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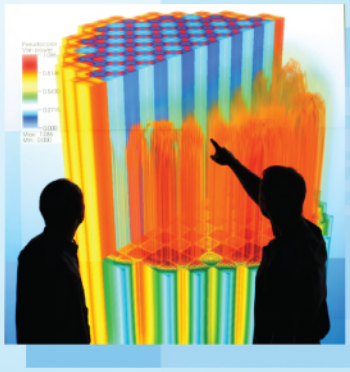

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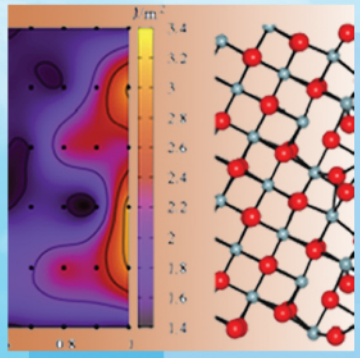

Fundamental science

Plant operational data

CASL
Consortium for Advanced Simulation of LWRs

Operational Reactor Model Demonstration with VERA: Watts Bar Unit 1 Cycle 1 Zero Power Physics Tests

Jess C Gehin, ORNL
Andrew T Godfrey, ORNL
Fausto Franceschini, Westinghouse

Advanced Modeling Applications

Thomas M Evans, ORNL
Benjamin S Collins, UM
Steven P Hamilton, ORNL

Radiation Transport Methods

Revision 1

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REVISION LOG

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0	6/7/2013	All	Original Release
1	8/23/2013	iii-vii, 22, 35-36, 43-44, 64-71, 73	Updated NEXUS and Insilico results and added correction for thermal expansion. The NEXUS results were improved by a change in the radial reflector model and the Insilico calculations were redone after finding and fixing a bug in the homogenized cross section generation.

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Randy Summers, VRI Deputy Lead
Zeses Karoutas, AMA Deputy Lead
Steve Hess, AMA Deputy Lead
Rose Montgomery, Product Applications Coordinator

EXECUTIVE SUMMARY

The Consortium for Advanced Simulation of Light Water Reactors (CASL) is developing a collection of methods and software products known as VERA, the Virtual Environment for Reactor Applications. VERA will provide coupled, high fidelity nuclear reactor analysis capabilities in multiple areas of physics such as neutronics, thermal-hydraulics, fuel mechanics, and others. A key milestone for this endeavor is to validate VERA against measurements from operating nuclear power reactors. This document demonstrates the capabilities of VERA to accurately simulate the initial startup physics tests of Watts Bar Nuclear Power Station, Unit 1 (WBN1), demonstrating the many achievements that have been made by the CASL partners over the past year.

Zero power physics tests are performed at the startup of each fuel cycle prior to escalating power and placing the unit on the electrical grid. Key measurement parameters include the soluble boron concentration and control rod positions for initial criticality, control rod reactivity worth, differential soluble boron reactivity worth and isothermal temperature reactivity coefficient. Since the measurements are performed at zero power conditions, simulation of thermal-hydraulics is not needed. For the initial reactor startup, all the fuel in the core is fresh and depletion capability is also not needed. As a result, the zero power physics tests can be simulated by performing neutronics-only eigenvalue calculations.

CASL staff have performed numerous tasks to support this demonstration, including the collection of measured data, generation of new multi-group cross section libraries, enhancements of 3D neutron transport methods, development of a practical and intuitive reactor-based input format, and significant testing and analysis for a set of newly defined PWR benchmark problems leading up to this analysis. Significant achievements have also been made in development of continuous energy Monte Carlo models for a numerical reference solution for VERA comparison. Furthermore, models have also been created and results analyzed using the Westinghouse advanced nodal neutronics methods in the NRC-licensed code package NEXUS. The results of these methods are included alongside the VERA results for each of the WBN1 physics tests.

VERA calculations were performed with the Insilico code being developed at ORNL, which uses cross section processing from the SCALE system and S_N and SP_N transport capabilities within the Denovo transport code (this work utilized the SP_N method). The calculations were performed with ENDF/B-VII.0 cross sections in 252 groups (collapsed to 23 groups for the 3D transport solution). Additional VERA calculations were performed with the Michigan PArallel Characteristics based Transport (MPACT) code developed at the University of Michigan, included in Appendix A.

The key results of the comparison of calculations with measurements are as follows:

- *Initial Criticality*: For the initial criticality test, the Insilico result agrees with the measured conditions with a 19 pcm reactivity difference (or 2 ppm soluble boron).
- *Control Rod Worth Critical Configurations*: For the control rod worth measurements, Insilico matches ten selected critical conditions, each with a unique control bank

configuration, with an average reactivity difference of 89 pcm and maximum of 147 pcm.

- *Control Rod Worth:* For the actual rod worths, Insilico agrees with the measured worths, adjusted by consistent rod shadow factors, to within 3.0% with differences in individual bank worths of up to 7.5%.
- *Differential Boron Worth:* Insilico predicts the measured differential boron worth with a difference of 0.7 pcm/ppmB.
- *Isothermal Temperature Reactivity Coefficient:* Insilico predicts the isothermal temperature coefficient with a difference of 1.7 pcm/°F. This value is unexpectedly large and requires further investigation.

All of these results are well within the acceptance criteria needed for operation of the reactor and are in excellent agreement with the reference Monte Carlo calculations and results obtained with the Westinghouse design and analysis tools, except for the more negative temperature coefficient.

This work marks a significant achievement in the development of VERA including the following accomplishments:

1. The VERA common input provides a usable engineering interface that can be used to model operational reactors while supporting several different computational codes (in this case Insilico and MPACT).
2. The collection and documentation of an extensive set of validation data from the CASL physical reactor, TVA's Watts Bar Nuclear Unit 1.
3. Successful completion of AMA Core Physics Progression Problem #5, "Physical Reactor Zero Power Physics Tests"
4. Excellent agreement of VERA results for Watts Bar Nuclear Unit 1, Cycle 1, for initial criticality, control rod worth, and differential boron worth in comparison to plant measurements. The isothermal temperature coefficient prediction is not as good and requires some additional investigation.
5. Excellent agreement of VERA results in comparison to reference continuous energy Monte Carlo results as well as results from Westinghouse's NEXUS core physics package, other than the temperature coefficient.
6. Demonstration of ability to extract, process, and display detailed results from VERA using a standardized output format file and freely-available visualization tools (VisIt in this case).

The development of the VERA core simulation capabilities is well underway with ongoing activities to provide the coupled neutronics, thermal-hydraulics, and rod mechanics capabilities needed to model power ascension and steady-state operation. This capability will be demonstrated as part of the AMA core physics progression problems.

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This CASL Level 1 milestone was completed only through the significant contributions from many individuals from laboratory, university, and nuclear power industry organizations. The authors would like to express gratitude especially to the individuals and organizations below:

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ACRONYMS

1D	One Dimensional
2D	Two Dimensional
3D	Three Dimensional
AMA	Advanced Modeling Applications
ANS	American Nuclear Society
ARO	All Rods Out
BOC	Beginning of Cycle
CASL	Consortium for Advanced Simulation of Light Water Reactors
CE	Continuous energy
CFM	Centerline Fuel Melt
CMFD	Coarse Mesh Finite Difference
CP	Collision Probability
DBW	Differential Boron (reactivity) Worth (pcm/ppmB)
DNB	Departure from Nucleate Boiling
ESSM	Embedded Self-Shielding Method
HDF	Hierarchical Data Format
HZP	Hot Zero Power
IFBA	Integral Fuel Burnable Absorber
ITC	Isothermal Temperature (reactivity) Coefficient (pcm/°F)
KBA	Koch-Baker-Alcouffe wavefront parallel algorithm
LWR	Light Water Reactor
MG	Multi-group (as in cross sections)
MOC	Method of Characteristics
MPACT	Michigan PArallel Characteristics based Transport (computer code)
MTC	Moderator Temperature Coefficient (pcm/°F)
OLCF	Oak Ridge Leadership Computing Facility
ORNL	Oak Ridge National Laboratory
PCI	Pellet-Clad Interaction
PCM	Percent Mille (in this case, 10^5 times Δk or $\Delta\rho$)
PWR	Pressurized Water Reactor
RCCA	Rod Cluster Control Assembly
RNSD	Reactor and Nuclear Systems Division (at ORNL)
RSICC	Radiation Safety Information Computational Center
RTM	Radiation Transport Methods
TVA	Tennessee Valley Authority
UM	University of Michigan
UTK	University of Tennessee Knoxville
NRC	Nuclear Regulatory Commission
VERA	Virtual Environment for Reactor Applications
VRI	Virtual Reactor Integration
WBN1	Watts Bar Nuclear Unit 1
ZPPT	Zero Power Physics Testing

1. INTRODUCTION

The Consortium for Advanced Simulation of Light Water Reactors (CASL) is developing a collection of methods and software products known as VERA, the Virtual Environment for Reactor Applications. VERA will provide coupled, high fidelity nuclear reactor analysis capabilities in multiple areas of physics such as neutronics, thermal-hydraulics, fuel mechanics, and others. A key milestone for this endeavor is to validate VERA against measurements from operating nuclear power reactors. This document will demonstrate the capabilities of VERA to accurately simulate the startup physics tests of an operational reactor, demonstrating the many achievements that have been made by the CASL partners over the past year.

There are many aspects of nuclear analysis and reactor methods benchmarking that are faced by industry engineers on a daily basis. Unlike basic research, the application of advanced software to practical nuclear reactor analysis requires a combined understanding of reactor operation, measurement techniques, model development, physics simulation and analysis methods. CASL is uniquely positioned to both develop state-of-the-art software tools as well as perform detailed fuel and core analysis due to the breadth of the expertise of the consortium members. The members that contributed to this report, listed in the Acknowledgements section, have provided many significant contributions, including:

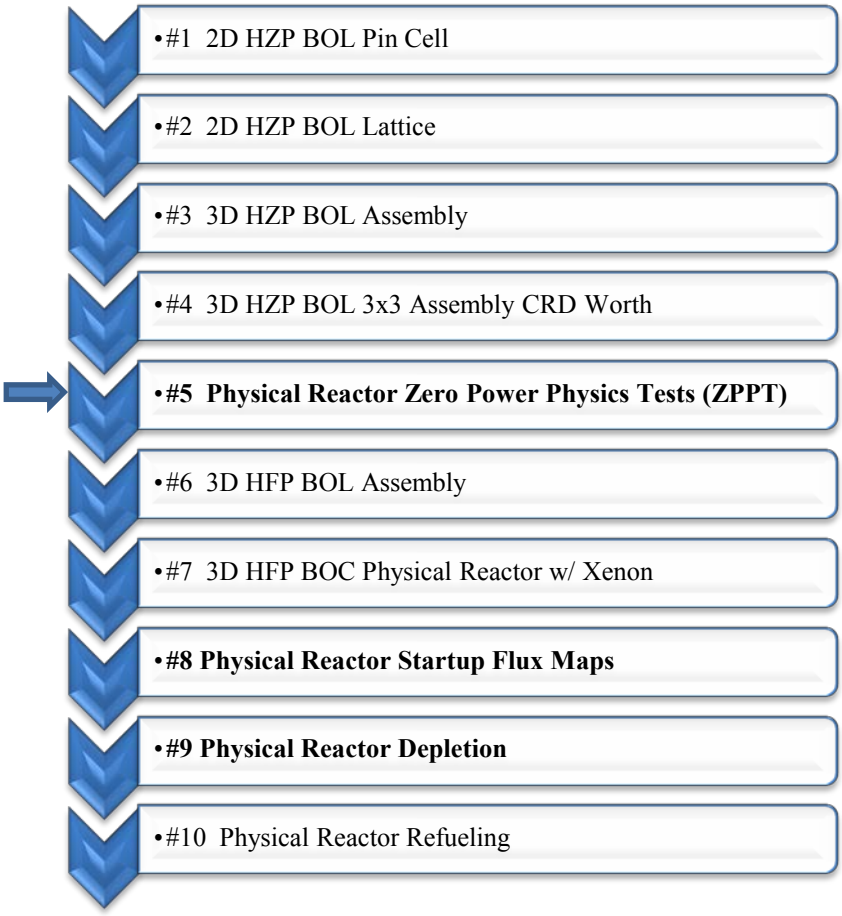
- Gathering and documentation of historical reactor operation data and plant procedures and mentoring staff on reactivity measurement methodologies practiced by the nuclear industry
- Development of a detailed model specification for the operational reactor based solely on publicly available data that can be used by the entire nuclear community for methods and software verification and benchmarking
- Generation of new 60 and 252 group cross section libraries that produce results in close agreement to continuous energy (CE) Monte Carlo methods
- Development of a common ASCII input format to VERA that is based on reactor geometric specifications and is practical to use for three dimensional (3D) core analysis
- Development of software object models and metadata that interpret basic engineering parameters for reactor fuel and core geometries into models and meshes for high fidelity, massively parallel 3D neutron transport and thermal-hydraulic codes
- Development of several 3D neutron transport methodologies for eigenvalue and power distribution calculations using hundreds to several thousands of computing cores
- Development of a HDF5 common binary output that permits post processing and data visualization
- Simulation of the operating reactor using an established continuous energy (CE) Monte Carlo particle transport method to obtain a numerical reference solution
- Simulation of the operating reactor using a well validated and NRC-licensed methodology that is representative of the current industry state-of-the-art

- Engineering analysis and documentation of the ability of each software product to predict the measured data from the operational reactor

Each of these aspects is addressed in this document and represents a significant achievement by CASL and its partners, and the combination of these items together provides an excellent demonstration of the accuracy and usability of VERA to simulate operating nuclear power reactors. Section 2 provides an overview of the AMA Core Physics Benchmark Progression Problems, which include the specific operational reactor zero power physics test benchmark problem that is being considered in this report. A description of the data collection and the benchmark problem geometry is provided in Section 3. The computer codes and cross section libraries used in this work are discussed in Section 4. Section 5 provides an overview of a numerical reference solution to the operational reactor benchmark problem and Section 6 discusses the solution obtained with industry codes. The calculated results and comparisons with measured plant data is presented in Section 7. Conclusions and future plans are included in Sections 8 and 9.

2. CORE PHYSICS BENCHMARK PROGRESSION PROBLEMS

The CASL Advanced Modeling Applications (AMA) focus area has developed a series of ten problems which provide a method for developing and demonstrating increasing capabilities for reactor physics methods and software. They provide a model-based approach to prioritization of requirements (Ref. 1), and create clear metrics to communicate development status. Figure 1 provides a listing of the ten problems, with bold items representing cases where measured reactor data are available.



* **Bold** indicates comparisons against measured data

Figure 1: Ten AMA Core Physics Benchmark Progression Problems (Ref. 2)

Currently, the first five problems have detailed specifications and CE Monte Carlo reference solutions, and are documented in the CASL report 'VERA Core Physics Benchmark Progression Problem Specifications', Reference 2. All of the fuel and reactor geometry data in this document are based on the Physical Reactor selected by CASL, the Tennessee Valley Authority (TVA) Watts Bar Unit 1 Nuclear Plant, but was compiled from publicly available sources. Therefore this document may be used across the nuclear industry for testing and validation of nuclear core analysis methods.

The work documented in this report represents analysis of Problem 5, Physical Reactor Zero Power Physics Tests (ZPPT). The VERA capabilities required for this problem include the neutronics components of cross section methodology and neutron transport, as well as problem input/output in a manner useable by industry engineers and analysts. This problem does not require coupled thermal-hydraulics, instrumentation, depletion, or fuel shuffling, though these capabilities will be available in VERA in the future and will be applied to Problems 6-10. Analysis of the Cycle 1 ZPPT, which contains only fresh fuel, allows the first comparisons of CASL neutronics tools with reactor operational data, before these other features are available.

For a more detailed description of the Core Physics Benchmark Progression problems or the models used for their reference solution, please refer to Reference 2, which is publicly available on the CASL website, www.casl.gov.

3. CASL PHYSICAL REACTOR AND DATA COLLECTION

CASL has selected the Tennessee Valley Authority's Watts Bar Nuclear Plant for its initial Physical Reactor for validation and benchmarking. Watts Bar Nuclear Unit 1 (WBN1) began construction in the 1970's and was the last nuclear plant in the United States to come online in the 20th century, beginning commercial operation in May of 1996 (Ref. 3). It is a typical Westinghouse-designed 4-loop Pressurized Water Reactor (PWR) originally licensed for 3411 MW_{th} operation with 193 17x17-type fuel assemblies (Ref. 4).

Figure 2: TVA's Watts Bar Nuclear Plant, Spring City, TN
(Ref. 3)

Watts Bar has many sister plants throughout the nuclear industry, making it an ideal selection for CASL. In addition, Unit 2 is currently under construction and will provide a unique opportunity for CASL to obtain measured data from a modern startup core. Finally, Watts Bar's physical location in east Tennessee provides another advantage for CASL staff at Oak Ridge National Laboratory (ORNL) to interact with TVA Nuclear Fuel Engineering and Reactor Engineering personally and more frequently. The partnership and collocation of TVA and ORNL staff has proven to be a significant advantage of the CASL project.

3.1 Zero Power Physics Testing

During the startup of each fuel cycle, following the core reload, extensive testing is performed prior to escalating power and placing the unit on the electrical grid. ZPPT, also referred to as Low Power Physics Testing, is performed for a variety of purposes, including:

1. To confirm the reactor core is loaded as designed (i.e. detect fuel misloadings)
2. To ensure the reactor core meets technical specification limits for temperature reactivity coefficients
3. To validate the reactivity parameters and uncertainties assumed in safety and accident analyses performed for the fuel cycle

The series of ZPPT tests typically performed for PWRs are:

- Criticality
- Control rod reactivity worths
- Differential soluble boron reactivity worth
- Isothermal temperature reactivity coefficient (or indirectly, the moderator temperature coefficient)

The core analysis team provides predictions for each of the test states in advance of the ZPPT series that is used as criteria for acceptance of further power escalation in operation. The measured data captured during ZPPT tests are some of the most common sources of data for validation and licensing for modern nuclear analysis codes. Therefore VERA's ability to perform these calculations accurately is considered by CASL to be a key demonstration of capabilities for common analysis practices of actual plant conditions.

TVA staff gathered the data obtained from the startup of eleven WBN1 fuel cycles and provided this data to CASL through its Technology Control Process (Ref. 5). Each cycle's report contains the results of each of the physics tests described above. The Cycle 1 report is used extensively for this document, and the subsequent cycle reports will be utilized when VERA has the capability to model multiple fuel cycles. Also provided for Cycle 1 was the detailed testing procedure from the 1996 startup which includes all the precise system conditions of each test. Additional interactions with TVA and Westinghouse staff to answer additional questions and provide additional data were also invaluable.

More details are provided in subsequent sections of this document regarding details of the ZPPT testing and the measured data for WBN1 Cycle 1.

3.2 WBN1 Cycle 1 Core Configuration

WBN1 Cycle 1 was a typical startup core for the Westinghouse four-loop series of ice condenser plants. It utilized 193 Westinghouse 17x17 VANTAGE (V5H) fuel assemblies and was designed to operate at 2250 psia producing 3411 MW of thermal energy in the reactor core. At zero power full flow conditions the reactor system is at the hot operating inlet temperature of 557°F (Ref. 4).

Each V5H assembly consists of 264 fuel rods, 24 control rod guide tubes, and 1 central instrument tube (Figure 3). These rods and tubes are connected via eight spacer grids, which also serve to improve coolant mixing and provide tangential support between adjacent assemblies. Top and bottom nozzles provide a base for contact with the upper and lower core plates and serve as a filter to prevent unwanted debris in the reactor system from entering the core region and potentially causing fuel rod damage (Figure 4). Each fuel rod contains a 144-inch (cold) stack of enriched UO_2 pellets with an upper plenum for fission gas collection and a stainless steel spring to maintain compression of the fuel stack.

For more detailed specification of the WBN1 Cycle 1 model used in this report, please see the "VERA Core Physics Benchmark Progression Problem Specifications", Reference 2.

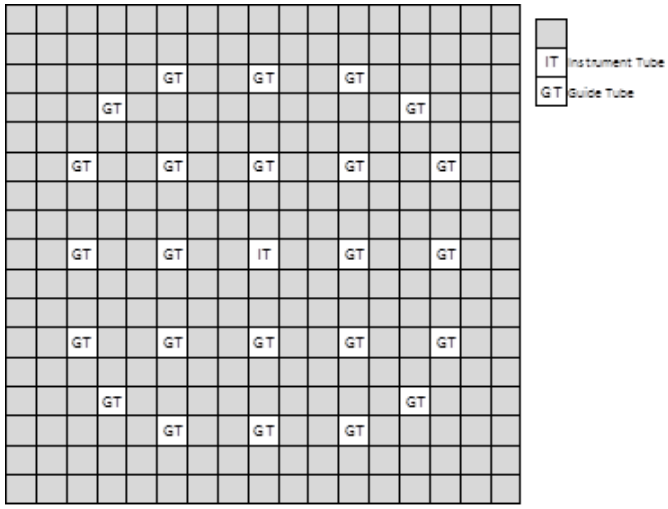


Figure 3: 17x17 VANTAGE (V5H) Lattice Fuel Rod and Thimble Arrangement
(Ref. 4 Figure 4.2-1)

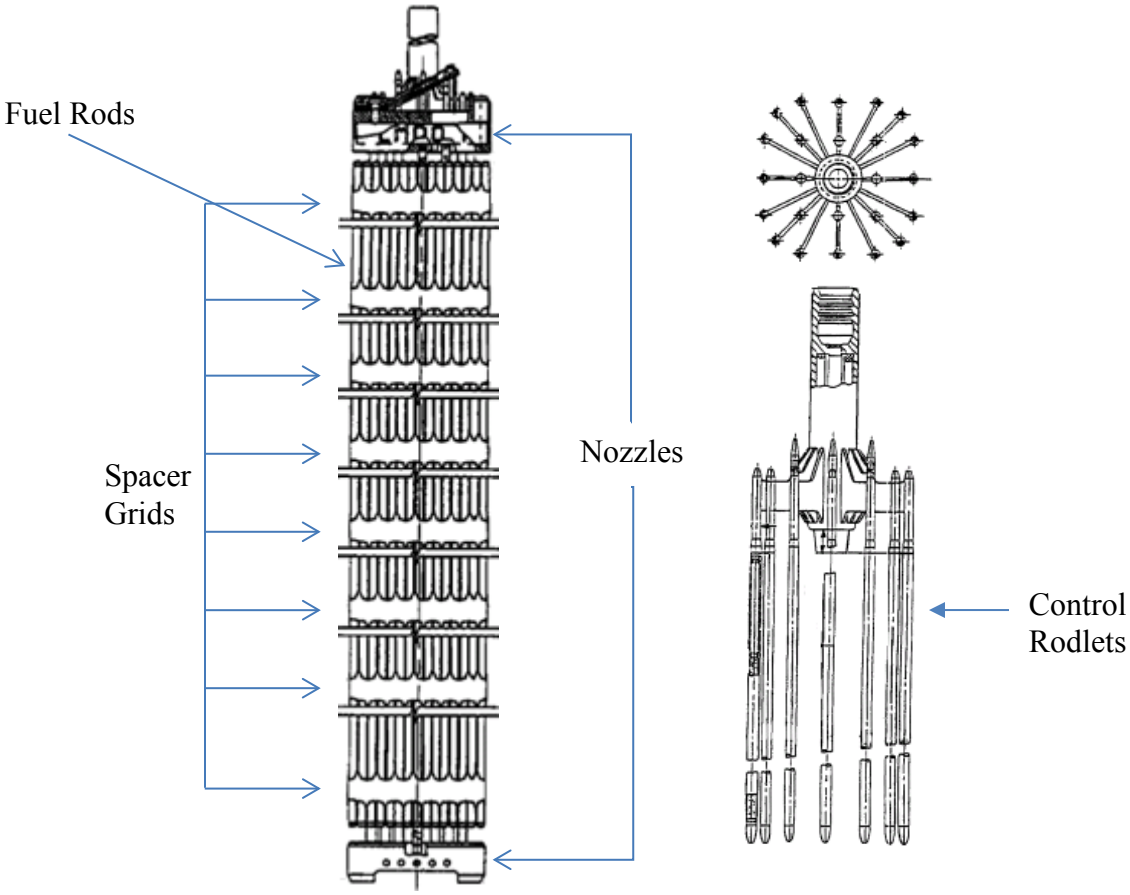


Figure 4: 17x17 Fuel Assembly and RCCA Arrangement
(Ref. 4 Figure 4.2-2 and Figure 4.2-15)

The WBN1 Cycle 1 core design consisted of three batches of fuel assemblies with as-built uranium enrichments of 2.110%, 2.619%, and 3.100% ^{235}U. Excess reactivity was suppressed with approximately 7,000 discrete burnable poison rods composed of annular borosilicate glass (Pyrex) in five unique patterns, as well as with the use of soluble boron as a chemical shim. The core loading pattern is shown with quarter core symmetry in Figure 5.

