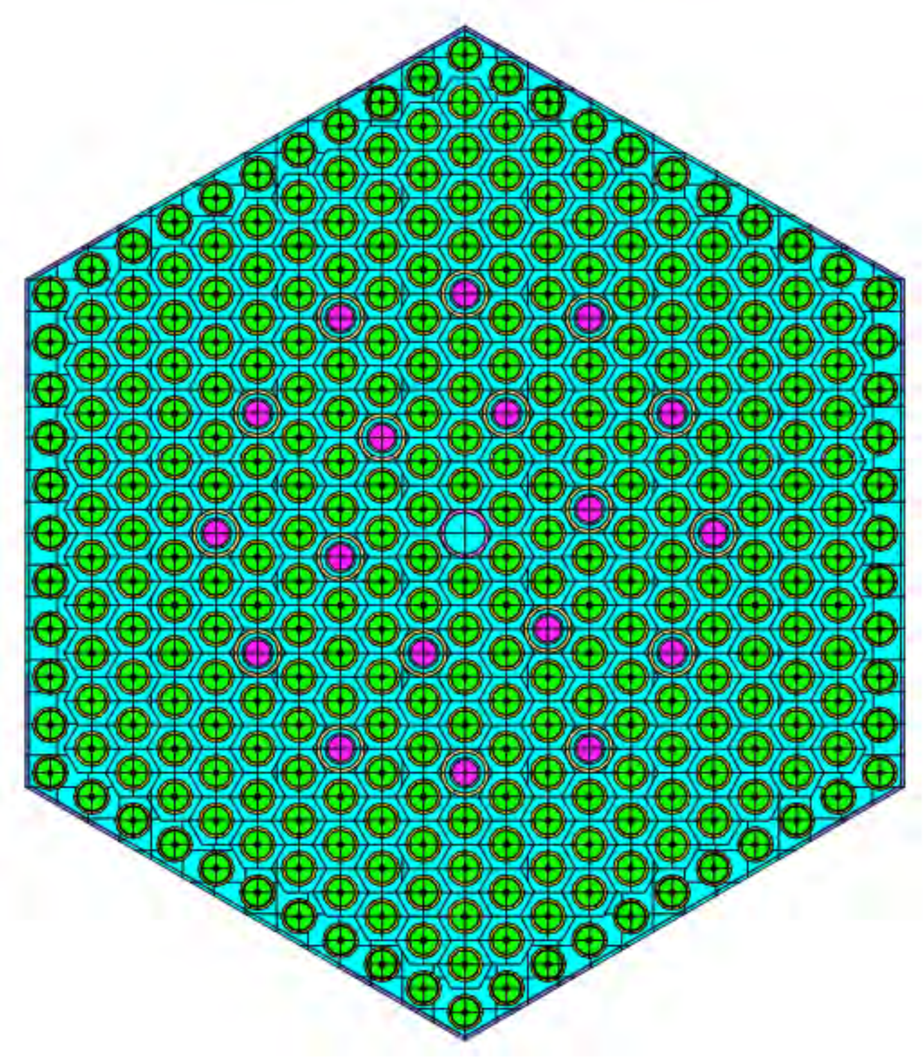
Core Specifications

Property	Value
Number of assemblies used in 1st cycle:	
13au	48
22au	42
30av5	37
39awu	24
390go	12
Number of assemblies with control rods	61
Control rod groups	10
Active Fuel Height [cm]	355.0
Thermal Power [MW]	3000.0
Coolant inlet temperature [K]	563.15
Coolant outlet temperature [K]	592.75
Core pressure [MPa]	15.7

Lattices Modeled Using TRITON

Designation	Number of Pins	Pin Enrichment (%)	Pin Gd_2O_3 (wt%)
13au	312	1.30	0.0
22au	312	2.20	0.0
30av5	303	2.99	0.0
	9	2.40	5.0
39awu	243	4.00	0.0
	60	3.60	0.0
	9	3.30	5.0
390go	240	4.00	0.0
	66	3.60	0.0
	6	3.30	5.0

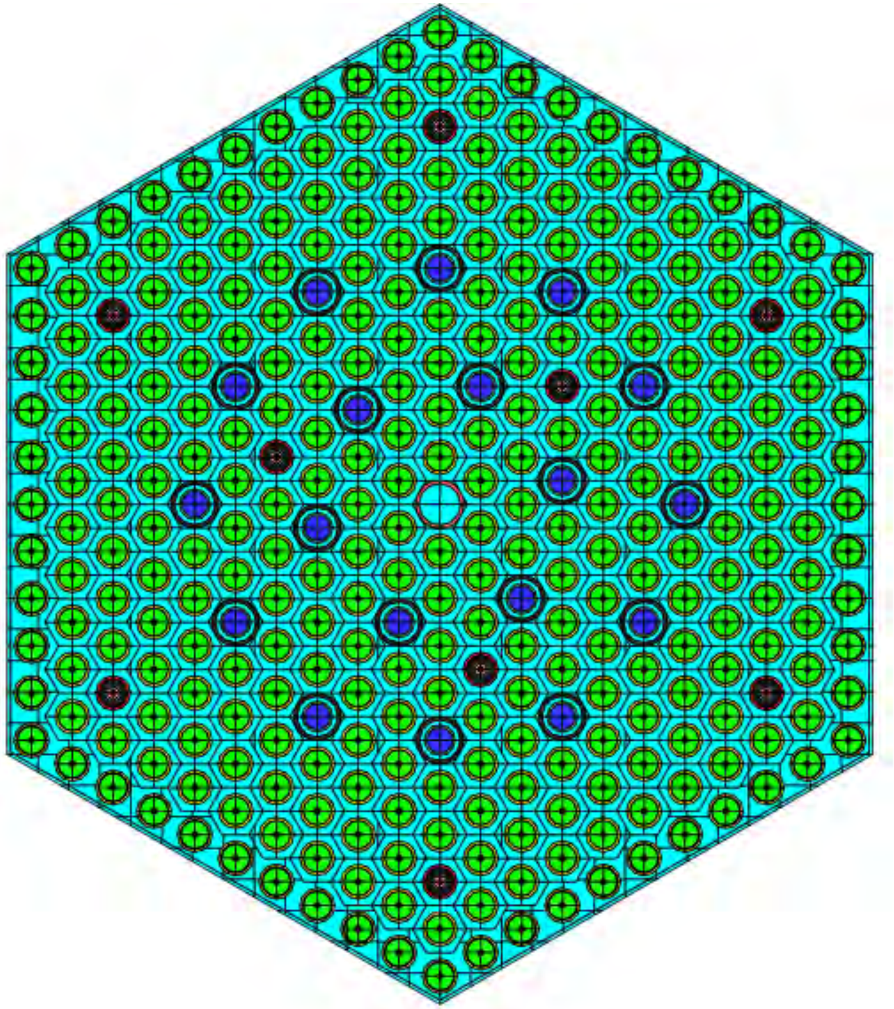
Lattices Modeled Using TRITON



1.3% ^{235}U, 0 Gd_2U_3 0%

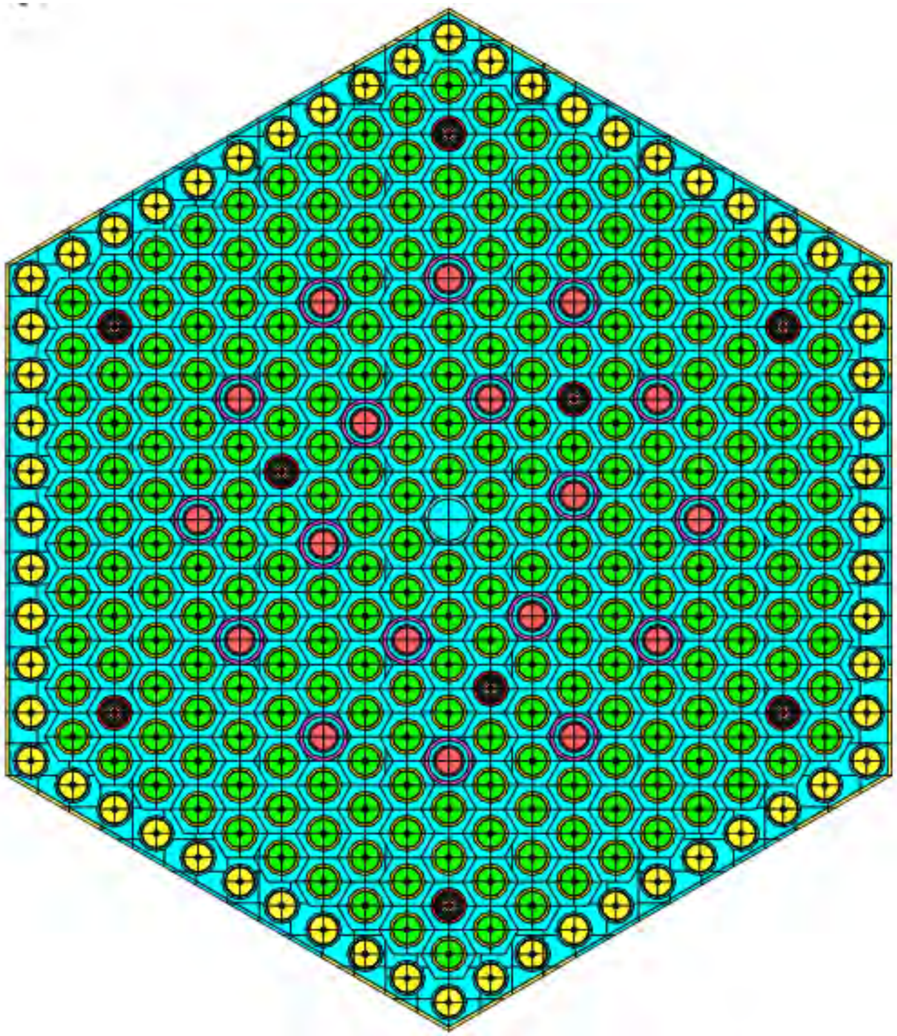
2.2% ^{235}U, 0 Gd_2U_3 0%

Lattices Modeled Using TRITON



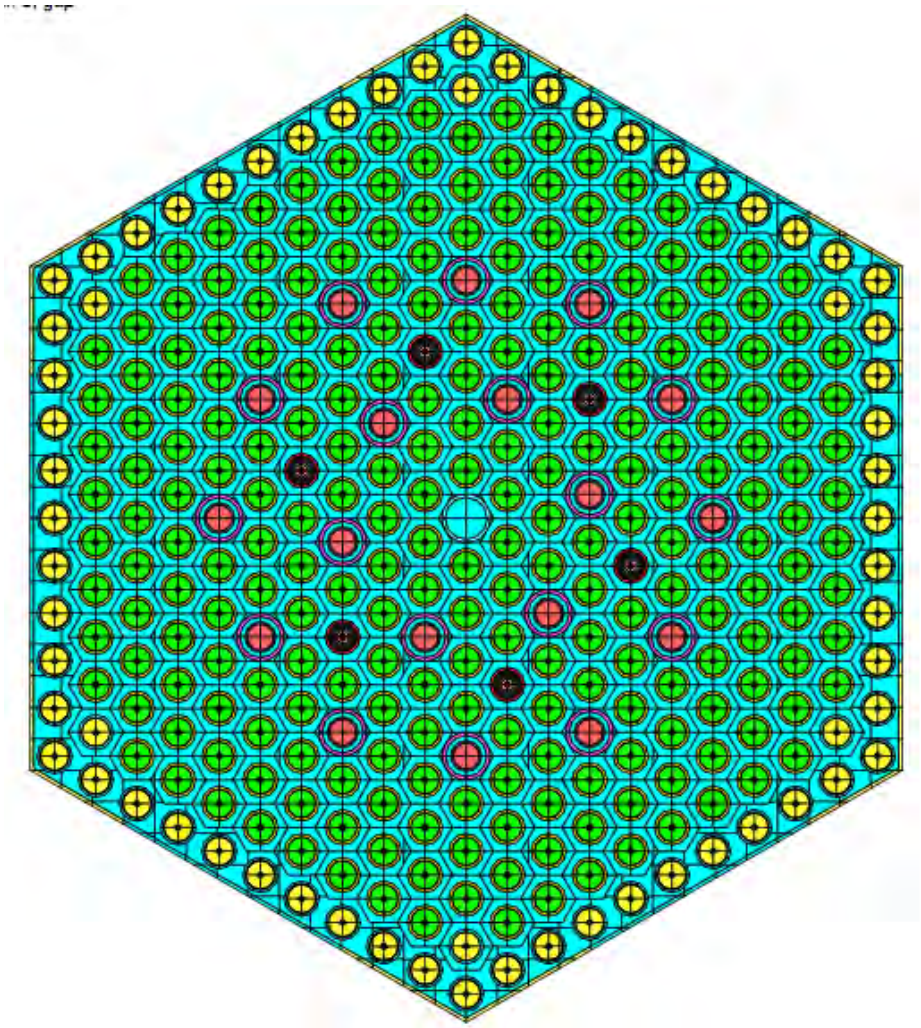
2.99% ^{235}U, 9 2.4% Enrich Gd_2U_3 5% Gd

