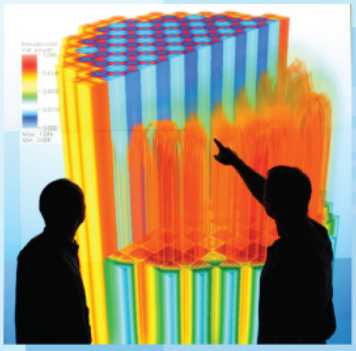
Power uprates
and plant life extension

CASL-U-2014-0051-000

Consortium for Advanced Simulation of LWRs

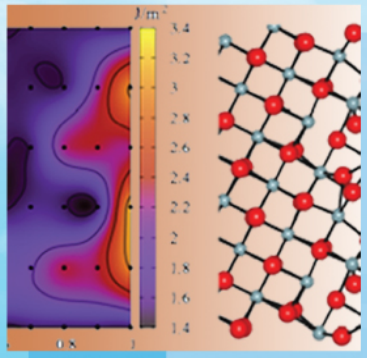


Engineering design
and analysis

Demonstration of Neutronics Coupled to Thermal-Hydraulics for a Full-Core Problem using COBRA-TF/MPACT

Science-enabling
high performance
computing

April 1, 2014



Fundamental science

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Plant operational data

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Oak Ridge National Laboratory

in partnership with

Electric Power Research Institute

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ACRONYMS

AMA	Advanced Modeling Applications
CASL	Consortium for Advanced Simulation of Light Water Reactors
CTF	COBRA-TF
DOE	U.S. Department of Energy
DOE-NE	U.S. Department of Energy Office of Nuclear Energy
DTK	Data Transfer Kit
FA	Focus Area
HFP	Hot Full Power
HPC	high-performance computing
HZP	Hot Zero Power
INL	Idaho National Laboratory
LANL	Los Alamos National Laboratory
LWR	light water reactor
MPO	Materials Performance and Optimization
ORNL	Oak Ridge National Laboratory
PCI	pellet-cladding interaction
PCM	percent mille (10^{-5})
PNNL	Pacific Northwest National Laboratory
PPM	parts per million (usually boron)
PSU	Pennsylvania State University
PWR	pressurized water reactor
RTM	Radiation Transport Methods
SNL	Sandia National Laboratories
T-H	thermal-hydraulics
TPL	third-party library
V&V	verification and validation
VERA	Virtual Environment for Reactor Applications
VRI	Virtual Reactor Integration

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1. Introduction

This report documents the completion of Milestone L3:RTM.P7.05 – MPACT running a realistic full core at beginning of life, hot full power, with critical boron and Equilibrium Xe/Sm treatment. (AMA Benchmark 7). The purpose of this milestone is to demonstrate the modeling of a full-core PWR core with a multiphysics coupling of neutronics (including cross section and neutron transport) and thermal-hydraulics. The neutronics solution is provided by the MPACT code from the University of Michigan, and the thermal-hydraulic solution is provided by the COBRA-TF (CTF) code from Penn State University (PSU). The neutronics and T/H are coupled with the LIME and DTK toolkits.

This demonstration is "Problem 7" of the AMA Progression Benchmark Problems [1]. The original milestone desciption implies running with critical boron search and equilibrium xenon treatment. However, the critical boron search and equilibrium xenon components are left for future work, as demonstrating the neutronics and T/H coupling is more important. The progression problems were defined to help drive development of the VERA Core Simulator capability. The progression problems serve several different functions. The first function is to help developers determine schedule and priorities for implementing features into the core simulator. This is achieved by defining a useful capability in discrete steps ranging from a single pincell up to a full-core depletion. The second function is to inform users when capabilities will be available and provide specific deliveries when users can start verification and validation studies of completed components. The third function, which was not envisioned initially, is to provide measurable metrics that management can use to gauge progress. The VERA Core Simulator is a multi-year development project and it is important to provide management with a long-term schedule and metrics to determine how well progress is being made.

The ten AMA Progression Benchmark Problems are listed in Table 1-1. The purpose of this Milestone report is to document the completion of Problem 7.

Table 1-1 AMA Progression Benchmark Problems

- #1 2D HZP Pincell
- #2 2D HZP Lattice
- #3 3D HZP Assembly
- #4 HZP 3x3 Assembly CRD Worth
- #5 Physical Reactor Zero Power Physics Tests (ZPPT)
- #6 HFP BOL Assembly (begin Challenge Problem coupling)
- #7 HFP BOC Physical Reactor w/ Xenon
- #8 Physical Reactor Startup Flux Maps
- #9 Physical Reactor Depletion
- #10 Physical Reactor Refueling

Note that progression problems 1-5 are at hot zero power (HZP) conditions. At HZP, there is no sensible heat generation, and therefore, no thermal-hydraulic feedback. Problem 6 is the first progression problem that includes heat generation and requires coupled thermal-hydraulic feedback, and was documented in Milestone L3:VRI.PSS.P7.03 [2]. Problem 7 extends Problem 6 to a full-core and adds boron search capabilities.

Section 2 of this report provides a summary of the individual computer codes that were coupled together. Section 3 provides information on how the code coupling is performed. Section 4 contains a description of the test problem used in this Milestone. Section 5 provides results for the single assembly test cases used in Problem 6. Section 6 provides results for full-core problem used in Problem 7. Finally, Section 7 contains a conclusion, discussion of future work, and recommendations going forward.

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In addition, this Milestone would not have been possible without the use of the Eos computer at ORNL. This research used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725.

2. Physics Component Descriptions

This section includes descriptions of the individual physics components (CTF and MPACT) and the VERA Common Input module.

2.1 VERA Common Input (VERAIn)

The VERA Common Input (VERAIn) is a single common input used to drive all of the physics codes in the VERA Core Simulator (VERA-CS). Early in the development of the core simulator, it was recognized that it would be unreasonable to require users to generate input decks for each of the individual physics codes. This is especially true if the core simulator allows multiple codes to solve each physics problem (i.e. multiple subchannel codes, multiple neutronics solvers). In addition to the ease-of-use aspects, it is critical in multiphysics applications that all of the different code systems have consistent input. Having a single common input simplifies the user experience and helps ensure that all of the physics applications are solving a consistent geometry.

The common input is based on a single ASCII input file. The input file uses a free-form input format that is based on keyword inputs. The format of the input file was designed by engineers with broad experience with current industry core design tools, so the format of the input file will be easy for industry users to understand. The ASCII input file provides several advantages to the users:

- Allows users to easily transfer input and output between different computer systems.
- Allows users ability to easily edit the file on remote computers.
- Provides a format that users can readily read and understand.
- ASCII input files are an approved archive format recognized by the NRC (ASCII, PDF, or TIFF).
- Allows users to “diff” input files on a variety of remote computers
- Allows users to archive inputs in standard source code repositories and/or directories with read-only permissions.

The input file contains a description of the physical reactor geometry, including: fuel assemblies, removable poison assemblies, control rods, non-fuel structures, detectors, baffle, etc. The input file also contains a description of the current reactor statepoint including: power, flow, depletion, search options, etc.

In order to translate the user input to input needed for the individual code packages, a multistep process is used. First, an input parser reads the text input file and converts it into an XML file. Some physics codes, such as Insilico and MPACT, can read the XML file directly using readily-available XML libraries. Other codes, such as CTF and Peregrine, require an intermediate step that converts the XML file into the native code input. This process allows the common input file to be used for existing physics codes where we do not want to make extensive modifications to the input.

Currently, the following physics codes can interface with the VERA common input:

- Insilico
- MPACT
- COBRA-TF (CTF)
- Peregrine

Examples of VERA common input files are shown in “Appendix B – Single-Assembly Input File” and “Appendix C – Full-Core Input File”.

It should be noted that there is one class of input that cannot be readily generated by the VERA common input. Some physics codes, such as CFD, require a detailed mesh that is usually generated from a CAD file. For these codes, it is expected that the user will still have to attach an externally generated mesh file and make sure that the mesh file is consistent with the common input.

2.2 COBRA-TF (CTF)

COBRA-TF (CTF) is a thermal-hydraulic simulation code designed for Light Water Reactor (LWR) analysis) [3]. CTF has a long lineage that goes back to the original COBRA program developed in 1980 by Pacific Northwest Laboratory under sponsorship of the Nuclear Regulatory Commission (NRC). The original COBRA began as a thermal-hydraulic rod-bundle analysis code, but versions of the code have been continually updated and expanded over the past several decades to cover almost all of the steady-state and transient analysis of both PWR’s and BWR’s. CTF is currently being developed and maintained by the Reactor Dynamics and Fuel Management Group (RDFMG) at the Pennsylvania State University (PSU).

CTF includes a wide range of thermal-hydraulic models important to LWR safety analysis including flow regime dependent two-phase wall heat transfer, inter-phase heat transfer and drag, droplet breakup, and quench-front tracking. CTF also includes several internal models to help facilitate the simulation of actual fuel assemblies. These models include spacer grid models, a fuel rod conduction model, and built-in material properties for both the structural materials and the coolant (i.e. steam tables). CTF uses a two-fluid, three-field representation of the two-phase flow. The equations and fields solved are:

- Continuous vapor (mass, momentum and energy)
- Continuous liquid (mass, momentum and energy)
- Entrained liquid drops (mass and momentum)
- Non-condensable gas mixture (mass)

Also more recently, several improvements were made to CTF to improve performance and parallelism [16]. Some of the reasons for selecting CTF as the primary T/H solver in the VERA core simulator are the reasonable run-times compared to CFD (although CFD will be available as an option), the fact that it is being actively developed and supported by PSU, and for the ability to support future applications of VERA such as transient safety analysis and BWR and SMR applications.

2.3 MPACT

MPACT is one of the neutronics solvers in the VERA Core Simulator (along with Insilico). For the nuclear data it uses a multi-group cross section library pre-generated using components of the SCALE code system that provide microscopic cross section data as a function of temperature for 100's of isotopes. Reference [4] and [5] contains a detailed description of the methods used in MPACT as a part of the VERA Core Simulator.

In the work reported here the 2-D/1-D method in MPACT is used to obtain the solution of the neutron flux, although a 3-D method of characteristics (MOC) transport solver is also available. In the 2-D/1-D method, the 2-D MOC solver is used for the radial (x,y) domain and a 1-D nodal diffusion method is used to solve the flux in the axial direction. Higher order 1-D transport based methods are currently being developed for problems when a higher degree of accuracy in the axial direction is warranted. The cross section feedback model includes an in-line resonance calculation based on the subgroup method. In the subgroup method the explicit geometric configuration and spatial distribution of the material densities and temperatures within the problem are accounted for. Therefore, the cross section feedback model can be considered direct as it does not rely on any pre-computed or tabulated macroscopic cross sections or simplified models to generate the macroscopic cross sections from the microscopic cross section data.

3. Code Coupling

3.1 Introduction

This Milestone is a demonstration of coupling the two codes MPACT and COBRA-TF (CTF) together to calculate the temperature, fission rate, and neutron flux distribution within a PWR core. All neutronics aspects of the problem (cross-sections, neutron transport, and power release) are solved using MPACT and all thermal-hydraulic aspects (including fuel rod conduction) are solved using CTF. The coupling of these codes to create a single-executable multiphysics coupled-code application is achieved using the VERA infrastructure tools LIME [6] and DTK [7].

3.2 Building a Single Executable

To couple the physics codes CTF and MPACT together, both programs are combined and compiled in a single executable using the subroutine interface to CTF and MPACT along with a top-level LIME problem manager. The LIME problem manager serves as the "main" program, controls the iteration strategy, calls the CTF and MPACT subroutines as needed, and transfers data between the codes using LIME model evaluators and DTK (See Figure 2-1 below).

The single coupled executable is named "VRIPSScobra_mpact_coupled.exe" and contains all of the coupling codes. This program is located in the VERA GIT repository "PSSDrivers":

```
PSSDriversExt/VRIPSS/drivers/cobra_mpact/VRIPSScobra_mpact_coupled.exe
```

Compiling different physics codes together can be a complicated task, especially when the packages are large and rely on additional third-party libraries (TPL's). To overcome these complications, the TriBITS build system is used. In addition to providing the build system, TriBITS also provides an integrated testing platform to help automated developer testing.

TriBITS stands for the "Tribal Build, Integrate, and Test System" and was originally developed for Trilinos, but was later extended for VERA, SCALE and other projects. TriBITS is based on the well-known Kitware open-source toolset CMake, CTest, and CDash. Some additional features of TriBITS include the following:

- Built-in CMake-based package architecture support for partitioning a project into "Packages" with carefully regulated dependencies with numerous features including:
    - Automatic enabling of upstream and downstream packages (critical for large projects like Trilinos, SCALE, and CASL)
    - Integrated MPI and CUDA support
    - Integrated TPL support (coordinate common TPLs across unrelated packages, common behavior for user configuration, etc.)
    - Removal of a lot of boiler-plate CMake code for creating libraries, executables, copying files, etc.
- Powerful TRIBITS_ADD_[ADVANCED]_TEST(…) wrapper CMake functions to create advanced tests

- Integrated support for add-on repositories with add-on packages.
- TribitsCTestDriver.cmake testing driver:
    - Partitioned package-by-package output to CDash and reporting on a package-by-package basis
    - Failed packages don't propagate errors to downstream packages
    - Integrated coverage and memory testing (showing up on CDash)
    - Nightly and continuous integration (CI) test driver.
- Pre-push synchronous CI testing with the Python checkin-test.py script
- In addition: TribitsDashboardDriver system, download-cmake.py and numerous other tools

TriBITS is an open-source project and is available for download from the internet [8].

3.3 LIME

The Lightweight Integrating Multiphysics Environment for coupling codes (LIME) is used to integrate the two physics codes [3][4]. LIME is designed to integrate separate computer codes, which may be written in different languages, into a single package to solve multiphysics problems. LIME provides high-level routines to create a "Problem Manager" to control the overall-iterations and perform communication through "Model Evaluators" for each of the separate physics codes. LIME is an open-source project and is available for download from the internet [9]. A description of how LIME is used to couple CTF and MPACT is provided in Section 3.5.

3.4 Data Transfer Kit (DTK)

The Data Transfer Kit (DTK) library is used to transfer data between the two physics codes. DTK is based on the Rendezvous algorithm [7] and facilitates the transfer of data between multiple codes with different meshes partitioned on different parallel processors. From the DTK website:

> *"The Data Transfer Kit (DTK) is a software component designed to provide parallel services for mesh and geometry searching and data transfer for arbitrary physics components. In many physics applications, the concept of mesh and geometry is used to subdivide the physical domain into a discrete representation to facilitate the solution of the model problems that describe it. Additionally, the concept of the field is used to apply degrees of freedom to the mesh or geometry as a means of function discretization. With the increased development efforts in multiphysics simulation, adaptive mesh simulations, and other multiple mesh/geometry problems, generating parallel topology maps for transferring fields and other data between meshes is a common operation. DTK is being developed to provide a suite of concrete algorithm implementations for these services."*

DTK is an open-source project and is available for download from the internet [10].