	H	G	F	E	D	C	B	A
8	2.1	2.6 20	2.1	2.6 20	2.1	2.6 20	2.1	3.1 12
9	2.6 20	2.1	2.6 24	2.1	2.6 20	2.1	3.1 24	3.1
10	2.1	2.6 24	2.1	2.6 20	2.1	2.6 16	2.1	3.1 8
11	2.6 20	2.1	2.6 20	2.1	2.6 20	2.1	3.1 16	3.1
12	2.1	2.6 20	2.1	2.6 20	2.6	2.6 24	3.1	
13	2.6 20	2.1	2.6 16	2.1	2.6 24	3.1 12	3.1	
14	2.1	3.1 24	2.1	3.1 16	3.1	3.1		
15	3.1 12	3.1	3.1 8	3.1				

Enrichment
Number of Pyrex Rods

Figure 5: WBN1 Cycle 1 Assembly and Poison Loading Pattern
(Ref. 4 Figures 4.3-1 & 4.3-5)

Additionally, eight Rod Cluster Control Assembly (RCCA) Banks consisting of 1368 hybrid AIC/B_4C rods were positioned in the core to control reactivity during power maneuvers and to maintain shutdown margin. During each cycle's startup, the reactivity worth of each bank is measured. The control rod banks and locations are shown in Figure 6.

	H	G	F	E	D	C	B	A
8	D		A		D		C	
9						SB		
10	A		C				B	
11				A		SC		
12	D				D		SA	
13		SB		SD				
14	C		B		SA			
15								

Figure 6: WBN1 Cycle 1 RCCA Bank IDs and Positions
(Ref. 4 Figure 4.3-36)

4. VERA SUMMARY AND COMPONENTS

The Virtual Environment for Reactor Applications (VERA) will contain methods for many aspects of nuclear reactor modeling and simulation, including tightly coupled solutions for the key physics areas: neutronics, thermal-hydraulics, and fuel rod mechanics. For CASL to provide meaningful solutions to the CASL Challenge Problems (CRUD, PCI, RIA, etc.), these tools need to improve the resolution and accuracy over what is available from current analysis methods.

VERA will have the capability to perform high-fidelity steady-state fuel cycle depletion as well as time-depending transient analyses, using engineering scale input and output interfaces. A few of the advanced features expected for VERA for use in reactor core analysis are provided in Table 1 and contrasted with typical analytical capabilities commonly used in the nuclear industry. Though many of these features are not yet available in VERA, they are planned or in development.

Several aspects of VERA have been improved recently to support a practical analysis of an operating nuclear power reactor. These components are discussed in this section, including:

1. VERA Common Input – Provides an effective, common interface for typical nuclear engineers and analysts to develop high-fidelity core models for the VERA physics codes.
2. Enhanced SCALE cross section libraries – Improved multi-group (MG) cross section libraries have been developed by the SCALE team at ORNL which are capable of achieving nearly the same accuracy as continuous energy (CE) methods for LWR problems.
3. Development has continued on the University of Michigan neutron transport code MPACT, which now supports 3D core geometries defined through the VERA input.
4. Improvement in XSProc and Denovo at ORNL, including pin cell homogenization techniques and implementation of a SP_N method, have produced accurate results for geometries much larger than was previously allowed with the pin "resolved" S_N method.
5. Initial use of a VERA common output file in the HDF5 binary format allows development of practical post-processing, analysis, and visualization tools by typical industrial users, and has allowed AMA to perform detailed analyses of the performance of VERA codes and methods.

Note that the VERA components used in this analysis, and described below, represent the current development versions that will be included in the VERA 3.1 snapshot to be completed in July 2013.

Table 1: VERA Capabilities for Reactor Physics Analysis
(*italics* represents items under development)

Capability	VERA	Typical Nodal Methods
Neutron Transport	3D (or hybrid) whole-core transport based on actual fuel, core, and support structure geometry	Transport-based 2D infinite lattice physics + 3D nodal diffusion theory with approximate reflectors
Cross Section Energies	Finer energy group structures such as 8, 23, or 64 groups	Lattice physics in many groups with 3D diffusion in few groups (2-3)
Pin-by-pin Powers	Explicit 3D pin powers *(and intra-pin powers)*	3D pin average powers reconstructed from 2D infinite lattice calculations and nodal solution
Thermal Hydraulics	*Direct coupling sub-channel two-phase for each flow channel (pin-by-pin) with cross flow*	Simplified models for neutronics with detailed sub-channel bounding analyses uncoupled
Fuel Mechanics	*Directly coupling for intra-pin fuel temperature feedback and cladding stress calculations*	Simplified average fuel temperature models for neutronics with detailed risk analyses uncoupled
Instrumentation	*Direct incore and excore response models*	Incore response from 2D infinite lattice calculations; no excore models
Short Lived Fission Product Poisons	*Explicit pin-by-pin buildup, decay, and burnout of Xenon and Samarium*	Average Xenon and Samarium concentrations tracked nodally and do not affect pin power distributions
Depletion	*Explicit pin-by-pin (and intra-pin) depletion at actual local spectral conditions, including component depletion such as control rods and instrumentation, and including explicit pin-by-pin shutdown decay calculations*	Depletion performed explicitly at 2D lattice levels for various anticipated spectral and geometric conditions and pin exposures inferred at 3D level from node-average exposure for approximate spectral conditions
Spacer Grids	Direct effects on pin powers, *depletion, and instrument response*	Typically not explicitly resolved or included in pin powers or depletion
Safety Analysis	*Direct calculations for parameters such as DNB, PCI, CFM, etc*	Bounding analyses performed separate from neutronics, sometimes with manual iteration between physics
Neutron Fluence	*Direct accumulation in structural components for lifetime evaluations*	Approximated from few group nodal flux in nearest fuel locations

4.1 Input

The CASL Virtual Reactor Integration (VRI) focus area has successfully created an input interface to VERA that is easy to use, consistent with typical input styles of modern industry methods, and capable of conforming to potential users QA programs. With this common ASCII-based input, it is possible to conveniently create full core models of typical PWR power plants with a simple and minimal input structure. From a user perspective, this input provides a high

level usability that allows complex three-dimensional multi-physics models to be easily generated.

The VERA common input is a free-format, simple ASCII text file with minimal delimiters that is simple for nuclear engineers to create and modify, even on remote systems. The input quantities are intuitive to nuclear engineers familiar with modern core analysis tools, and are based on engineering drawing or specification quantities. The main section of input is specific to the model geometry and is not dependent on the component of VERA being executed. The input is in separate 'blocks' and can include comments following an exclamation mark (!). An example of each block of input is provided in the subsequent sections with data based on the WBN1 model discussed in this report.

The VERA input is parsed as a pre-processing step before execution of the individual physics code. The user data are converted to a common geometry model for use by all VERA codes, and stored in a Teuchos parameter list (Ref. 6) in an XML file format. The abstraction of this data layer will support other types of input in the future, but the ASCII input described here is the simplest type and most familiar to potential users today. The advantages of using the simple common input verses direct XML manipulation are:

- Significant reduction of extraneous characters
- Elimination of repetitive declarations
- Simple interfaces for 1D and 2D arrays
- Use of symmetry for lattices and core maps
- Free format supports arrangement of input for improved QA and error reduction

4.1.1 Materials

VERA supports the use of common PWR materials without explicit isotopic specification. The composition of each is derived from the standard SCALE (Ref. 7) materials database. Each unique material is given a character label and density. Each input block can have a unique set of material definitions. For WBN1 Cycle 1, non-fuel materials are declared for helium (gaps and plena), Zircaloy-4, Inconel, stainless steel, Pyrex (borosilicate glass), and the silver-indium-cadmium and boron carbide control rod absorbers.

```
mat he     0.0001786       ! id, density (g/cc), library key (if different)
mat zirc   6.56 zirc4
mat inc    8.19
mat ss     8.0
mat pyrex  2.25 pyrex-vera
mat aic    10.2
mat b4c    1.76
```

4.1.2 Assemblies

The ASSEMBLY block allows the description of each unique type of fuel assembly. This data structure is similar to the input for modern lattice physics codes. Each assembly type is provided a name, number of fuel rods in each direction, and constant pin pitch.

```
title "Westinghouse 17x17"
npin 17
ppitch 1.260
```

For each unique fuel enrichment, a fuel type is defined using an alphanumeric identifier. The fuel uranium isotopic compositions are calculated automatically by VERA based on the single input of ^{235}U enrichment. In this case, WBN1 Cycle 1 has three unique fuel enrichments, each with the same effective fuel density, which are named 'U21', 'U26', and 'U31'.

```
fuel U21 10.257 94.5 / 2.110          ! ID, density, theoretical density
fuel U26 10.257 94.5 / 2.619          ! and enrichment
fuel U31 10.257 94.5 / 3.100
```

For each unique fuel pellet, a 2D fuel cell is defined using another alphanumeric identifier, based on the identifiers for input materials and fuel. For WBN1 Cycle 1, there are simply six different cell types, accounting for three fuel enrichments, guide and instrument tubes, and fuel rod plenum and end plugs. In this case, the guide and instrument tubes are assumed to be the same geometrically. Each cell is defined using a listing of radii and materials for that cell, with the core coolant (mod) being assumed to be the outer-most region. The non-fuel reflector regions are defined in the same manner as fuel regions.

```
cell 1     0.4096 0.418 0.475 / U21 he zirc       ! fuel, gap, clad
cell 2     0.4096 0.418 0.475 / U26 he zirc
cell 3     0.4096 0.418 0.475 / U31 he zirc
cell 4            0.561 0.602 / mod    zirc       ! guide/instrument tube
cell 5            0.418 0.475 /     he zirc       ! plenum
cell 6                  0.475 /        zirc       ! end plug
```

After definition of the 2D cells, the radial arrangement of these cells is made into 2D lattices. The input may take advantage of symmetry. In this case, octant symmetry is used to simplify the input and reduce user errors. Lattices may also be defined for the plenum and plug (if desired) non-fuel regions.

```
lattice LAT21
     4
     1 1
     1 1 1
     4 1 1 4
     1 1 1 1 1
     1 1 1 1 1 4
     4 1 1 4 1 1 1
     1 1 1 1 1 1 1 1
     1 1 1 1 1 1 1 1 1
```

```
lattice LAT26
     4
     2 2
     2 2 2
     4 2 2 4
     2 2 2 2 2
     2 2 2 2 2 4
     4 2 2 4 2 2 2
     2 2 2 2 2 2 2 2
     2 2 2 2 2 2 2 2 2

lattice LAT31
     4
     3 3
     3 3 3
     4 3 3 4
     3 3 3 3 3
     3 3 3 3 3 4
     4 3 3 4 3 3 3
     3 3 3 3 3 3 3 3
     3 3 3 3 3 3 3 3 3

lattice PLEN
     4
     5 5
     5 5 5
     4 5 5 4
     5 5 5 5 5
     5 5 5 5 5 4
     4 5 5 4 5 5 5
     5 5 5 5 5 5 5 5
     5 5 5 5 5 5 5 5 5

lattice PLUG
     4
     6 6
     6 6 6
     4 6 6 4
     6 6 6 6 6
     6 6 6 6 6 4
     4 6 6 4 6 6 6
     6 6 6 6 6 6 6 6
     6 6 6 6 6 6 6 6 6
```

Following definition of the 2D rod arrays, each of these is “stacked” axially to form the representation of the full 3D assembly. Axial elevations are provided relative to the bottom core plate (the fuel assembly seat). In this case, three assembly types are defined as ‘1’,’2’, and ‘3’, each formed by its corresponding cell enrichment.

```
axial  1  10.281 PLUG 11.951 LAT21 377.711 PLEN 393.711 PLUG 395.381
axial  2  10.281 PLUG 11.951 LAT26 377.711 PLEN 393.711 PLUG 395.381
axial  3  10.281 PLUG 11.951 LAT31 377.711 PLEN 393.711 PLUG 395.381
```

Spacer grids are defined and placed based on simple engineering inputs of material, mass, and height. The axial elevations of each grid are provided from the lower core plate to the center of the spacer grid. In this case, the WBN1 Cycle 1 assemblies have Zircaloy-4 'mid' (or intermediate) grids and slightly larger Inconel 'end' grids at the top and bottom. The spacer grids need not lie in the fuel region, but are required to lie in the axial region defined by the 'axial' input cards. In Insilico, the spacer grid material is homogenized into the coolant at each axial location.

```
grid END inc  1017 3.866     ! grid ID, material, mass (g), and height (cm)
grid MID zirc 875  3.810

grid_axial
    END  13.884
    MID  75.2
    MID 127.4
    MID 179.6
    MID 231.8
    MID 284.0
    MID 336.2
    END 388.2
```

Finally, optional inputs are provided for the assembly nozzles (or end fittings). Specifications of material, mass, and height allow for simple homogenization of the nozzles with the reactor coolant in the volume bounded by the assembly pitch, nozzle height, and adjacent core plate. Any region that is not defined by either the 'axial' cards or the nozzle is filled by borated moderator.

```
lower_nozzle  ss 6.053 6250.0  ! nozzle material, height (cm), mass (g)
upper_nozzle  ss 8.827 6250.0
```

4.1.3 Inserts (Discrete Burnable Poisons)

Data for guide tube inserts, control rods, and instruments are not included with the fuel definition because the VERA methodology does not require a cross section pre-parameterization and therefore there is no need to input each combination of fuel and insert type. For simplicity, each unique type of insert is defined separately and VERA is responsible for combining the insert with the fuel assembly where they are collocated, while assuring compatibility with the guide tube dimensions (else an error message is generated). This also minimizes the number of required inputs and easily supports insert shuffling from one assembly to another.

For each insert type a name and lattice size is provided. This lattice size must be consistent with the fuel assembly in which the insert is located.

```
  title "Pyrex"
  npin 17
```

2D cells of each unique poison/insert rod are defined consistent with the fuel definition. In this example cells are defined for poison, plenum, and rodlet end plug regions. Note that only the rod parameters are included here, and the guide tubes specification for the assembly is not repeated.

```
cell 1  0.214 0.231 0.241 0.427 0.437 0.484 / he ss he pyrex he ss ! Pyrex
cell 2                          0.437 0.484 /                he ss ! plenum
cell 3                                0.484 /                   ss ! plug
```

As with the fuel, the cells are arranged as 2D lattices. Only locations of rodlets are defined, which are verified to align with fuel assembly guide tubes. A dash ('-') is used to identify undefined locations. In WBN1 Cycle 1, five unique Pyrex patterns exist, but only one (sixteen rodlets) is shown below for example.

```
rodmap  PY16
  -
  - -
  - - -
  1 - - -
  - - - - -
  - - - - - 1
  - - - 1 - - -
  - - - - - - - -
  - - - - - - - - -

rodmap  PLEN16
  -
  - -
  - - -
  2 - - -
  - - - - -
  - - - - - 2
  - - - 2 - - -
  - - - - - - - -
  - - - - - - - - -

rodmap  PLUG16
  -
  - -
  - - -
  3 - - -
  - - - - -
  - - - - - 3
  - - - 3 - - -
  - - - - - - - -
  - - - - - - - - -
```

\

Consistent with the fuel assembly construction, the 2D lattices are placed into "stacks" with the input axial boundaries. The elevations are relative to the lower core plate (fuel assembly seat) and are not required to align with the fuel boundaries.

```
axial   8  13.221 PLUG8  15.761 PY8  376.441 PLEN8  398.64
axial  12  13.221 PLUG12 15.761 PY12 376.441 PLEN12 398.64
axial  16  13.221 PLUG16 15.761 PY16 376.441 PLEN16 398.64
axial  20  13.221 PLUG20 15.761 PY20 376.441 PLEN20 398.64
axial  24  13.221 PLUG24 15.761 PY24 376.441 PLEN24 398.64
```

4.1.4 Controls (RCCAs)

Control rod clusters (RCCAs) are defined in exactly the same manner as inserts – completely independent of the fuel in which they are inserted. Unlike inserts, RCCAs can be positioned axially in the model based on input parameters on the STROKE card.

```
title "B4C with AIC tips"
npin 17
stroke  365.125 230       ! total travel length (cm), max number of steps
```

2D cells of each unique control rodlet are defined consistent with the fuel definition. In this example cells are defined for poison, plenum, and end plug regions. Note that only the rod parameters are included here, and the guide tubes specification for the assembly is not repeated. VERA will ensure that each defined control rod will fit in the designated control rod guide tube.

```
cell 1  0.382 0.386 0.484 / aic he ss
cell 2  0.373 0.386 0.484 / b4c he ss
cell 3        0.386 0.484 /     he ss     !plenum
cell 4              0.484 /        ss     !plug
```

As with the fuel, the cells are arranged as 2D lattices. Only locations of rodlets are defined, which are verified to align with fuel assembly guide tubes. A dash ('-') is used to identify undefined locations.

```
rodmap AIC
  -
  - -
  - - -
  1 - - 1
  - - - - -
  - - - - - 1
  1 - - 1 - - -
  - - - - - - - -
  - - - - - - - - -
```

```
rodmap B4C
  -
  - -
  - - -
  2 - - 2
  - - - - -
  - - - - - 2
  2 - - 2 - - -
  - - - - - - - -
  - - - - - - - - -

rodmap PLEN
  -
  - -
  - - -
  3 - - 3
  - - - - -
  - - - - - 3
  3 - - 3 - - -
  - - - - - - - -
  - - - - - - - - -

rodmap PLUG
  -
  - -
  - - -
  4 - - 4
  - - - - -
  - - - - - 4
  4 - - 4 - - -
  - - - - - - - -
  - - - - - - - - -
```

Consistent with the fuel assembly construction, the 2D lattices are placed into “stacks” with the input axial boundaries. The elevations are of the RCCA when fully inserted, relative to the lower core plate (fuel assembly seat). In this example, WBN1 Cycle 1 has hybrid RCCAs consisting of predominately B_4C regions with AIC tips.

```
axial  1       15.131
         PLUG  17.031
          AIC 118.631
          B4C 377.711
         PLEN 388.411
```

4.1.5 Instrumentation

VERA permits the definition and placement of the incore instrumentation thimbles, which are stainless steel tubes that displace moderator and provide a guide for the movement of neutron detectors. These are inserted into a portion of the fuel assemblies from below the vessel during core loading. The user input is consistent with the insert block, as shown below. The thimble is defined as a “stack” of 2D lattices, in this case extending from the bottom to the top core plates. For 17x17 fuel, the instrument location is in the center cell, and all other unused locations are identified with a dash (“-“). Note that incorporation of the effects of the instrument thimble on

the core neutronics is an advanced feature which is typically not included in current nodal methods.