Lattices Modeled Using TRITON



4.0% ^{235}U, Outer Ring 3.6% ^{235}U, 9 3.3% Enriched Gd_2U_3 5% Gd

Lattices Modeled Using TRITON



4.0% ^{235}U, Outer Ring 3.6% ^{235}U, 6 3.3% Enriched Gd_2U_3 5% Gd

Models Include Stiffening Plates

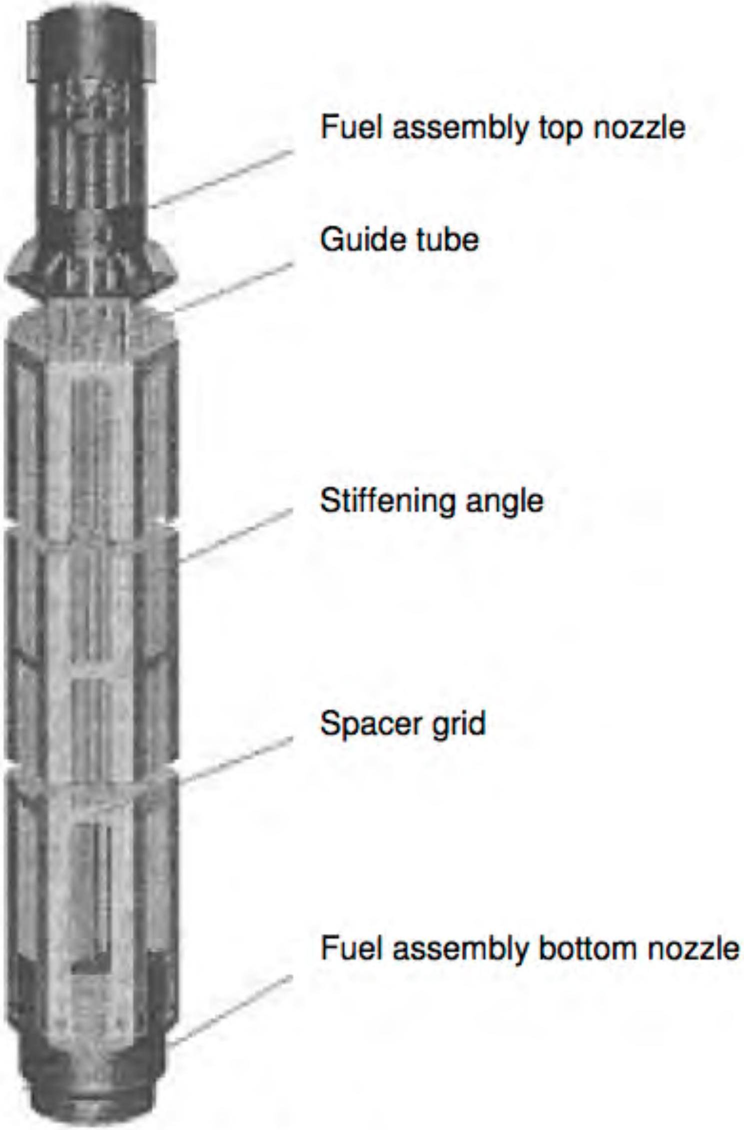
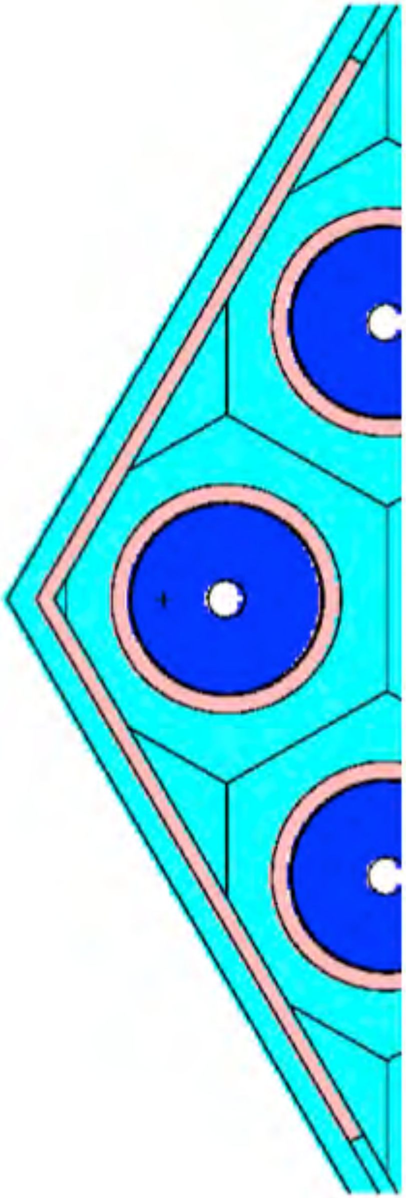
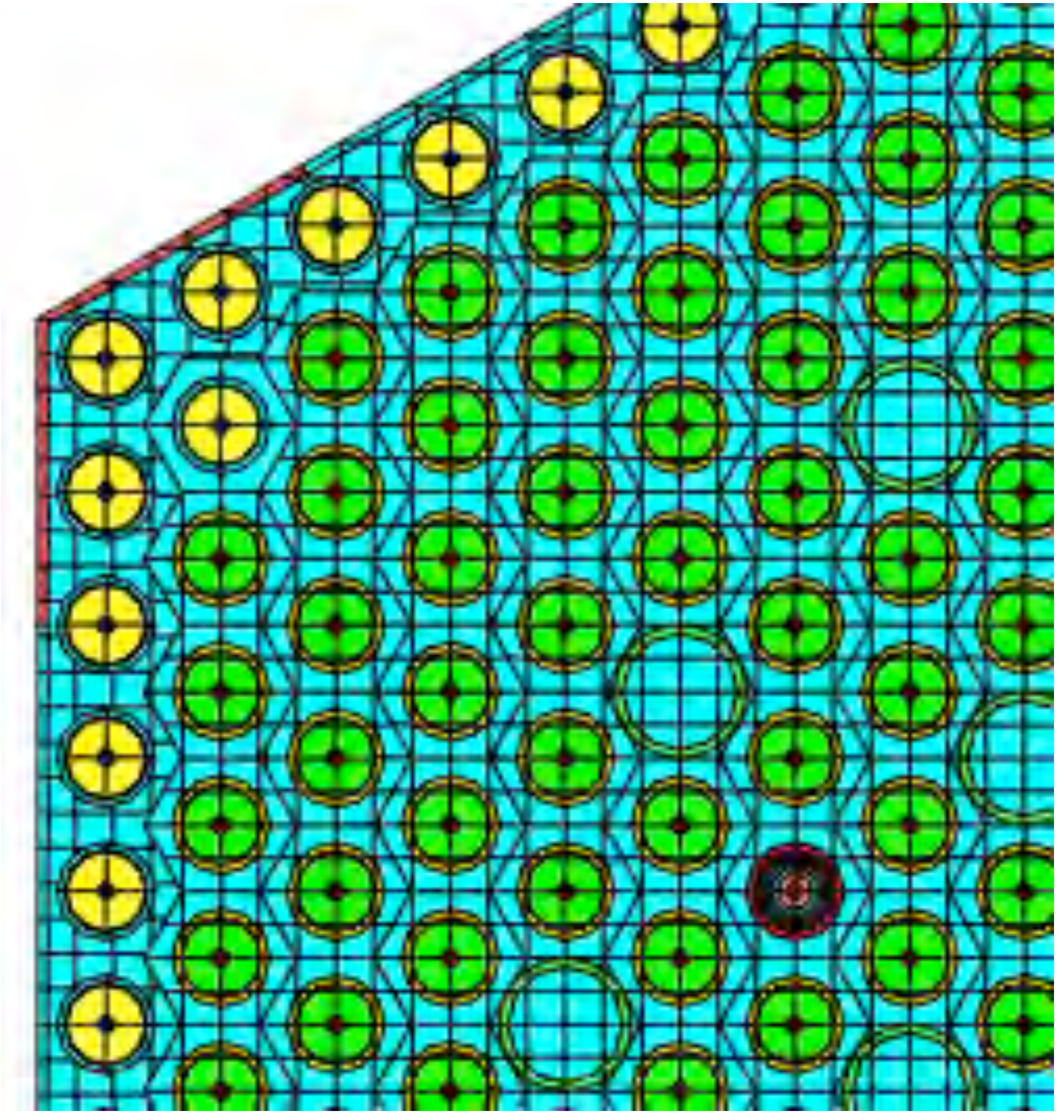