3.5 Coupling Strategy

A challenging aspect of coupling neutronics and thermal-hydraulics is that the different physics associated with these two codes are strongly coupled and nonlinear. By strongly coupled we mean that the quantities calculated

in each physics code and passed to the other have a significant impact on the solution of the other physics code. By nonlinear we mean that a change in values calculated in one code do NOT result in a "linearly-proportional" change to values in the other. Figure 2-1 illustrates key aspects of the single-executable coupled-code (MPACT-CTF) simulation capability created within VERA to solve this problem.

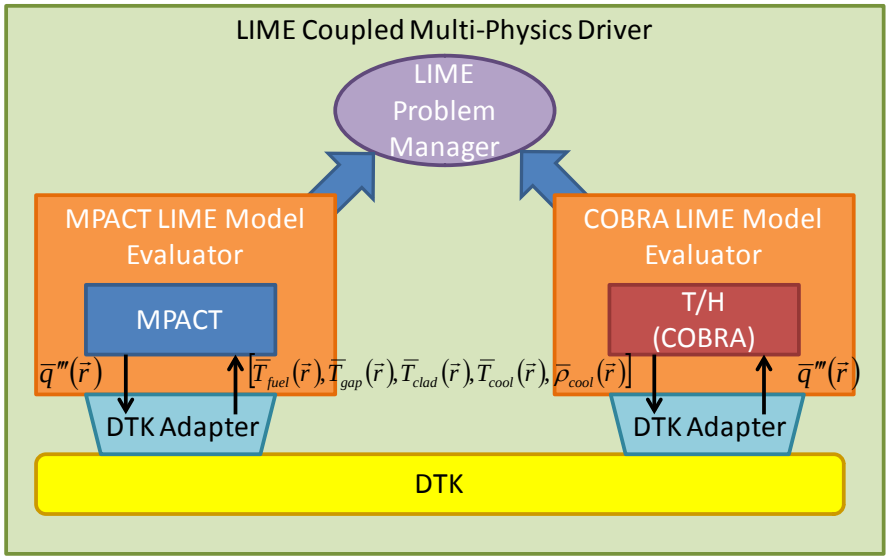


Figure 2-1 Key components of a coupled MPACT-CTF application created to solve the example problem.

To solve the neutronics part of the overall problem, MPACT must be provided with values for the following quantities associated with each rod at each axial level:

1. average fuel temperature, T_f
2. average clad temperature, T_c
3. average coolant temperature surrounding the rod, T_w
4. average coolant density surrounding the rod, ρ_w

Additionally, the average exit conditions of the coolant at the top of the active fuel are needed to approximate the T/H conditions of all the core regions above the active fuel (e.g. plenum, upper tie plate, upper reflector, etc.). Figure 2-2 below shows the regions of the core and how the T/H properties are mapped within MPACT.

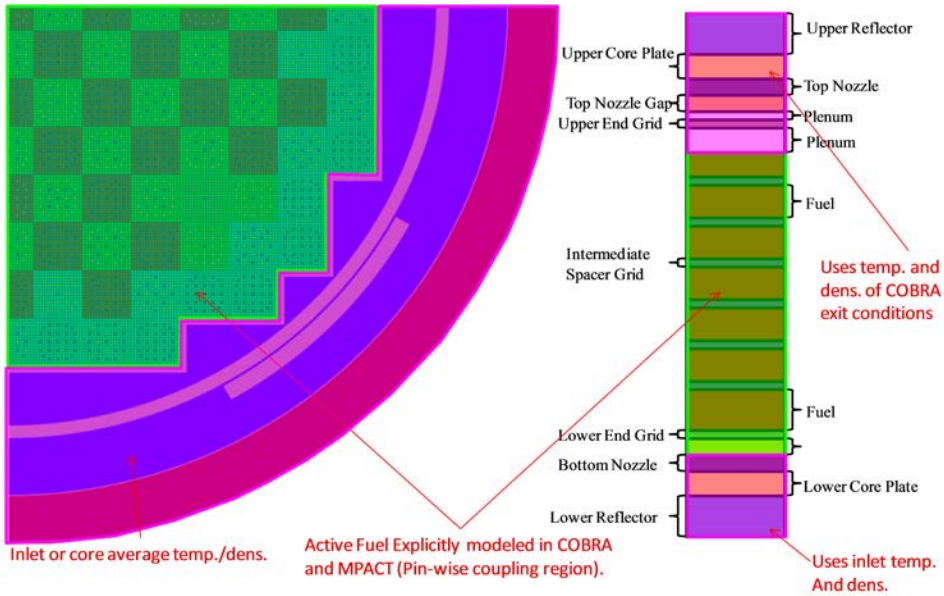


Figure 2-2 T/H Coupling of Core Regions in MPACT

For the active fuel region the following types of pin cell geometries for regular fuel pins and rodded/unrodded guide tubes must be considered for mapping T/H solution data. Rather than create new data containers for the guide tube geometries, either rodded or unrodded, the existing data containers are reused. This is illustrated in Figure 2-3.

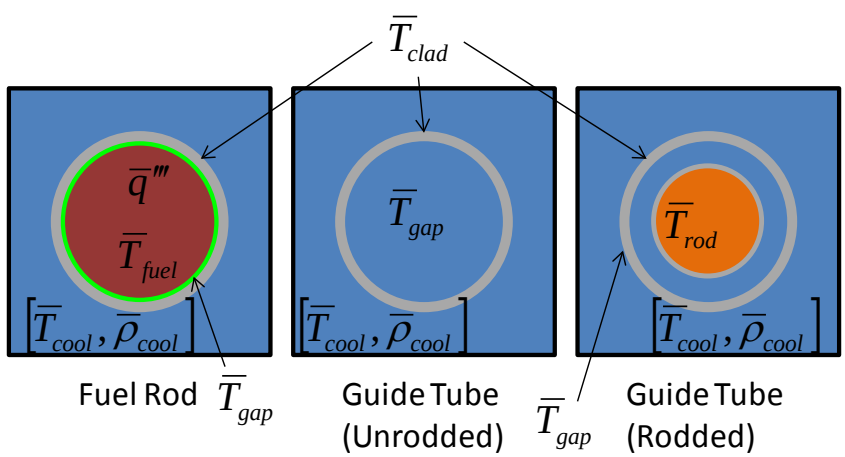


Figure 2-3 Pin Cell Coupling Models used in MPACT

These quantities are calculated in the CTF code and stored in the following two-dimensional arrays in the "transfer_io" module.

`cool_avg_den(n,jh)`	Average Coolant Density
`cool_avg_tmp(n,jh)`	Average Coolant Temperature
`clad_avg_tmp(n,jh)`	Average Clad Temperature
`fuel_avg_tmp(n,jh)`	Average Fuel Temperature

Here *n* denotes the fuel rod and *jh* the axial heat transfer level. Values in these arrays are transferred to MPACT at designated times during the overall solution procedure. Of note is that MPACT is itself solving a multiphysics neutronics problem that involves calculating cross sections, doing neutron transport, and computing energy release.

To solve the thermal hydraulics part of the problem, CTF requires the energy release rate *Q* in each fuel rod at each axial level. These values are computed by MPACT and transferred to CTF. Note that CTF also solves several coupled-physics equation sets internally, i.e. conservation of mass, momentum and energy in the fluid together with heat transfer to fuel rods where energy is being released and conducted within the rods.

The transfer of data between MPACT and CTF is enabled and directed by several additional software components represented in Figure 2-1 (e.g. MPACT and CTF Model Evaluators and DTK adaptors). These small components leverage LIME and DTK and provide the additional functionality needed to create the overall coupled-code simulation capability. In particular, they address the details of how and where the transfer data is stored in each code, and how to correctly transfer that data in the form required by both the "source" and the "target" during each transfer operation.

As described in references [6] and [11], LIME supports several different types of nonlinear solution strategies (i.e. Newton, JFNK, fixed point) depending on the capabilities available from the physics codes being coupled. In this case, we solve the overall coupled nonlinear system using a simple "Fixed Point Iteration" algorithm. This is an iterative method where each physics code is sequentially solved independently within a global iteration loop, and updated transfer-data is passed between physics codes immediately after each physics code solution. In addition, the change in transferred values between iterations can be "relaxed" so as to improve the convergence speed of the approach.

The simplified execution diagram in Figure 2-2 illustrates the fixed point algorithm executed by the LIME problem manager for the example problem.

The first time CTF is asked to perform a solution the power release is internally specified based on a typical power profile that has the correct overall power. Thereafter, the power is specified by the transfer-data received from the most recent MPACT calculation.

Because neither MPACT nor CTF can currently provide a residual vector to LIME, the convergence criteria used here is based on checking that key global metrics associated with the solutions in each code have reached a steady invariant condition within a user-specified tolerance. Currently the following parameters are checked for convergence:

1. Eigenvalue
2. Maximum change in local power
3. Maximum change in local fuel temperature
4. Maximum change in local clad temperature
5. Maximum change in local coolant temperature

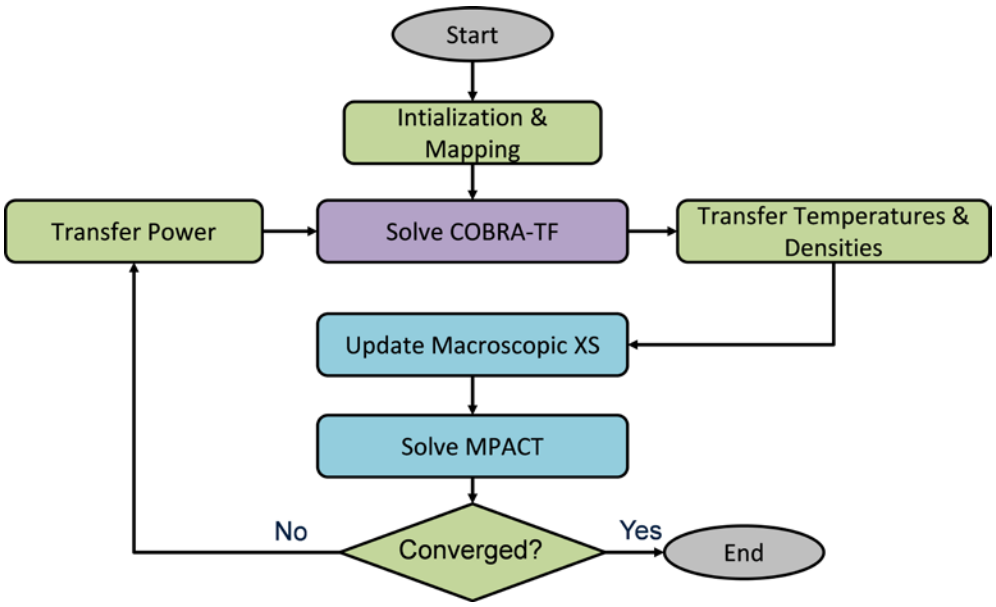


Figure 2-4 Simplified flow chart illustrating the coupled code "Seidel" fixed point algorithm

4. Problem Description

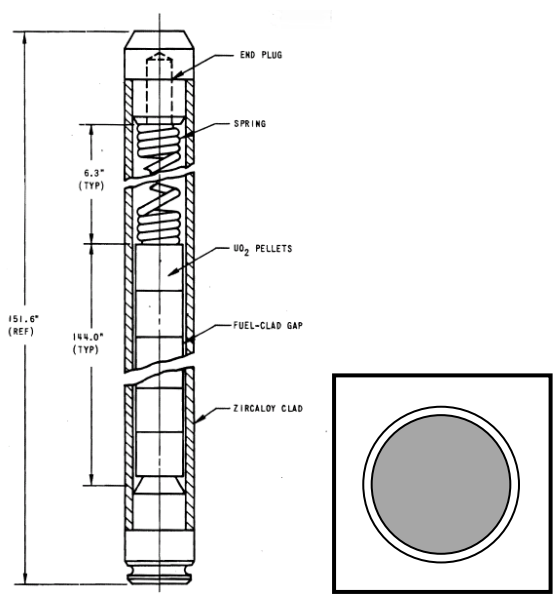
This Milestone report contains results for both single-assembly and full-core calculations. The geometries are described by the AMA Progression Benchmark Problems [1] and are based on the dimensions and state conditions of Watts Bar Unit 1 Cycle 1. The single-assembly coupled problem corresponds to Problem 6, and the full-core coupled problem corresponds to Problem 7. All dimensions are non-proprietary and are derived from the publically available Watts Bar Unit 1 FSAR [12].

4.1 Single-Assembly Description

The first example problem used in this Milestone is a PWR single assembly corresponding to AMA Progression Benchmark Problem 6. Results are shown for different boron concentrations (0, 600, and 1300 ppm) and power levels (70, 100, 130, and 150% power).

The assembly is a standard 17x17 Westinghouse fuel design with uniform fuel enrichment. There are no axial blankets or enrichment zones. The assembly has 264 fuel rods, 24 guide tubes, and a single instrument tube in the center. There are no control rods or removable burnable absorber assemblies in this problem.

The primary geometry specifications of the fuel rod and guide tube materials are given in Figure 4-1 and Table 4-1. The geometry specification for the assembly is given in Figure 4-2 and Table 4-2. For a complete description of the geometry, including spacer grid and nozzle specifications, refer to Reference [13]. The complete input listing for this problem is shown in Appendix B – Single-Assembly Input File.



All dimensions in Figure are in inches

Figure from Reference [12], Figure 4.2-3

Figure 4-1 Fuel Rod Diagram

Table 4-1 Fuel Rod and Guide Tube Descriptions

Parameter	Value	Units
Fuel Pellet Radius	0.4096	cm
Fuel Rod Clad Inner Radius	0.418	cm
Fuel Rod Clad Outer Radius	0.475	cm
Guide Tube Inner Radius	0.561	cm
Guide Tube Outer Radius	0.602	cm
Instrument Tube Inner Radius	0.559	cm
Instrument Tube Outer Radius	0.605	cm
Outside Rod Height	385.10	cm
Fuel Stack Height (active fuel)	365.76	cm
Plenum Height	16.00	cm
End Plug Heights (x2)	1.67	cm
Pellet Material	UO_2	
Clad / Caps / Guide Tube Material	Zircaloy-4	

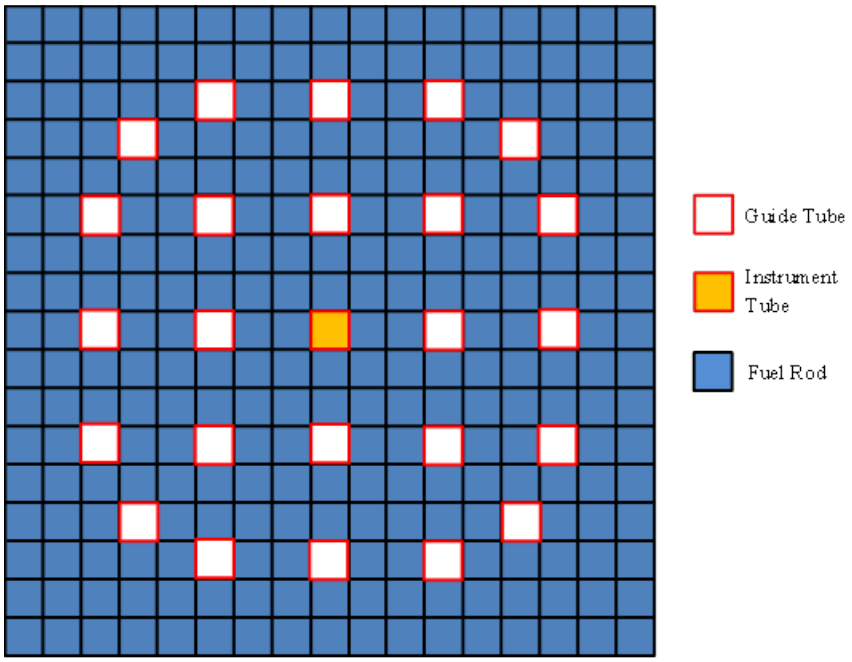


Figure 4-2 Assembly Layout Showing Guide Tubes (GT) and Instrument Tube (IT) placement.