Excore instrumentation is currently not supported in VERA.

```
title "Incore instrument thimble"
npin 17

cell 1  0.258 0.382 / he ss

rodmap  LAT
   1
   - -
   - - -
   - - - -
   - - - - -
   - - - - - -
   - - - - - - -
   - - - - - - - -
   - - - - - - - - -

axial 1  0.0 LAT 406.337
```

4.1.6 Core Geometry

The CORE block is the primary input structure for assembling the core components such as fuel, burnable poisons, and control rods, and allows definition of core level properties that are common to all components. These data are most similar to the input for modern 3D nodal diffusion codes, and should be intuitive to engineers with experience in core design and analysis. The core size, assembly pitch, rated power and flow, and core height (usually defined here as distance between the core plates) are specified simply as:

```
size 15                ! number of fuel assemblies across core
rated 3411 131.68      ! thermal power (MW), core flow (Mlbs/hr)
apitch 21.5            ! assembly pitch (cm)
height 406.337         ! distance between core plates (cm)
```

For each new reactor core model, the fuel assembly locations in the square grid are required. By provided the code with the core "shape", subsequent core maps can be input with flexible symmetry options and minimal characters.

```
core_shape
  0 0 0 0 1 1 1 1 1 1 1 0 0 0 0
  0 0 1 1 1 1 1 1 1 1 1 1 1 0 0
  0 1 1 1 1 1 1 1 1 1 1 1 1 1 0
  0 1 1 1 1 1 1 1 1 1 1 1 1 1 0
  1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
  1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
  1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
  1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
  1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
  1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
  1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
  0 1 1 1 1 1 1 1 1 1 1 1 1 1 0
  0 1 1 1 1 1 1 1 1 1 1 1 1 1 0
  0 0 1 1 1 1 1 1 1 1 1 1 1 0 0
  0 0 0 0 1 1 1 1 1 1 1 0 0 0 0
```

The fresh fuel assembly type layout (or loading pattern) is supplied below using octant symmetry. This map refers to fuel assemblies only.

```
assm_map
  1
  2 1
  1 2 1
  2 1 2 1
  1 2 1 2 2
  2 1 2 1 2 3
  1 3 1 3 3 3
  3 3 3 3
```

Unlike many modern methods, the VERA input allows the user to define and load fuel assembly inserts such as discrete burnable absorbers separately from the fuel assemblies themselves. This reduces the amount of input burden on the user and more easily supports component depletion, shuffling, and tracking. This capability is enabled because VERA does not use the typical two-step methods approach of many nodal diffusion methods, so the 3D geometry can be assembled and shuffled in-line with the cross section processing and neutron transport calculations. The map below demonstrates the independent placement of the five Pyrex burnable absorber patterns in the WBN1 Cycle 1 core, with locations without inserts defined with a dash ("-"). It is noted that though numeric IDs are used in this case, all of the VERA input identifiers are alphanumeric and may be defined by the user to be almost any string found to be useful.

```
insert_map
   -
  20  -
   - 24  -
  20  - 20  -
   - 20  - 20  -
  20  - 16  - 24 12
   - 24  - 16  -  -
  12  -  8  -
```

Like the previous insert map, the control rod type layout is specified in the exact same manner. For WBN1, all of the RCCAs are the same type (hybrid B_4C/AIC). VERA will also ensure that each insert or RCCA rodlet defined will physically fit into the fuel assembly guide tubes and that inserts and control rodlets do not occupy the same fuel assembly location.

```
crd_map
  1
  - -
  1 - 1
  - - - 1
  1 - - - 1
  - 1 - 1 - -
  1 - 1 - 1 -
  - - - -
```

The user input for the RCCA banks is similar to the previous data, except that the bank definition controls the grouping of RCCA movement during simulation of operation. PWRs typically move control rod assemblies in groups, or banks, rather than individually, and startup testing confirms the reactivity of these groups prior to power escalation. In this case, WBN1 has eight total RCCA banks, four used for normal operation control, A-D, and four for ensuring safe shutdown margin, SA-SD. Bank D is the nominal regulating bank and also has the highest reactivity worth. Note that all the banks are octant symmetric except for Shutdown banks SC and SD, so therefore the input must be in quarter, also called quadrant, symmetry. Locations not containing RCCAs are indicated with a dash ("-").

```
crd_bank
  D  -  A  -  D  -  C  -
  -  -  -  -  - SB  -  -
  A  -  C  -  -  -  B  -
  -  -  -  A  - SC  -  -
  D  -  -  -  D  - SA
  - SB  - SD  -  -  -
  C  -  B  - SA  -
  -  -  -  -
```

The core locations of incore detector thimble tubes are specified with the input below. Though VERA does not currently support incore detector response models, it does account for the presence of the thimble (stainless steel and displaced moderator) in the instrument tube of the specified assemblies. For WBN1, these locations are not symmetric, and therefore must be entered in full geometry. Non-instrumented locations are indicated with a dash ("-").

```
det_map
          - - 1 - - 1 -
      1 - - 1 - 1 - - - - -
    - - - - - - 1 - 1 - 1 - 1
    1 1 - - - - 1 - - - - - -
  - - - - 1 - - - 1 - 1 - 1 - -
  1 - 1 - - 1 - 1 - - - - - 1 -
  - - - 1 - - 1 - - 1 - - 1 - -
  1 - 1 - 1 - 1 - - 1 - 1 1 1 -
  - 1 - - - - - - 1 - 1 - - - 1
  - - - - 1 - 1 - - - - 1 - - -
  1 - - - 1 - - 1 - - 1 - - - 1
    - - - - 1 - - 1 - - 1 - -
    - 1 - 1 - - 1 - - - - - 1
      1 - - - 1 - - 1 - 1 -
          1 - - 1 - - -
```

Core structure components such as baffle and core plate characteristics are also provided. VERA will perform volume weighted homogenization with the core coolant for each item. Models for the core barrel, neutron pads, and vessel have not been implemented.

```
baffle ss 2.85 0.19       ! material, thickness (cm), and gap (cm)
lower_plate ss  5.0 0.5   ! material, thickness (cm), volume fraction
upper_plate ss  7.6 0.5

xlabel  R P N M L K J H G  F  E  D  C  B  A      ! core location labels
ylabel  1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
```

Additional depths of generic axial reflector regions can be defined beyond the core plate regions. In this case some additional thickness of moderator is added above and below the model.

```
lower_ref  mod 25.0 1.0   ! material, thickness (cm), and volume fraction
upper_ref  mod 25.0 1.0
```

4.1.7 State Data

The input STATE block provides VERA with the statepoint conditions of the reactor for each instantaneous time step. These parameters include relative core power, relative core flow, soluble boron concentration, and for cases without thermal-hydraulic feedback, the user can also input the average fuel temperature and moderator density. For the WBN1 Cycle 1 model the inputs below describe the approximate initial criticality conditions.

```
power  0.0            ! %
flow                  ! %
tinlet 557.33         ! F - 565K
tfuel  565.0          ! K - 565K
boron  1293           ! ppmB
modden 0.743          ! g/cc
```

The control rod bank positions for each statepoint are provided in terms of steps withdrawn for each defined bank in the core geometry.

```
rodbank  SA 230
         SB 230
         SC 230
         SD 230
          A 230
          B 230
          C 230
          D 167        ! Bank D at 167 steps withdrawn
```

Finally, the zero power cases are calculated without thermal-hydraulic feedback and using quarter symmetry to reduce the computational requirements.

```
feedback off
sym qtr
```

4.1.8 Code Specific Input

In addition to the geometry specifications provided above, user input for specific physics codes is also provided in separate blocks. This allows all the relevant codes to access geometrically consistent models and significantly reduces the burden on the user to develop multiple models. However, many of the code specific inputs currently require advanced knowledge of the code methods. In the future it is expected that these inputs will be optional with default presets for standard LWR analyses. The section below provides an example of the current input provided to Insilico for the WBN1 model.

```
cell_homogenize true
Pn_correction true
eq_set        spn_fv
SPN_order     5
Pn_order      3
tolerance     1e-6
dimension     3
mesh          2
max_delta_z   2.54

mat_library casl_comp_r2.sh5
xs_library  lib252_hetbondoneabs-noabssigp

num_blocks_i  26
num_blocks_j  26
num_z_blocks  1
num_groups    23
num_sets      1

azimuthals_octant  4
polars_octant      4
quad_type          qr

silo_output  p5
```

```
new_grp_bounds
  8.2085e+05  1.1109e+05  5.5308e+03  1.8644e+02
  3.7612e+01  3.5379e+01  2.7697e+01  2.1684e+01
  2.0397e+01  1.5968e+01  7.1500e+00  6.7000e+00
  6.3000e+00  1.0970e+00  1.0450e+00  9.5000e-01
  3.5000e-01  2.0600e-01  1.0700e-01  5.8000e-02
  2.5000e-02  1.0000e-02  1.0000e-05
```

4.2 SCALE Multi-Group Cross Section Libraries

The SCALE (Ref. 7) cross section team at ORNL has made significant advances in the development of ENDF/B-VII multi-group (MG) self-shielded cross section libraries for LWR applications. Several new libraries have recently been developed and provided to CASL for use with Insilico and MPACT. These are:

- A 252 group library for Insilico calculations
- A 60 group subgroup library for MPACT calculations
- A prototype 64 group library for both Insilico and MPACT calculations

Each library was generated from ENDF/B-VII.0 data using the AMPX code system (Ref. 8). Insilico calculations utilize the Bondarenko self-shielding method. MPACT calculations can utilize either the subgroup method or the embedded self-shielding method (Ref. 9). The AMPX code system has been enhanced to generate more accurate nuclear data for all self-shielding methods employed by CASL. These enhancements include the following:

- A point-wise (PW) spectrum corresponding to typical PWRs was used in averaging the MG data.
- Temperature-dependent PW flux weight functions were used to process thermal scattering kernels
- The thermal upscattering cut-off was increased from 3 eV to 5 eV
- A new method was developed for truncation of upscattering to provide smoother transition from thermal to epithermal energy regions
- The Bondarenko self-shielding factors are tabulated with increased number of temperatures and increased number of background cross sections
- Intermediate resonance (IR) parameters (i.e. “lambdas”) have been included on the AMPX libraries.

- Enhancements have been made to the CENTRM computational module utilized in the AMPX and SCALE code systems to generate PW flux spectra. The enhancements include the new capability to compute PW flux spectra for 2D pin cell configurations, which provides more accurate weight functions for MG cross section generation than volume-equivalent 1D pin cell configurations.
- The Bondarenko self-shielding factors for nuclides with atomic masses Z > 39 were calculated with CENTRM PW flux spectra rather than the analytical methods based on the Narrow Resonance (NR) approximation. Two types of CENTRM models were used. Heterogeneous models of water-moderated lattices spanning the range of expected self-shielding were used to calculate shielding factors for ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu. Homogeneous models were used to compute shielding factors for the remaining nuclides with Z>39.

Reference 10 contains detailed information regarding the new SCALE MG libraries. These libraries were also used in Core Physics Progression Problems 1-4 (ranging from single pin cell and 2D lattices to 3D assembly and multi-assembly configurations) and have demonstrated excellent agreement in comparison to continuous energy Monte Carlo results for Problems 1 and 2. Analysis of subsequent problems is still ongoing.

Figure 7 provides an example showing the PW CE total cross section for ^{238}U and its representation with the 252 group structure for the 4 – 250 eV energy range.

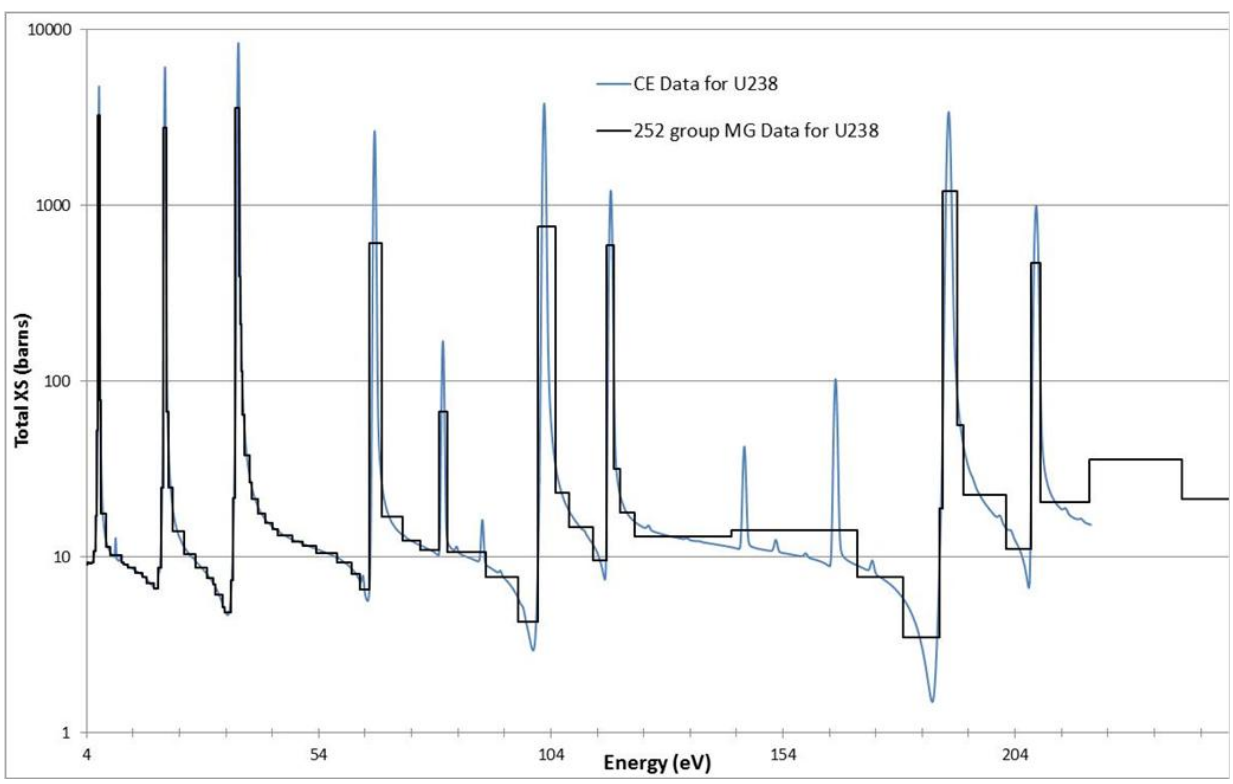


Figure 7: 252 Energy Group Structure Comparison for ^{238}U Total Cross Section

4.3 MPACT

The MPACT (Michigan PArallel Charactistics based Transport) code has been developed by the University of Michigan (UM) to perform pin resolved Light Water Reactor (LWR) neutronics analyses using whole-core transport calculations. This section will provide a brief overview of MPACT.

Several transport capabilities are available within MPACT including 2D and 3D Method of Characteristics (MOC), as well as the 2D/1D method. The code supports parallelism with both MPI and OpenMP for decomposing the problem by space, angle, and characteristic rays. The code is capable of running on $O(10^5)$ processors and can be used on multiple platforms such as Windows and Linux. References 11 and 13 provide the detailed description of MPACT and its capabilities as of version 1.2. This section will briefly highlight the important features for the full core solution to include the 2D/1D kernel, CMFD acceleration, and the available cross section libraries.

The cross section library used in MPACT is the ENDF/B-VII.0 ORNL 60 group cross-section library as described previously and in Reference 12. This library has been developed by ORNL using the SCALE AMPX (Ref. 8) code system in order to provide CASL a releasable cross section capability. This library can be used with both sub-group and Embedded Self-Shielding (ESSM) cross-section methodologies (Ref. 9). Currently MPACT use sub-group methodology for spatially dependent self-shielding.

In the 2D/1D solution, the 3D domain is decomposed into 2D planes and the MOC transport equation is solved for each 2D plane. The benchmarking of the 2D MOC solver was previously reported and is summarized in Reference 13. The planes are coupled together through a transverse leakage source and the axial variation in the flux is currently modeled using a nodal diffusion approximation. The 3D solution is accelerated using a Coarse Mesh Finite Difference (CMFD) solver. The 2D MOC transport sweeper in MPACT has been utilized by AMA for analysis of Core Physics Progression Problem 1 and 2 (Reference 14) and provides the foundation of the 2D/1D solution. The source term in the MOC sweeper has been altered to account for axial leakage between planes and the current assumption in the baseline 2D/1D method is that the axial source is isotropic. Ongoing research is investigating computationally efficient methods to include the angular shape of the axial leakage in the 2D/1D solution (References 15 and 16).

The neutron flux distribution in the axial direction of the 2D/1D solution is calculated using a low order approximation to the transport equation. Several nodal diffusion kernels have been implemented in MPACT but typically the Nodal Expansion Method (NEM) kernel is used. The NEM kernel assumes the intra-nodal flux is a fifth order Legendre polynomial in space and then enforces current and flux continuity between nodes. The remaining coefficients are solved using a set of three weighted residual equations. A two-node formulation is used to solve the nodal equations, which enhances the stability of the nodal solver over previously implemented one-node formulations. In the two-node formulation, a NEM system is constructed for every axial interface and the current and surface flux are solved at the interface of the two nodes. The boundary condition for the two node problem is the average flux in both of the adjacent nodes. Fixing the average flux of each node serves to stabilize the local iteration and helps to

prevent the two node solutions from becoming out of phase with the global solution. Since the dominant parallel decomposition in the 2D/1D problem is by axial planes, the axial solution is highly decomposed. In the axial iteration scheme, the shape of the source, cross sections, and the average flux are passed via MPI communication to the processor which solves the two node problem and then the flux shape and interface current are passed back. In MPACT, each process will solve the interface on the top of its subdomain. In the case of the bottom boundary of the core, the processor who owns the bottom node will also solve for that interface

A principle feature of the 2D/1D solution is the CMFD acceleration scheme which not only accelerates the convergence of the entire solution but also provides stability to the radial and axial sweeps. Since the radial and axial equations are solved alternately, data propagation in the axial direction can become very slow as the planes become thin. CMFD mitigates this effect by coupling all planes together and solving a global diffusion-like system of equations. The elliptic nature of the diffusion system tightly couples the interior of the core to the boundary. It should also be noted that if nonlinear correction factors are not used in the axial direction, then the CMFD accelerator can be used to provide a computationally inexpensive finite difference 3D solution. However, the unique feature of MPACT is the 2D MOC which provides intra-pin geometric resolution as depicted in Figure 8.

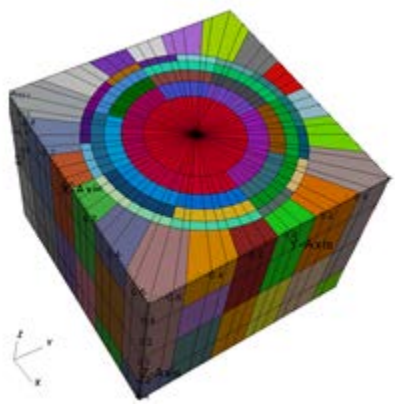


Figure 8: MPACT Intra-pin Geometric Resolution

The global iteration scheme used for the baseline 2D/1D scheme is for the CMFD system to accelerate the calculation of the eigenvalue and eigenvector of the system. Once CMFD has sufficiently converged, the fission source is fixed and the axial solution is performed. The axial solver obtains estimations for the axial leakage which is then used in the 2D MOC planar solutions. Once the leakage source is fixed, the 2D MOC solver is called to determine the new flux distribution. When the planar MOC solutions are complete, the homogenized cross sections and nonlinear correction factors for CMFD are updated and the iteration continues. The iteration is complete when the eigenvalue and flux are sufficiently converged.

The current status of the MPACT development and capabilities is provided in Appendix A. At the present time, MPACT results are not provided for the WBN1 ZPPT tests.

4.4 Insilico

Insilico uses the SCALE (Ref. 7) code XSProc to generate multi-group cross sections and the ORNL 3D neutron transport code Denovo (Ref. 17) to perform eigenvalue and flux calculations. The combination of these codes provides VERA a high fidelity true 3D transport capability for nuclear reactor geometries. Insilico has been used by AMA to generate solutions to Core Physics Problems 1-5, with accuracy depending on the solvers and mesh refinements used.

The steps performed by Insilico are:

1. Process a reactor engineering specification converted into XML format
2. Convert input specification into arguments for XSProc
3. Generate a geometric representation of the reactor needed by XSProc
4. Build and partition a Denovo discrete mesh representation of the reactor geometry
5. Broadcast XSProc geometry to each processor domain
6. Run XSProc to generate macroscopic cross sections
7. Map the cross sections to Denovo computational mesh cells
8. Run Denovo S_N or SP_N to calculate scalar fluxes
9. Integrate scalar fluxes with fission reaction rate data to calculate the normalized pin power distributions
10. Perform parallel output

Further description of the Insilico components is given below.

4.4.1 XSProc

The XSProc module used by Insilico is based on techniques in the SCALE code system (Ref. 7) for the generation of problem-dependent multi-group (MG) cross section data and has been incorporated into VERA for use in neutronics calculations. XSProc performs resonance self-shielding with full range Bondarenko factors using either the narrow resonance approximation or the intermediate resonance approximation. For uniform fuel lattices, Dancoff factors are automatically generated from the user-input geometry and material descriptions. XSProc also allows user-input Dancoff factors to treat non-uniform lattice effects. The fine energy group structure of the resonance self-shielding calculation can optionally be collapsed to a coarse group structure through a one-dimensional (1D) discrete ordinates transport calculation internal to XSProc.

The SCALE 6.2 252 group ENDF/B-VII.0 neutron cross section data library described previously is utilized for the WBN1 calculations. This library contains data for 417 nuclides and 19 thermal-scattering moderators. Thermal scattering data for most nuclides are available at five temperatures, where other nuclides provide data for as many as ten temperatures. Bondarenko factors are tabulated at five different temperatures and thirty background cross sections.

The XSProc module provides the following capabilities:

- Material processing
- Temperature interpolation
- Problem-dependent resonance self-shielding
- Macroscopic mixing of multi-group (MG) cross section data
- Energy collapse of cross section data based on the local pin spectra
- Pin cell macroscopic cross section homogenization based on the local pin spectra
- Serialize/deserialize unit cells and cross section data
- Infinite lattice Dancoff factor calculation, with option to use user defined values

XSProc uses Bondarenko calculations for resonance self-shielding using the BONAMI module of the SCALE system (Ref. 7). A wide variety of options are provided for different lattices and cell geometries through the use of Dancoff approximations. Linear interpolation is performed to determine self-shielded two-dimensional thermal scattering cross sections at the requested temperature.

The SCALE Material Information Processor capabilities are included in XSProc to convert user input material data into atom number densities needed for cross section processing; convert user-input of fuel lattices, region-wise, and infinite medium into a form suitable for cross section processing; calculate Dancoff factors for uniform lattices; allow user input Dancoff factors for non-uniform lattices; and generate an appropriate spatial mesh for 1D transport calculations.

The SCALE XSDRNPM transport solver (Ref. 7) provides flux-weighting of cross section data and generates energy group collapsed and cell-homogenized data for subsequent multi-dimensional transport calculations. XSDRNPM is a discrete-ordinates code that solves the 1D Boltzmann equation in slab, cylindrical, or spherical coordinates.

4.4.2 Denovo

Denovo is a two and three-dimensional deterministic radiation transport code package under development at ORNL. Denovo provides two deterministic transport solvers that are currently integrated into VERA:

- Discrete ordinate (S_N)
- Simplified P_N (SP_N)

Each method solves stable, consistent discretizations of the eigenvalue form of the linear, Boltzmann transport equation. Details about each method can be found in References 17 and 18.

The S_N method is a collocation method in angle that solves the first-order form of the Boltzmann transport equation. The spatial differencing schemes used by the S_N solver include linear-discontinuous and tri-linear-discontinuous finite element on 3D grids, bilinear-discontinuous finite element on 2D grids, and step-characteristics/slice balance on 2D and 3D grids. Weighted diamond-difference and theta-weighted diamond-difference are also available. All spatial discretizations are implemented on orthogonal Cartesian grids. Denovo provides three inline quadrature options: level-symmetric, Gauss-Legendre product, and quadruple range. Additionally, the user can input unique angular quadratures if desired. Denovo uses the Trilinos library to implement state-of-the-art numerical solvers, including Krylov linear solvers for within-group and multigroup linear problems as well as Arnoldi and generalized Davidson eigenvalue solvers for the k-eigenvalue problem. Standard fixed-point iteration methods such as DSA-accelerated source iteration for within-group iterations in a Gauss-Seidel multigroup outer iteration and power iteration for eigenvalue problems are also available.