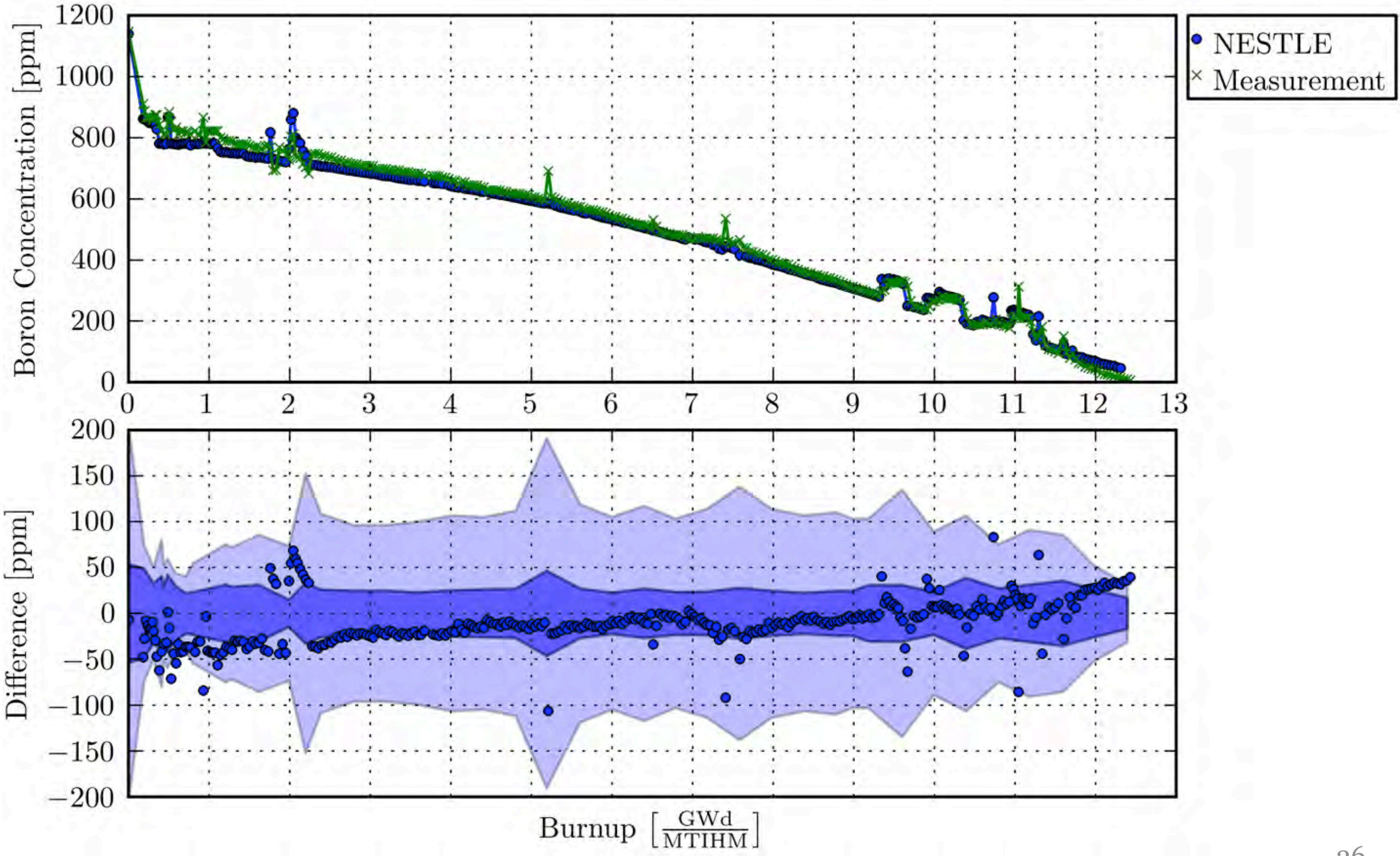
Fig. 1: General view of the TVSA



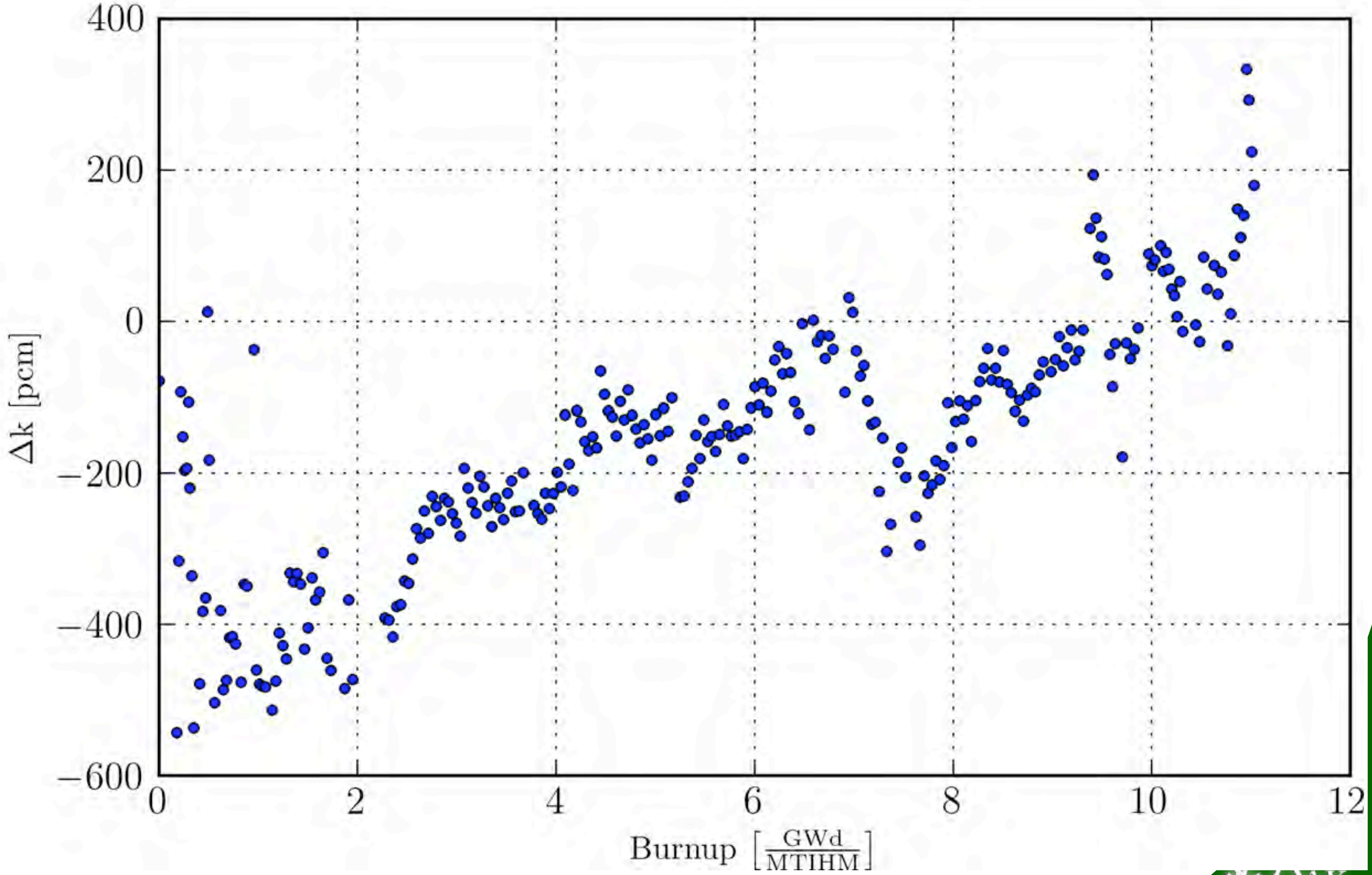
390go Lattice Detail in TRITON



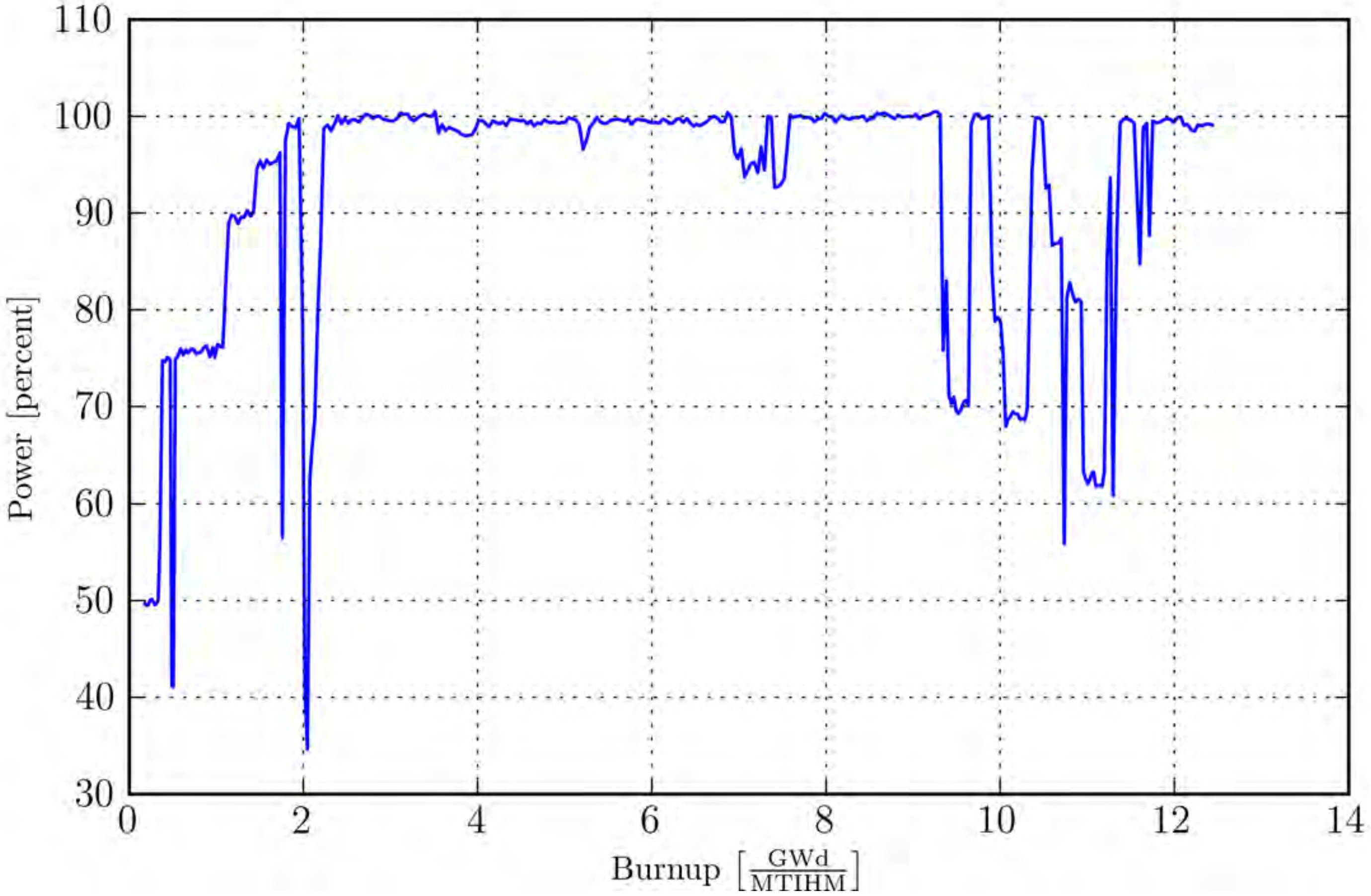
Khmelnitsky-2 Cycle 1 Boron



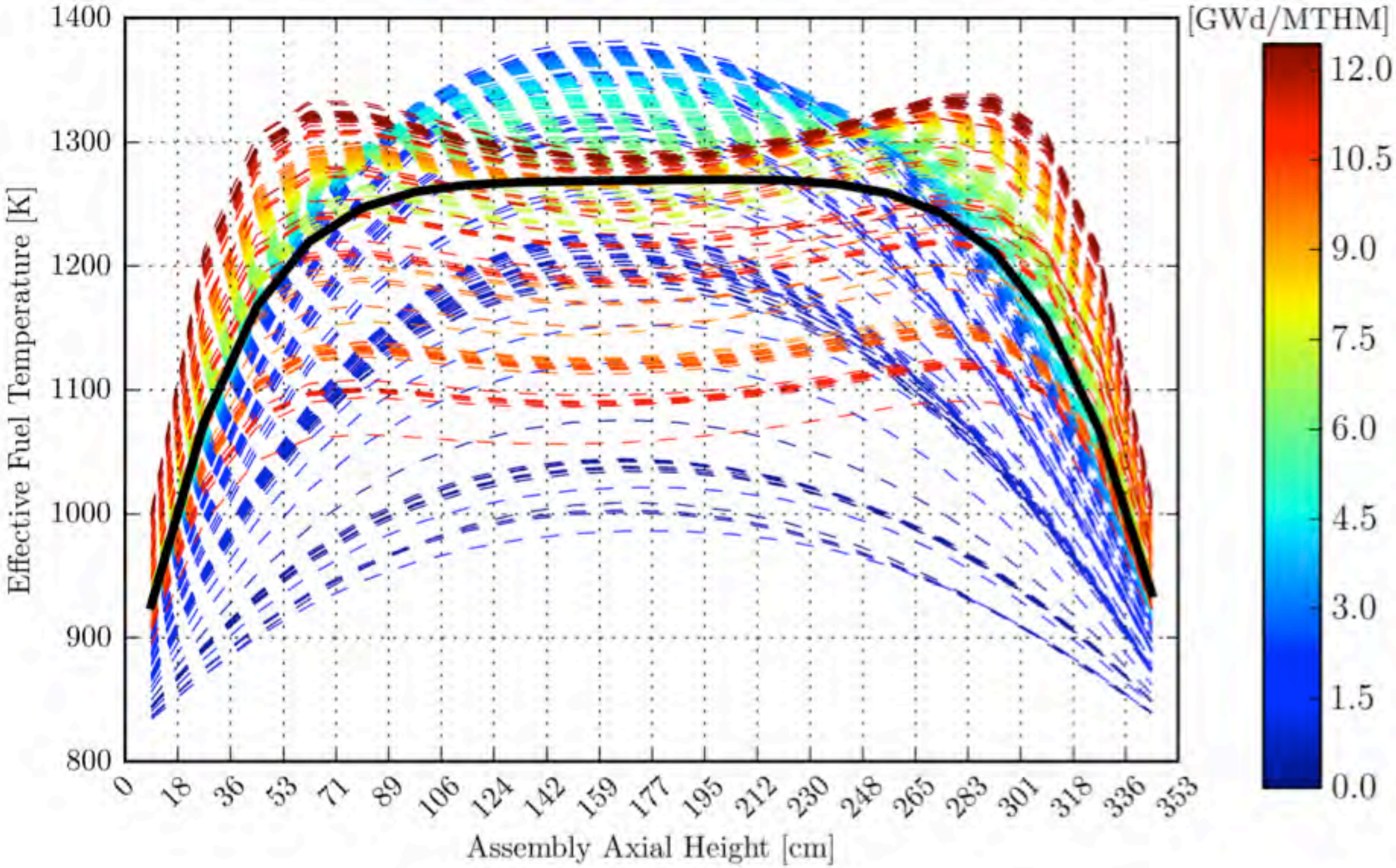
k_{eff} Difference Through Cycle



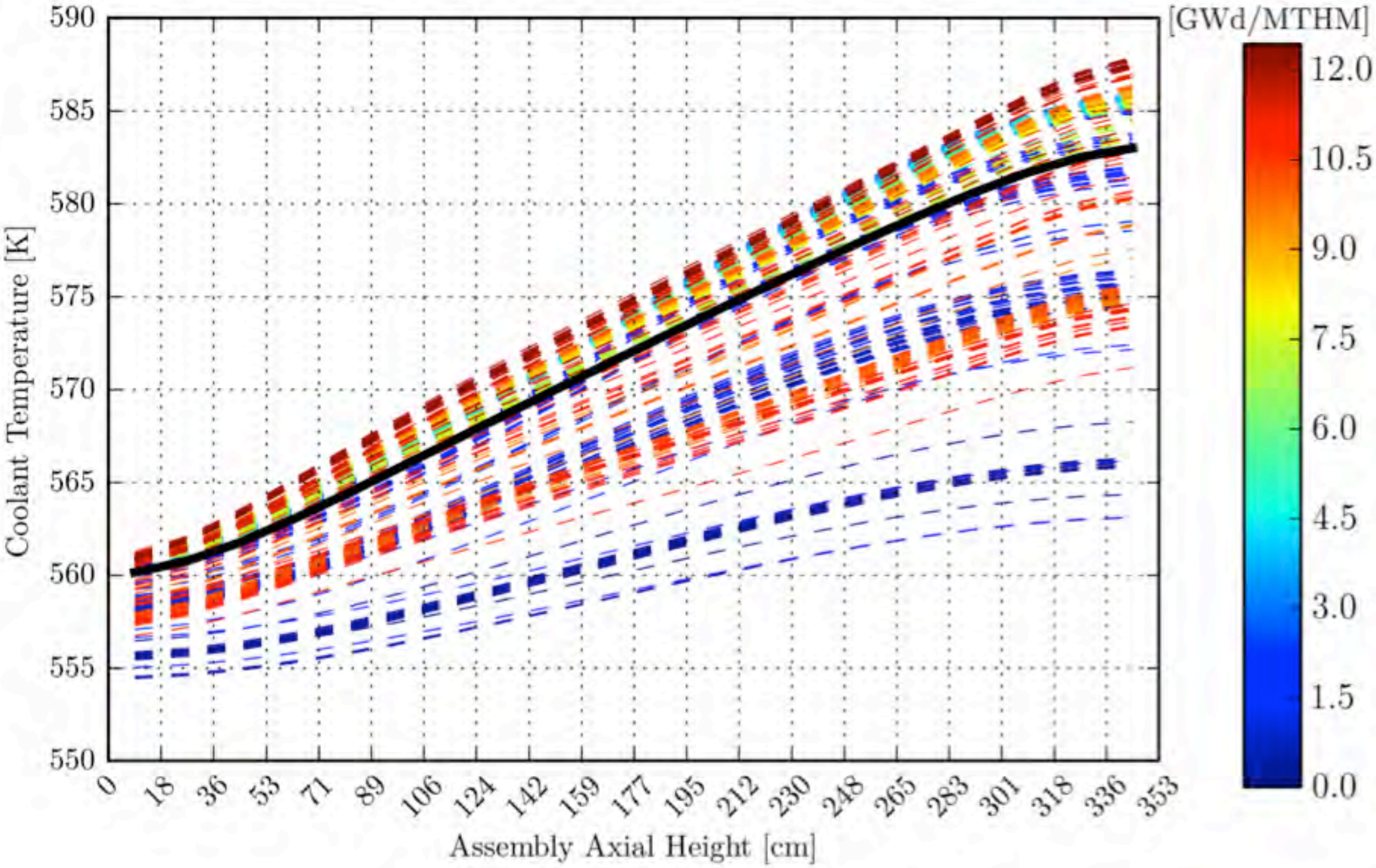
Power History for Khmelnitsky-2



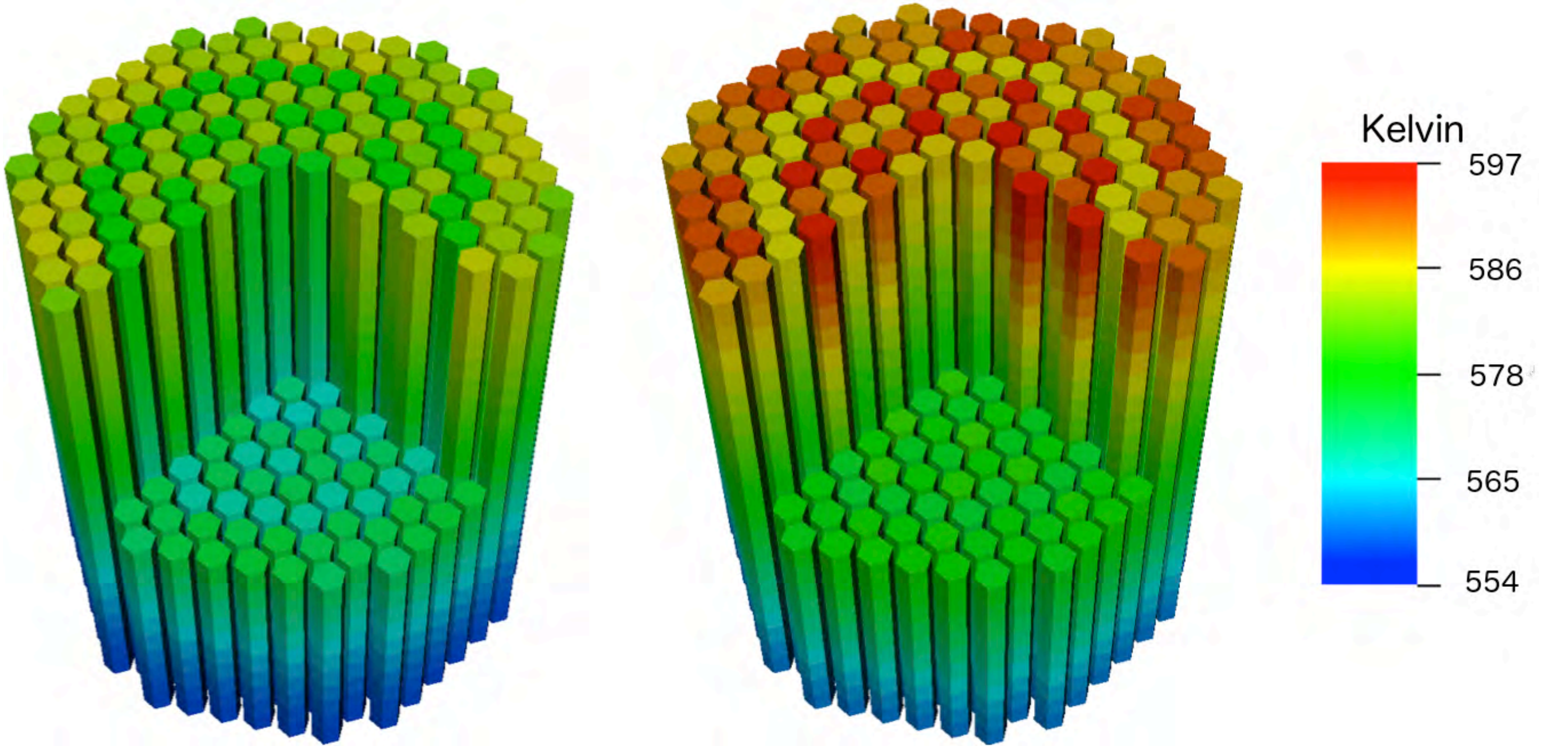