Table 4-2 Assembly Description

Parameter	Value	Units
Rod Pitch	1.26	cm
Assembly Pitch	21.5	cm
Inter-Assembly Half Gaps	0.04	cm
Geometry	17x17	
Number of Fuel Rods	264	
Number of Guide Tubes (GT)	24	
Number of Instrument Tubes (IT)	1	

The thermal-hydraulic specifications for this problem are shown in Table 4-3. The thermal-hydraulic conditions and feedback are the essential difference between Progression Problems 3 and 6.

Table 4-3 Nominal Thermal-Hydraulic Conditions for a Single-Assembly

Parameter	Value	Units
Inlet Temperature	559	degrees F
System Pressure	2250	psia
Rated Flow (100% flow)	0.6824	Mlb/hr
Rated Power (100% power)	17.67	MWt

4.2 Full-Core Description

The second example problem used in this Milestone is a full core PWR corresponding to AMA Progression Benchmark Problem 7. This problem corresponds to Watts Bar Unit 1 Cycle 1. The assembly geometry descriptions for the Watts Bar core are the same as the previous section. The full-core contains 3 enrichment zones (2.1, 2.6, and 3.1% U-235) and several configurations of Pyrex burnable absorber rods. The enrichment zones and Pyrex configurations are shown in Figure 4-3. Additional Core Parameters are shown in Table 4.4. A detailed description of this reactor core is given in [7]. A partial input listing for the full-core problem is shown in Appendix C – Full-Core Input File.

	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 4-3 Core Layout for Watts Bar Unit 1 Cycle 1

Table 4-4 Full-Core Description

Parameter	Value	Units
Number of Fuel Assemblies	193	
Assembly Pitch	21.5	cm
Inlet Temperature	559	degrees F
System Pressure	2250	psia
Rated Flow (100% flow)	131.68	Mlb/hr
Rated Power (100% power)	3411	MWt
Boron Concentration	1225	ppm
Baffle Gap	0.19	cm
Baffle Thickness (stainless steel)	2.85	cm

5. Single-Assembly Results

5.1 Modeling Options

In the neutronics solution, the MPACT solver is used with the “Chebyshev-Gauss” quadrature set (16 azimuthal angles and 4 polar angles per octant) and the ray spacing used was 0.05 cm. For the scattering source a "limited" transport corrected P_0 approximation was used which helps to insure the positivity of the total MOC region source by limiting the traditional out-scatter approximation of the higher order scattering source to be positive, but is “limited” to the fast energy groups above 1 MeV. The cross section library used was the "declib56g_e7_v3.0_0708.fmt" library provided by ORNL to UM. Axial boundaries are positioned at each material and edit interface. The neutron flux is calculated from below the lower core plate to above the upper core plate in order to accurately capture the axial leakage effects. The MOC meshing used for the radial domain is illustrated in the Figure 5-1 below.

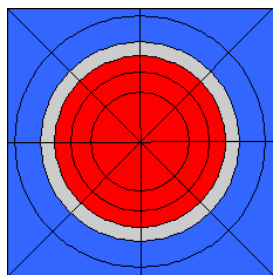


Figure 5-1 2-D MOC mesh for a fuel pin

In the T/H solution, CTF has 49 axial levels over the active fuel region. The axial levels are defined to explicitly include the spacer grid, and to use uniform mesh spacing between the spacer grids. The maximum axial mesh is approximately 7 cm. The exact axial levels used in CTF are listed in the `[EDITS]` block of the sample input file. The CTF fuel rod heat conduction model uses 3 radial rings in each fuel rod. Data transfer between MPACT and CTF occurs at each fuel rod on each axial level of the mesh.

Because this problem uses the same discretization as that used for the reference AMA problem 3 results [14], it is expected that the discretization should provide reasonably accurate results. The purpose of this Milestone is to demonstrate the coupling between neutronics and T/H, so no comparisons are made to other solutions. Instead the results are evaluated against expectations based on engineering experience.

5.2 Single-Assembly Results

A typical iteration summary for the single-assembly at 600 ppm boron is shown in Table 5-1.

- The first column shows the coupled iteration count.
- The second column (its) shows the number of MPACT iterations taken per coupled iteration.
- The third column (keff) shows the reactor eigenvalue.
- The fourth column (ΔK-eff) shows the change in eigenvalue between coupled iterations.

- The fifth column shows the maximum coolant temperature (degrees F, which are native CTF units) averaged over a single subchannel mesh and axial mesh.
- The sixth and seventh columns show the maximum clad and fuel temperatures (degrees F, which are native CTF units) averaged over a single fuel rod and axial mesh.
- The eighth through tenth columns show the change in peak temperatures between iterations for the coolant, clad, and fuel respectively.

Table 5-1 Iteration Summary at 600 ppm boron and 100% power

Iter.	K-iters	K-eff	ΔK-eff	Cool. Temp.	Clad Temp.	Fuel Temp	Cool. ΔT	Clad. ΔT	Fuel. ΔT
1	14	1.2524522		622.22	691.56	1501.75	63.22	91.26	102.16
2	16	1.2501686	-228.36	623.08	690.37	1884.50	0.86	-1.19	382.75
3	16	1.2495716	-59.70	623.36	696.31	1990.58	0.28	5.95	106.09
4	15	1.2493939	-17.77	623.37	697.97	2017.66	0.00	1.65	27.08
5	15	1.2493439	-5.00	623.36	698.34	2026.14	-0.01	0.38	8.48
6	15	1.2493262	-1.77	623.37	698.54	2028.37	0.01	0.20	2.23
7	15	1.2493198	-0.64	623.38	698.61	2029.10	0.01	0.07	0.74
8	15	1.2493172	-0.26	623.38	698.64	2029.34	0.01	0.03	0.24
9	15	1.2493140	-0.32	623.43	698.73	2029.35	0.05	0.09	0.01

The eigenvalue convergence is set to 5 pcm ($1x10^{-5}$ delta-k), however, the convergence criterion for temperatures are relatively tight. The most limiting convergence criteria is the maximum change in peak fuel temperature, which has a convergence criteria of 0.1 degrees F. All of the coupled iteration parameters are set in the `[COUPLED]` block of the input file. The normalized radial fission rate distribution integrated over the axial direction is shown in Figure 5-2. Note that the results are octant symmetric and there is no power in the guide tubes or instrument tubes.

0.943	0.938	0.942	0.952	0.962	0.972	0.970	0.971	0.975	0.971	0.970	0.972	0.962	0.952	0.942	0.938	0.943
0.938	0.936	0.945	0.963	0.983	1.011	0.988	0.988	1.011	0.988	0.988	1.011	0.983	0.963	0.945	0.936	0.938
0.942	0.945	0.973	1.017	1.038		1.028	1.027		1.027	1.028		1.038	1.017	0.973	0.945	0.942
0.952	0.963	1.017		1.054	1.047	1.011	1.007	1.033	1.007	1.011	1.047	1.054		1.017	0.963	0.952
0.962	0.983	1.038	1.054	1.036	1.047	1.014	1.011	1.037	1.011	1.014	1.047	1.036	1.054	1.038	0.983	0.962
0.972	1.011		1.047	1.047		1.040	1.038		1.038	1.040		1.047	1.047		1.011	0.972
0.970	0.988	1.028	1.011	1.014	1.040	1.013	1.012	1.039	1.012	1.013	1.040	1.014	1.011	1.028	0.988	0.970
0.971	0.988	1.027	1.007	1.011	1.038	1.012	1.012	1.038	1.012	1.012	1.038	1.011	1.007	1.027	0.988	0.971
0.975	1.011		1.033	1.037		1.039	1.038		1.038	1.039		1.037	1.033		1.011	0.975
0.971	0.988	1.027	1.007	1.011	1.038	1.012	1.012	1.038	1.012	1.012	1.038	1.011	1.007	1.027	0.988	0.971
0.970	0.988	1.028	1.011	1.014	1.040	1.013	1.012	1.039	1.012	1.013	1.040	1.014	1.011	1.028	0.988	0.970
0.972	1.011		1.047	1.047		1.040	1.038		1.038	1.040		1.047	1.047		1.011	0.972
0.962	0.983	1.038	1.054	1.036	1.047	1.014	1.011	1.037	1.011	1.014	1.047	1.036	1.054	1.038	0.983	0.962
0.952	0.963	1.017		1.054	1.047	1.011	1.007	1.033	1.007	1.011	1.047	1.054		1.017	0.963	0.952
0.942	0.945	0.973	1.017	1.038		1.028	1.027		1.027	1.028		1.038	1.017	0.973	0.945	0.942
0.938	0.936	0.945	0.963	0.983	1.011	0.988	0.988	1.011	0.988	0.988	1.011	0.983	0.963	0.945	0.936	0.938
0.943	0.938	0.942	0.952	0.962	0.972	0.970	0.971	0.975	0.971	0.970	0.972	0.962	0.952	0.942	0.938	0.943

Figure 5-1 Normalized Radial Fission Rate Distribution at 600 ppm and 100% power

A map of the coolant density in the top axial elevation of the core is shown in Figure 5-2. The coolant density shown in this map is the average density surrounding each rod, and not the density in each CTF channel. The calculation for this density is described in Appendix A. Note that the exit density is lower in the center of the assembly, corresponding to the higher fuel rod powers shown in Figure 5-2.

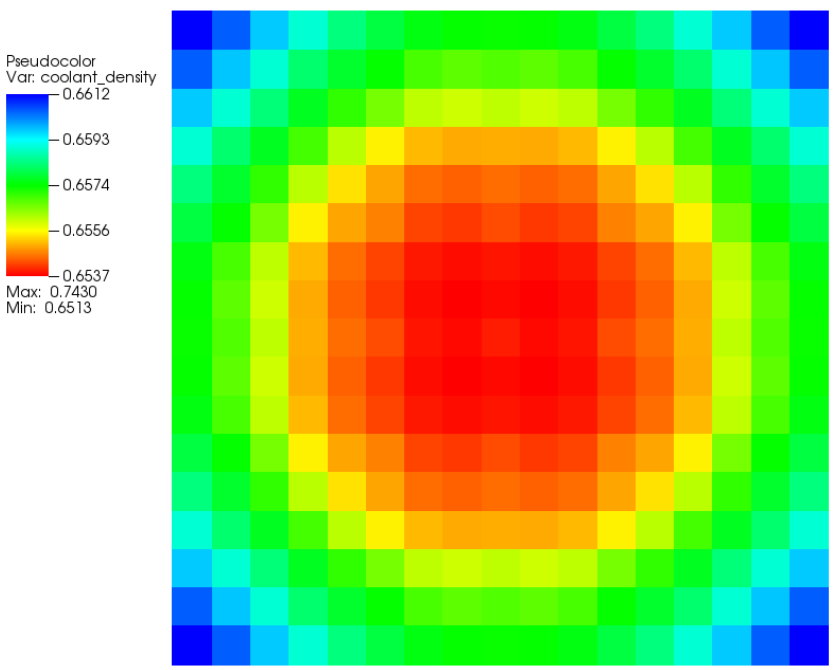


Figure 5-2 Exit Coolant Density (g/cc) at 600 ppm and 100% power

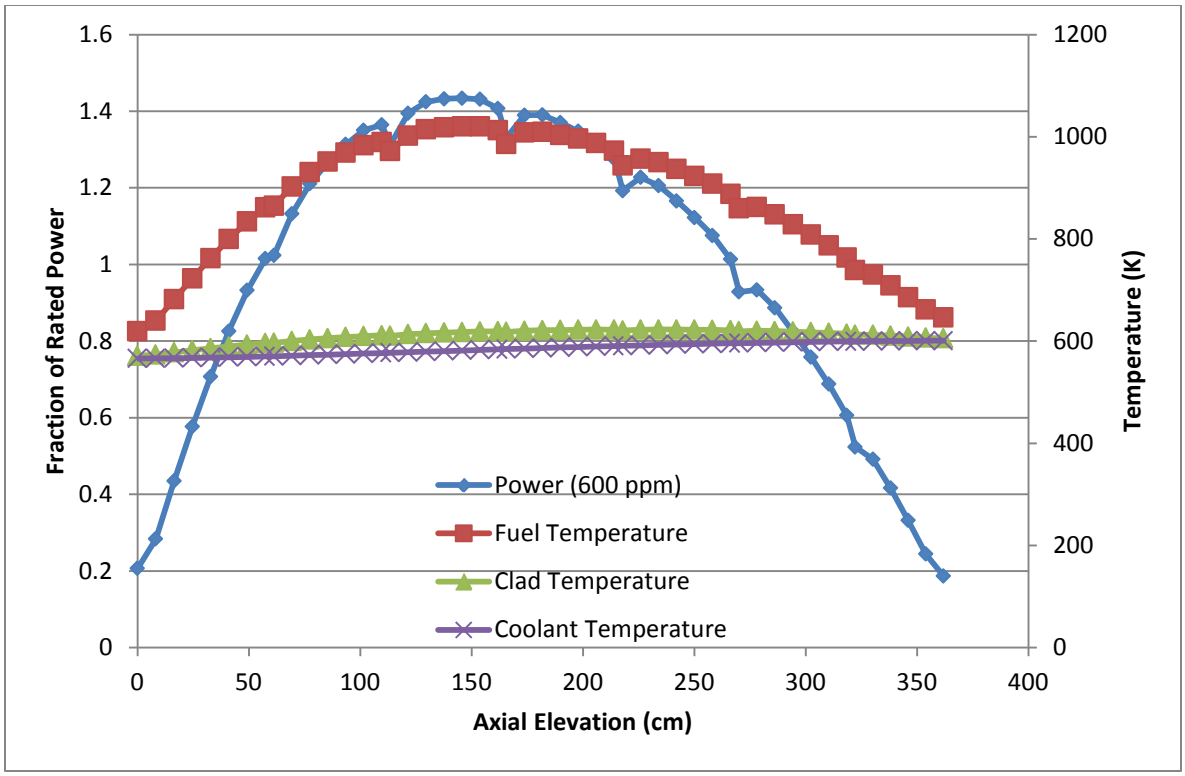


Figure 5-3 Axial Distributions at 600 ppm and 100% power (with fuel temperature shown)