The S_N method employed in Denovo is parallelized over space-angle using the Koch-Baker-Alcouffe (KBA) wavefront parallel algorithm. Parallelization over energy is provided by "sets" of energy groups in which the space-angle partitioned grid is replicated within each set. This multi-level parallel decomposition over space-angle and energy has demonstrated reasonable scaling using 200,000 processors on the Jaguar XT5 at the Oak Ridge Leadership Computing Facility (OLCF).

As opposed to the S_N method, which is a consistent discretization of the continuous Boltzmann transport equation in space, angle, and energy, the SP_N method is a numerically-consistent, low-order space-angle approximation that, in general, will not converge to the true transport solution as angle (represented by Legendre moments) and space are refined. The advantage of SP_N is that the matrix representing the transport operator can be explicitly formed, whereas this is not possible for 3D S_N. The ability to form the matrix opens many possibilities for parallel decomposition, preconditioning, and solvers. Thus, the SP_N equations are generally much easier to solve than S_N equations, and each iteration requires much less work. Comparing the two methods, the number of unknowns that is solved in an S_N calculation is

$$N_c \times N_u \times N_a \times (N+1)^2 \times N_g$$

where N_c is the number of computational cells, N_u is the number of spatial unknowns per computational cell (4 for linear-discontinuous finite element, 1 for step-characteristics), N_a is the number of angles, N is the number of angular flux moments, and N_g is the number of groups. The SP_N solver uses a second-order accurate finite volume spatial discretization. The number of unknowns for SP_N is

$$N_c \times \left(\frac{N+1}{2}\right) \times N_g$$

Here, N is the SP_N expansion order (currently supported options are 1, 3, 5, or 7). As mentioned above, SP_N will not converge to the true transport solution as the SP_N expansion is increased, but has been widely used and shown to be a significant improvement over diffusion theory for reactor problems.

Both deterministic methods in Denovo are unconditionally convergent; however, accuracy is governed by the discrete resolution in space, angle, and energy. For high-order methods such as S_N, the resolution required for accuracy may be prohibitive for many problems. For example, a 3D 17 × 17 assembly may require the solution of $O(10^{10})$ unknowns for a pin-resolved transport solution. Because the SP_N method solves a low-order approximation to the transport equation, the computing requirements are much smaller. However, SP_N requires cross-section homogenization to obtain accurate solutions.

Both an Arnoldi and a generalized Davidson eigensolver from Trilinos have been studied for use with the SP_N discretization. An important feature of the generalized Davidson solver is that, unlike the Arnoldi method, it is able to directly solve a generalized eigenvalue problem, eliminating the need for an inner iteration requiring the solution of a linear system of equations involving the multigroup transport problem. Instead, each Davidson iteration requires only the application of a preconditioner that approximates the process of solving a linear system. A multigrid in energy preconditioner was developed to fill this role for the Denovo SP_N discretization. Numerous numerical studies have been performed comparing the performance of the Arnoldi and Davidson solvers, with the Davidson solver yielding a lower time to solution in every problem considered so far, typically reducing the run time by a factor of four to six relative to the Arnoldi solver. Because of this, the Davidson solver has been selected as the default solver for the SP_N equations and was used for all of the SP_N results presented in this report.

SP_N was implemented for future work to provide a low-order transport option for coupling 2D Method of Characteristics (MOC) with 3D transport. However, it has been shown to be efficient and accurate when using pin-homogenized cross sections for the ZPPT analysis of WBN1.

Insilico has been utilized to accurately solve multi-assembly 2D and 3D problems on thousands of compute cores using the very accurate S_N solver and "resolving" fuel rods with a 12x12 Cartesian radial mesh. The results of these calculations agree very well with CE Monte Carlo methods, except for cases with large absorbers (such as control rods) or thin absorbers (such as IFBA).

For the WBN1 cases in this document, the SP_N solver was used to perform full 3D quarter-core calculations using pin-homogenized macroscopic cross sections. The calculations presented in this report used a 2x2 radial mesh per pin and a maximum axial mesh cell height of 1 inch. (mesh cells are automatically refined to resolve geometric features such as spacer grids and assembly components), resulting in a mesh with 18 million computational cells. All calculations were performed using 23 energy groups, collapsed from the previously described SCALE 252 group library by XSProc. An SP_5 angular approximation was employed, which has three degrees of freedom per space-energy location. Thus, the total number of degrees of freedom for the WBN1 cases is slightly over 1.2 billion and the number of nonzero entries in the matrix representing the SP_N operator exceeded 57 billion. The WBN1 calculations were executed on the Oak Ridge Leadership Computing Facility's (OLCF) supercomputer TITAN using 676 computational cores and approximately 5.3 TB of memory. The solution of the initial critical configuration required 33 minutes of total processing time. Of this time, approximately 26% was spent in the generation of cross sections by XSProc, 21% was spent in setup operations such as matrix and

preconditioner construction, and 50% was spent in the SP_N eigenvalue calculation. A plot of the thermal neutron flux distribution in the core as computed by the Denovo SP_N solver is shown in Figure 9.

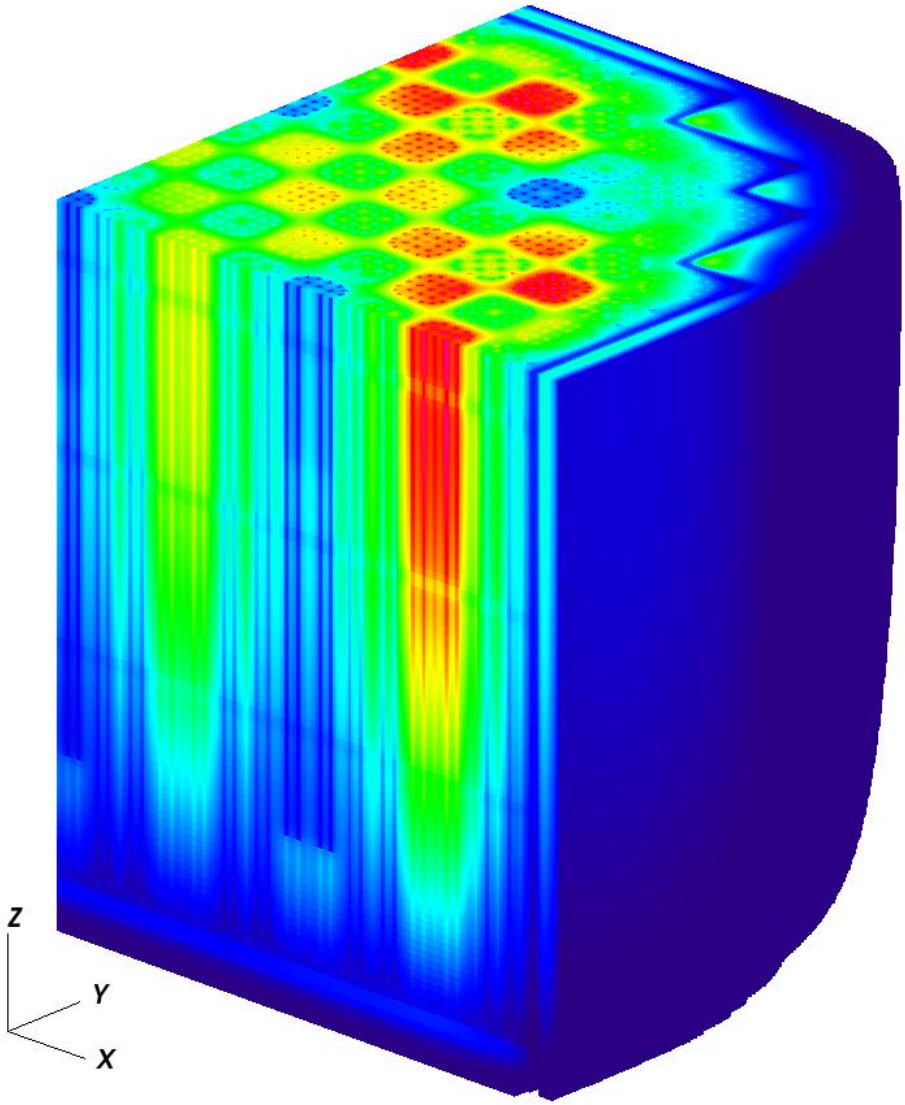


Figure 9: Insilico Watts Bar 1 3D Thermal Flux Distribution
(Bank D inserted – Core Octant)

4.5 Output

The preliminary VERA common output is a binary HDF5 (hierarchical data format) file type (Ref. 19) commonly used for scientific data storage and I/O. Considerable effort has been spent to define a standard output format for all codes and to develop post-processing codes to generate standard core analysis edits, such as axial power distribution or radial peaking factors. The HDF5 file is accessible by novice developers and engineers through many software languages such as FORTRAN, C/C++, Java, Matlab, etc. AMA has itself developed several FORTRAN and C++ utilities to compare multiple files and perform typical statistical analyses associated with core design and methods validation and benchmarking. In addition, a utility has also been

developed to convert the HDF5 file data into a SILO file format suitable for various visualizations with VisIt (Ref. 20).

While the HDF5 output is still preliminary, many codes and converters are being developed to use the same common format, including Insilico, COBRA-TF, MPACT, KENO-VI, ANC9, and MCNP5. Having all the codes produce data in the same format makes data analysis and sensitivity studies much easier. In this section several figures are provided to demonstrate the current analysis capabilities that are available with the VERA output format.

One of the advantages of the HDF5 format is availability of software tools to view and modify the data. One such tool is HDFView (Ref. 21), shown below.

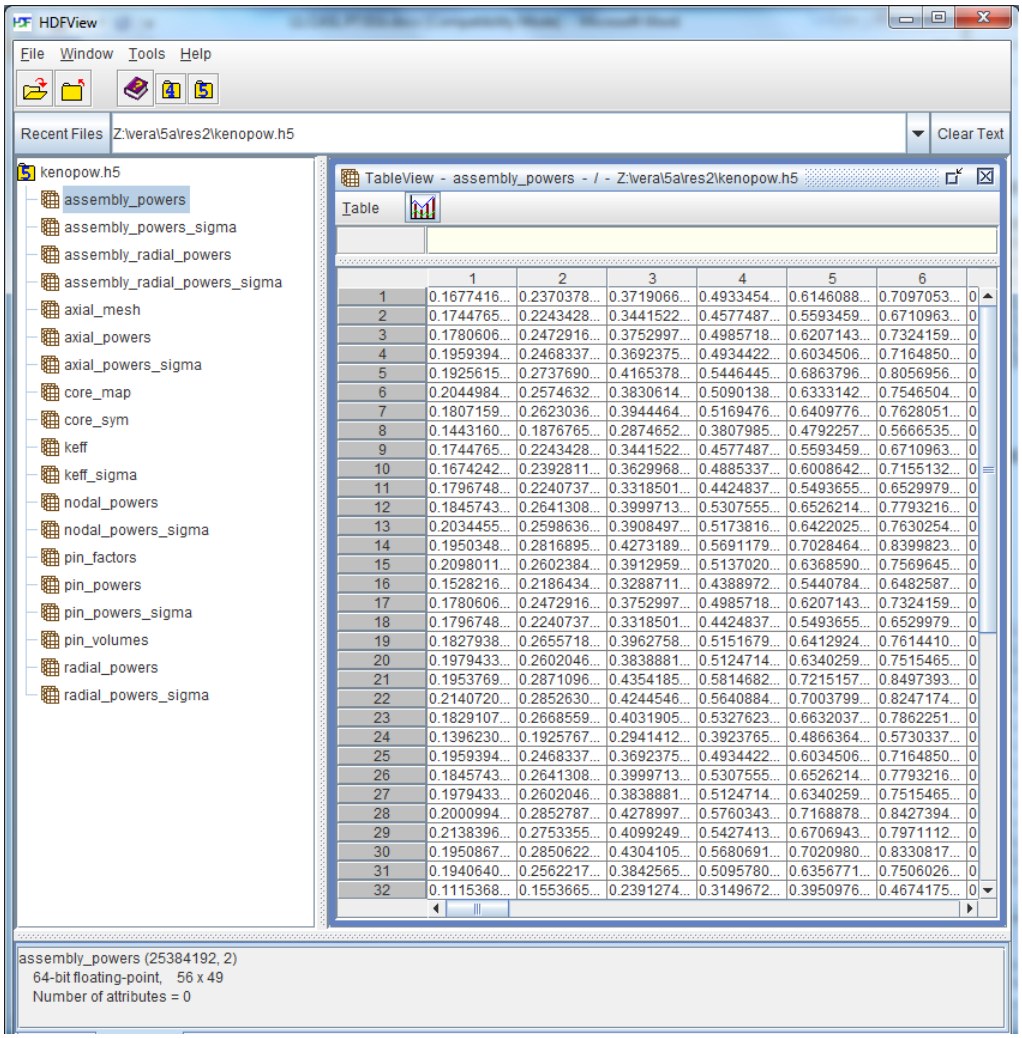
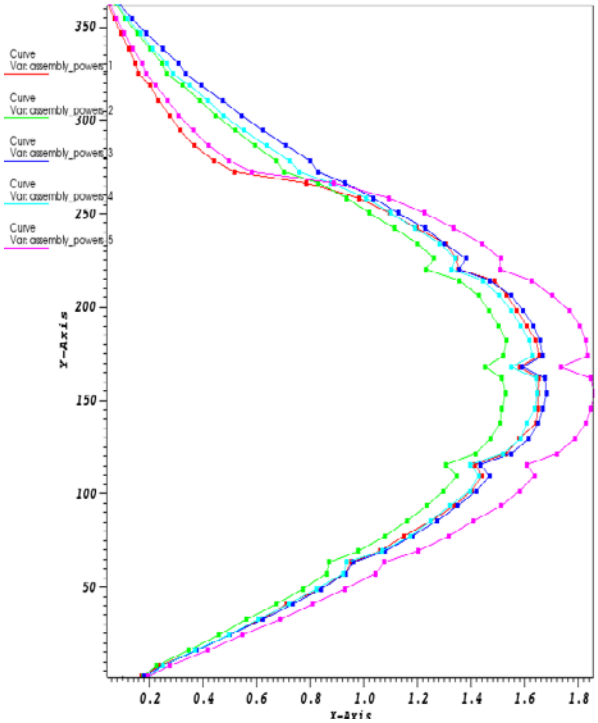
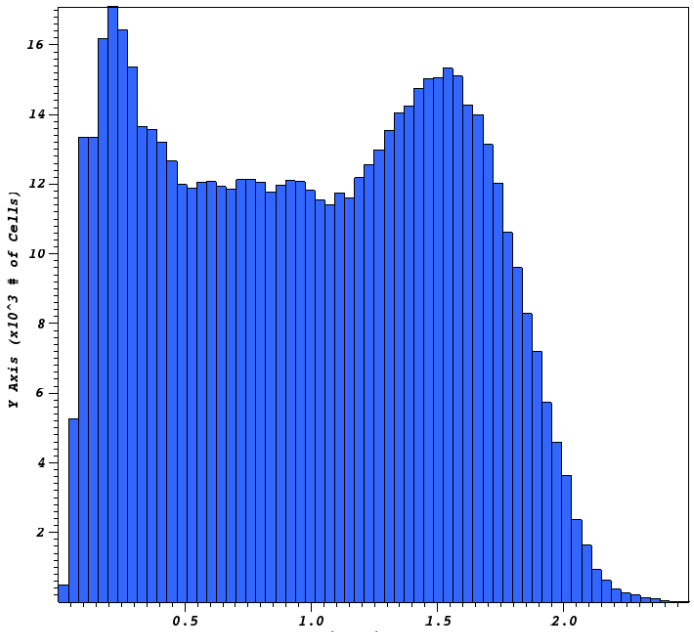


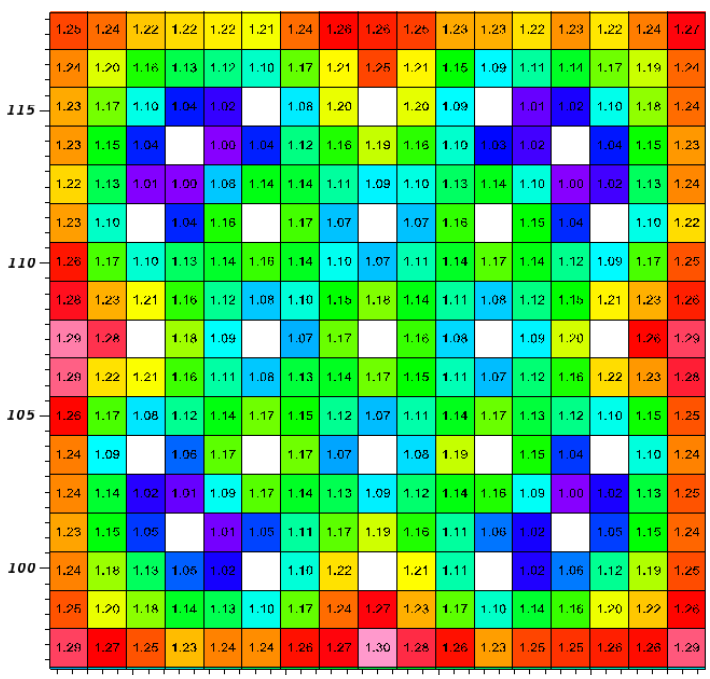
Figure 10: Screenshot of HDFView with HDF5 File from KENO-VI Post-Processor



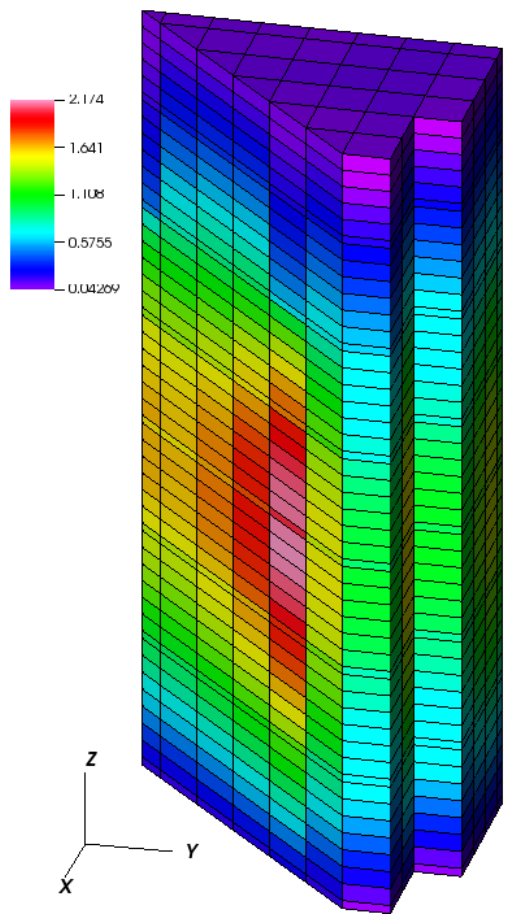
Axial Assembly Power Shapes



Histograms of Distributions



2D Lattice Views with Value Labels



3D Assembly Average Powers
(Octant Symmetry)

Figure 11: VisIt Visualizations of HDF5 Output Data for WBN1

5. NUMERICAL REFERENCE SOLUTION

A portion of the VERA testing and V&V activities performed by the AMA focus area has included the model development of the WBN1 fuel and core geometries with an independent continuous energy (CE) Monte Carlo neutron transport reference solution. The model has been extensively used to create the publicly available reference solutions for the first five of the Core Physics Progression Problems (Ref. 2) previously discussed, as well as some additional benchmark problems that have assisted cross section and neutron transport code developers to identify and correct software accuracy issues. This model is considered the reference numerical prediction for the Watts Bar 1 Cycle 1 ZPPT tests because of the detail of the model and rigor in the CE Monte Carlo method.

Monte Carlo tools in the SCALE 6 (Ref. 7) system, which has been developed and maintained by ORNL since 1969, are commonly used in criticality safety calculations as well as sensitivity and uncertainty (S/U) analyses, depletion, and criticality alarm system analyses. The SCALE code system includes the KENO V.a and KENO-VI (Ref. 22) Monte Carlo criticality codes; both offer continuous energy (CE) and multi-group (MG) energy treatments to calculate physical parameters of fissile systems. The major difference between these two codes is their geometry processors; KENO V.a uses very simple geometric components but KENO-VI uses the SCALE Generalized Geometry Package (SGGP) which allows more complex geometric modeling.

KENO-VI is usually used within SCALE's CSAS6 control sequence, which was originally developed to provide automated multi-group cross section processing for MG KENO-VI transport. Later, CSAS6 was redesigned to support CE KENO-VI calculations for transport as an input and material preprocessor. More recently, KENO-VI has been extensively applied to lattice physics problems and compared successfully to the well-known Monte Carlo code MCNP5 (Ref. 23). In summary, KENO-VI was selected by AMA for the neutronics reference solution because:

- The Monte Carlo approach to particle transport has no geometric approximations like deterministic solution techniques that use spatial discretization approaches.
- The use of Continuous Energy (CE) transport and cross sections are more rigorous than self-shielding cross section methods and multi-group (MG) treatments.
- The new KENO-VI parallel version (SCALE 6.2) permits simulations with an extremely large number of particles histories, which are required to limit the reaction rate uncertainties for large problems.
- KENO-VI allows solutions for large geometrically complex problems whose computer storage requirements and geometric complexity preclude solution by previous versions of KENO
- Association with SCALE and ORNL, including familiarity of analysts and proximity of developers for support.

The SCALE Generalized Geometry Package permits construction of the models used in this document and in Reference 2 by combining geometric shapes such as cylinders and cuboids, or

any volume that can be constructed with quadratic equations. For larger models, this input can become complicated, but software has been developed by AMA which permits the input of basic fuel and core design parameters for WBN1, and produces the large input files required for the model. In this report, the KENO models were all constructed using core quadrant symmetry to decrease the computer resources required to solve these problems by geometrically reducing the calculated reaction rate statistical uncertainties. However, the KENO-VI boundary conditions do not support rotational (or cyclic) symmetry, so reflective symmetry is assumed. The effects of this are minimal for this first cycle core except for when safety banks SC or SD are inserted.

In addition to reactivity, KENO-VI can also provide reaction rate tallies by region, allowing the user, with some post-processing challenges, to extract the normalized fission reaction rate distribution for reactor physics problems. For this activity, AMA has developed a post-processing procedure for extracting the calculated fission rates and uncertainties for each unique fuel region and calculating the volume-weighted normalized power distribution for comparison to other codes, including pin, assembly, radial, and axial powers, for example. In some cases, credit is taken for octant symmetry, effectively doubling the sampling for symmetric rods and reducing the Monte Carlo estimated uncertainty for their fission rate.