NESTLE: AER Benchmark Cycle 1



NESTLE: AER Benchmark Cycle 1



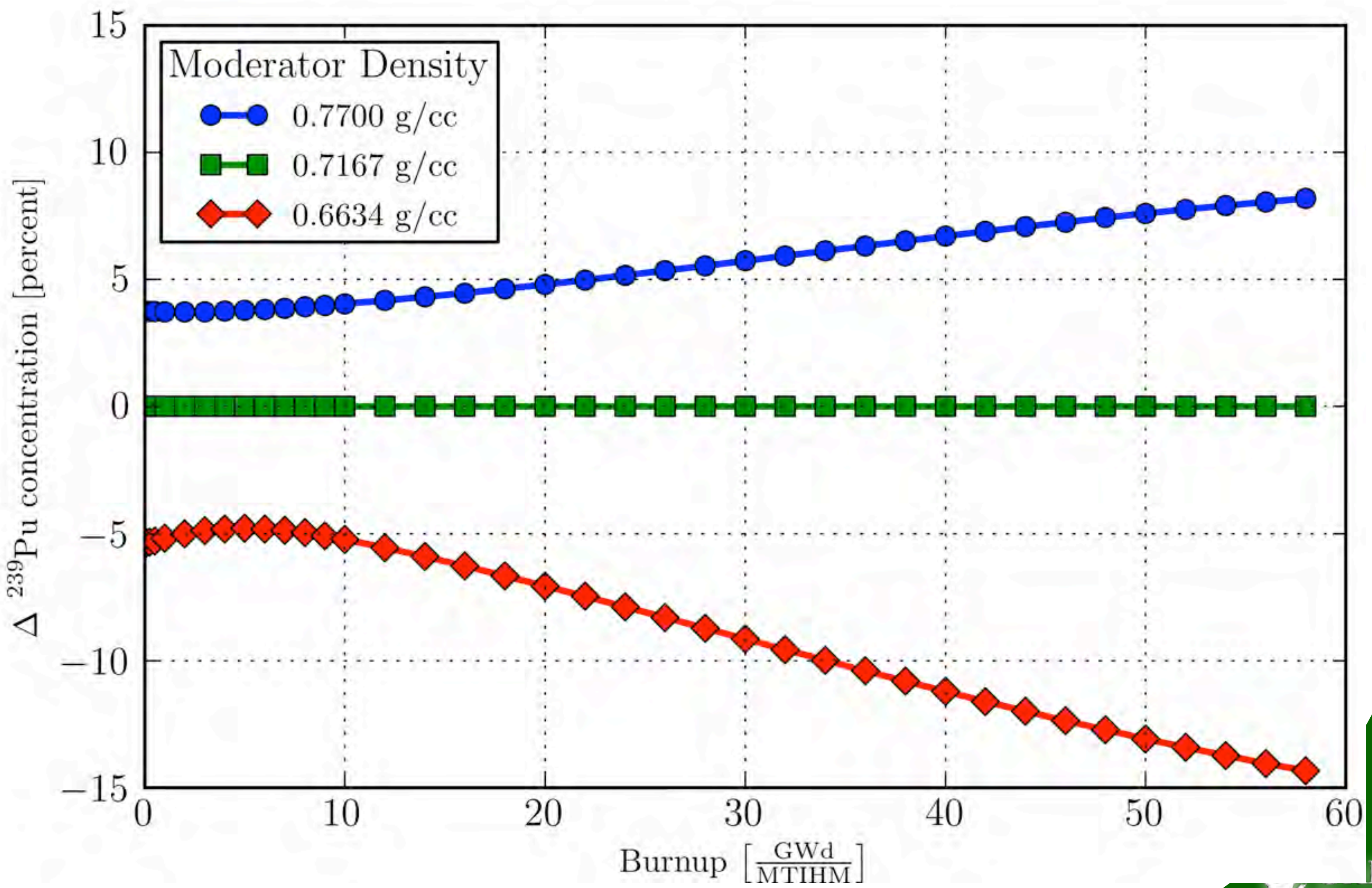
Coolant Temperature Distributions



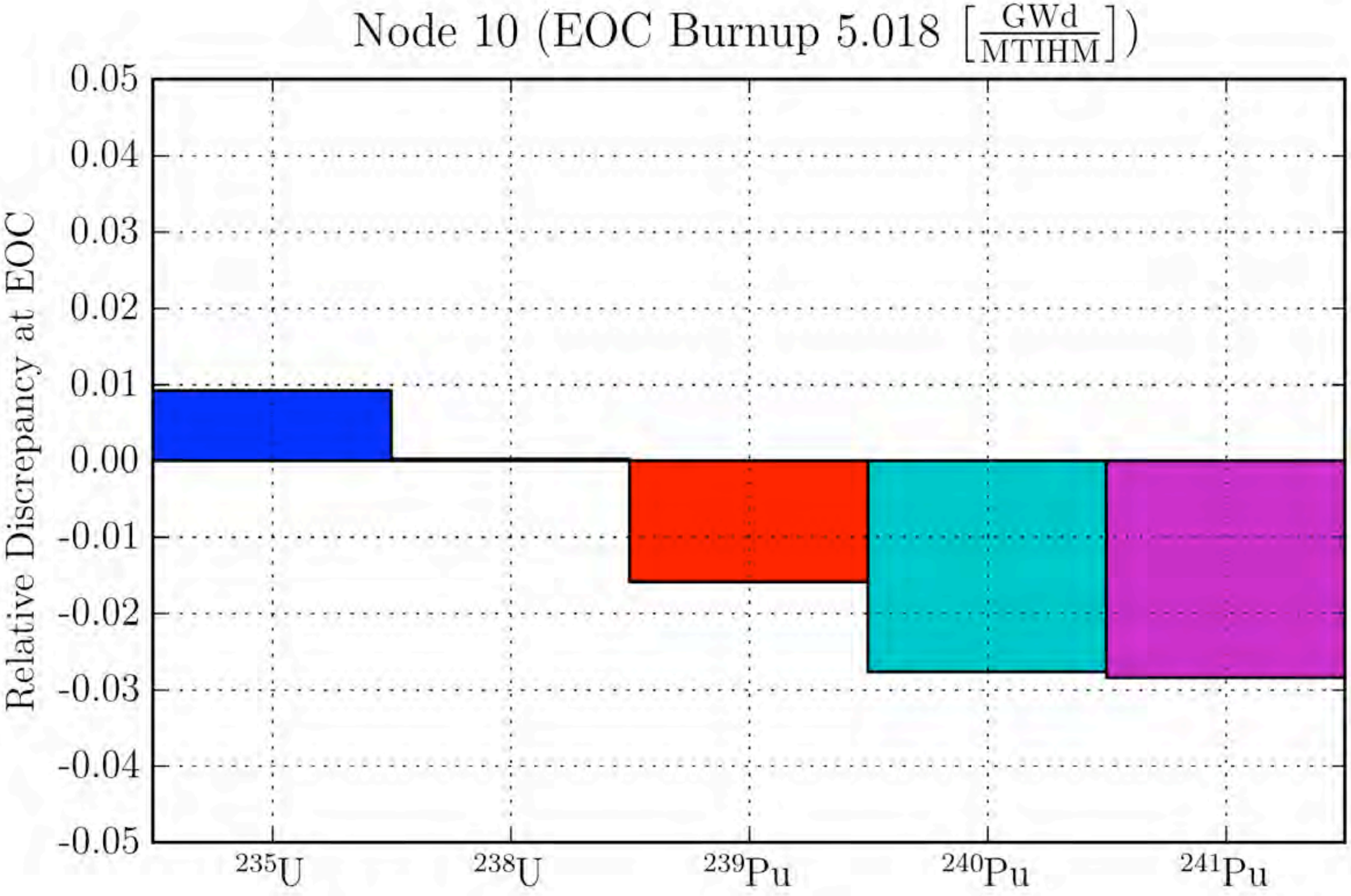
BOC

EOC

^{239}Pu Concentration Due to Moderator Density



Difference in Content Using Axially Flat Temperature Profile



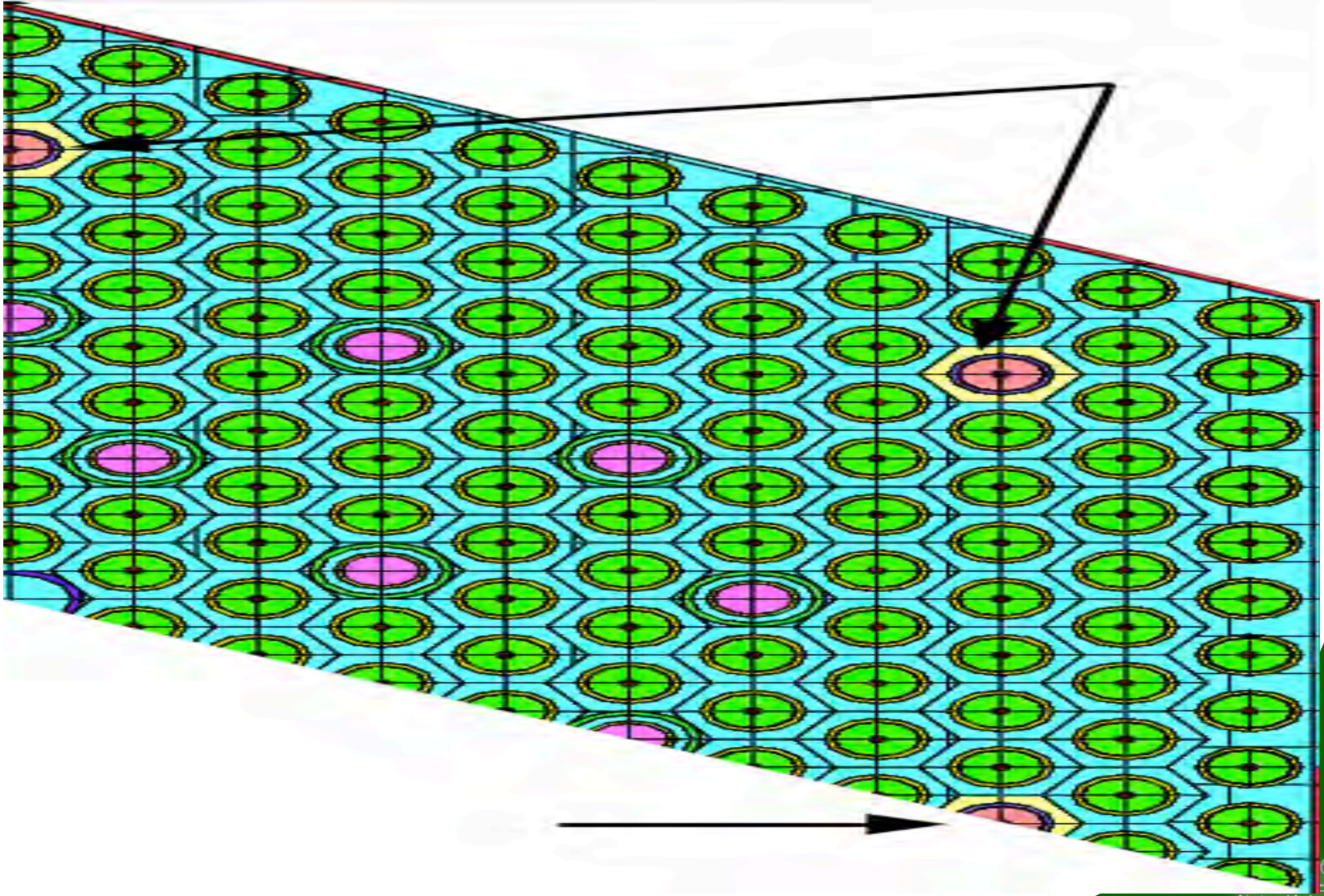
NESTLE-ORIGEN Pin Depletion

NESTLE-ORIGEN: Recollapse