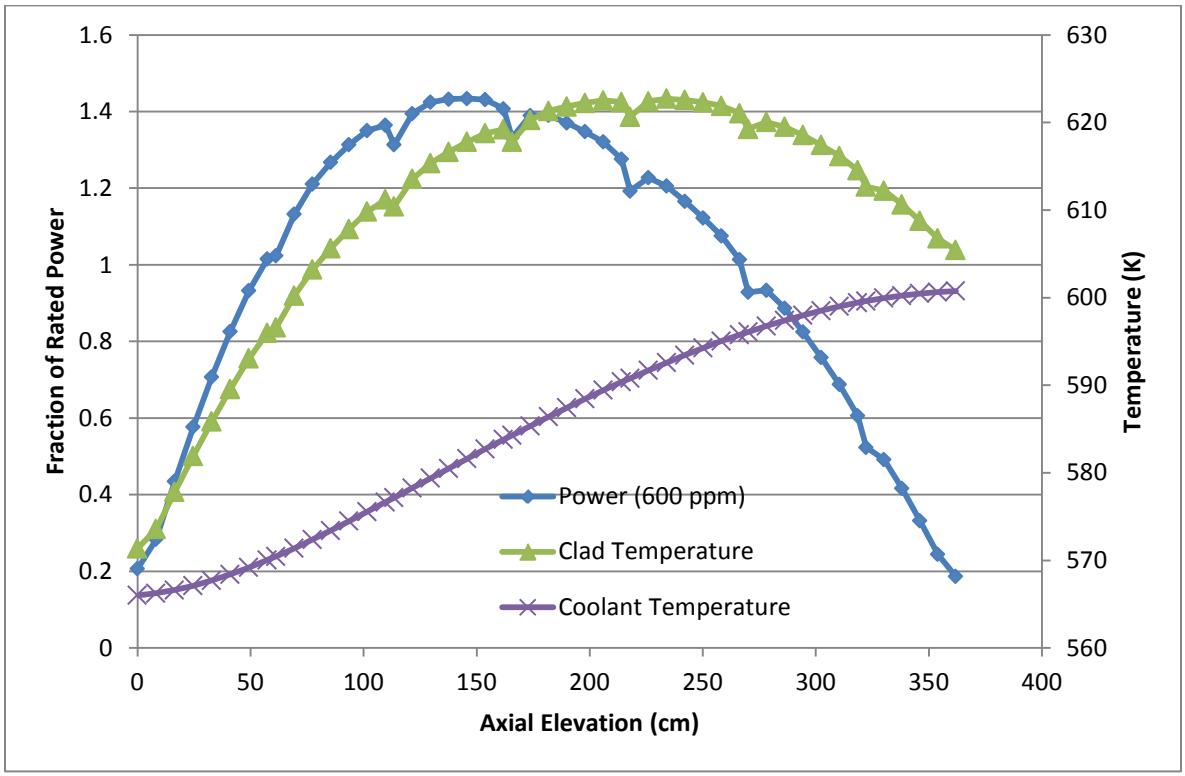


Figure 5-4 Axial Distributions at 600 ppm and 100% power (without fuel temperature)

5.3 Boron Perturbations

In order to examine the effects of different boron concentrations on the results, the single-assembly case was run at three different boron concentrations – 0, 600, and 1300 ppm boron. The eigenvalues and wall-clock times for these cases are listed in Table 5-2.

Table 5-2 Iteration Summary for Boron Cases

Boron Concentration	Eigenvalue	Wall Time (HH:MM:SS)	Coupled Iterations
0 ppm	1.32907	4:50:24	8
600 ppm	1.24710	4:39:58	9
1300 ppm	1.16467	5:04:01	10

The fission rate and fuel temperature profiles for three different boron concentrations are shown in Figure 5-6. With T/H feedback, the fission rate shape is shifted lower in the core from the normal cosine-shaped distribution which occurs with no T/H feedback. The reason for this downward shift in the fission rate is that the coolant density is higher at the bottom of the core, and the higher coolant density increases the neutron moderation. As more boron is added, the additional neutron absorption counters the higher moderation, and less power shift towards the bottom of the core is observed.

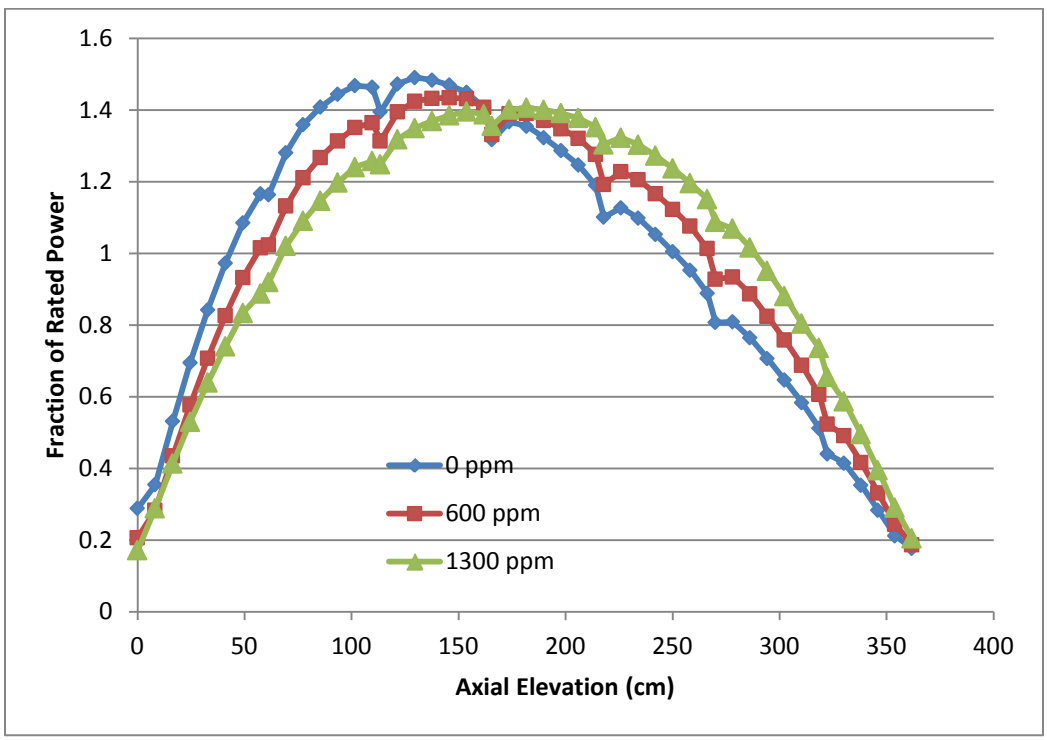
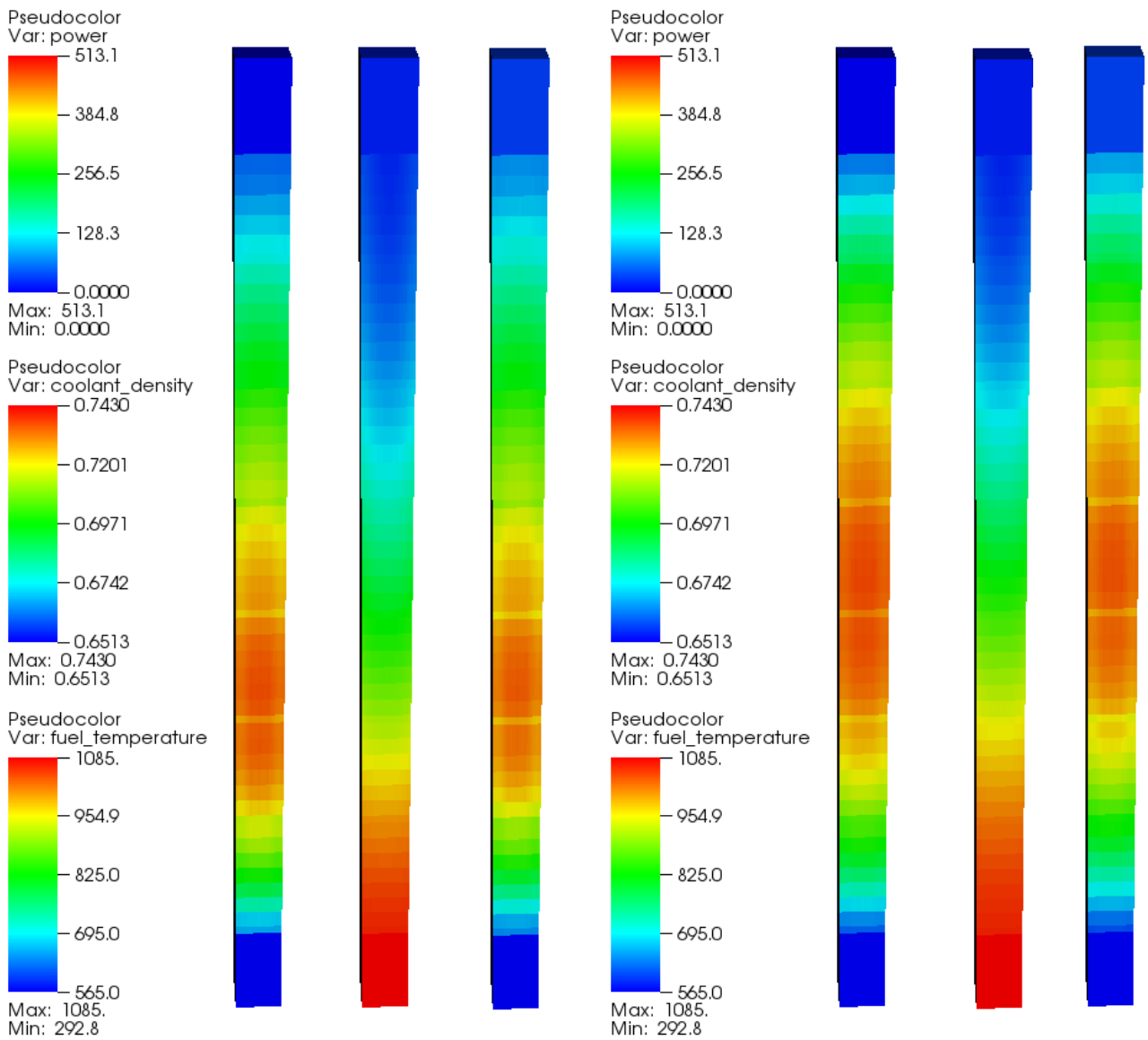


Figure 5-5 Axial Plot of Fission Rates at Different Boron Concentrations

In order to display 3D distributions, the coupled code also produces output in the form of SILO files. These files can be used by visualization tools, such as VisIt or ParaView, to look at 3D plots of the output. Figure 5-7 shows an example of 3D distributions of the fission rate, coolant density, and fuel temperature for cases at 0 ppm and 1300 ppm boron. (Note that the results in this figure were generated with different code options and are not consistent with the results in the other figures.)



0 ppm 1300 ppm

Figure 5-6 Graphical Output of the Fission Rate, Coolant Density, and Fuel Temperatures at 0 and 1300 ppm Boron

5.4 Power Perturbations

In order to observe the effects of different power levels on the results, the nominal single-assembly case was run at four different power levels – 70, 100, and 130% power. The eigenvalues and wall-clock times for these cases are shown in Table 5-3.

Table 5-3 Iteration Summary for Power Cases

Power Level	Eigenvalue	Wall Time (HH:MM:SS)	Coupled Iterations
70%	1.25301	4:35:52	9
100%	1.24710	4:39:58	9
130%	1.24080	5:20:52	10

The fission rate profiles for the four power cases are shown in Figure 5-7. At higher power levels, the fission rate shape is shifted lower in the core from the normal cosine-shaped distribution you would see with no T/H feedback.

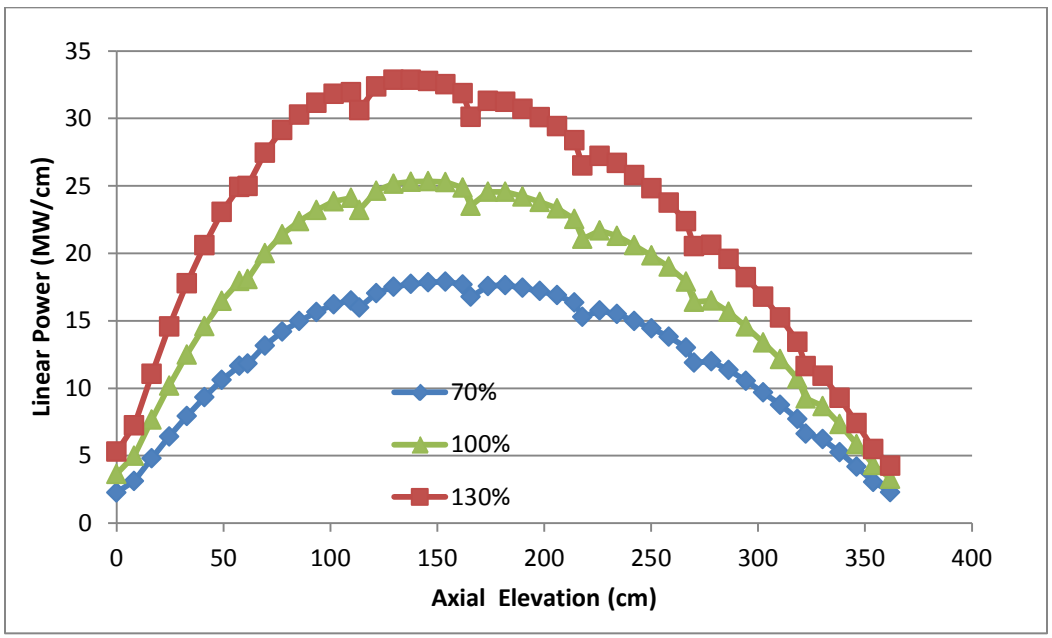


Figure 5-7 Axial Plot of Fission Rates at Different Power Levels

6. Full-Core Results

This section reports the results for a full-core 3D model (quarter core symmetric) calculation with a coupled MPACT-CTF solver described earlier.

6.1 Full-Core Development

In the development of the full core coupled model, the primary challenge was to ensure consistent mapping between CTF and MPACT. Previously in [2] the mapping was demonstrated for a single assembly, however, for the full core model there are several addition considerations. These include the treatment of the radial reflector and baffle, multiple fuel assemblies, symmetry, and parallel decomposition of the radial spatial domain. The initial implementation of the mapping could also account for the radial reflector/baffle assemblies and multiple assemblies. However, significant modifications were needed to handle symmetry and the radial decomposition. A principal issue encountered was with symmetry and radial decomposition since MPACT will split the fuel pins along the symmetry line of the assembly into halves or quarters for all assemblies. It was then necessary to condense this information to a single entry for mapping. When using parallelism, multiple domains would have part of the information for the same pin. So a communication scheme was required which determined which process owned the pin data for mapping needed so that the same pin was not mapped multiple times within CTF. The current implementation of DTK only supported a 1-to-1 mapping and not a many-to-1. This is due to the problem of how to reduce the solution field data when mapping. It was determined that this operation should be defined by the individual physics solvers, rather than the data transport library since the method of the reduction operation may differ for different physics solvers.