To reduce the uncertainty in the fission rates of individual fuel rods, especially lower powered ones, an extremely large number of particles is required. For the WBN1 core, the problem size is prohibitively large to obtain normalized pin powers with uncertainties less than a few percent. Reference 2 contains reference power distributions for Problems 1 through 4 and for other problems such as a 2D quarter core. However, only core eigenvalues (k-effective) and derived quantities are calculated for the quarter core problems. It is also noted that the KENO-VI power distributions are based on fission rate only and do not consider any redistribution due to gamma sources and neutron kinetic energy.

The KENO-VI version used for this analysis is a development version to be released in SCALE 6.2. The development version was utilized to take advantage of several new features and bug fixes, the most important to this effort being parallelization of the particle transport. This KENO-VI version will be released to SCALE users through RSICC later in 2013. Development testing has shown good agreement between the latest version of KENO-VI and MCNP5 for PWR 2D lattices.

ENDF/B-VII.0 CE cross section libraries have been used to provide reference solutions for the Core Physics Progression Problems. The ENDF/B-VII cross sections are the latest cross sections sets, which were generated by the AMPX code system (Ref. 8), and are targeted for use in CASL. All the results used for WBN1 comparisons in this document utilize this library. A CE cross section library at a temperature of 565 K was generated to specifically match that at which the ZPPT measurements were performed to avoid the need for temperature corrections. Revisions to SCALE CE data libraries have improved both S(α,β) data, resulting in significant bias reduction for thermal systems, and the probability tables that provide CE treatment in the unresolved resonance range, resulting in reduced biases for systems that are sensitive to the intermediate energy range. All these updates improve the data accuracy and enhance the solution's fidelity.

For the WBN1 models, the KENO-VI pre-processor developed by AMA generates 3.5 million line ASCII input files containing 300,000 unique geometry units. Most core features are modeled with explicit features using cold dimensions, while regions above and below the fuel are treated as homogenized regions. A detailed listing of the features of the KENO-VI model for WBN1 are described below.

- Explicit representation of fuel rod stack, plenum, and end plugs. The end plug geometry is a simplified cylinder, and is similar for each of the fuel, poison, and control rods. The plenum spring itself is not modeled.
- Semi-explicit representation of all spacer grids, by dividing the grid mass equally amongst the 289 lattice cells in each assembly, and placing that mass in an equivalent volume box on the outside of each cell. The spacer grid spacer sleeves are ignored, which are less than 10% of the total grid mass. Figure 12 depicts the KENO-VI spacer grid model.
- Guide tubes and instrument tubes are assumed to extend from the bottom nozzle to the top nozzle, and the lower dashpot region of the guide tubes is ignored.
- Homogenization of the top and bottom nozzles of each assembly.
- Explicit modeling of Pyrex and RCCA stacks, axial locations, end plugs, and plenum regions below the top nozzle. RCCA geometry in and above the top nozzle is ignored. Fully withdrawn RCCAs are also included in the model up to the upper nozzle.
- Explicit inclusion of thimble plugs in upper regions of guide tubes, which do not contain RCCA rodlets or Pyrex rodlets.
- Non-symmetric inclusion of incore instrumentation thimbles. Though this invalidates the quarter symmetry, the effect is expected to be small and inclusion somewhat accounts for the correct effect on the core average reactivity due to displaced moderation. See Reference 2 for the exact core wide instrument thimble locations.
- Exclusion of primary and secondary source rods.
- Explicit treatment of the core baffle, assuming solid stainless steel.
- Homogenization of upper and lower core plates assuming 50% coolant volume fraction.
- Inclusion of core support structure and containers such as the neutron pads, core barrel, vessel liner, and the carbon steel vessel itself.
- 50 cm axial buffer of moderator between the core plates and axial vacuum (non-reentrant) boundary to assure proper calculation of the core axial leakage.
- The AMA KENO-VI preprocessor permits input and positioning of each of the eight RCCA banks, used for the bank reactivity worth calculations performed for the results in this report.

Each eigenvalue calculation performed by KENO-VI for the WBN1 models utilized 1,200 generations and 200,000 particles per generation, skipping the first 100 generations. This resulted in a one-standard deviation statistical uncertainty in eigenvalue of less than 6 pcm (percent-mille, or 10^{-5}). Each calculation was performed on the Reactor and Nuclear Systems

Division (RNSD) cluster Cpile2 at ORNL, and took about 3,000 core-hours. As previously discussed, this was not sufficient to obtain adequate reaction rate uncertainties to support a power distribution calculation, however this is not required for the ZPPT analyses.

Figures 12-15 are provided to demonstrate the high fidelity of the CE KENO-VI models used for Watts Bar. Figure 12 provides a detailed view of the semi-explicit "equal cell" spacer grid model, which divides the spacer grid mass uniformly among the lattice cells and locates the mass at the outer boundary of the square cell, avoiding homogenization with the moderator. Each of eight spacer grids per assembly is treated in this manner.

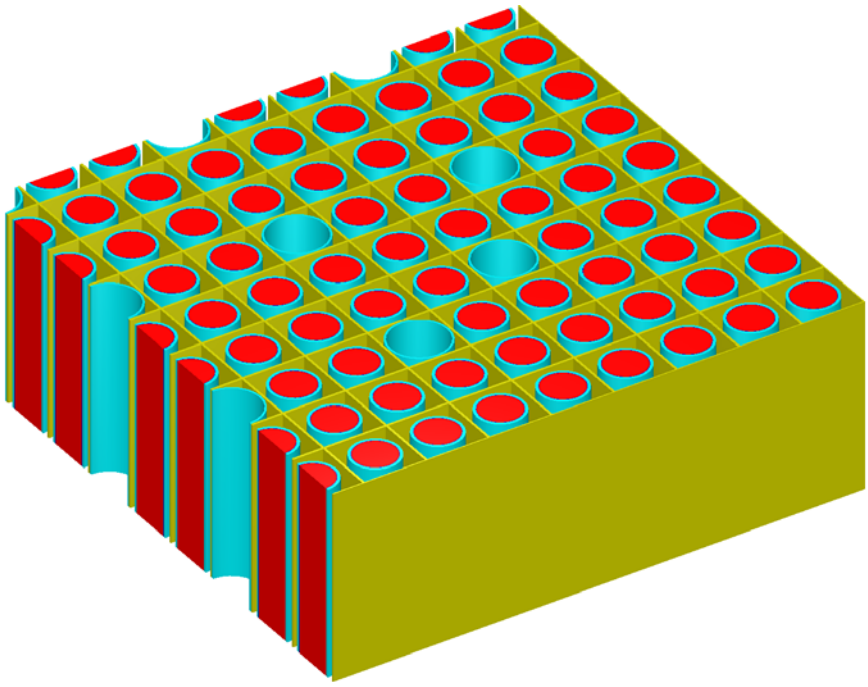


Figure 12: KENO-VI Semi-Explicit Spacer Grid Model
(Quarter Symmetry – "Equal Cell" approach)

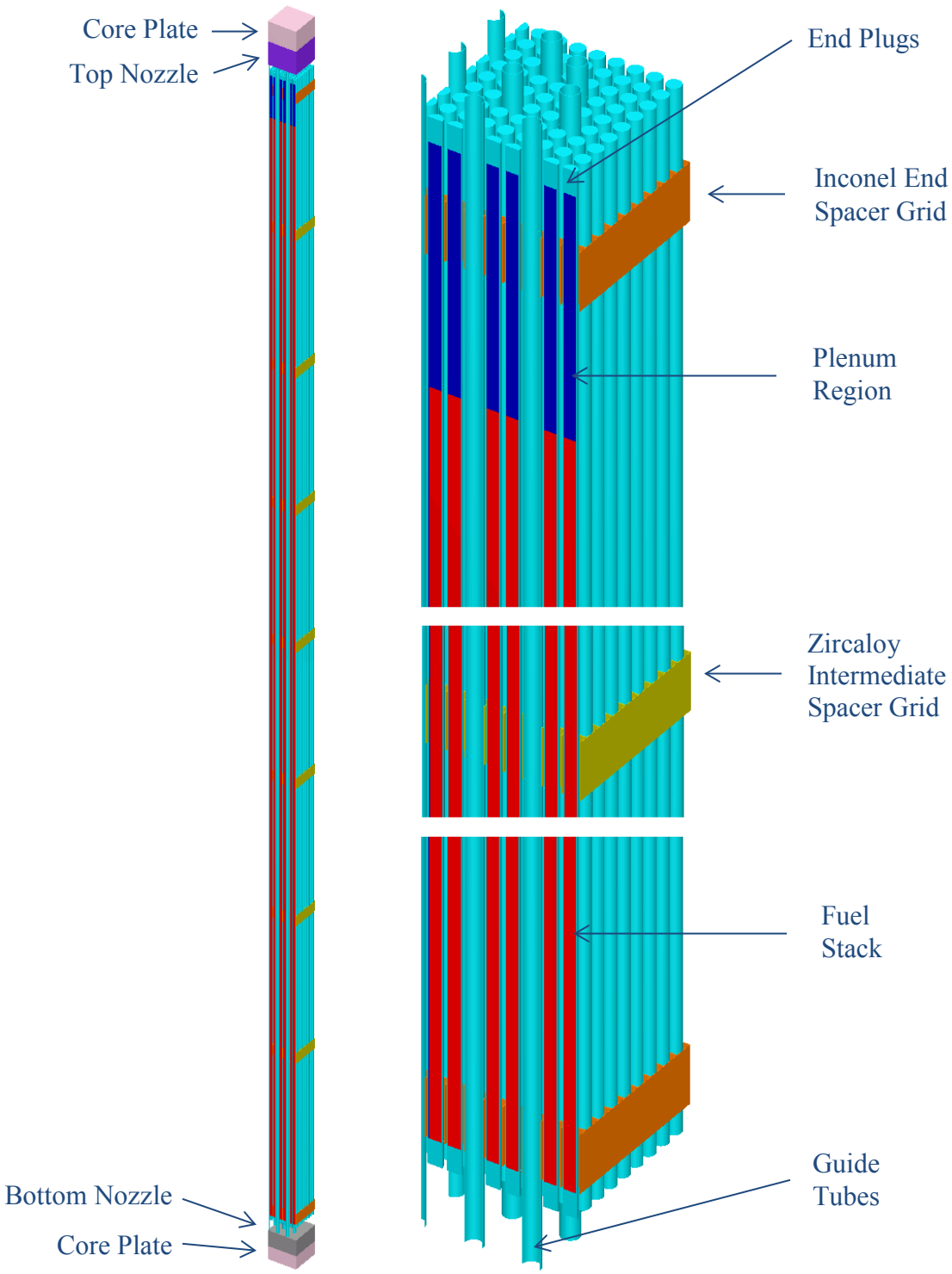


Figure 13: KENO-VI 3D Fuel Assembly Model
(Quarter Symmetry)

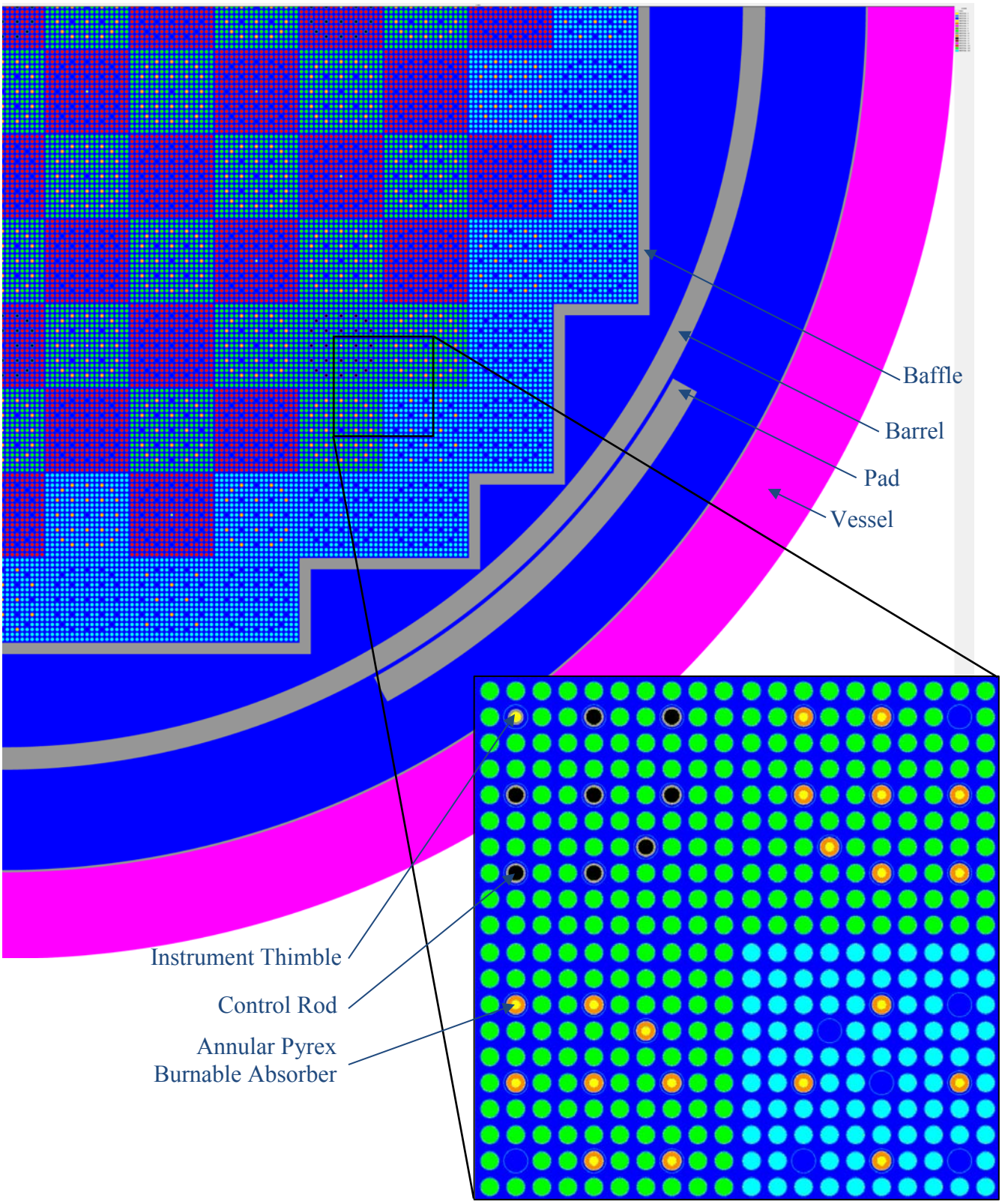


Figure 14: KENO-VI Watts Bar 1 Model – Radial View

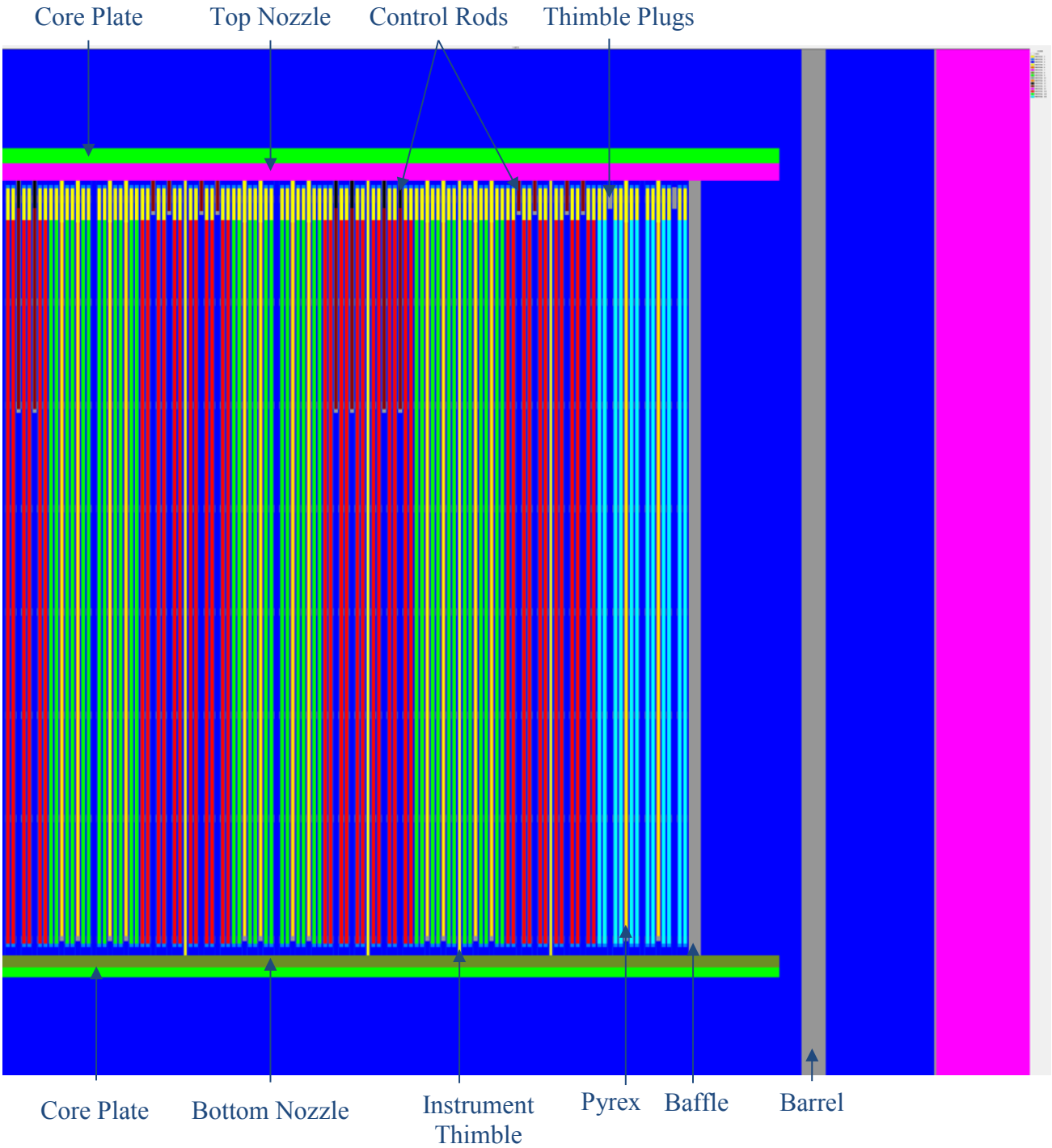
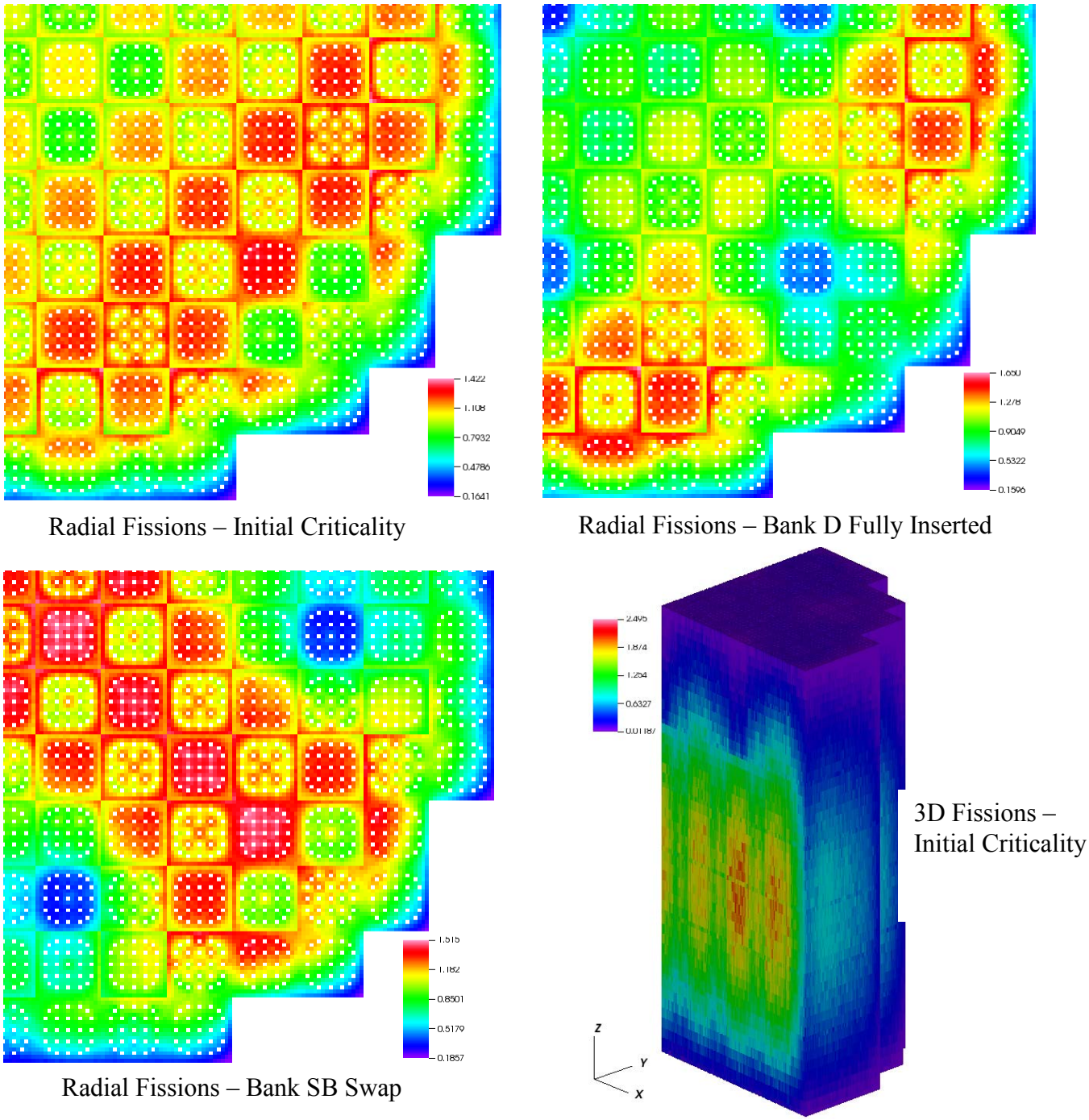


Figure 15: KENO-VI Watts Bar 1 Model – Axial View

The post-processing application developed by AMA permits reactor analysis of the KENO results by production of 3D normalized reaction rates and corresponding uncertainties for common reactor analysis tool edits, such as radial powers, axial powers, assembly averaged powers, etc. This tool also produces data files in the same binary HDF5 format as VERA, permitting direct post-processing comparisons of the large pin power distributions, as well as visualization of these distributions with VisIt (Ref. 20). Figure 16 demonstrates the visualization capability developed by AMA for KENO-VI output.