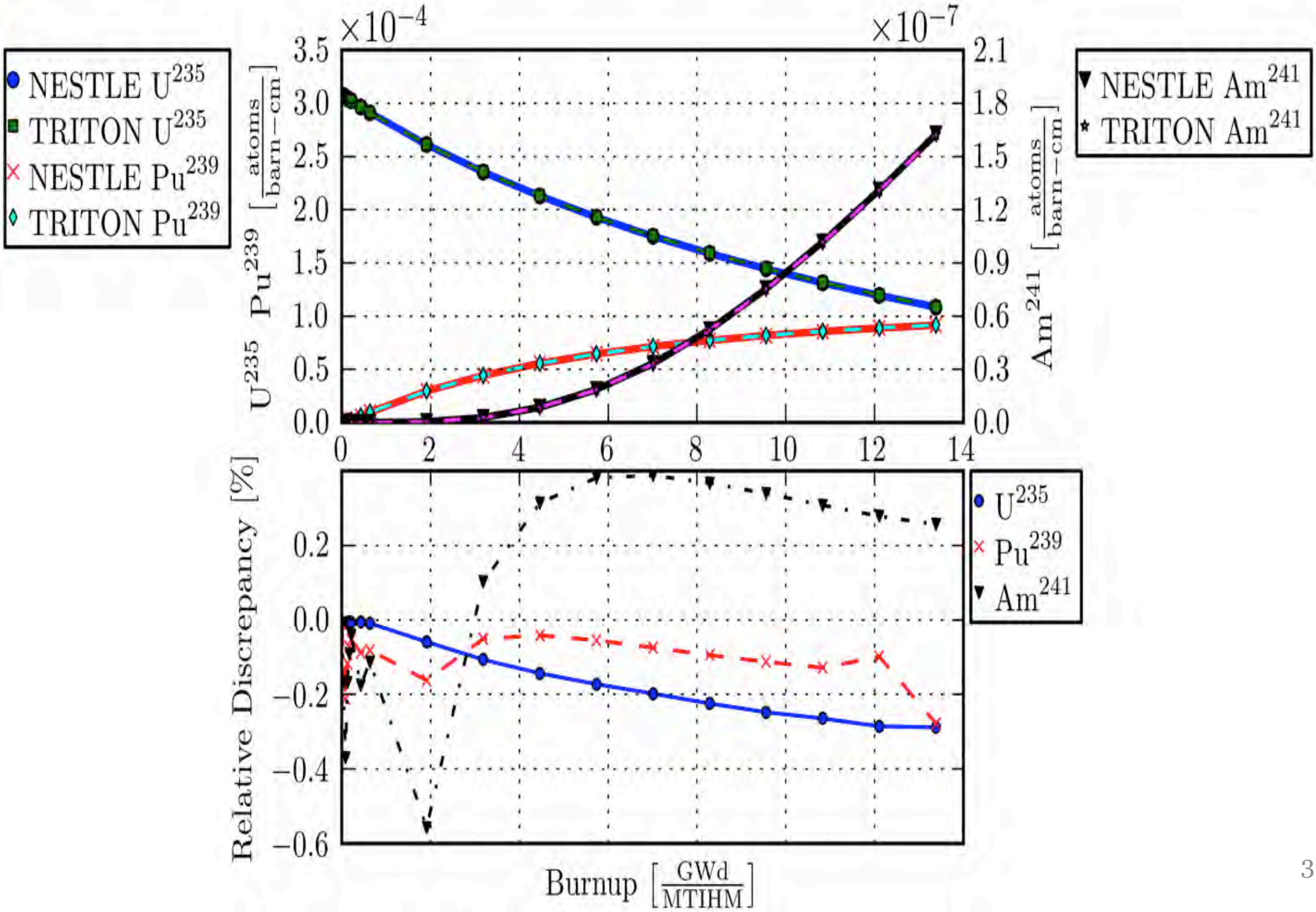
$$\sigma = \frac{\sum_{g=1}^{G} \Phi_g \sigma_g}{\sum_{g=1}^{G} \Phi_g}$$

- Cross sections originally collapsed weighted by TRITON flux
  - 238 groups --> few groups (2-4)
  - Lattice calculation bias present in few-group cross sections
- Recollapse in NESTLE
  - Few-groups (2-4) --> 1 group --> ORIGEN
  - Captures spectral effect to extent possible

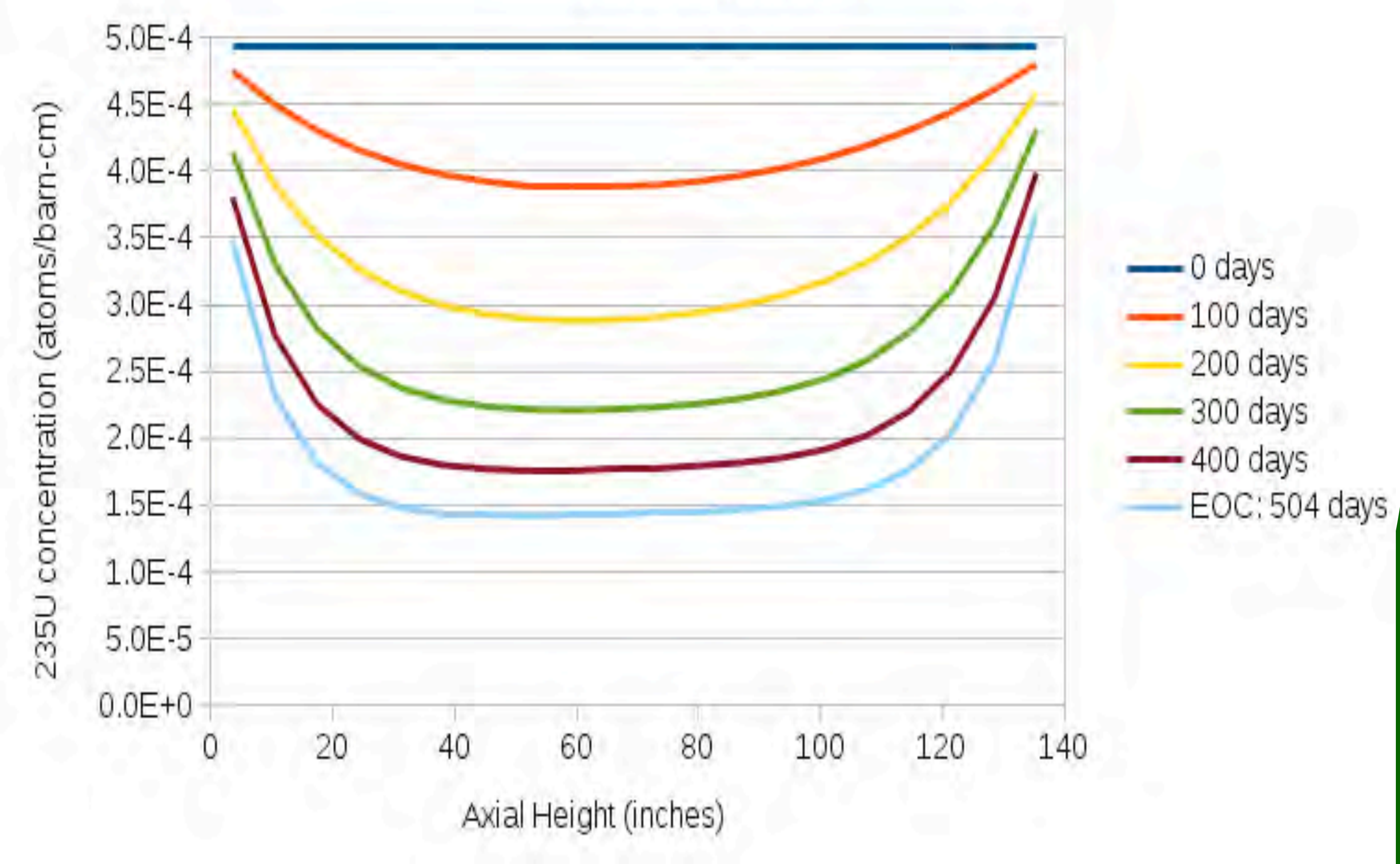