Additionally, it was expected that a restart file capability would be needed to run the coupled problem to convergence within the wall time limits of the target platform. However this did not turn out to be the case because the simulation was able to converge within the allowable wall time. However, significant progress was made in the implementation of a restart file capability. This capability will be needed in future AMA benchmark problems (most likely problem 8 and definitely problem 9).

6.1.1 Progress towards restart capability

The resart or "checkpoint" capability was implemented to the point of integral testing. The checkpoint file is differentiated from a restart capability in the sense that a checkpoint file is used to "pause" a simulation that will be continued at a later time, essentially being run in the exact same fashion. The restart file can be thought of as a more general case of the checkpoint file whereby new calculations restarted from a restart file can use a different mesh, or different state of the reactor. The checkpoint file requires, and enforces, a consistent input, mesh and state between the simulations reading and writing the file. In terms of their usage, the checkpoint file may be written after each outer iteration of a steady-state eigenvalue problem at any point in the simulation. The restart file is only written for a converged steady state solution. The user has some control on when a checkpoint file is written, in order to facilitate job monitoring in queue or batch systems on large super computers. If a file named "`MPACT_CHECKPOINT`" is placed in the working directory of the simulation then MPACT will write a checkpoint file at the end of the next outer iteration. This allows users to not lose the progress of their simulations if the job was specified with an insufficient wall time, to be able to do this after the

simulation has started running is useful because it is not always known *a priori* how long it will take the simulation to converge.

6.2 Full-Core Modeling Options

This section describes the modeling options used to model the full-core reactor. The full-core results were run with a VERA build from 3/28/2014. The results were run on Eos using 2,784 cores (48 radial by 58 axial). The cross section data used was a 56 energy group library generated by ORNL on September 4, 2013.

For this problem, most of the same geometry and thermal-hydralic conditions shown in Figure 4-3 and Table 4-4 were used. This core has 8 control rod banks, 4 of which are operational banks and the other 4 are shutdown banks. In these cases, all control rod banks were withdrawn, and a boron concentration of 1285.2 ppm was used. The axial mesh modeled 58 planes including the upper and lower core plates, a top and bottom axial reflector, upper and lower nozzles, a homogenized lower assembly gap and plug, a homogenized upper assembly gap and plug, 3 upper plenum regions, and 49 fuel planes. The maximum axial mesh is 8.827 cm and the minimum is 3.578 cm. The pin mesh has three sub-radii for the fuel and center guide tube regions, and one sub-radius for all other radial material regions. The pins are also divided azimuthally into octants. The azimuthal discretization of the pin mesh may be adjusted automatically to ensure at least one ray traverses the region. The ray parameters used were 0.05 cm ray spacing, 8 azimuthal angles, and 3 polar angles. The Chebyshev quadrature was used in the azimuthal direction and the 1-D Gauss quadrature was used in the polar direction. This mesh was similar to that used in [15], but no mesh parametrics were performed to ensure a mesh converged solution for the reported results since the objective of the milestone is to demonstrate the capability.

The parallel partitioning for this problem consisted of only decomposing in space. In the radial direction, 48 regions were specified, the smallest of which was a 2 by 2 region of quarter assemblies, or a full assembly. The largest was a 3 by 3 region, which is 2.25 full assemblies. The problem was fully decomposed axially.

For COBRA-TF, the solution is generated with CTF using 49 axial levels in the active fuel region. The axial levels are defined to explicitly include the spacer grid heights, and to use uniform mesh spacing between the spacer grids. The maximum axial mesh is approximately 8 cm. The exact axial levels used in CTF are listed in the `[EDITS]` block of the sample input file. The CTF fuel rod heat conduction model uses 3 radial rings in each fuel rod. Data transfer between MPACT and CTF occurs at each fuel rod on the 49 axial level mesh, also known as the "coupling mesh".

The iteration controls for this problem varied, but the convergence criteria were relatively tight. For MPACT, there were several options enabled to aide in the stability and convergence of the problem. The 2D-1D options

used were NEM for the axial solver, transverse leakage splitting, and under relaxing the transport sweeper solution by a factor of 0.5 on top of the automatic under relaxation normally performed. For CMFD, Weilandt shift was not used and the maximum number of iterations for CMFD is set to 200. The solver type sweeper was a 1-Group sweeping of the linear system. The scattering treatment method used was P_2 and the boundary update method for the incoming angular flux was P_0. The eigenvalue tolerance was set to 1.0E-7 and the fission source tolerance was set to 1.0E-5.

6.3 Results

A typical iteration summary for the full core calculation is shown in Table 6-1.

- The first column shows the coupled fixed point iteration count.
- The second column (K-iters) shows the number of MPACT steady-state eigenvalue iterations taken per coupled fixed point iteration.
- The third column (K-eff) shows the reactor eigenvalue.
- The fourth column (ΔK-eff) shows the change in eigenvalue between coupled iterations.
- The fifth column shows the maximum coolant temperature (degrees C) averaged over a single subchannel mesh and axial mesh.
- The sixth and seventh columns show the maximum clad and fuel temperatures (degrees C) averaged over a single fuel rod and axial mesh.

The eigth through tenth columns show the change in peak temperatures between iterations for the coolant, clad, and fuel respectively. As with the single assembly problem the limiting criteria was that placed on the change in the maximum fuel temperature. Furthermore the total number of iterations to reach convergence were basically the same as the single assembly problem (9 vs. 10).

Table 6-1 Iteration Summary of Full Core Calculation

Iter.	K-iters	K-eff	ΔK-eff	Cool. Temp.	Clad Temp.	Fuel Temp	Cool. ΔT	Clad. ΔT	Fuel. ΔT
1	20	0.988204	---	327.75	366.85	817.21	35.90	52.04	58.55
2	17	0.985898	-230.51	334.48	382.74	1274.25	6.72	15.88	457.05
3	12	0.985248	-65.08	336.86	389.58	1415.16	2.38	6.85	140.91
4	10	0.985039	-20.84	337.38	391.36	1453.84	0.52	1.78	38.68
5	8	0.984974	-6.5	337.50	391.77	1465.36	0.12	0.41	11.52
6	9	0.984951	-2.35	337.60	391.95	1468.77	0.10	0.18	3.41
7	9	0.984942	-0.89	337.64	392.01	1469.93	0.04	0.06	1.16
8	6	0.984936	-0.58	337.82	392.12	1470.38	0.18	0.11	0.45
9	2	0.984935	-0.12	337.85	392.11	1470.44	0.02	-0.01	0.06
10	5	0.984935	0.02	337.86	392.11	1470.46	0.02	-0.01	0.02

Table 6-2 provides a more detailed break down of the time spent in each phase of the coupled calculation. The total walltime was 12 hours and 11 minutes on 2784 processors. The sums of the first three columns are displayed in the pie chart of Figure 6-1 to show the relative fractions spent in each major phase of the calculation. CTF required relatively little time compared to the other phases of the coupled calculation. The time for each subgroup calculation is essentially constant for each iteration since this this a fixed source problem. As noted in Table 6-1 the number of eigenvalue iterations for each fixed point iteration is generally reduced with increasing fixed point iteration, this correlates to shorter times for the eigenvalue calculation in MPACT. The time per eigenvalue iteration also tends to change as the CMFD typically takes less iterations as the coupled calculation progresses. The time spent in CMFD versus MOC for the eigenvalue calculation was not measured explicitly, but is presently estimated to be around 80% in MOC and 20% in CMFD. Reducing the computational requirements of MPACT is a clear priority for reducing the overall execution time for coupled problems. There appear to be some simple changes that could reduce the MPACT computational time without changing the accuracy of the neutronics solution (e.g. calling the subgroup less frequently, perhaps for the last 5 iterations, could reduce the simulation time by roughly 2.5 hours).

Table 6-2 Run-Time Summary of Full Core Calculation (seconds)

Iter.	CTF*	Subgroup	Eigenvalue	Total MPACT	Total F.P. Iter
1	303	1434	6804	8238	8540
2	293	1425	5436	6861	7154
3	292	1424	3890	5314	5606
4	212	1427	3027	4454	4666
5	131	1426	2064	3490	3621
6	126	1425	1961	3386	3512
7	128	1423	1752	3175	3303
8	163	1424	1262	2686	2849
9	127	1424	397	1821	1948
10	116	1425	963	2388	2504
Total	1891	14257	27556	41813	43703

* - CTF times also include all time needed for data transfers

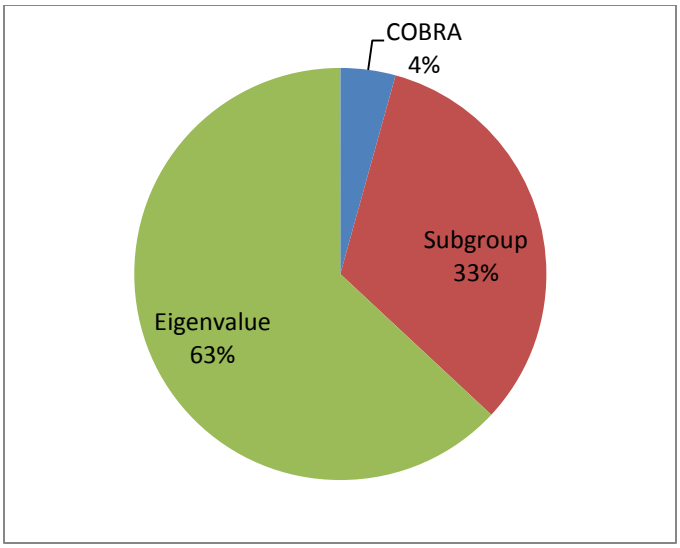


Figure 6-1 Relative Time Spent in each Phase of Calculation

The power is summarized in Figures 6-2 through 6-5. In Figure 6-2 it is noted that the power distribution is not symmetric about the diagonal, although the model is 1/8th symmetric. This suggests some issue in the model, coupled mapping, edit, or the solution methodology of MPACT that requires further investigation.

	H	G	F	E	D	C	B	A
8	1.0690	0.9921	1.0625	1.0295	1.1292	1.0472	1.0463	0.7767
9	0.9922	1.0564	0.9505	1.1084	1.0656	1.1375	1.0325	0.8803
10	1.0626	0.9525	1.0894	1.0556	1.1630	1.1245	1.0583	0.7866
11	1.0293	1.1055	1.0556	1.1559	1.0847	1.1204	1.0179	0.6529
12	1.1304	1.0667	1.1641	1.0856	1.2684	0.8967	0.9280	
13	1.0499	1.1431	1.1245	1.1251	0.8955	0.9090	0.6301	
14	1.0492	1.0355	1.0637	1.0202	0.9293	0.6325		
15	0.7785	0.8821	0.7864	0.6542				

Figure 6-2 2D Assembly Power Results

Table 6-2 and Figure 6-3 show a summary of the location of the min and max rod powers and their axial shape compared to the core average. The power surpression near the grid spacers in the core average appears to be over-estimated which may be an issue with the edit or the model. The power is slightly peaked below the core mid-plane as expected and in general the shape of the power in the peak rod follows the shape of the core average.

Table 6-2 Pin Power Results

	Power	Pin Location	Axial Plane Midpoint	Assembly
2D min rod	0.1647	(17,17)	---	C-14
2D max rod	1.3885	(5,6)	---	D-12
3D min	0.0312	(17,17)	18.884 cm	C-14
3D max	1.9661	(5,6)	170.5975 cm	D-12

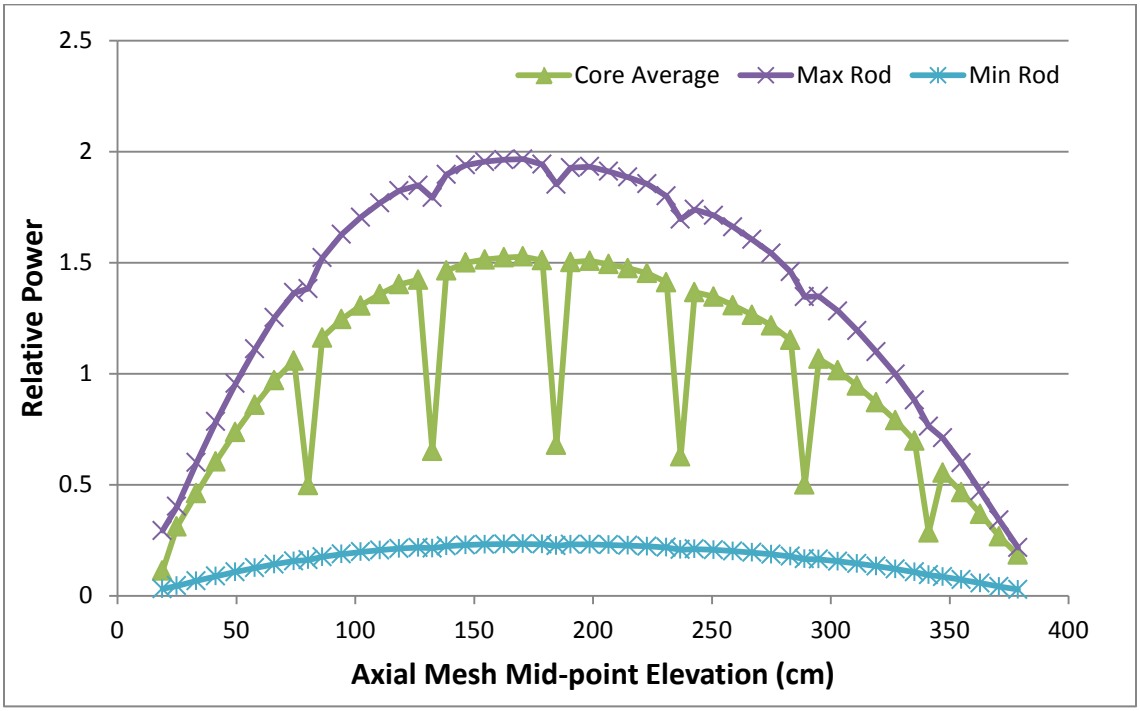


Figure 6-3 Axial Plots of Maximum, Minimum, and Average Rod Powers

Figure 6-4 shows the 3D power distribution for this problem. The cutout is provided to show the power at the interior of the core.