Radial Fissions – Initial Criticality

Radial Fissions – Bank D Fully Inserted

Radial Fissions – Bank SB Swap

3D Fissions – Initial Criticality

Figure 16: KENO-VI Watts Bar 1 Results – Normalized Fission Rate Distributions

6. INDUSTRIAL REACTOR PHYSICS SOLUTION

The nuclear industry routinely performs reactor analysis to support the operating fleet, as well as product development, using well proven and qualified core physics packages. Besides an adequate level of accuracy, these tools need to be simple, flexible, reliable, and computationally efficient to satisfy the needs of the nuclear industry and allow daily usage from core designers for reload analyses. These requirements have resulted in the development of a two-step methodology to perform industrial core physics analysis, with pre-generation of some lattice parameters as the first step to be then used in a 3D nodal core simulator as the second step of the analysis. The Westinghouse core physics package incorporates this common nodal methodology. Many developments have been performed over the course of the years to improve and expand its prediction capabilities without forgoing any of the other key requisites: simplicity, flexibility, reliability, and computational efficiency.

This section reviews the reactor physics methods currently in use at Westinghouse and provides an overview of its state-of-the-art core simulator NEXUS/ANC9 (Refs. 24-27). This information is provided in some detail so that the reader can have a better understanding of current industry practice including the emphasis on usability. This is followed by a description of the lattice data generation and core model employed in NEXUS for the simulation of Watts Bar Unit 1, Cycle 1, and in particular of its startup physics tests.

6.1 Introduction

The standard methodology adopted by the industry for performing core physics analysis is based on a two-step process. First, a two-dimensional lattice physics calculation is performed for a fuel segment using reflective boundary conditions. The resultant neutron spectrum is used to collapse and homogenize the fine-group cross sections to few-group macroscopic cross sections over the fuel lattice domain. Such a lattice physics calculation is performed for all unique fuel types in the core. In order to cover all possible core conditions, for each fuel segment type, the lattice calculation is repeated at different thermal-hydraulic and control feedback parameters (fuel temperature, moderator temperature, moderator density, etc.) and different burnup conditions. These calculations generate the homogenized cross section data as well as the pin form factors for each individual lattice type. These data are processed through tabulation or fitting to a parameterized library which is used to characterize the core in the next calculation step.

The second step is the core calculation. A nodal method is traditionally used to solve the two-group diffusion theory equations and generate 3D node-wise flux and power distributions in the core. From the node-wise distribution and using the pin form factors, the pin-by-pin power distribution is also calculated for each fuel node through pin power reconstruction techniques. The node-wise cross sections are constructed utilizing the above pre-generated cross section library adjusted to account for the local core conditions.

The traditional method works well under the assumption that the pin-by-pin parameters from lattice calculations adequately represent the pin data of the fuel assembly at actual core operation conditions. This does not always happen as the interaction between fuel assemblies is not always

negligible, e.g. UO_2/MOX cores or peripheral assemblies with strong asymmetric radial gradients, or in case of significant heterogeneity changes in the radial or axial direction of a fuel assembly, e.g. from prolonged depletion with inserted control rods and/or in proximity of the tip of a partially inserted control rod. However, for conventional PWRs operated with UO_2 fuel at all rods out (ARO) conditions the assumptions at the basis of the traditional methods are valid, and the reactivity and power distribution obtained are typically accurate.

The traditional methods are challenged when applied to heterogeneous fuel and core conditions, and for Westinghouse plants this occurs in the **AP1000**®[a] due to the advanced MSHIM™ operational strategy (Refs. 29 and 30). These issues can be fundamentally resolved through direct pin-by-pin transport calculations in conjunction with 3D pin-by-pin isotopic tracking. These schemes have been widely considered as the next generation methods (NGM), and are currently under development in CASL and through other efforts. However these direct methods are still in the research and development phase, and the computer power required still precludes implementation in standard core design applications. Westinghouse has developed a new methodology to overcome the above difficulties which has been implemented in the NEXUS system, the Westinghouse state-of-the-art core physics package. The trademark feature of this new methodology is a 3D Pseudo Pin-by-Pin Calculation ("P3C") which enables accurate prediction of the pin-by-pin power distribution properly accounting for the control rod history and environmental effects.

A review of the NEXUS code system together with its components, functionalities, and latest developments to address some of the issues of traditional nodal methods is given in the following.

6.2 NEXUS

NEXUS is an automated once-through cross section system designed to provide nuclear data to core simulators. NEXUS has been implemented, qualified, and licensed for PWR core analysis in the United States (Refs.26-28). The PWR NEXUS system consists of several computer codes: NEXrun, NEXpre/ALPHA, PARAGON, NEXlink and ANC9. These are briefly described below and interface according to the flowchart in Figure 17.

- NEXrun is the overall system controller. This program executes each of the following codes and controls the data transfer between these codes. For typical production calculations, the user only needs to provide the NEXpre input and execute NEXrun to obtain cross sections for the core simulator. At the conclusion of NEXrun execution, the cross section data file will be generated and ready for use with the core simulator.
- NEXpre/ALPHA work together to provide the user input interface with the code system and generate all the input necessary for the lattice code. NEXpre is linked to a controlled database which supplies most of the data needed to develop the lattice code input

[a] AP1000 and MSHIM are trademarks or registered trademarks of Westinghouse Electric Company LLC in the United States and may be registered in other countries throughout the world. All rights reserved. Unauthorized use is strictly prohibited.

including cycle specific fuel and plant data from the Westinghouse database of cores and reload information, material and fuel temperature information based on their thermo-mechanical properties and expected irradiation behavior. In typical production calculations the NEXpre input file is very simple and limited to data specific to a given fuel type, though flexibility is provided to suit the needs of development applications.

- PARAGON (Ref. 31) is the Westinghouse lattice transport code used to generate the lattice nuclear data. PARAGON was licensed in the U.S. in 2004 (Ref. 32) and is also used in PWR nuclear design as part of the Westinghouse APA nuclear code system. More details on PARAGON are given in a standalone section.
- NEXlink is the implementation of the NEXUS cross section representation methodology, processing the nuclear data from the lattice codes and generating the fitted data and other nuclear data needed by the simulator. NEXlink has been written in a general manner. The user does not have to input any details about the calculation matrix that NEXlink will fit. NEXlink determines the details of the calculations that it is being asked to fit at runtime. NEXlink generates backfitting statistics to keep the user informed as to the quality of the fitting. NEXlink writes the final fitting data as well as pin data and other nuclear data needed by the simulator to a cross section data file in HDF5 format.
- ANC (Ref. 41) is the Westinghouse advanced nodal core simulator used for all nuclear core design calculations. More details on ANC are given in a subsequent section.

These codes are run in the order listed above, with NEXrun controlling the entire cross section generation calculation. The system has been designed to be completely automated. NEXUS reads most of the inputs needed to generate simulator nuclear data from a configured database in XML format which includes data for all current plant and assembly designs. Required user input has been minimized to only those data unique to a particular assembly design, i.e. enrichment pattern and burnable absorber loading and placement. Flexibility has been built into the system allowing the user to override any parameter from the database and also to run new designs that are not yet part of the database.

NEXUS includes features needed for the simulation of next generation PWRs. It generates data for the new pin power methodology developed in ANC to capture the effects on pin powers of prolonged control rod insertion. NEXUS also provides the core simulator with the data necessary to deplete control rods.

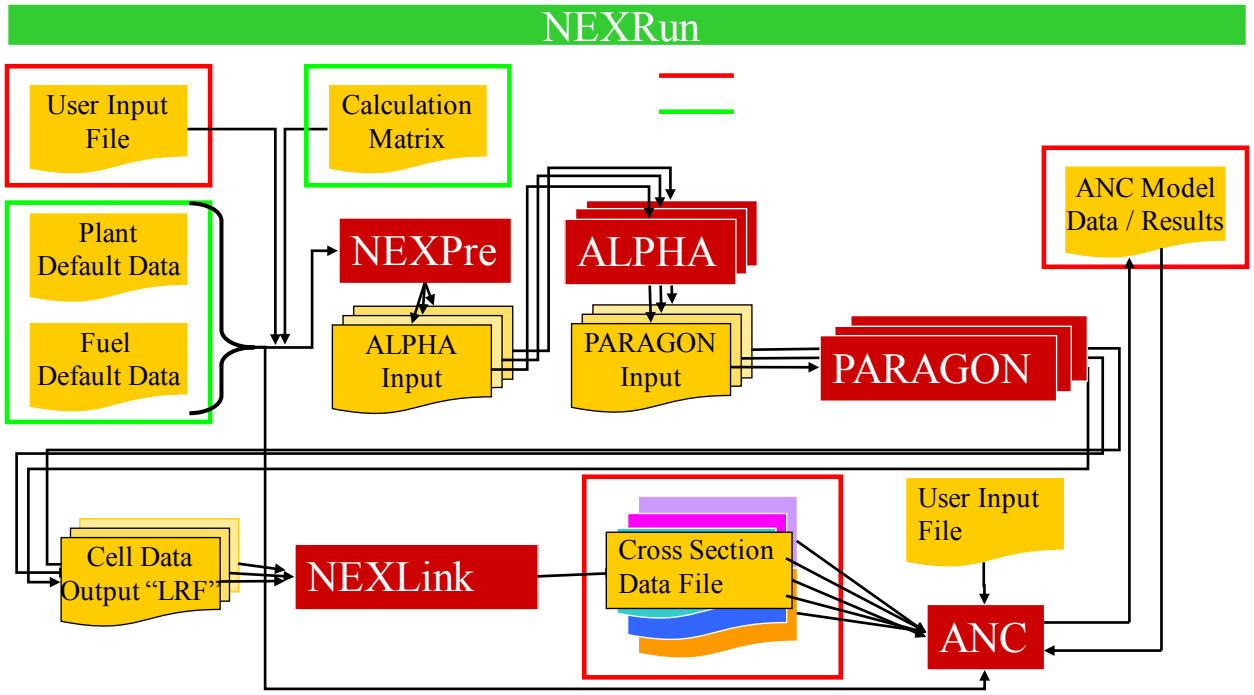


Figure 17: Flowchart for the NEXUS system

6.3 PARAGON

PARAGON is Westinghouse's lattice transport code (Ref.31). It provides lattice data for the ANC core simulator. These data include macroscopic cross sections, microscopic cross sections for feedback adjustments, pin factors for pin power reconstruction calculations, and nodal discontinuity factors. PARAGON uses collision probability (CP) theory with the interface current cell coupling method to solve the integral transport equation. Throughout the entire calculation, PARAGON uses the exact heterogeneous geometry of the assembly and the same energy groups as in the cross section library to compute the multi-group fluxes for each micro-region location of the assembly. In order to generate the multi-group data, PARAGON goes through four steps of calculations: resonance self-shielding, flux solution, burnup calculation, and homogenization.

The 70 group PARAGON cross section library used for production calculations is based on the ENDF/B-VI.3 basic nuclear data. This library has an extensive validation basis and it has been applied for design and analysis of commercial PWR cores for several years. A 70 group ENDF/B-VII.0 based library is also available (Refs.33 and 34) and has been employed for these WBN1 calculations. Both ENDF/B-VI.3 and ENDF/B-VII.0-based libraries implement a reduction in the U-238 resonance integral as recommended in Reference 35 and discussed in Reference 36. The ENDF/B-VII library includes an increase in the upper bound for the upscattering effects from 2.1eV to 4.0 eV to improve MOX fuel predictions, while showing similar overall accuracy for UO_2 core calculations, as discussed in Reference 36.

The 70 group PARAGON library includes explicit multi-group cross sections and other nuclear data for 174 isotopes, without any lumped fission products or pseudo cross sections. PARAGON

and its 70 group cross section library are benchmarked, qualified, and approved both as a standalone transport code and as a nuclear data source for a core simulator in a complete nuclear design code system for core design, safety, and operational calculations. Ref. 32 addresses the qualification of the basic methodology used in PARAGON within a nuclear design system. The basic methodology and its implementation in PARAGON have been qualified through comparisons to critical experiments and isotopic measurements. These include the Strawbridge experiments with Urania-Gadolinia fuel. Additionally, reactivity and power distribution comparisons between PARAGON and Monte Carlo (MCNP, Ref. 23) calculations for single assembly problems have been performed. Comparisons have also been successfully demonstrated for the 2nd Core Physics Progression Problem in Reference 14. Various assembly designs similar to those currently in use in PWR cores have been included in these comparisons. Isotopic comparisons have been made between PARAGON and the Yankee and Saxton isotopic measurements.

6.4 ANC

ANC (Ref.37-43) is a multi-dimensional advanced nodal code for nuclear core design calculations. ANC predicts core reactivity, assembly power, rod power, detector thimble flux, and other relevant core characteristics. ANC was originally released in 1987 (Ref. 41) and has had numerous small and three large version updates since. The third large version update – Version 9.1 – incorporated the NEXUS methodologies into ANC in addition to a large number of other improvements. New input and output interfaces have been developed based on JAVA technologies to provide a more user-friendly experience. ANC has been updated to use a new data storage mechanism that is faster and easier to use. Moreover, in order to further improve the accuracy of ANC predictions and add flexibility in modeling complex fuel and core conditions, a number of major functionality changes have been made in ANC.

The ANC version 9 series makes use of the Primary Input Processor, known as PIP, developed at Westinghouse. This language is a hierarchical structured ASCII input language which supports all data formats – strings, integers, real numbers, Boolean values, dates, lists, maps and structures. This new language reads structured ASCII input and translates it to an XML document that is read by ANC. ANC makes use of a FORTRAN-based XML library to validate and read the transformed user input. This new language has many advantages. The first is that input is now more human readable and easily verifiable, and thus, reduces the likelihood of human errors. Also, as new needs arise for input processing, user input can be easily translated into other formats using XSL transformations without recoding the input processor. ANC9 also makes use of JAVA technologies to produce its output and of a code called DEPORT to generate all ASCII output. The integration with DEPORT also serves the integration of ANC and BEACON™, the Westinghouse on-line core monitoring system. This integration spurred improvements also in the data storage system, which must be capable of reading and writing multiple depletion-steps worth of data in a timeframe consistent with on-line core monitoring needs. ANC9 makes use of a new data storage mechanism known as CoreStore developed at Westinghouse. This storage system was built using HDF5 and allows for platform independent storage of data and meets all performance requirements of an on-line core monitoring system.

ANC 9 includes a number additional physics models and features compared to earlier versions. Briefly, these include:

- An improved methodology of cross section representation which is based on representing both macroscopic and microscopic cross sections primarily as a function of three parameters: 1) spectrum index, the ratio of fast to thermal group node-average fluxes, 2) fuel temperature, and 3) moderator temperature.

- The new 3D Pseudo Pin-By-Pin Calculation (P3C) Methodology (Ref. 38), which uses pin-cell cross sections and fluxes for heterogeneous assemblies in combination with the tracking of individual fuel rod depletion histories to compute pin-by-pin fluxes.

- A new control rod depletion model (Ref. 43) which in synergy with the P3C methodology enables accurate prediction of the reactivity feedback and the impact on pin powers resulting from repeated control rod insertion and withdrawal sequences.

6.5 QUALIFICATION OF NEXUS

NEXUS received approval from the U.S. Nuclear Regulatory Commission (NRC) for use on UO_2 PWR cores in February, 2007. Subsequently, the new pin power reconstruction method has also been approved by the NRC and is currently adopted for all production calculations.

The qualification of the NEXUS/ANC system demonstrates the capability of the system to perform accurate nuclear design calculations for PWR cores. The approach used for the qualification is described in Reference 27. The core qualification included ten plants covering 45 cycles of operation. These plants included six Westinghouse designed plants and four Combustion Engineering designed plants. The plants included out-in loading patterns, low-leakage loading patterns and three first core designs. Burnable absorbers included IFBA, erbia, gadolinia, and discrete Pyrex. Cycle lengths varied from annual to near 24 month cycles. Enrichments varied from low enriched (0.74 w/o) ^{235}U to near 5 w/o ^{235}U. Lattice designs included 14x14 through 17x17 for Westinghouse designs and both 14x14 and 16x16 for Combustion Engineering designs. Fuel rod sizes varied from 0.360 inch diameter through 0.420 inch diameter. Core parameters compared against measurement included BOC HZP critical boron, BOC HZP isothermal temperature coefficient, BOC HZP control rod bank worths, and at-power critical boron and axial offsets throughout the cycles. In addition, the results from the NEXUS system were compared to those from the APA Westinghouse nuclear design system for shutdown margin, rod ejection, and other parameters that are not directly measured including Doppler and power coefficients and defects. The qualification calculations gave satisfactory results and the system was qualified for design calculations of PWR cores. These results include comparisons of measured to predicted results for the startup parameters which are relevant for this report. Accurate measurements of these parameters are generally performed for every cycle and a large database exists in Westinghouse.

6.5.1 Startup Parameters

The startup measured parameters that are used for the qualification of PWR core physics simulation packages usually include: 1) Hot zero power (HZP), beginning of cycle (BOC) critical boron, BOC HZP isothermal temperature coefficient (ITC) and BOC HZP control rod worths. NEXUS/ANC calculations are performed for all these parameters for all cycles in the qualification plant database where existing measurement data are available.

Figure 18 shows a histogram of the differences between measured data and NEXUS/ANC-calculated BOC HZP critical boron results. These results show very good performance, with an average difference very close to zero and a standard deviation on the order of 20 ppm.

Results for HZP ITC with NEXUS/ANC for the benchmark cores are also very good. The mean for all cores is very close to zero with a standard deviation of about 0.5 pcm/°F.

BOC HZP rod worths calculations also demonstrate very good agreement with measurement. The average difference between measured and calculated rod worths for individual control rod banks is about 0.1% with a standard deviation of nearly 6%.

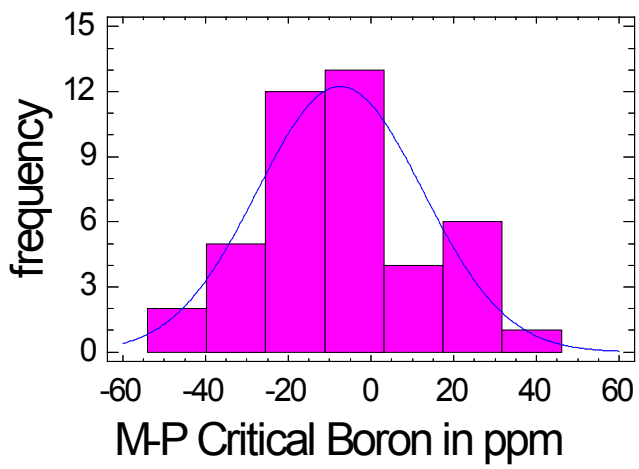


Figure 18: Histogram of HZP BOC Measured – Predicted differences for NEXUS/ANC

6.6 NEXUS WBN1 Model

An ANC 9 WBN1 core model has been setup with lattice data parameters generated using PARAGON within the NEXUS system (Figure 17). The cross section library used is based on ENDF-BVII.0 (Reference 34). These modeling parameters are sufficiently close to those adopted in the CASL deterministic codes for the WBN1 startup tests simulations. Generic 4-loop axial and radial reflector cross sections available in the Westinghouse database have been employed. It should be noted that the Westinghouse NEXUS models have not undergone independent verification and prototypical version of the codes and library have been adopted for this study.

Sample BOC nodal radial power and pin power distributions obtained with ANC 9 for WBN1 are given in Figure 19. The characteristic power distribution with the radial peak occurring in the ring of assemblies about two-third of the way from the core center to the periphery is visible. The calculations performed for this study focus on the BOC HZP eigenvalue with the measured soluble boron concentration for the initial criticality and the rod worth calculations, with results discussed in Section 7. Automated sequences are available in ANC 9 to perform these calculations, with results generated using a single input deck and very short execution time.

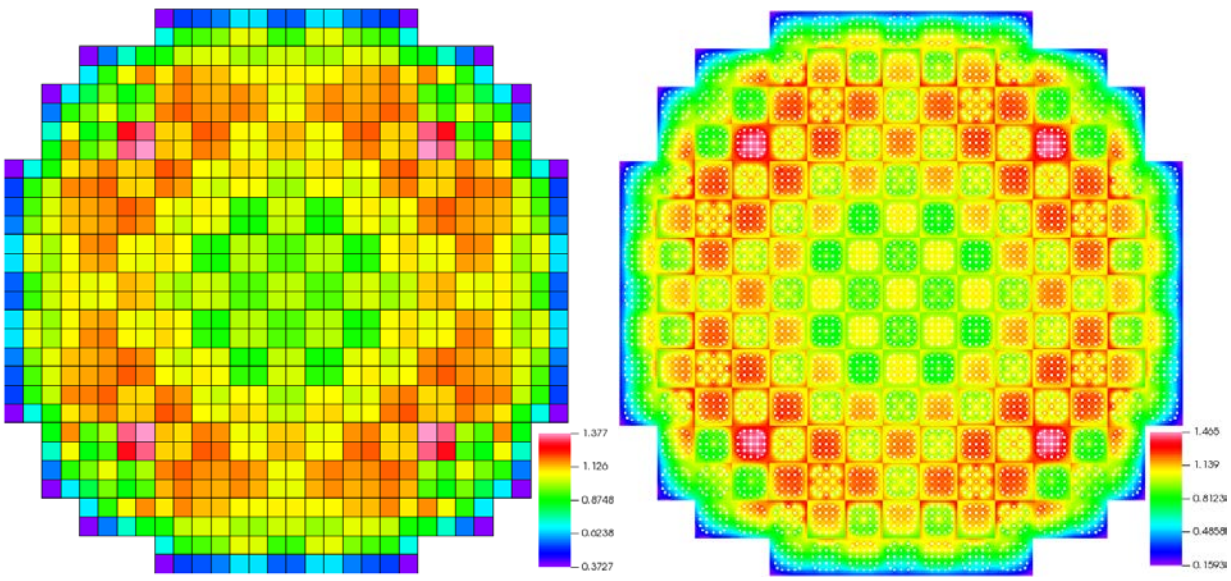


Figure 19: NEXUS Watts Bar 1 Results –Radial Nodal and Pin Power Distributions

7. DEMONSTRATION AND ANALYSES OF ZERO POWER PHYSICS TESTS

TVA's Watts Bar Nuclear Unit 1 Cycle 1 reached initial reactor criticality on January 18th, 1996 and completed a series of zero power physics tests on January 22nd, 1996. The test's results were documented in TVA plant procedures and regulator communications (Ref. 44) and have been provided to CASL through its partnership with TVA. The WBN1 Cycle 1 ZPPT tests will be described in detail in this section and the results will be presented from simulations with VERA codes and the other methods previously described to demonstrate the capability developed by CASL to accurately model physical nuclear power reactors. The tests that will be simulated are:

1. Initial Criticality
2. RCCA Bank Reactivity Worth
3. Differential Soluble Boron Worth
4. Isothermal Temperature Reactivity Coefficient

Note that ZPPT tests do not include incore flux mapping due to very low power and flux (and thus instrument response) in the system. Typical incore detector systems are unavailable until after power escalation has begun. This data will be analyzed in a later report when VERA is capable of thermal-hydraulic feedback for full core problems.