Lattice 22au Selected Pins for Depletion



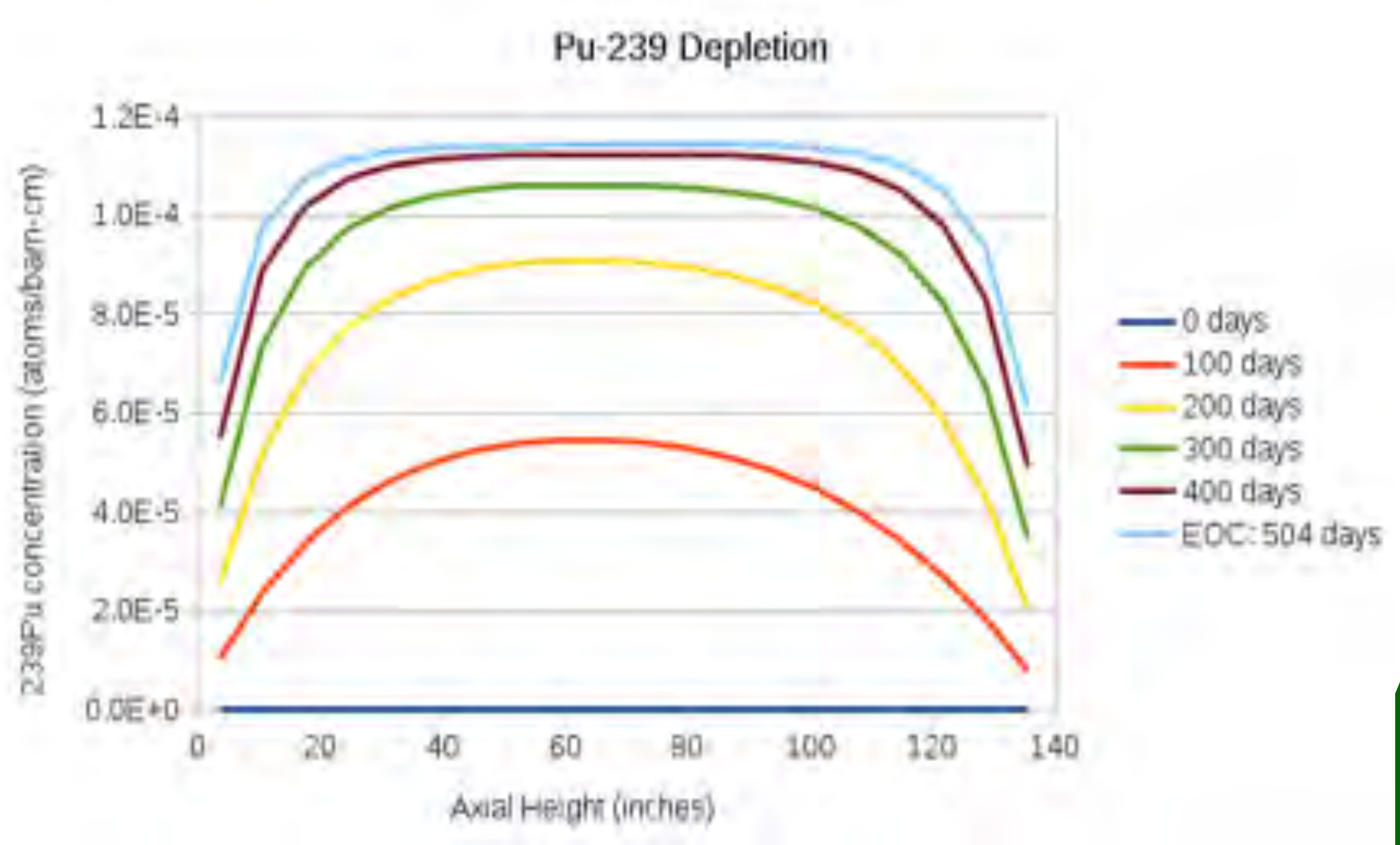
ORIGEN Depletion



Time Dependent ^{235}U Concentration

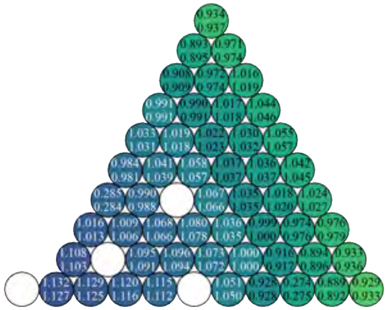


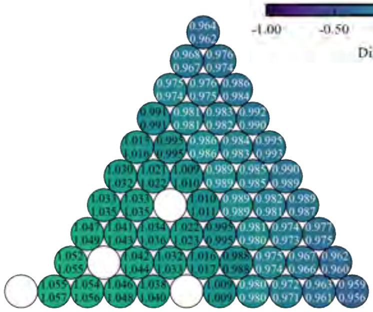
Time Dependent ^{239}Pu Concentration

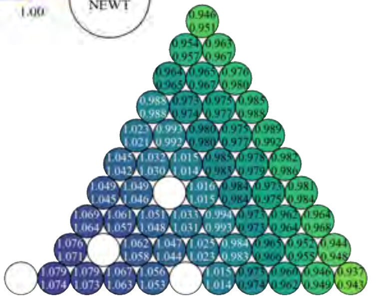


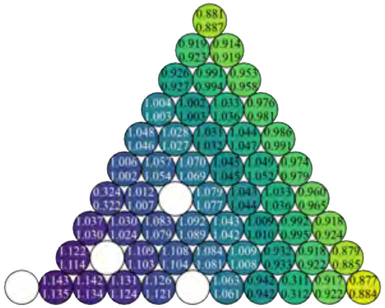
Pin Power Reconstruction V&V (Poster Session: Wed 5-7pm)