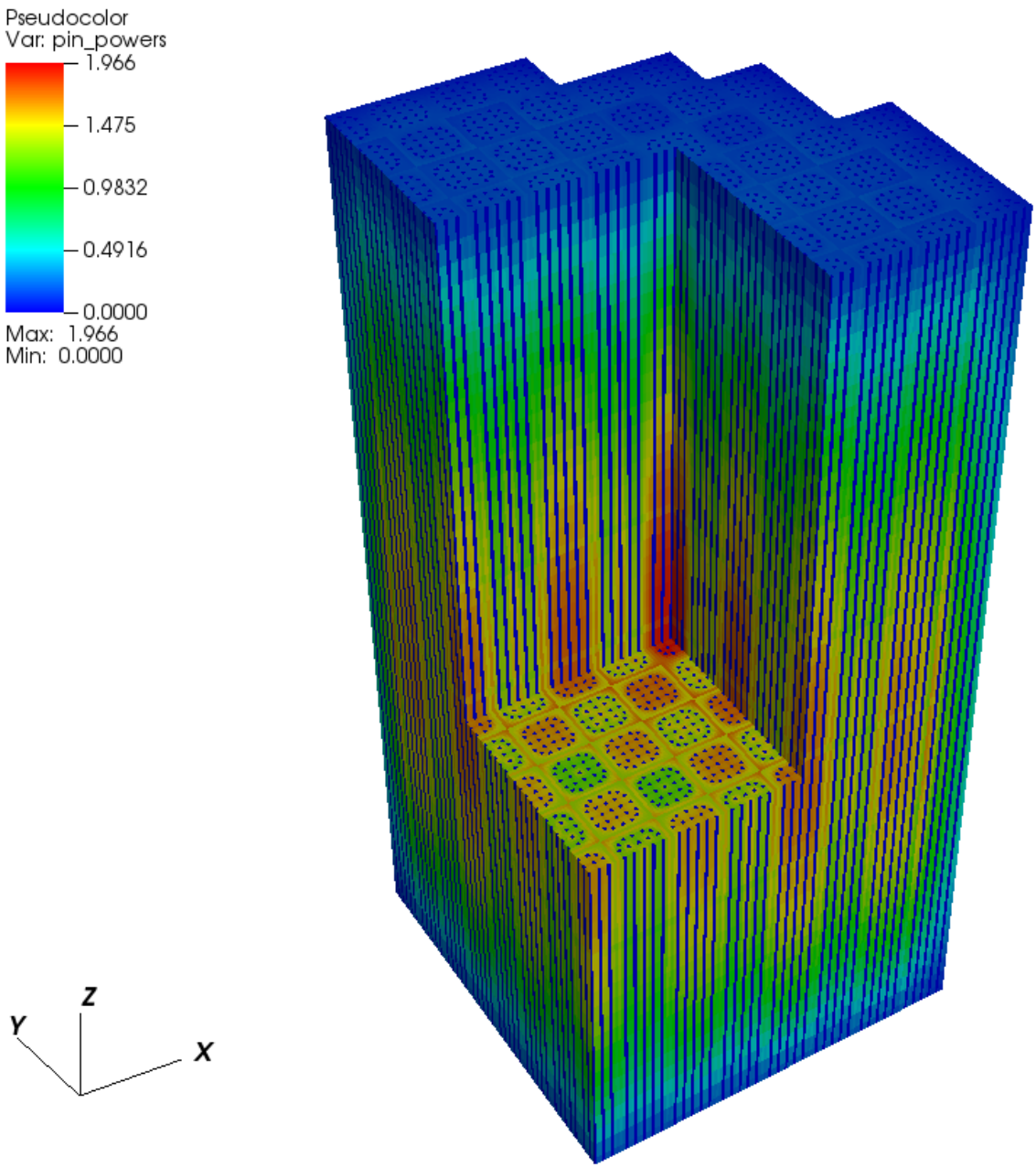


Figure 6-4 3D Power Distribution with a cutout at the top of the core

Figure 6-5 shows a 3D figure of the coolant enthalpy in the active fuel region. This figure shows that the enthalpy rise is not uniform and is closely related to the assembly powers.

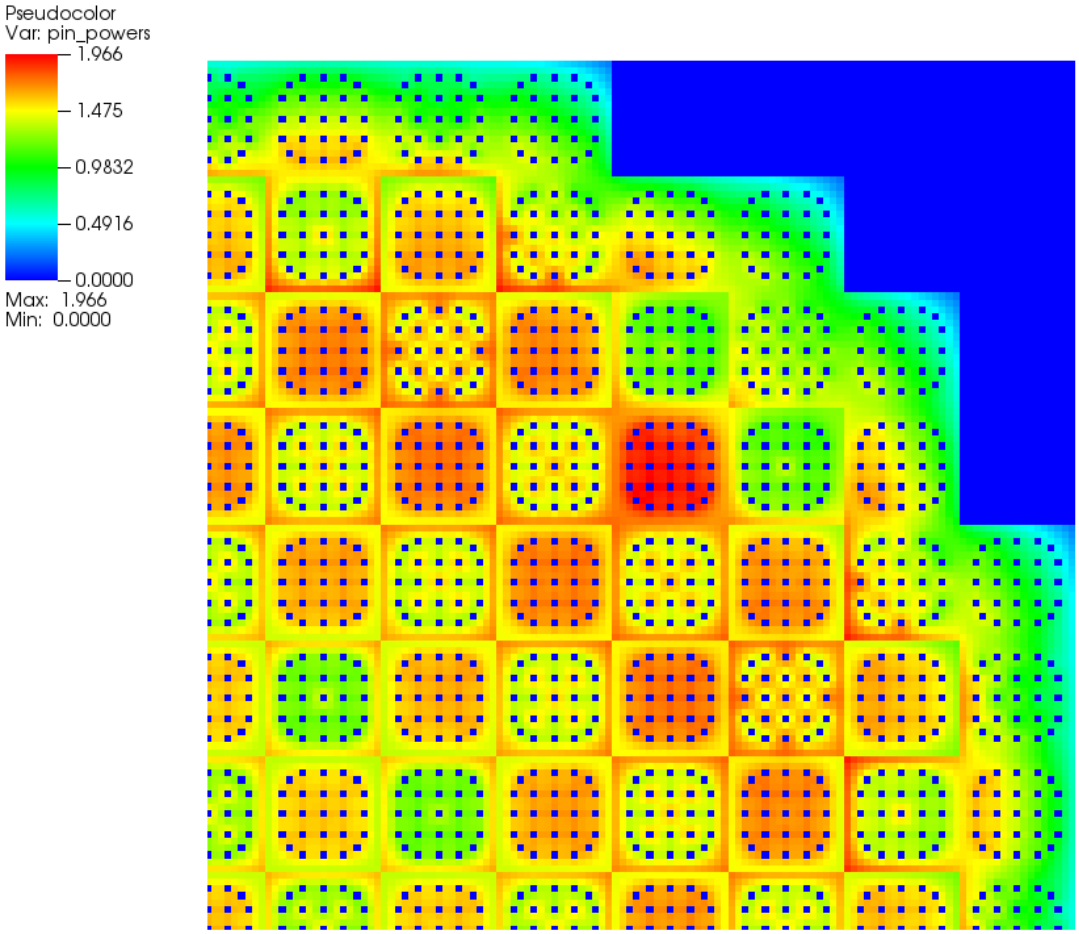


Figure 6-5 2D Slice of Power Distribution near the Core Midplane

Figure 6-6 shows a 2D figure of the coolant enthalpy at the core exit. Note the large enthalpy gradients at the core periphery.

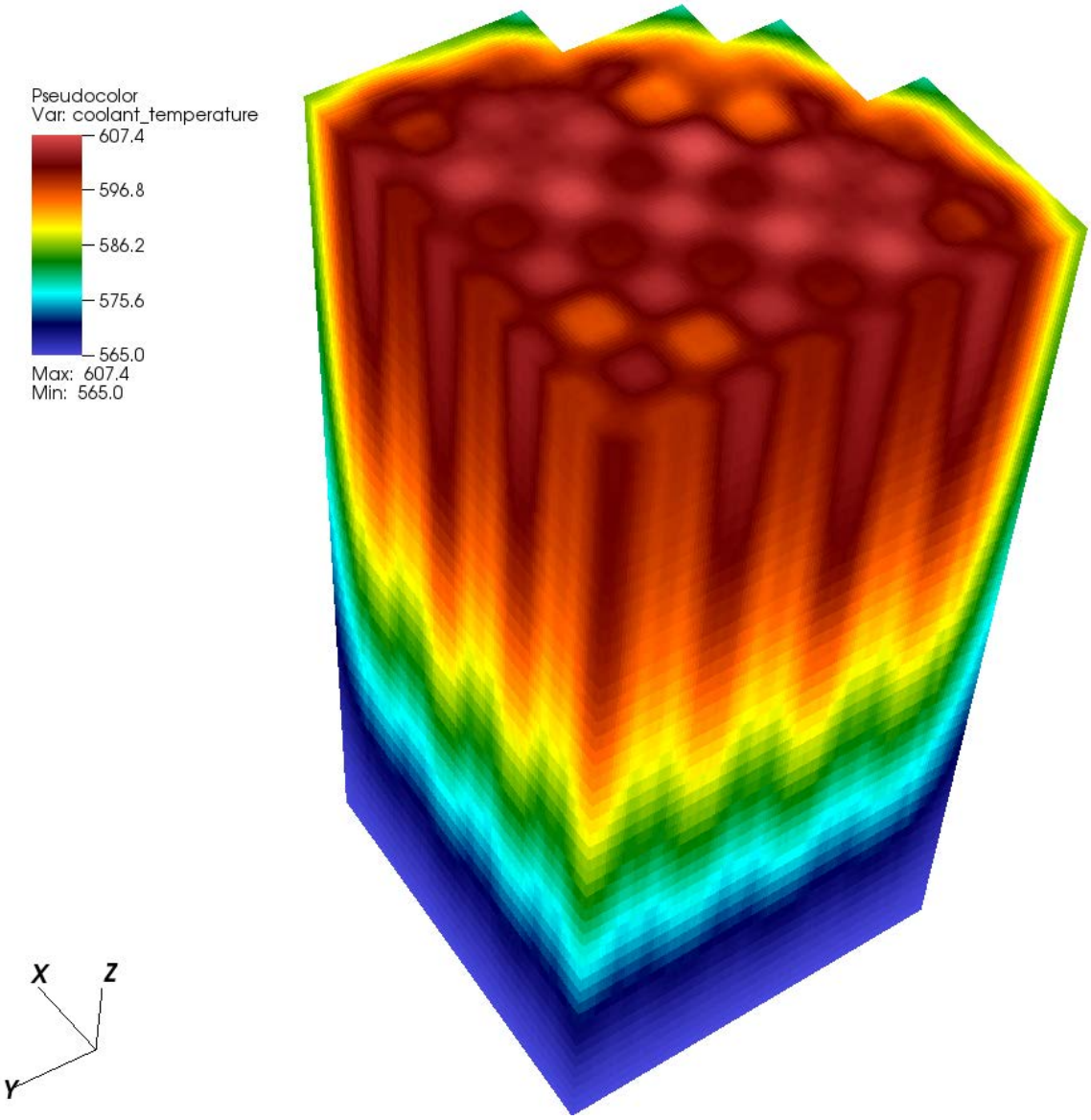


Figure 6-6 3D Coolant Temperature Distribution (K) in the active fuel region

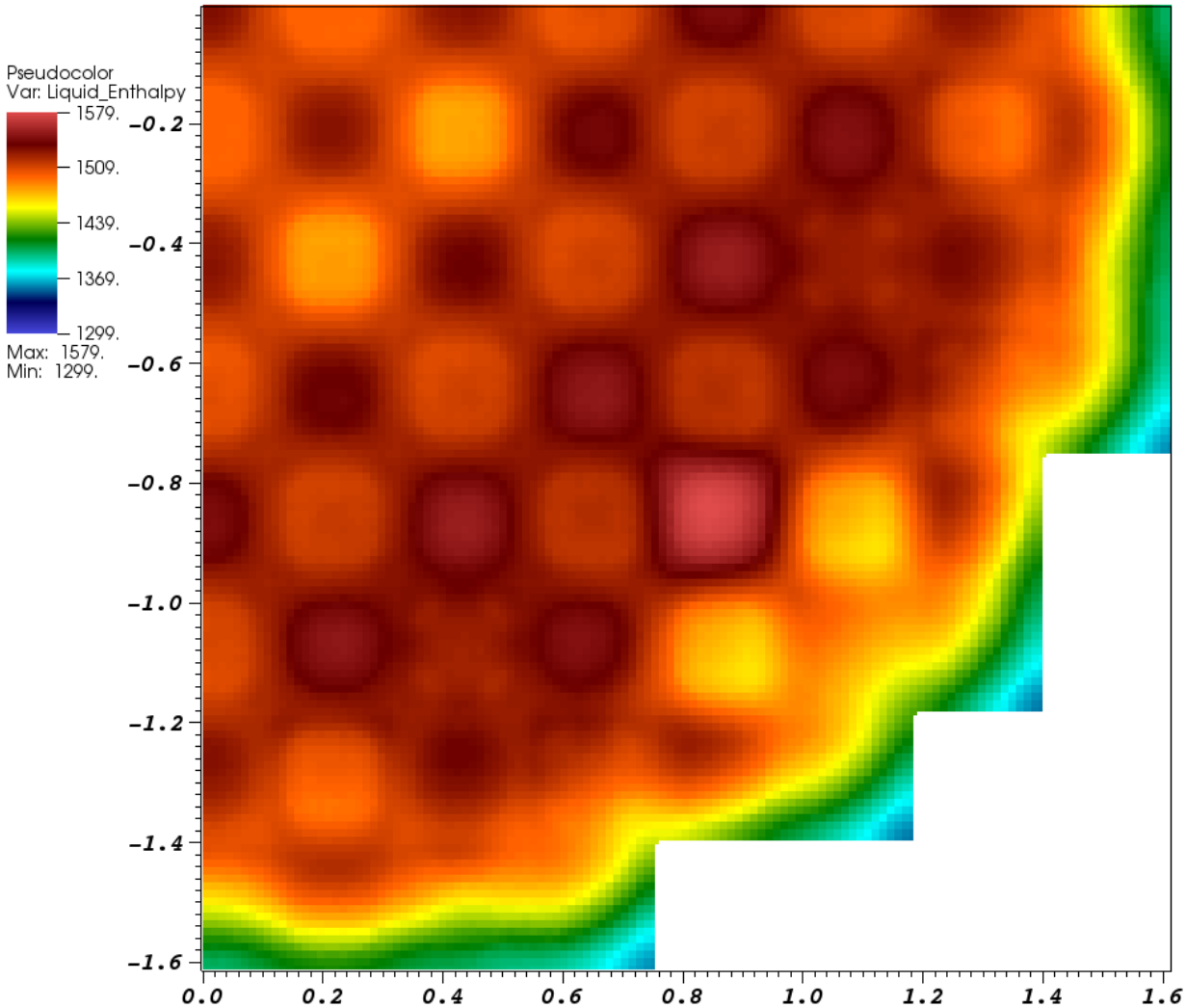


Figure 6-6 Coolant Enthalpy Distribution at the Core Exit

7. Conclusion and Recommendations

This Milestone demonstrates the successful multiphysics coupling of the MPACT neutronics code to the thermal-hydraulics code COBRA-TF. Multiphysics results are shown for several single-assembly cases (AMA Benchmark 6) and for a full-core operating reactor based on Watts Bar Unit 1 Cycle 1 (AMA Benchmark 7).