7.1 Initial Criticality

The approach to initial criticality for a nuclear power reactor core is performed in a cautious and controlled manner. This test is the first opportunity to demonstrate to plant staff and operators that the reactor will perform as designed by the core design engineers. Human errors in fuel manufacturing, core design and analysis, and fuel assembly and control component core placement could lead to a deviation in core behavior from design values which could penalize operation. Therefore, it is paramount to the successful startup of a reactor and its eventual electrical generation that the initial criticality goes smoothly and as predicted by core analysis software.

The criticality test for WBN1 Cycle 1 began by placing the source and intermediate range monitors and reactivity computer into operational service per prior plant procedures. The initial test conditions were nominal operating system temperature and pressure including substantial sub-criticality with all RCCA banks fully inserted and a soluble critical boron concentration of approximately 2000 ppm. Then the four safety RCCA banks (SA-SD) were fully withdrawn, and the control RCCA banks (A-D) were withdrawn in an overlapped manner until Bank D was about two-thirds withdrawn (all other banks fully withdrawn). Finally, non-borated water was injected into the reactor coolant system to dilute the soluble boron concentration to a range in which criticality could be achieved by further withdrawal of Bank D. During this time, source range excore detectors were monitored to assess the rate of positive reactivity addition as the point of criticality was approached. Finally, Bank D was withdrawn to 167 steps to achieve criticality at a system soluble boron concentration of 1293 ppmB.

The acceptance criterion for this test was a measured boron concentration within 100 ppm, which corresponds to a ~1000 pcm (percent mille) discrepancy for WBN1 at the beginning of Cycle 1 (BOC1) (as it will be shown later, the boron worth for WBN1 BOC1 is about 10 pcm/ppmB). The review criterion is 50 ppm critical boron, corresponding to about 500 pcm. The measurement uncertainty for soluble boron is about 5 ppm (or 50 pcm for WBN1).

This test was simulated by each of the codes and methods described in this report. Bank D and the system boron concentrations were set to their critical values, and the core average eigenvalue (or k-effective) was calculated. These results are shown below, along with the reactivity difference from critical calculated as:

$$\rho = \frac{k_{eff} - 1}{k_{eff}} \times 10^5 \; [pcm]$$

Note that a correction (78 pcm) was applied to the results from the KENO-VI calculations to account for the difference between the estimated ^{10}B fraction of the boron contained in the reactor coolant system and that used by SCALE. While these codes assume 19.9 at% ^{10}B in B, the WBN1 data suggests about 19.78 at%. The Insilico calculations were performed at a boron concentration corrected for the ^{10}B abundance discrepancy, and the NEXUS calculations were performed with the measured isotopic distributions.

An additional correction (-57 pcm) was applied to the results from KENO-VI and Insilico to account for thermal expansion of the fuel. This value was determined from NEXUS calculations performed with and without thermal expansion enabled.

Table 2: WBN1 Cycle 1 Initial Criticality Results

Result	k-effective	Reactivity Difference (pcm)	Effective Critical Boron Difference (ppmB)†
Measured	1.00000	--	--
CE KENO-VI	0.99957 ± 0.00005	-43 ± 5	-4 ± 1
NEXUS	0.99813	-187	-19
VERA	0.99981	-19	-2

† calculated using the calculated ARO DBW for each code, to the nearest ppmB

Each of the results is well within the review criteria. The values predicted by KENO-VI and VERA are within the measurement uncertainty of the criticality test.

7.2 RCCA Bank Reactivity Worths

Following initial criticality of Cycle 1, Watts Bar Nuclear 1 testing continued by measurement of the nuclear reactivity worth of each of the control rod (or RCCA) banks. This included verification of the core design values for the ARO critical boron concentration, the critical boron concentration with Bank D fully inserted, and the measurement of the differential reactivity worth of Bank D as well as the integral worth of all of the banks. The predicted RCCA worth is one of the input parameters to the safety analysis, such as for shutdown margin calculations, and

the accuracy of predicted RCCA worths are used for justification of uncertainties in some accident analyses. Therefore, the ability to accurately predict the worth of control rods in a reactor core is a requirement of any core analysis software.

The Bank D worth for WBN1 was measured directly by the reactivity computer monitoring system during a reactor system dilution. The all-rods-out (ARO) boron concentration was established following criticality by addition of soluble boron (boration) until Bank D was nearly fully withdrawn. Then the system was diluted at a constant rate though addition of unborated water while Bank D was inserted to maintain criticality (also known as 'boron swap'). The change in reactivity for each bank D movement was measured using the reactivity computer monitoring system, and the integral Bank D worth was directly calculated by summation of all the differential worths over the full range of Bank D movement.

The remaining RCCA bank worths were measured by reactivity exchange against Bank D, known as the 'rod swap' method. As the highest worth bank, Bank D was chosen as the reference bank for the swaps, and thus was measured first with the reactivity computer. Then each of the other banks (the "test" bank) was alternately inserted while Bank D was withdrawn to compensate for the reactivity change and maintain criticality. At the end of each test bank insertion, a new critical condition was established and measured by the reactivity computer. The measured reactivity worth of each of the rod swap banks is inferred based on the endpoint critical position of the reference bank. This calculation will be described in more detail in a subsequent section.

The demonstration of the VERA capabilities will be divided into two parts to account for the specifics of the rod swap methodology and associated set of measurements available for benchmarking. The first is a statistical comparison to each of ten critical configurations identified during the rod swap procedure. These include initial criticality, ARO criticality, and criticality with each of the rod banks fully inserted. Because the reactor core is critical throughout the testing, this provides a consistent set of measured data to compare against reactor simulations. The second part of this demonstration will be the simulation of the predicted bank reactivity worths, including modification of the "inferred" worths. This will provide a demonstration of each code's performance if adopted for nuclear design analysis, and namely to support the rod swap measurement methodology.

7.2.1 Direct Rod Swap Criticals

This section demonstrates the accuracy of each code and model to predict criticality with different RCCA bank configurations. Like the previous section on initial criticality, a 500 pcm review criteria is assumed and the measurement uncertainty is assumed to be approximately 50 pcm. Also, as was indicated previously, adjustments of approximately 70 pcm, depending on the measured boron concentration, are made to KENO-VI results to account for differences in ^{10}B abundance.

The measured value of interest for these tests is the final critical position of the reference bank following insertion of the test bank. If all of the tools had an option to search on Bank D position for criticality, the critical positions could be calculated and compared directly for each test bank. However, since this capability does not exist currently, the measured critical positions

are input into the codes directly and the reactivity difference is assumed to be the amount of predicted sub- or super-criticality. Table 3 contains the results of the measured rod swap criticals.

Table 3: WBN1 Cycle 1 Rod Swap Criticals

Critical Description	Critical Boron (ppmB)	Reference Bank Position (steps)	k-effective			Reactivity Difference (pcm)		
			KENO-VI‡	NEXUS	VERA	KENO-VI‡	NEXUS	VERA
Initial	1293	167	0.99957	0.99813	0.99981	-43 +/- 5	-187	-19
ARO	1299	230	1.00016	0.99853	1.00024	16 +/- 5	-147	24
Bank D In	1177	18	0.99894	0.99749	0.99884	-106 +/- 6	-251	-116
Bank C In	1177	119	0.99886	0.99743	0.99884	-114 +/- 5	-257	-116
Bank B In	1177	113	0.99906	0.99717	0.99927	-94 +/- 6	-284	-73
Bank A In	1177	97	0.99863	0.99759	0.99853	-138 +/- 5	-242	-147
Bank SD In*	1177	71	0.99878	0.99725	0.99878	-122 +/- 5	-276	-122
Bank SC In*	1177	71	0.99873	0.99725	0.99876	-127 +/- 5	-276	-124
Bank SB In	1177	134	0.99911	0.99749	0.99921	-89 +/- 5	-252	-79
Bank SA In	1177	69	0.99872	0.99711	0.99883	-128 +/- 6	-289	-117
Average			**0.99906**	**0.99755**	**0.99911**	**-94 +/- 5**	**-246**	**-89**
St. Deviation			**0.00047**	**0.00045**	**0.00054**	**48**	**45**	**54**

‡ all CE KENO-VI eigenvalue uncertainties are less than 6 pcm
*A bias of -53 pcm is applied to cases where banks SC or SD are inserted to account for lack of rotational symmetry

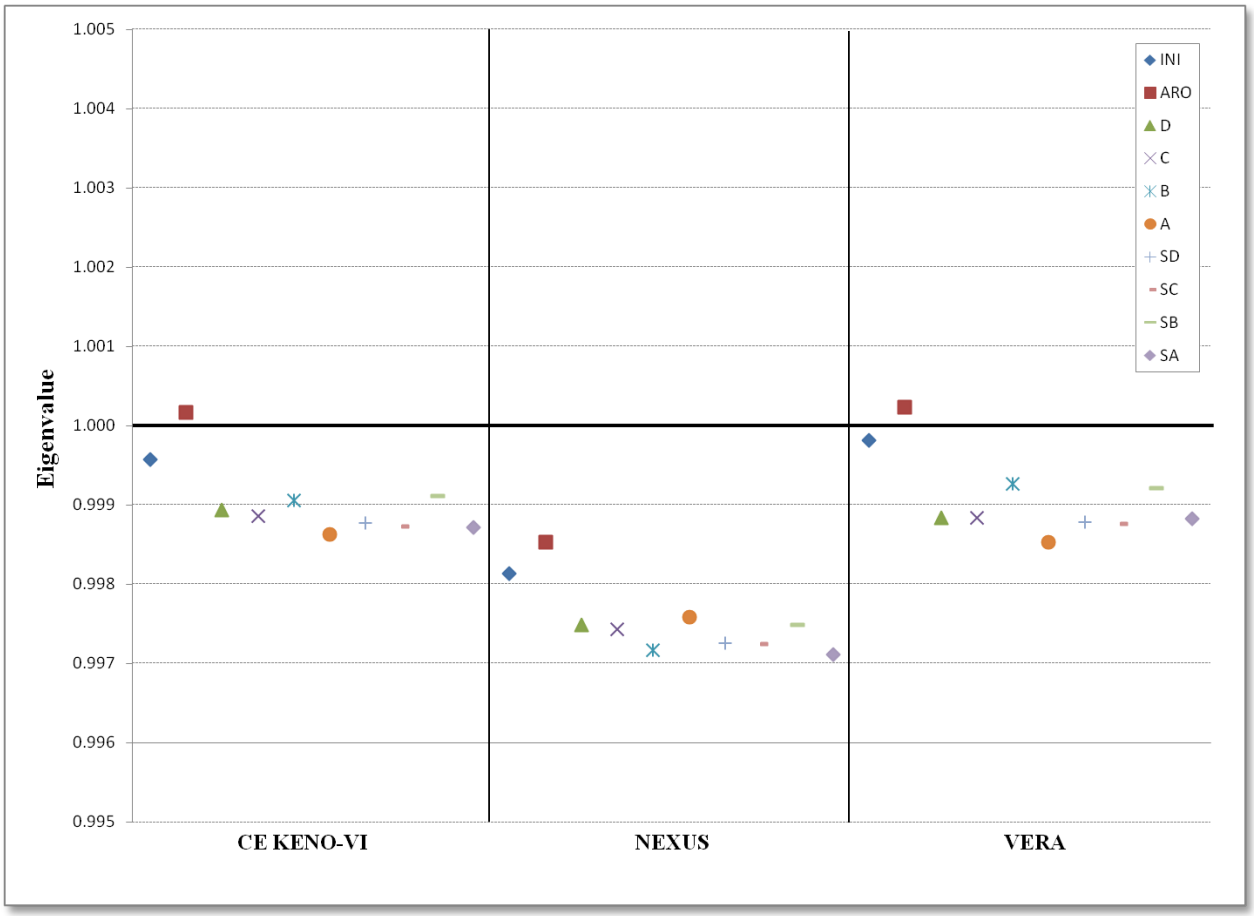


Figure 20: WBN1 Cycle 1 Rod Swap Criticals

Another small correction or bias is applied for the Bank SC and SD calculations. These banks are rotationally quarter core symmetric, not reflective (or mirror) symmetric. However, only the NEXUS methodology supports rotational symmetry. Based on NEXUS calculations, this effect is worth approximately -50 pcm versus the reflective geometry used by the other codes. Therefore, these cases are adjusted for now until this capability becomes available.

For each code, the average and standard deviation of the ten criticality differences is calculated and reported in the subsequent results. These results are excellent and demonstrate good agreement with measured conditions. VERA results also agree very well with KENO-VI, and clearly demonstrate the ability to accurately predict many different RCCA configurations for the WBN1 Cycle 1 core. Figure 20 presents these results graphically.

7.2.2 Inferred RCCA Bank Worths

Direct comparison of predicted bank reactivity worths is not possible. The WBN1 Cycle 1 ZPPT utilized the rod swap technique to calculate the 'inferred' bank worths from the final reference bank critical position after each bank insertion. In particular, the calculation of the test bank worth is based on the measured integral and differential reactivities of the reference bank

(Bank D) and a pre-calculated 'shadow factor' that accounts for the change in reference bank worth due to the presence of the test bank. The WBN1 Cycle 1 shadow factors were calculated by the Westinghouse design and analysis methods prior to the startup based on predicted critical configurations.

Each simulation code discussed in this document was used to recalculate shadow factors for the actual bank configuration of each test bank measurement. This results in new inferred bank worths that are provided and compared below in Table 4. Note that Bank D was not measured with the rod swap method. It was measured independently and directly by the reactivity computer during dilution and is not impacted by the rod shadow corrections.

Note that the corrections for rotational symmetry of Banks SC and SD are also included in the calculation of the new shadow factors of those banks.

Table 4: WBN1 Cycle 1 Inferred Bank Worths for Rod Swap
(pcm with change from original value in (%))

Bank	Original	KENO-VI	NEXUS	VERA
D†	1342	--	--	--
C	940	963 (+2.4%)	944 (+0.4%)	953 (+1.4%)
B	871	871 (+0.0%)	868 (-0.4%)	881 (+1.1%)
A	830	850 (+2.4%)	840 (+1.2%)	844 (+1.7%)
SD	495	480 (-3.0%)	481 (-2.9%)	484 (-2.3%)
SC	494	487 (-1.3%)	481 (-2.7%)	484 (-2.1%)
SB	1048	1045 (-0.3%)	1050 (+0.2%)	1058 (+0.9%)
SA	431	424 (-1.7%)	429 (-0.4%)	434 (+0.7%)
Total	6451	6461 (+0.2%)	6433 (-0.3%)	6479 (+0.4%)

†The Bank D worth is not inferred, but was directly measured

The predicted RCCA bank reactivity worths are calculated from inserting the test bank alone from All-Rods-Out (ARO) conditions (i.e. the reference bank is fully withdrawn). For Bank D, which was measured directly during dilution, the bank worth is calculated at the beginning and end of the dilution and the values are averaged. For the rod swap banks, the calculation is performed once at the dilution endpoint concentration. For these calculations the traditional form of the reactivity change equation is used:

$$\Delta\rho_{test} = \left({}^{1}/_{k_{test}} - {}^{1}/_{k_{ARO}}\right) \times 10^5 \; [pcm]$$

For the rod worth comparisons, the ARO-based worth is compared to the inferred measured worth associated with the same methods code. This is consistent with the comparison used during plant startup to verify compliance of the predicted rod worth with the acceptance and review criteria. It also allows comparison from future codes and methods without the need to recalculate the shadow factors. Should comparisons to measurement be desired, the inferred worth calculated from the CE KENO-VI shadow factors can be assumed to be the best available.

Table 5 provides the predicted WBN1 RCCA bank worths for each code, as well as the absolute and relative differences from the measured values.

Table 5: WBN1 Cycle 1 RCCA Bank Reactivity Worths

Bank	Reactivity Worth (pcm)			Worth Difference (pcm)			Relative Worth Error (%)		
	KENO	NEXUS	VERA	KENO	NEXUS	VERA	KENO	NEXUS	VERA
D	1387 ± 8	1358	1400	45	16	58	**3.3%**	**1.2%**	**4.3%**
C	983 ± 8	971	990	20	27	37	**2.1%**	**2.9%**	**3.9%**
B	870 ± 8	919	869	-1	51	-11	**-0.1%**	**5.9%**	**-1.3%**
A	894 ± 8	849	908	44	10	64	**5.1%**	**1.1%**	**7.5%**
SD*	489 ± 8	508	498	**9**	**28**	**14**	2.0%	5.8%	3.0%
SC*	501 ± 8	508	500	**14**	**28**	**16**	2.9%	5.8%	3.4%
SB	1051 ± 8	1074	1068	7	25	10	**0.6%**	**2.3%**	**1.0%**
SA	446 ± 8	469	441	**22**	**40**	**7**	5.2%	9.3%	1.7%
Total	6622 ± 22	6657	6675	160	224	196	**2.5%**	**3.5%**	**3.0%**

*A bias of -39 pcm is applied to cases where banks SC or SD are inserted to account for lack of rotational symmetry

The criteria for the WBN1 Cycle 1 control rod worth tests were as follows:

Measurement	Review Criteria	Acceptance Criteria
Bank D	10%	15%
Banks A, B, C, SB	15%	30%
Banks SA, SC, SD	100 pcm	200 pcm
Total Banks Worth	10%	10%

Each of the codes would pass the rod worth review criteria for the WBN1 Cycle 1 startup testing with a comfortable margin. The excellent performance of VERA should be noted. These results clearly demonstrate VERA's ability to simulate the criticality and control rod worth testing of an operating LWR. Figure 21 also provides the relative errors graphically.

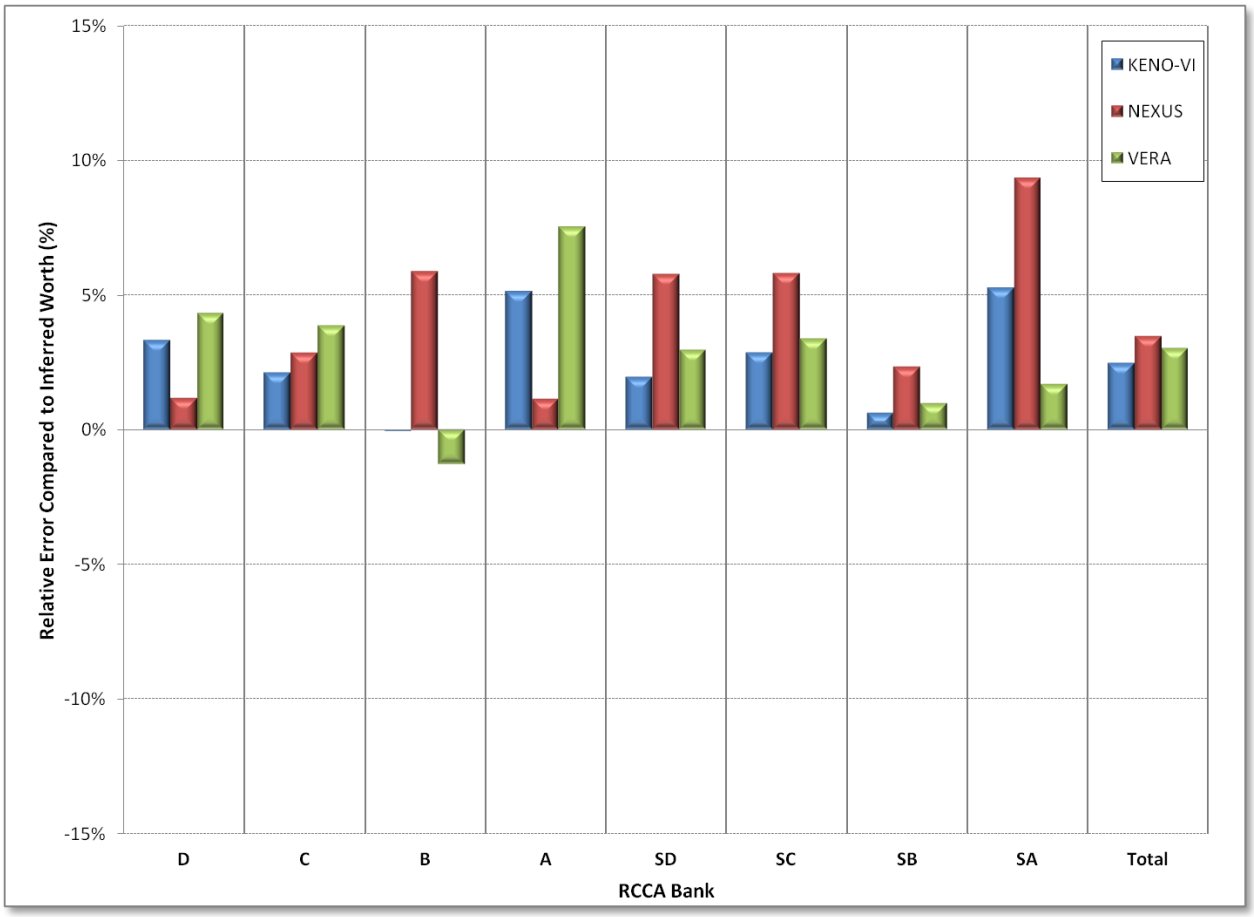


Figure 21: WBN1 Cycle 1 Control Bank Worth Deviations

7.3 Differential Soluble Boron Reactivity Worth

The average Differential Boron Worth (DBW) for WBN1 Cycle 1 was determined during the worth measurement of RCCA Bank D. The integral worth of Bank D was measured by the reactivity computer during dilution of the reactor system. Because the reactor remained critical, the reactivity worth of the change in soluble boron concentration is equal to the integral Bank D worth, and the average DBW is the measured Bank D worth divided by the change in boron, in units of pcm per ppmB.

The predicted DBW is calculated by determining the reactivity change due to single perturbations in boron concentration for given fixed conditions. Because the measured value is an average over the range of insertion of Bank D, the predicted values are calculated as an average of the DBW with Bank D withdrawn and the DBW with Bank D inserted. However, for WBN1 these values are very insensitive to the presence of Bank D, and can be ignored.

$$DBW = \frac{\Delta\rho}{\Delta C_B} = \frac{{}^{1}/_{k_1} - {}^{1}/_{k_2}}{C_{B2} - C_{B1}} \times 10^5 \left[{}^{pcm}/_{ppmB}\right]$$

The DBW results are provided in Table 6. A minor correction is made to the KENO-VI results data to account for the slight difference between the ^{10}B abundance assumed in the codes versus the actual WBN1 value (a 0.6% difference).