Test problems of benchmark specified 2D lattices were computed with NEWT and used to verify the pin power reconstruction calculation in a nodal simulator. The spatial distributions of the pin power factors are shown below. The nodal simulators reconstructed pin powers generally compare well with the pin powers computed by NEWT for the reflected lattices. The results are consistent with similar published results that tested the same pin power reconstruction method, which stated that for assemblies away from the edge of the core pin powers were reconstructed within 0.2% RMS and 1.0% maximum.

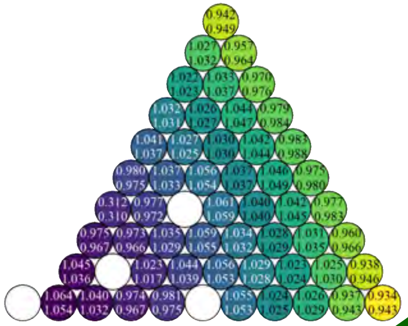








Lattice	Minimum Difference [%]	Maximum Difference [%]	Root Mean Square Deviation [%]
13au	0.312	0.270	0.154
22au	-0.517	0.603	0.301
30av5	-0.410	0.481	0.238
30awu	-0.730	0.868	0.431
390go	-0.885	0.981	0.501

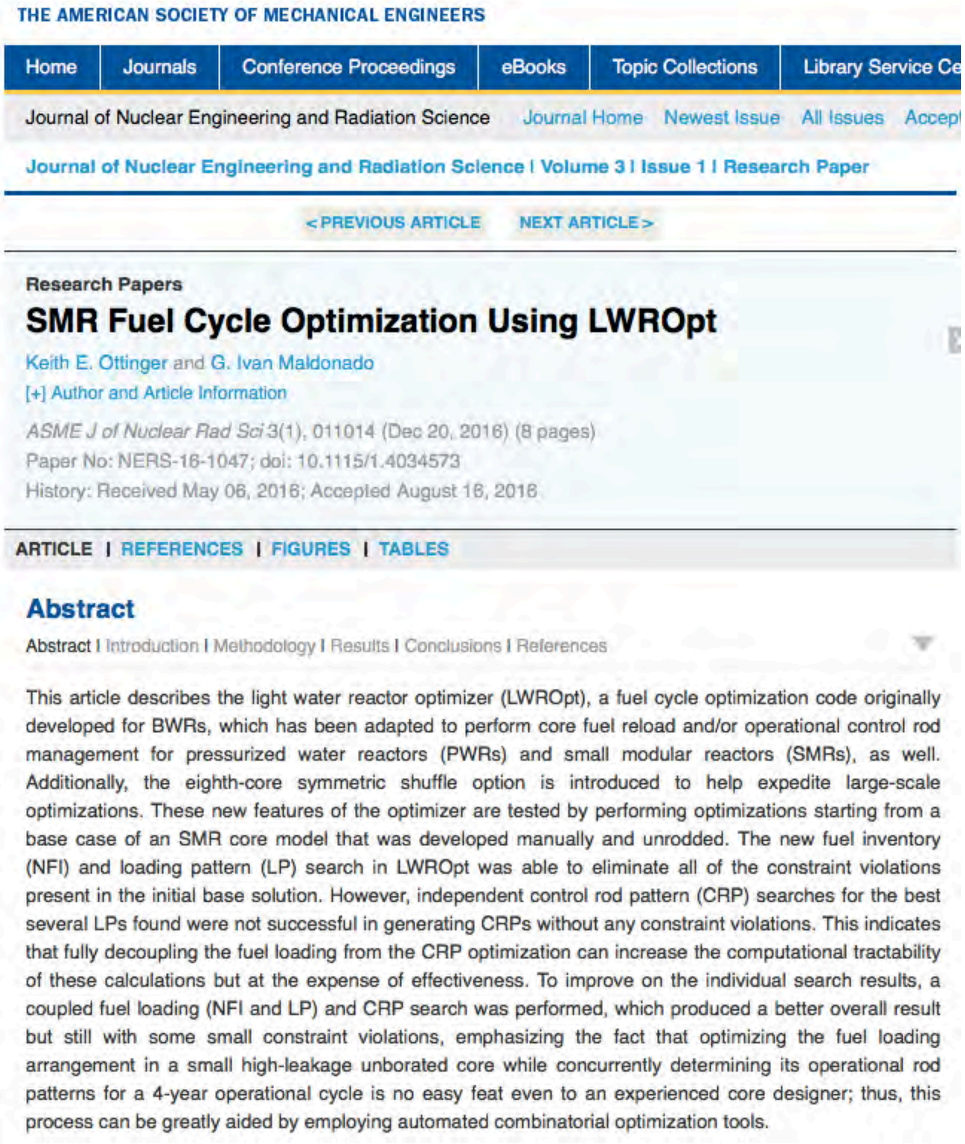


Selected SCALE to NESTLE Project Illustrations

SMR Modeling and Optimization

Keith Ottinger

SMR Optimization with LWROpt



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Research Papers

SMR Fuel Cycle Optimization Using LWROpt

Keith E. Ottinger and G. Ivan Maldonado

[+] Author and Article Information

ASME J of Nuclear Rad Sci 3(1), 011014 (Dec 20, 2016) (8 pages)
Paper No: NERS-16-1047; doi: 10.1115/1.4034573
History: Received May 06, 2016; Accepted August 16, 2016

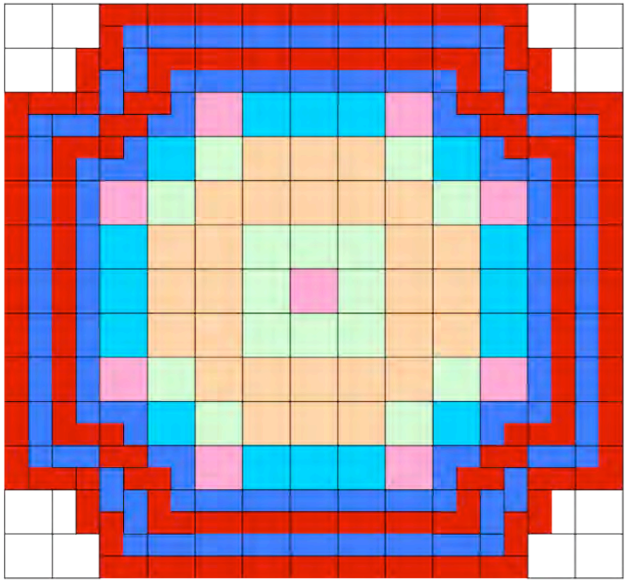
Abstract

This article describes the light water reactor optimizer (LWROpt), a fuel cycle optimization code originally developed for BWRs, which has been adapted to perform core fuel reload and/or operational control rod management for pressurized water reactors (PWRs) and small modular reactors (SMRs), as well. Additionally, the eighth-core symmetric shuffle option is introduced to help expedite large-scale optimizations. These new features of the optimizer are tested by performing optimizations starting from a base case of an SMR core model that was developed manually and unrodded. The new fuel inventory (NFI) and loading pattern (LP) search in LWROpt was able to eliminate all of the constraint violations present in the initial base solution. However, independent control rod pattern (CRP) searches for the best several LPs found were not successful in generating CRPs without any constraint violations. This indicates that fully decoupling the fuel loading from the CRP optimization can increase the computational tractability of these calculations but at the expense of effectiveness. To improve on the individual search results, a coupled fuel loading (NFI and LP) and CRP search was performed, which produced a better overall result but still with some small constraint violations, emphasizing the fact that optimizing the fuel loading arrangement in a small high-leakage unborated core while concurrently determining its operational rod patterns for a 4-year operational cycle is no easy feat even to an experienced core designer; thus, this process can be greatly aided by employing automated combinatorial optimization tools.

SMR Modeling and Simulation (Base Model)

- 17 Lattice types modeled with TRITON
- 4 assembly types, axial zoning
- Based on Physor '12 paper on mPower design

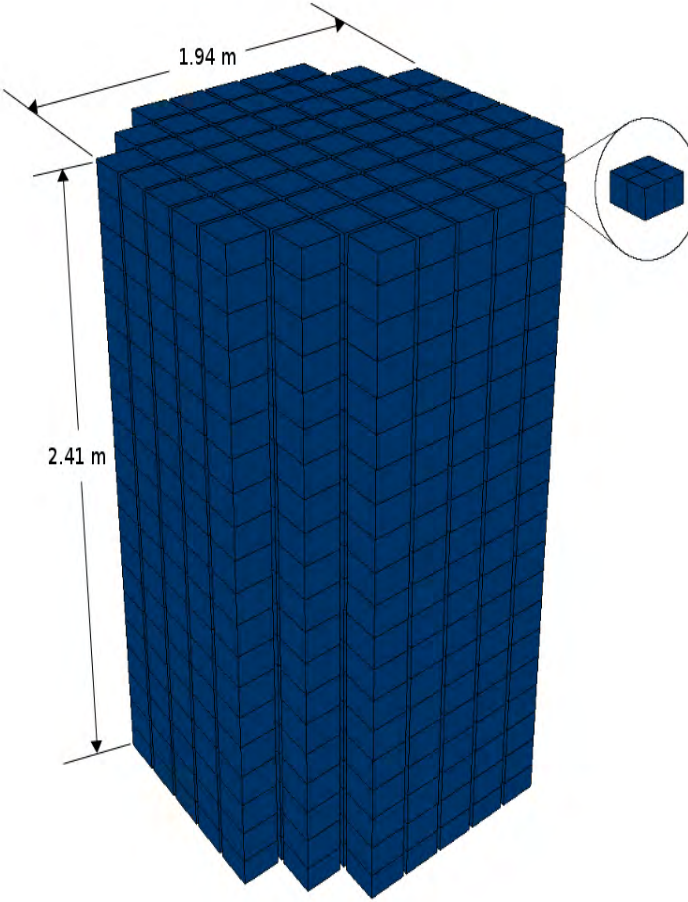
Node	1	2	3	4
1	100	200	300	400
2	130	230	320	430
3	130	230	353	430
4	130	293	353	494
5	130	293	353	494
6	193	293	353	494
7	193	293	353	494
8	193	293	353	494
9	193	283	353	494
10	193	283	353	494
11	193	283	353	494
12	193	283	353	494
13	193	283	353	494
14	193	283	353	494
15	193	283	353	494
16	193	283	353	494
17	193	283	353	494
18	193	283	353	494
19	193	283	353	494
20	110	210	310	410



Key
Assemby Type 1
Assemby Type 2
Assemby Type 3
Assemby Type 4
304 Steel
Water

SMR Optimization with LWROpt

- A non-proprietary small PWR core design was developed using available open literature for a single four-year cycle
- The design specifies the non-use of soluble poisons therefore primary reactivity control is achieved through the movable Ag-In-Cd CRs.
- The core consists of 69 fuel assemblies each using a standard 17×17 pin lattice on a 21.5 cm pitch. The tot assembly height is 241.3 cm.
- The lattice includes 24 control rodlet locations, and one central instrument tube. Fuel rods or burnable poison rods (BPRs) were placed in the remaining 264 pin locations.
- To achieve the four-year cycle length, the standard UC fuel pin is a relatively high 4.95% enrichment.
- Integral burnable poisons (UO_2-Gd_2O_3) and BPRs (B_4C-Al_2O_3) are used in the lattices to reduce maximum relative pin power peaking to ≤ 1.1.
- The UO_2-Gd_2O_3 pins use a reduced enrichment of 3.95% and contain 3.0% Gd2O3 by weight. The BPRs contain 4.0% B_4C by weight.