This milestone delivers important capability to CASL which includes the ability to model full-core reactors at HFP conditions with:

- 3-D pin-resolved transport,
- Direct on-the-fly cross section feedback for local temperature and density effects,
- 3D subchannel T/H calculations for each rod subchannel in the core, and
- 3D pin-by-pin fuel temperature distributions.

The successful completion of the AMA 7 benchmark demonstrates the functionality necessary to solve subsequent problems in the AMA benchmark progression, to include AMA8 / Start-up Physics, AMA9 / Full 3D Core Depletion, and AMA10 / Multi-cycle Depletion.

7.1 Recommendations

While this Milestone successfully meets all the objectives of coupling the multiphysics codes MPACT and COBRA-TF, there are still several areas that require further study and code development. The following recommendations are provided for the near term:

1. **Resonance Treatment:** It has been suggested [17] that the subgroup calculation may only need to be called during the first 4 iterations when the T/H distribution is still changing quite a bit. This would help reduce the the overall execution time of the coupled calculation.
2. **Convergence Analysis:**
   a. Presently MPACT fully converges its steady-state eigenvalue calculation before running COBRA again. Iterating with partial convergence during the initial iterations would help reduce the overall execution time.
   b. Investigate switching from the fixed point Gauss-Seidel coupled iteration scheme to a Jacobi fixed point iteration scheme. This has been the approach used by KAERI with DeCART and MATRA-TH and also by SNU with nTracer and MATRA-TH. Furthermore, KAERI runs the subchannel and neutronics problems in parallel, rather than sequential as is done in the present approach.
   c. Better convergence checking should be performed for the coupled solution. Some work has already been done on this, but was not used in the results shown.
3. **General performance improvements**: Several possible improvements in MPACT are possible such as implementing a better P_0 transport correction so that the P_0 MOC kernel can be used in place of P_2 . This would reduce the MOC time by at least a factor 2, possibly up to a factor of 10.
4. **Mesh parametric study**. In this work only one disctretization was used to demonstrate the capability. Future work should assure the mesh discretization is providing an accurate solution.
5. **Additional Physics Analysis**: Critical boron search and equilibrium xenon enabled.

8. References

[1] A. T. Godfrey, "VERA Core Physics Benchmark Progression Problem Specifications", CASL-U-2012-0131-002, Rev. 2, March 29, 2013.

[2] B. Kochunas, et. al, "Coupled Single Assembly Solution with COBRA-TF/MPACT (Problem 6)", CASL-U-2013-0230-000, November 30, 2013.

[3] M. N. Avramova. CTF: A Thermal Hydraulic Sub-Channel Code for LWR Transient Analyses, User's Manual, Pennsylvania State University, February 2009.

[4] MPACT Theory Manual, version 1.0, University of Michigan, October, 2013.

[5] MPACT User Manual, version 1.0, University of Michigan, October, 2013.

[6] R. Schmidt, N. Belcourt, R. Hooper, R. Pawlowski, An Introduction to LIME 1.0 and it's Use in Coupling Codes for Multiphysics Simulation, Sandia National Laboratories, SAND2011-8524, November 2011.

[7] S. R. Slattery, P. P. H. Wilson and R. P. Pawlowski, "The Data Transfer Kit: A Geometric Rendezvous-Based Tool for MultiPhysics Data Transfer," *International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering (M&C 2013)*, Sun Valley Idaho, May 5-9, 2013.

[8] TriBITS website: https://code.google.com/p/tribits/

[9] LIME website: http://sourceforge.net/projects/lime1/

[10] Data Transfer Kit (DTK) website: https://github.com/CNERG/DataTransferKit

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[15] A. T. Godfrey, "MPACT Testing and Benchmarking Results", CASL-U-2014-0045-000, Rev. 2, March 31, 2014.

[16] R. Salko, et al., “Initial COBRA-TF Parallelization”, CASL-I-2013-0180-000, Aug 2013.

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Appendix A – Property Averaging

This appendix describes how to compute average values in CTF for transfer to MPACT.

A.1 Average coolant properties

MPACT requires an average coolant density and average coolant temperature for each rod. Thus before values can be passed to MPACT, a weighted average of the four surrounding subchannel values must be calculated. These average values are computed in the avg_rod_props subroutine in CTF.

Figure A-1 illustrates how each rod within a PWR assembly is surrounded by four subchannels.

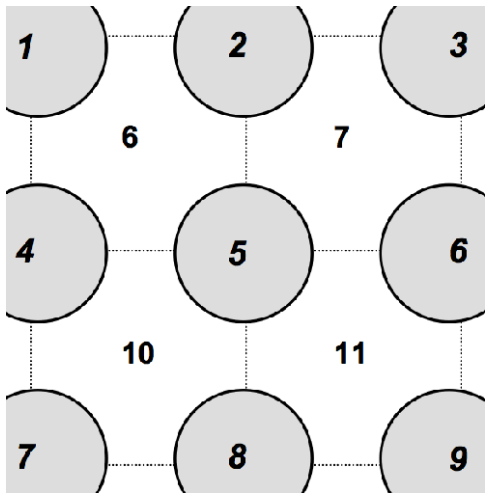

Figure A-1 Illustration of how a typical fuel rod is surrounded by four subchannels in a PWR square lattice fuel assembly.

The average coolant density surrounding fuel rod "n" at axial level "j" is calculated as an area-weighted average of the liquid and vapor densities in the surrounding subchannels (i=1,4) per the following equation.

$$\bar{\rho}_n = \sum_{i=1}^{4} \omega_i \left[(1-\alpha_i)\rho_{liq(i,j)} + \alpha_i \, \rho_{vap(i,j)}\right] \qquad (1)$$

where α_i is the volume fraction of the vapor phase, and the normalized weighting factor ω_i is defined in terms of the four surrounding cross sectional areas A_i as

$$\omega_i = \frac{A_i}{\sum_{i=1}^{4} A_j} \qquad (2)$$

The average coolant temperature surrounding fuel rod "n" at axial level "j" is calculated as a mass-weighted average of the liquid phase temperatures in the surrounding subchannels (i=1,4) per the following equation.

$$\overline{T}_{n,j} = \sum_{i=1}^{4} \psi_i T_{i,j} \qquad (3)$$

where the normalized mass-weighting factor Ψ_i is defined in terms of the mass of liquid in the four surrounding subchannels (i=1,4)

$$\psi_i = \frac{A_i \rho_{liq,i}}{\sum_{j=1}^{4} A_j \rho_{liq,j}} \tag{4}$$

Note that the vapor-phase contribution is currently neglected because of the very large density difference between vapor and liquid and because of the relative insensitivity of cross sections to small changes in *T*.

A.2 Average fuel rod properties

MPACT requires an average fuel temperature and average clad temperature for each rod at each axial level. These values must be computed (in the avg_rod_props subroutine) in CTF before they can be passed to MPACT.

CTF resolves the radial variation of temperature within a fuel rod using a finite difference grid as illustrated in Figure A-2. The number of nodes is problem dependent and defined by the user. In Figure A-2 there are five internal nodes together with the requisite fuel pellet surface node and the inner and outer cladding surface nodes (for a total of eight). CTF also has the option to model azimuthal variations with a coarse azimuthal grid that corresponds to the number of subchannels that surround the fuel rod (four in a square lattice).

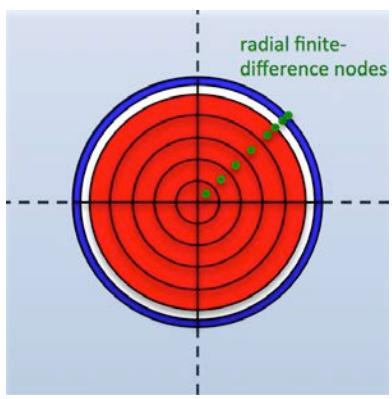

Figure A-2 Illustrative radial discretization of a fuel rod modeled by CTF

The average fuel temperature of fuel rod "n" at axial level "j" is calculated as an area-weighted average of the conduction node temperatures computed by the finite difference heat transfer solution within the fuel rod. This can be expressed as

$$\overline{T}_{f(n,j)} = \sum_{i=1}^{ic-2} \left(\frac{Ar_i}{Af_n} \right) \left[\frac{1}{kla} \sum_{k=1}^{kla} T_{i,n,j,k} \right] \tag{5}$$

where

Ar_i denotes the cross sectional area of radial finite difference node i,

Af_n denotes the total cross sectional area of the fuel,

kla denotes the number of azimuthal sections being modeled, and

ic denotes the total number of radial nodes in the fuel rod heat transfer model (the last 2 rings always refer to the clad material).

The average clad temperature of fuel rod "n" at axial level "j" is calculated in a similar fashion:

$$\overline{T}_{c(n,j)} = \sum_{i=ic-1}^{ic} \left(\frac{Ar_i}{Ac_n} \right) \left[\frac{1}{kla} \sum_{k=1}^{kla} T_{i,n,j,k} \right] \qquad (6)$$

where

Ac_n denotes the total cross sectional area of the clad,

and all other terms are as previously defined above.

Appendix B – Single-Assembly Input File

This appendix contains the input listing for a PWR assembly. All of the input for CTF, MPACT, and the coupled code is created through the VERA Common Input.

Input Listing

```
[CASEID]
  title 'CASL Problem 6a'
!==============================================================================
!  Sample input for Problem 6 (Single-assembly with T/H feedback)
!
!  Draft 1 - 9/28/2012 - starting with Problem 3 input deck
!     * changing power to 100%
!     * turn on T/H feedback
!     * remove "tfuel" and "modden" because these will be set by T/H feedback
!
!  Draft 2 - 10/13/2012
!     * added "mat" card in front of material cards
!
!  Update 11/19/2012
!     * added explicit lattice models for:
!         * lower_nozzle_gap_height
!         * lower_pincap_height
!         * upper_nozzle_gap_height
!         * upper_pincap_height
!         * upper_plenum_height
!
!  Update 03/18/2013
!     * fixed tinlet
!     * added sym and reflector cards
!     * updated dhfrac to default value
```

```
!
!  Update 04/10/2013
!     * add COUPLING block
!
!
!  To process:
!     ./react2xml.pl [file].inp [file].xml
!
!==============================================================================

[STATE]
  power  100.0         ! %
  tinlet 559.0         ! F
  boron  600          ! ppmB
  pressure 2250        ! psia

  tfuel  900.0         ! set to 900K with feedback
  modden 0.743         ! g/cc      Not used with T/H feedback!

  feedback on
  sym full

[CORE]
  size 1                ! 1x1 single-assembly
  rated 17.67   0.6824  ! MW, Mlbs/hr
  apitch 21.5
  height 406.328

  core_shape
    1
```

```
  assm_map
    A1

  lower_plate ss 5.0 0.5   ! mat, thickness, vol frac
  upper_plate ss 7.6 0.5   ! mat, thickness, vol frac
  lower_ref   mod 26.0 1.0
  upper_ref   mod 25.0 1.0


  bc_rad reflecting

  mat he     0.000176
  mat inc    8.19
  mat ss     8.0
  mat zirc   6.56 zirc4
  mat aic   10.20
  mat pyrex  2.23
  mat b4c    6.56

[ASSEMBLY]
  title "Westinghouse 17x17"
  npin 17
  ppitch 1.260

  fuel U31 10.257 95.0 / 3.1

!=== material label, key_name, density (lib_name defaults to key_name)
  mat he   0.000176
  mat inc  8.19
  mat ss   8.0
  mat zirc 6.56 zirc4
```

```
cell 1     0.4096 0.418 0.475 / U31 he zirc
cell 100          0.561 0.602 / mod    zirc       ! guide tube
cell 200          0.561 0.602 / mod    zirc       ! instrument tube
cell 7            0.418 0.475 / mod    mod        ! empty location
cell 8            0.418 0.475 /     he zirc       ! plenum
cell 9                  0.475 /        zirc       ! pincap

lattice FUEL1
   200
     1 1
     1 1 1
   100 1 1 100
     1 1 1   1 1
     1 1 1   1 1 100
   100 1 1 100 1   1 1
     1 1 1   1 1   1 1 1
     1 1 1   1 1   1 1 1 1

lattice LGAP1
   200
     7 7
     7 7 7
   100 7 7 100
     7 7 7   7 7
     7 7 7   7 7 100
   100 7 7 100 7   7 7
     7 7 7   7 7   7 7 7
     7 7 7   7 7   7 7 7 7
```

```
lattice PLEN1
   200
     8 8
     8 8 8
   100 8 8 100
     8 8 8   8 8
     8 8 8   8 8 100
   100 8 8 100 8   8 8
     8 8 8   8 8   8 8 8
     8 8 8   8 8   8 8 8 8

lattice PCAP1
   200
     9 9
     9 9 9
   100 9 9 100
     9 9 9   9 9
     9 9 9   9 9 100
   100 9 9 100 9   9 9
     9 9 9   9 9   9 9 9
     9 9 9   9 9   9 9 9 9

axial A1    6.050
    LGAP1  10.281
    PCAP1  11.951
    FUEL1 377.711
```

```
    PLEN1 393.711
    PCAP1 395.381
    LGAP1 397.501

 grid END inc  1017 3.866
 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

 lower_nozzle  ss 6.05  6250.0  ! mat, height, mass (g)
 upper_nozzle  ss 8.827 6250.0  ! mat, height, mass (g)

!! dancoff                   ! assembly_dancoff_map
!!   0.000
!!   0.287 0.315
!!   0.287 0.315 0.315
!!   0.000 0.287 0.286 0.000
!!   0.287 0.316 0.316 0.284 0.299
!!   0.288 0.317 0.316 0.287 0.267 0.000
!!   0.000 0.286 0.286 0.000 0.270 0.286 0.321
!!   0.287 0.319 0.319 0.286 0.315 0.335 0.333 0.337
!!   0.323 0.322 0.321 0.322 0.320 0.322 0.323 0.322 0.310
```

```
[EDITS]

!  3in intervals in active fuel
  axial_edit_bounds
          11.951
          15.817
          24.028
          32.239
          40.45
          48.662
          56.873
          65.084
          73.295
          77.105
          85.17
          93.235
          101.3
          109.365
          117.43
          125.495
          129.305
          137.37
          145.435
```

```
153.5
161.565
169.63
177.695
181.505
189.57
197.635
205.7
213.765
221.83
229.895
233.705
241.77
249.835
257.9
265.965
274.03
282.095
285.905
293.97
302.035
310.1
318.165
326.23
334.295
338.105
346.0262
353.9474
361.8686
369.7898
377.711
```

```
[MPACT]
  vis_edits         none
  ray_spacing       0.05
!quad_set
  quad_type         CHEBYSHEV-GAUSS
  polars_octant     4
  azimuthals_octant 16
!iteration_control
  flux_tolerance    1e-5
  num_inners        3
  k_tolerance       1e-5
  up_scatter        2
  num_outers        100
  scattering        LTCP0
!cmfd
  cmfd              cmfd
  cmfd_solver       mgnode
  k_shift           1.5
  cmfd_num_outers   20
!2D1D
  split_TL          true
  TL_treatment      lflat
  nodal_method      nem
!  under_relax       1.0
!parallel
  num_space         59
  num_angle         1
  num_energy        1
  num_threads       8
  par_method        PS
!xs_library
```

```
  xs_filename       declib56g_e7_v3.0_0708.fmt
  xs_type           ORNL
  subgroup_set      4
!mesh

  mesh fuel  3 1 1 / 8 8 8 8 8 8
  mesh gtube 3 1   / 8 8 8 8 8
  axial_mesh       20.0000
                    5.0000
                    6.0530
                    5.9010
                    3.8660
                    8.2110
                    8.2110
                    8.2110
                    8.2120
                    8.2110
                    8.2110
                    8.2110
                    3.8100
                    8.0650
                    8.0650
                    8.0650
                    8.0650
                    8.0650
                    8.0650
                    3.8100
                    8.0650
                    8.0650
                    8.0650
                    8.0650
```

```
8.0650
8.0650
3.8100
8.0650
8.0650
8.0650
8.0650
8.0650
8.0650
3.8100
8.0650
8.0650
8.0650
8.0650
8.0650
8.0650
3.8100
8.0650
8.0650
8.0650
8.0650
8.0650
8.0650
3.8100
7.9212
7.9212
7.9212
7.9212
7.9212
8.5560
3.8660
```

```
                    3.5780
                    3.7990
                    8.8270
                    7.6000

[COBRATF]
  nfuel   3             ! number of fuel rings in conduction model
  nc      1             ! conduction option - radial conduction
  irfc    2             ! friction factor correlation default=2
  dhfrac  0.02          ! fraction of power deposited directly into coolant
  hgap    5678.3        ! gap conductance
  epso    0.001
  oitmax  5
  iitmax  40
  gridloss END 0.9070   ! spacer grid loss coefficient
  gridloss MID 0.9065   ! spacer grid loss coefficient
  dtmin   0.000001
  dtmax   0.1
  tend    0.1
  rtwfp   1000.0
  maxits  10000
  courant 0.8

[COUPLING]
  epsk        5.0  ! pcm
  epsp        1.0e-4
  rlx_power   0.6
  rlx_tfuel   1.0
  rlx_den     1.0
  maxiter     100
```