Table 6: WBN1 Cycle 1 Differential Boron Worths

Result	DBW (pcm/ppmB)	Difference (pcm/ppmB)
Measured	10.8	--
CE KENO-VI	10.1	-0.7
NEXUS	10.1	-0.7
VERA	10.1	-0.7

7.4 Isothermal Temperature Reactivity Coefficient

The WBN1 Cycle 1 Isothermal Temperature Coefficient (ITC) measurement was made to verify the measured Moderator Temperature Coefficient (MTC) was less than or equal to zero. The MTC is inferred from the measured ITC and the design Doppler Temperature Coefficient, provided to the plant from the nuclear design codes at the time. The ITC measurement was performed by reducing the average reactor coolant system temperature by 4 °F achieved by increasing secondary load. The changes in reactivity were measured by the reactivity computer while holding the soluble boron concentration constant. Then the temperature was increased by 4 °F and the reactivity was measured again.

The purpose of the plant testing is to confirm a negative MTC. However, for benchmarking purposes, a desirable criterion is for agreement to be within 1 pcm/°F.

Table 7 contains the ITC results for the WBN1 Cycle 1 test. Due to the statistical nature of the Monte Carlo method in KENO-VI, it is difficult to predict a small reactivity effect with low enough uncertainties for a meaningful result. Therefore, KENO-VI results are not provided.

Table 7: WBN1 Cycle 1 Isothermal Temperature Coefficients

Result	ITC (pcm/°F)	Difference (pcm/°F)
Measured	-2.2	--
CE KENO-VI	--	--
NEXUS	-2.2	-0.1
VERA	-3.9	-1.7

The VERA ITC is significantly more negative than the measured value. This result is unexpected and is still being investigated.

8. CONCLUSIONS

Recent software development, testing, and data analysis efforts in CASL have led to the achievement of a full core simulation capability for PWRs such as TVA's Watts Bar Nuclear 1 demonstrated by results in this report. The CASL partners collaboratively bring together expertise in plant data and procedures, current analysis codes and methods, modern software development and supercomputing, advanced numeric and mathematical solvers, and reactor physics methods and analysis capabilities.

The WBN1 Cycle 1 zero power physics tests were analyzed with the current VERA capabilities and the results in this document demonstrate that VERA is able to accurately simulate the startup physics testing of an operating nuclear power reactor. The initial critical configuration, rod swap critical configurations, control rod worths, and the differential boron worth calculations with VERA are in excellent agreement with plant measurements. The isothermal temperature coefficient, however, shows an unexpected deviation from the measured value and requires further investigation.

The work presented in this document has also shown the commitment of CASL to develop the capabilities to better understand the performance of VERA and to educate CASL staff and industry partners on the advantages (e.g. accuracy and resolution) and limitations (e.g. computational burden) of using high-fidelity models and physics relative to currently applied methods. As part of these efforts, there has been a focus on the usability of VERA through the common input and standardized output. AMA has also developed a complete methodology for generation of CE KENO-VI models to provide a reference solution. Core models were also generated by AMA with the Westinghouse NEXUS/ANC9 system to compare the results to those obtained from industry state-of-the-art core physics tools. The results for each of these models have been provided in this document along with those from VERA, and these models will continue to add value to CASL analyses in the future.

9. FUTURE WORK

CASL is currently developing the capability for full core coupled thermal-hydraulics and AMA expects to apply that soon to Core Physics Progression Problems 7 and 8, representing full power operations. At that time CASL will be able to continue this benchmarking demonstration by simulation of the WBN1 power escalation testing, including T/H and Doppler feedback and incore flux distributions. Specifically, future development activities which are ongoing or will be soon initiated related to WBN1 simulation capability are:

- Investigation of the ITC results for the WBN1 startup testing
- Analysis of Core Physics Problems 3 and 4 with 2D/1D transport (MPACT)
- Addition of rotational (cyclic) symmetry for quarter core analyses
- Addition of reactivity feedback due to thermal expansion
- Completion of Core Physics Problem 5 capability and WBN1 analysis with MPACT
- 2D and 3D whole-core pin power distribution evaluations
- Improvement of Insilico cross section homogenization through the coupling of a 2D lattice physics capability with the Method of Characteristics (MOC)
- Development of Problem 6 and 7 capabilities using the coupling with COBRA-TF
- Incorporation of the fuel mechanics code Peregrine for at-power fuel temperature feedback
- Development of incore detector response capabilities and other support functions such as critical boron search and equilibrium xenon calculations.
- Addition of depletion capability

Upon the completion of the required development activities, VERA will be applied to the other progression problems. Problem 6, which includes coupling of neutronics and thermal hydraulics for a single assembly, is nearly completed. Problems 7-10, which represent full core operation at hot full power representing reactor operation will be analyzed and will provide additional opportunities for comparison of VERA calculated results with measured plant data.

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APPENDIX A: STATUS OF MPACT

The development and validation of the 2D MOC solver in MPACT was documented in Reference A.1 and provided the basis for the development of the 3D intra-pin transport capability based on the 2D/1D solution method. The 2D/1D method was designed to provide VERA with an efficient 3D core flux solution capable of resolving the heterogeneous intra-pin detail in the radial direction by taking advantage of the relative axial homogeneity in the typical PWR. The 2D/1D method utilizes the 2D MOC solver in the radial direction and a low order transport or diffusion approximations in the axial direction. Research into the stability of the 2D/1D method has also been completed Reference A.2 and has resulted in a robust 2D/1D method than can be used with fine axial mesh.

MPACT is currently under development for full core 3D applications, but in order to provide an update on the status of MPACT, this section will highlight some of the recent results obtained for selected VERA Core Physics benchmark problems.

A.1 VERA Core Physics Benchmark Problem 3

VERA Core Physics benchmark problem 3 was described in Reference A.3 and was designed to evaluate the ability of codes to model a 3D fuel assembly. Problem 3 consist of a fuel assembly with explicitly modeled fuel, grid spacers, upper plenum, top and bottom nozzles and the core plates as shown in Figure A.1.

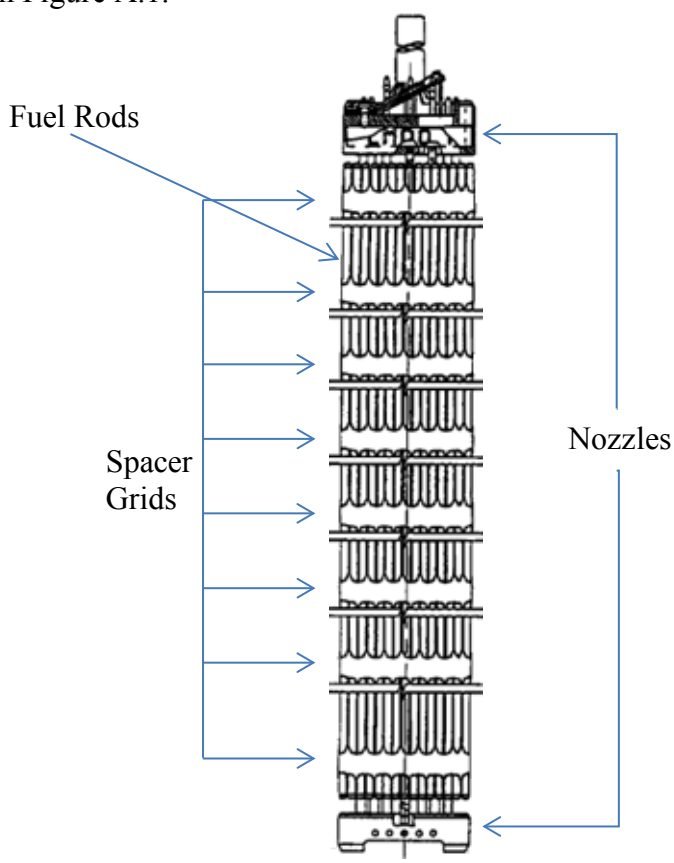


Figure A.1 VERA Core Physics Benchmark 3 Geometry

The eigenvalue for problem 3 is compared to the reference KENO solution in Table A.1. The normalized axial power profile obtained with MPACT is shown in Figures A.2 and A.3. As indicated the axial power is in good agreement with the KENO reference.

Table A.1 Eigenvalue Comparison for Problem 3

Reference	1.17629
MPACT	1.17486
Difference [pcm]	-143

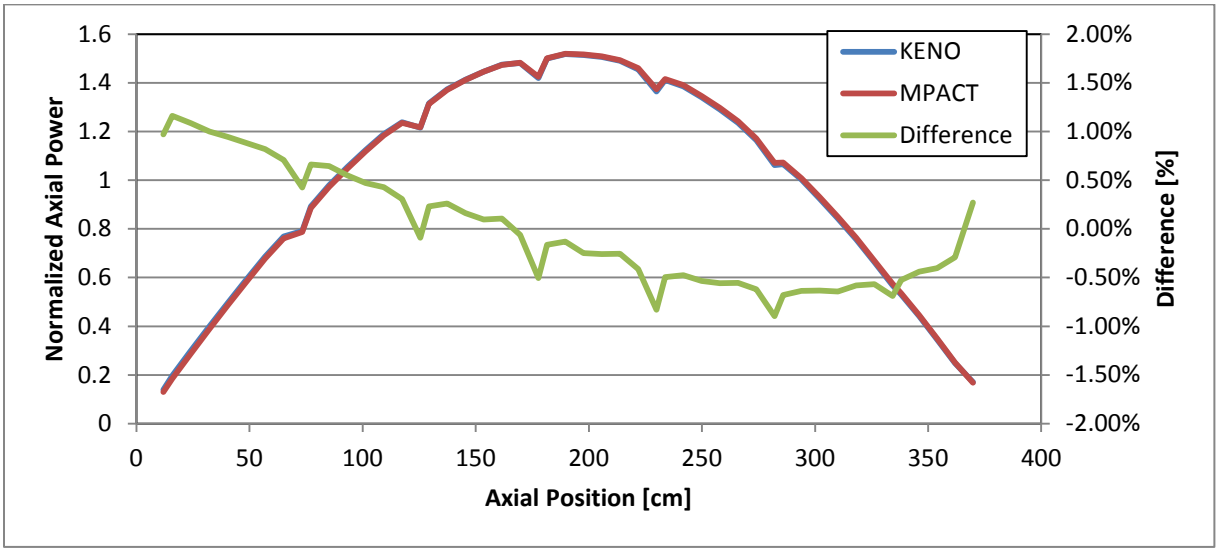


Figure A.2 MPACT Axial Power Shape for Problem 3

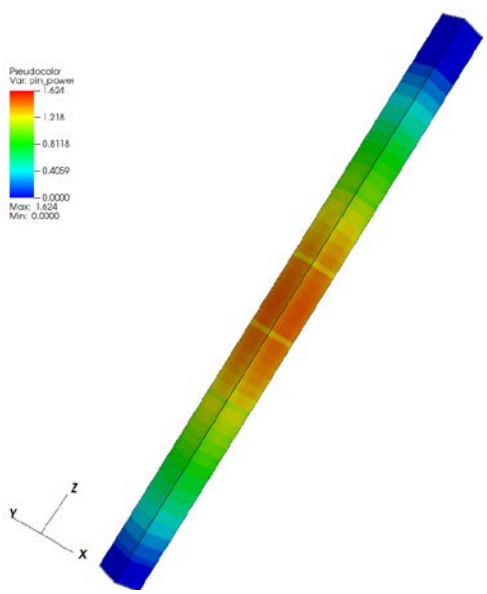


Figure A.3 MPACT Pin Power for Problem 3

A.2 VERA Core Physics Benchmark Problem 4

VERA Core Physics benchmark problem 4 was described in Reference A.3 and was designed to evaluate the ability to model a 3D fuel assembly cluster with a control rod inserted at prescribed positions. Problem 4 defines a control cell from the full core with all the axial geometric features in the single assembly. A control rod is placed in the center of the 3x3 control cell and Pyrex inserts are in the face adjacent assemblies as shown in Figure A.4. This problem represents the center of the full core problem discussed in the main paper.

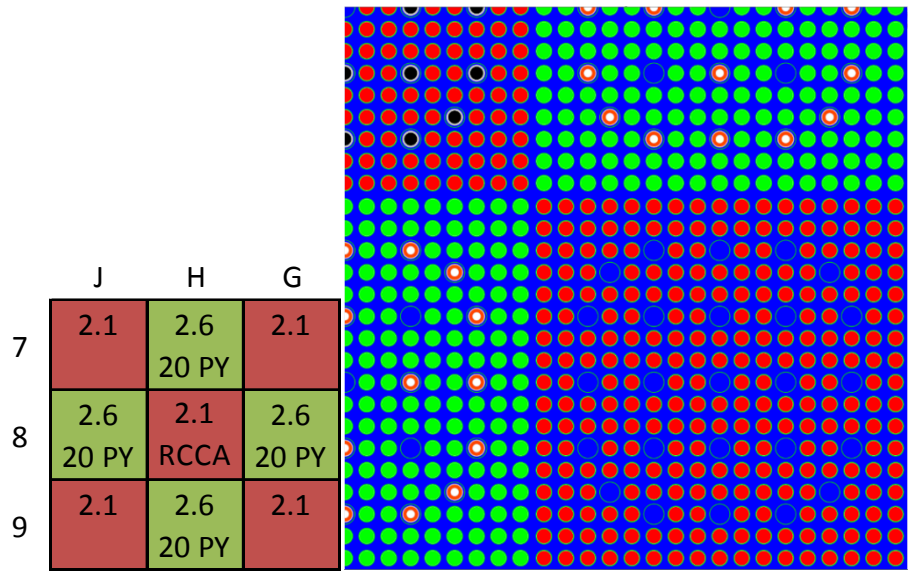


Figure A.4 Problem 4 Assembly layout

The eigenvalue comparisons for the unrodded and rodded cases are shown in Table A.2. The control rod worth shows a difference of 2.3%. The integral rod worth predicted by MPACT is shown in Figure A.5. As indicated the integral control rod worth is in good agreement with KENO.

Table A.2 Eigenvalue Comparison for Problem 4

	Unrodded	Rodded	Rod Worth
Reference	1.00264	0.97345	2991
MPACT	1.00181	0.97332	2922
Difference	83	13	-2.33%

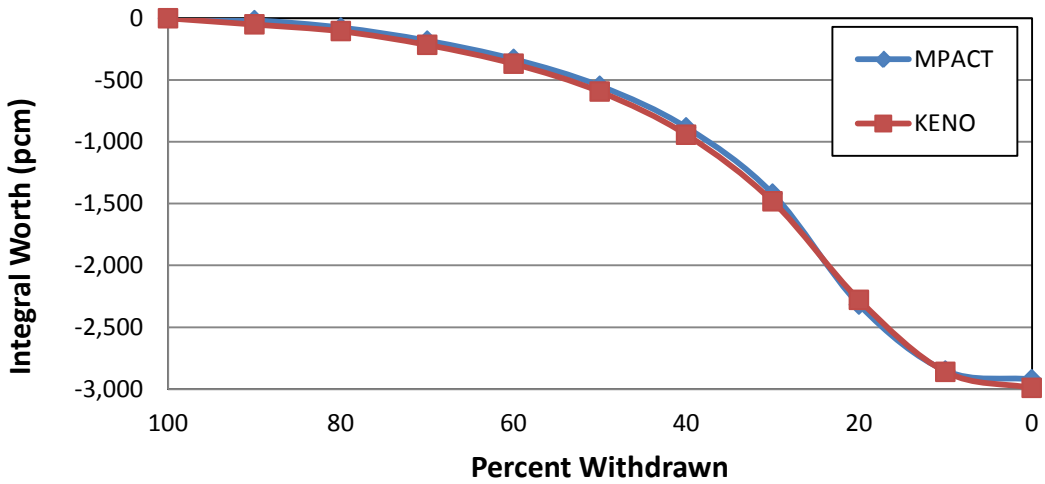


Figure A.5 MPACT Integral Rod Worth for Problem 4

A.3 VERA Core Physics Benchmark Problem 5

AMA benchmark problem 5 is described in the main section of this report and was designed to evaluate the ability to model a full 3D core with control rods inserted. The core loading pattern and control rod positions are described in Figure A.6

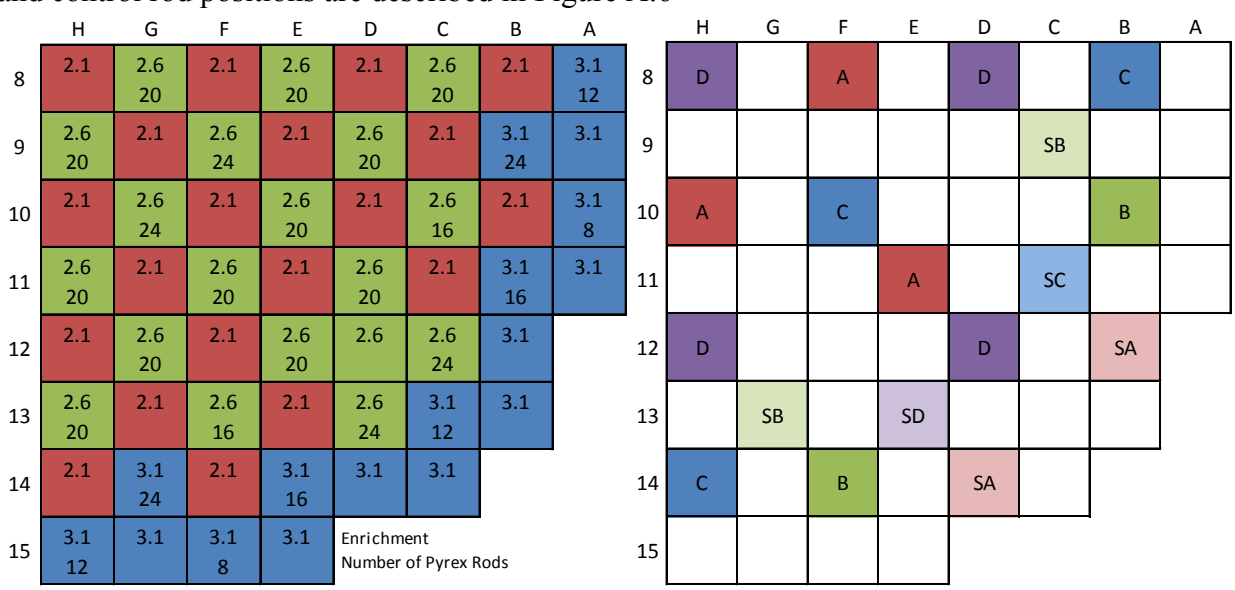
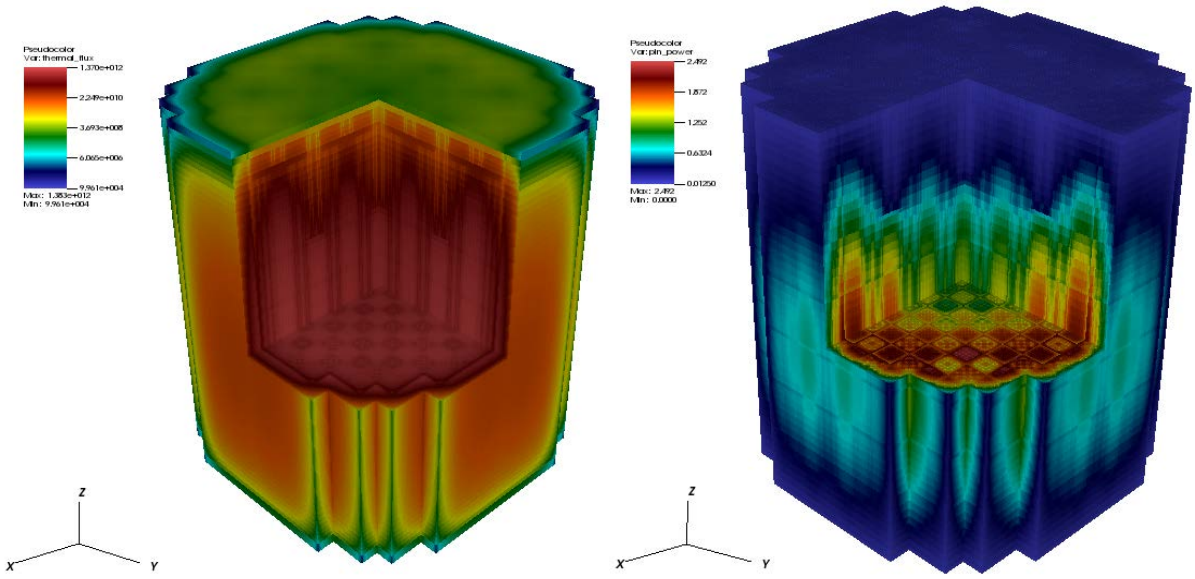


Figure A.6 MPACT Result for AMA Benchmark 4

Preliminary results for the thermal flux and pin powers predicted by MPACT are shown in Figure A.7 for the initial critical configuration where control bank D is partially inserted into the core.



Thermal Flux Pin Powers

Figure A.7 MPACT Result for Full Core Initial Criticality

Although MPACT has demonstrated the capability of converging a full core solution and the shape of the power and flux is reasonable, work is ongoing to verify the modeling of the full core reactor system. In particular, verification is being performed on the treatment of multiple insert types and the simultaneous movement of multiple control rod banks. The modeling of the jagged core boundary and the core baffle is also being verified. Work is also ongoing to evaluate the performance of selected methods, to include the treatment of anisotropic scattering considered for full core problems. Once all of the geometric complexities of the full core model and methods are verified, final results will be provided by MPACT for all of the critical configurations in the VERA Core Physics Benchmark Problem 5.

A.4 Summary

This appendix summarized the status of the MPACT full core transport code to perform 3D simulations using the 2D/1D methodology. Implementation of the VERA common input has been implemented and continues to be verified in order to ensure the accurate representation of the core-reflector geometry. Preliminary results suggest that the 2D/1D capability in MPACT provides an efficient and accurate method to model 3D reactor problems. The stabilization proposed by Larsen and Kelley provides a robust solution, even for very small axial mesh which previously had been an issue for the 2D/1D method. The results from the single assembly and the 3x3 control cell show that the 2D/1D method can provide accurate answers. Preliminary results on the full core also indicate that the code converges well for full core simulations. However, additional verification and analysis remains to be performed and upon completion of this work, MPACT will be ready to perform the full complement of startup physics testing as described in Problem 5.

A.5 References

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