SMR Optimization with LWROpt

- BWROpt renamed LWROpt and extended to PWRs and SMRs
- LWROpt performs New Fuel Inventory (NFI) and Loading Pattern (LP) optimization using Parallel Simulated Annealing (PSA) and can generate Control Rod Patterns (CRPs) using a heuristic search.
- Candidate “solutions” consist of a NFI, LP, and reactivity control strategy. These solution candidates are evaluated with a modern version of NESTLE.
- Candidate solutions are compared with an Objective Function (OF), C, that has the following user selectable components/constraints:
  - Fuel Cycle Cost (FCC),
  - minimum k_{eff},
  - maximum k_{eff},
  - maximum 2D (assembly) Relative Power Fraction (RPF),
  - maximum 3D (node) RPF,
  - maximum 2D exposure,
  - maximum 3D exposure.

SMR Optimization with LWROpt

$$C = C_0 + \sum_{n=1}^{N}\left[wf_n D_n FCC_n + \sum_{i=1}^{I} wc_{i,n} CV_{i,n}\right]$$

Where;

C_0 = calculated constant that ensures *C* is greater than zero;
N = number of cycles considered in the optimization;
I = number of constraints considered in the optimization;
wfn = FCC weight for cycle *n*;
Dn = discount factor used to weight cycle *n* FCC in the levelized FCC calculation;
FCCn = fuel cycle cost for cycle *n*;
$wc_{i,n}$ = weight for constraint *i* in cycle *n*;
$CV_{i,n}$ = constraint violation (or margin) for constraint *i* in cycle *n*.

SMR Optimization with LWROpt

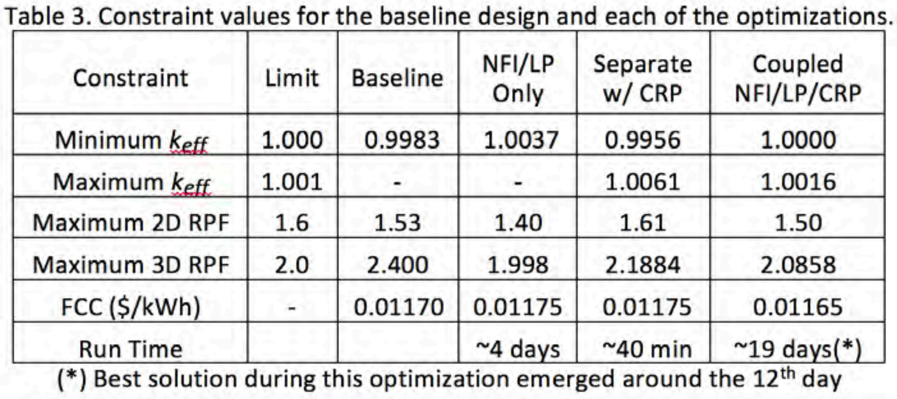


Table 3. Constraint values for the baseline design and each of the optimizations.

Constraint	Limit	Baseline	NFI/LP Only	Separate w/ CRP	Coupled NFI/LP/CRP
Minimum k_{eff}	1.000	0.9983	1.0037	0.9956	1.0000
Maximum k_{eff}	1.001	-	-	1.0061	1.0016
Maximum 2D RPF	1.6	1.53	1.40	1.61	1.50
Maximum 3D RPF	2.0	2.400	1.998	2.1884	2.0858
FCC ($/kWh)	-	0.01170	0.01175	0.01175	0.01165
Run Time			~4 days	~40 min	~19 days(*)

(*) Best solution during this optimization emerged around the 12th day

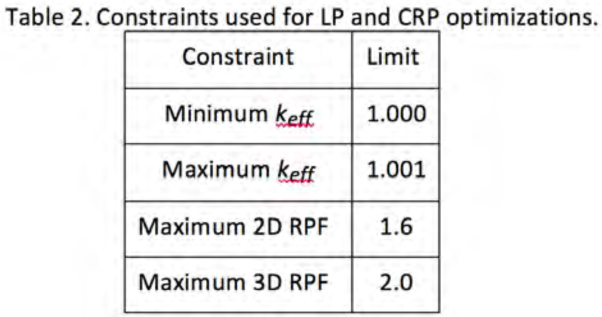
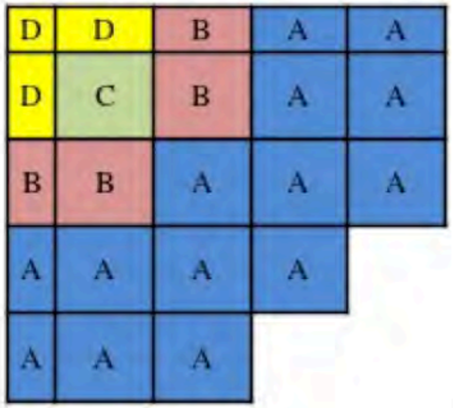


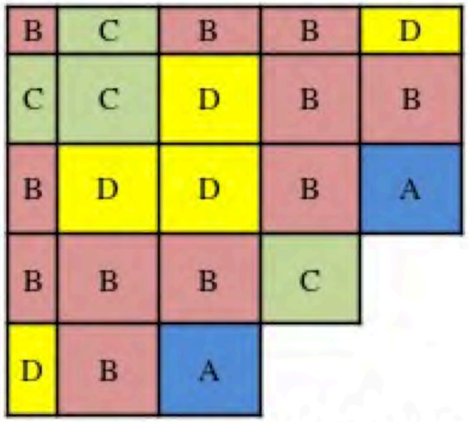
Table 2. Constraints used for LP and CRP optimizations.

Constraint	Limit
Minimum k_{eff}	1.000
Maximum k_{eff}	1.001
Maximum 2D RPF	1.6
Maximum 3D RPF	2.0



D	D	B	A	A
D	C	B	A	A
B	B	A	A	A
A	A	A	A	
A	A	A		

Fig. 5. Best LP found by LWROpt using only the LP optimization.



B	C	B	B	D
C	C	D	B	B
B	D	D	B	A
B	B	B	C	
D	B	A		

Fig. 8. Best LP found by LWROpt using the coupled LP/CRP optimization.

SMR Optimization with LWROpt

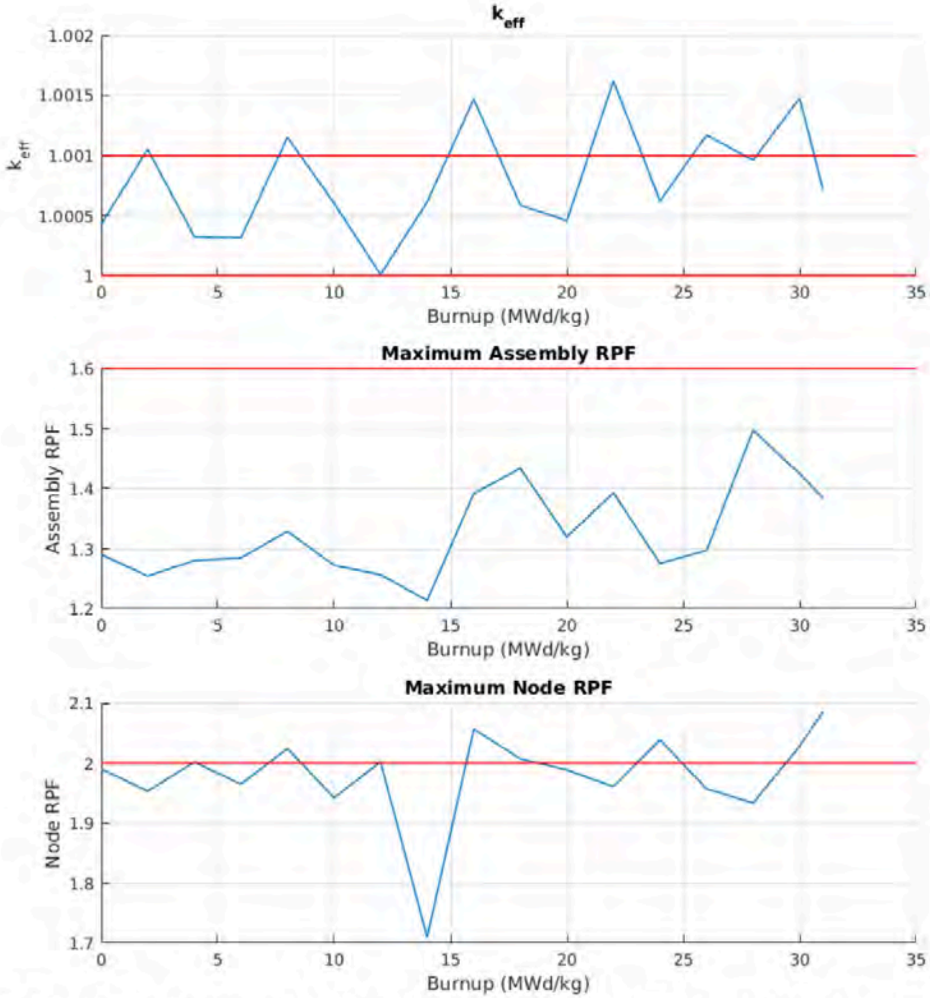


Fig. 9. Constraint values as a function of burnup for best LP/CRP for the coupled searches (constraint limits shown with horizontal lines).

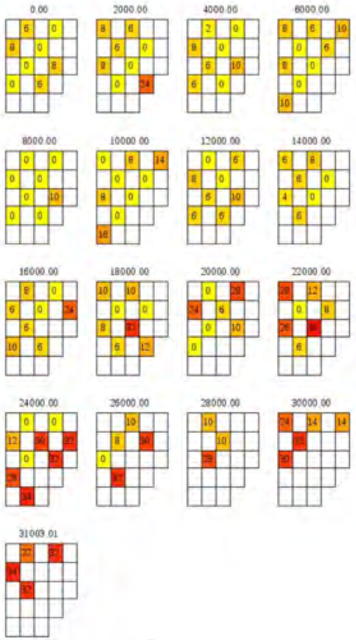


Fig. 10. CRPs generated for the coupled LP/CRP search (notches withdrawn, 40 total notches) for each burnup step (kWd/kg).