Appendix C – Full-Core Input File

This appendix contains a partial listing for a full-core PWR. All of the input for CTF, MPACT, and the coupled code is created through the VERA Common Input.

Input Listing

```
[CASEID]
  title 'CASL AMA Problem 7 - Watts Bar Unit 1 Cycle 1 - Public'

[STATE]
  title 'ARO'
  power    100.0          ! %
  tinlet   557.33       ! F - 565K
  tfuel    565.0        ! K
  boron    1285.2       ! ppmB 1293*19.78/19.9
  pressure 2250         ! psia
  modden   0.743        ! g/cc
  feedback on
  sym qtr

  rodbank SA 230
          SB 230
          SC 230
          SD 230
           A 230
           B 230
           C 230
           D 230

[CORE]
  size 15               ! assemblies across core
  rated 3411 131.68     ! MW, Mlbs/hr
  apitch 21.5
  height 406.337

  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

  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



  insert_map
     -
    20 TP
     - 24  -
    20 TP 20  -
     - 20 TP 20  -
    20  - 16  - 24 12
     - 24  - 16  - TP
    12 TP  8 TP

  crd_map
    1
    - -
    1 - 1
    - - - 1
    1 - - - 1
    - 1 - 1 - -
    1 - 1 - 1 -
    - - - -

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

! the detector map is upside down for denovo
  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 -

  baffle ss 0.19 2.85

  vessel  mod 187.96        ! barrel IR (cm)
           ss 193.68        ! barrel OR (cm)
          mod 194.64        ! neutron pad IR (cm)
           ss 200.4715        ! neutron pad effective OR (cm) (modelled as 90 by conserving
volume (32/90) and reducing actual OR
          mod 219.15        ! vessel liner IR (cm)
           ss 219.71        ! vessel liner OR / vessel IR (cm)
           cs 241.70        ! vessel OR (cm)

  lower_plate ss  5.0 0.5   ! mat, thickness, vol frac
```

```
  upper_plate ss  7.6 0.5   ! mat, thickness, vol frac

! lower_ref  mod 20.0 1.0 - ignore this for now
! upper_ref  mod 20.0 1.0 - ignore this for now

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

  mat he     0.0001786
  mat inc    8.19
  mat ss     8.0
  mat zirc   6.56 zirc4

[ASSEMBLY]
  title "Westinghouse 17x17"
  npin 17
  ppitch 1.260

  fuel U21 10.257 94.5 / 2.110
  fuel U26 10.257 94.5 / 2.619
  fuel U31 10.257 94.5 / 3.100

  cell 1     0.4096 0.418 0.475 / U21 he zirc
  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       ! plug
  cell 7                  0.475 /        mod        ! empty

  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

  lattice GAP
       4
       7 7
       7 7 7
       4 7 7 4
       7 7 7 7 7
       7 7 7 7 7 4
       4 7 7 4 7 7 7
       7 7 7 7 7 7 7 7
       7 7 7 7 7 7 7 7 7

  axial  1  6.053 GAP 10.281 PLUG 11.951 LAT21 377.711 PLEN 393.711 PLUG 395.381 GAP 397.51
  axial  2  6.053 GAP 10.281 PLUG 11.951 LAT26 377.711 PLEN 393.711 PLUG 395.381 GAP 397.51
  axial  3  6.053 GAP 10.281 PLUG 11.951 LAT31 377.711 PLEN 393.711 PLUG 395.381 GAP 397.51

  grid END inc  1017 3.866
  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

  lower_nozzle  ss 6.053 6250.0  ! mat, height, mass (g)
  upper_nozzle  ss 8.827 6250.0  ! mat, height, mass (g)

[INSERT]
  title "Pyrex"
  npin 17

  mat px 2.2452 pyrex-vera  ! slight mod to get 6.24 mgB10/cm

  cell X  0.214 0.231 0.241 0.427 0.437 0.484 / he ss he px he ss ! pyrex
```

```
cell P                          0.437 0.484 /            he ss ! plenum
cell G                                0.484 /               ss ! plug/cap
cell T                                0.538 /               ss ! thimble plug


rodmap  PY8
   -
   - -
   - - -
   X - - -
   - - - - -
   - - - - - X
   - - - - - - -
   - - - - - - - -
   - - - - - - - - -

rodmap  PY12
   -
   - -
   - - -
   X - - -
   - - - - -
   - - - - - -
   - - - X - - -
   - - - - - - - -
   - - - - - - - - -

rodmap  PY16
   -
   - -
   - - -
   X - - -
   - - - - -
   - - - - - X
   - - - X - - -
   - - - - - - - -
   - - - - - - - - -

rodmap  PY20
   -
   - -
   - - -
   X - - -
   - - - - -
   - - - - - X
   X - - X - - -
   - - - - - - - -
   - - - - - - - - -

rodmap  PY24
   -
   - -
   - - -
   X - - X
   - - - - -
   - - - - - X
   X - - X - - -
   - - - - - - - -
   - - - - - - - - -

rodmap  PL8
   -
   - -
   - - -
   P - - -
```

```
   - - - - -
   - - - - - P
   - - - - - - -
   - - - - - - - -
   - - - - - - - - -

rodmap  PL12
   -
   - -
   - - -
   P - - -
   - - - - -
   - - - - - -
   - - - P - - -
   - - - - - - - -
   - - - - - - - - -

rodmap  PL16
   -
   - -
   - - -
   P - - -
   - - - - -
   - - - - - P
   - - - P - - -
   - - - - - - - -
   - - - - - - - - -

rodmap  PL20
   -
   - -
   - - -
   P - - -
   - - - - -
   - - - - - P
   P - - P - - -
   - - - - - - - -
   - - - - - - - - -

rodmap  PL24
   -
   - -
   - - -
   P - - P
   - - - - -
   - - - - - P
   P - - P - - -
   - - - - - - - -
   - - - - - - - - -

rodmap  PG8
   -
   - -
   - - -
   G - - -
   - - - - -
   - - - - - G
   - - - - - - -
   - - - - - - - -
   - - - - - - - - -
```

```
rodmap  PG12
   -
   - -
   - - -
   G - - -
   - - - - -
   - - - - - -
   - - - G - - -
   - - - - - - - -
   - - - - - - - - -

rodmap  PG16
   -
   - -
   - - -
   G - - -
   - - - - -
   - - - - - G
   - - - G - - -
   - - - - - - - -
   - - - - - - - - -

rodmap  PG20
   -
   - -
   - - -
   G - - -
   - - - - -
   - - - - - G
   G - - G - - -
   - - - - - - - -
   - - - - - - - - -

rodmap  PG24
   -
   - -
   - - -
   G - - G
   - - - - -
   - - - - - G
   G - - G - - -
   - - - - - - - -
   - - - - - - - - -

rodmap  TP8
   -
   - -
   - - -
   P - - T
   - - - - -
   - - - - - P
   T - - T - - -
   - - - - - - - -
   - - - - - - - - -

rodmap  TP12
   -
   - -
   - - -
   P - - T
```

```
      - - - - -
      - - - - - T
      T - - P - - -
      - - - - - - - -
      - - - - - - - - -

  rodmap  TP16
      -
      - -
      - - -
      P - - T
      - - - - -
      - - - - - P
      T - - P - - -
      - - - - - - - -
      - - - - - - - - -

  rodmap  TP20
      -
      - -
      - - -
      P - - T
      - - - - -
      - - - - - P
      P - - P - - -
      - - - - - - - -
      - - - - - - - - -

  rodmap  TP24
      -
      - -
      - - -
      T - - T
      - - - - -
      - - - - - T
      T - - T - - -
      - - - - - - - -
      - - - - - - - - -


  axial   8  13.221 PG8  15.761 PY8  376.441 PL8  383.31 TP8  398.641
  axial  12  13.221 PG12 15.761 PY12 376.441 PL12 383.31 TP12 398.641
  axial  16  13.221 PG16 15.761 PY16 376.441 PL16 383.31 TP16 398.641
  axial  20  13.221 PG20 15.761 PY20 376.441 PL20 383.31 TP20 398.641
  axial  24  13.221 PG24 15.761 PY24 376.441 PL24             398.641
  axial  TP                                       383.31 TP24 394.31

[CONTROL]
  title "B4C with AIC tips"
  npin 17
  stroke  365.125 230     ! approx for 1.5875 step sizes and 230 max stroke

  mat aic 10.2
  mat b4c 1.76

  cell A  0.382 0.386 0.484 / aic he ss
  cell B  0.373 0.386 0.484 / b4c he ss
  cell P        0.386 0.484 /     he ss ! plenum
  cell G              0.484 /        ss ! plug

  rodmap AIC
      -
      - -
      - - -
      A - - A
```

```
      - - - - -
      - - - - - A
      A - - A - - -
      - - - - - - - -
      - - - - - - - - -

  rodmap B4C
      -
      - -
      - - -
      B - - B
      - - - - -
      - - - - - B
      B - - B - - -
      - - - - - - - -
      - - - - - - - - -

  rodmap PLEN
      -
      - -
      - - -
      P - - P
      - - - - -
      - - - - - P
      P - - P - - -
      - - - - - - - -
      - - - - - - - - -

  rodmap PLUG
      -
      - -
      - - -
      G - - G
      - - - - -
      - - - - - G
      G - - G - - -
      - - - - - - - -
      - - - - - - - - -

  axial  1    15.131
        PLUG  17.031
         AIC 118.631
         B4C 377.711
        PLEN 388.411
        PLUG 390.311

[DETECTOR]
  title "Incore instrument thimble"
  npin 17

  mat he 0.0001786
  mat ss 8.0

  cell 1  0.258 0.382 / he ss

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

```
  axial 1  0.0 LAT 397.51


[EDITS]
  axial_edit_bounds
      11.951
      15.817
      24.028
      32.239
      40.45
      48.662
      56.873
      65.084
      73.295
      77.105
      85.17
      93.235
      101.3
      109.365
      117.43
      125.495
      129.305
      137.37
      145.435
      153.5
      161.565
      169.63
      177.695
      181.505
      189.57
      197.635
      205.7
      213.765
      221.83
      229.895
      233.705
      241.77
      249.835
      257.9
      265.965
      274.03
      282.095
      285.905
      293.97
      302.035
      310.1
      318.165
      326.23
      334.295
      338.105
      346.0262
      353.9474
      361.8686
      369.7898
      377.711

[MPACT]
  vis_edits         none
  ray_spacing       0.05
  jagged            true
!quad_set
  quad_type         CHEBYSHEV-GAUSS
  polars_octant     3
```

```
  azimuthals_octant 8
!iteration_control
  flux_tolerance    1e-5
  num_inners        3
  k_tolerance       1e-6
  up_scatter        2
  num_outers        20
  scattering        P2
!cmfd
  cmfd              cmfd
  cmfd_solver       1gsweep
  k_shift           1.5
  cmfd_num_outers   60
!2D1D
  split_TL          true
  TL_treatment      lflat
  nodal_method      nem
!  under_relax       1.0
!parallel
  num_space         2784
  num_angle         1
  num_energy        1
  num_threads       1
  par_method        EXPLICITFILE
  par_file          part_p5-3d_48r_58z_2784np.txt
!xs_library
  xs_filename       declib56g_e7_09042013_p0mixed.fmt
  xs_type           ORNL
  subgroup_set      4
  xs_shielder       t
!mesh

  mesh fuel  3 1 1 / 8 8 8 8 8 8
  mesh gtube 3 1   / 8 8 8 8 8

  meshing_method    nonfuel
  automesh_bounds  2.0 20.0

[COBRATF]
  nfuel   3             ! number of fuel rings in conduction model
  nc      1             ! conduction option - radial conduction
  irfc    2             ! friction factor correlation default=2
  dhfrac  0.02          ! fraction of power deposited directly into coolant
  hgap    5678.3        ! gap conductance
  epso    0.001
  oitmax  5
  iitmax  40
  gridloss END 0.9070   ! spacer grid loss coefficient
  gridloss MID 0.9065   ! spacer grid loss coefficient
  dtmin   0.000001
  dtmax   0.1
  tend    0.1
  rtwfp   1000.0
  maxits  10000
  courant 0.8
  parallel 1
!  global_energy_balance    0.001 !% Total energy into water and out of water.
!  global_mass_balance      0.00003 !% Water in, Water out 3e-8
!  fluid_energy_storage     0.05  !% rho*c_p
!  solid_energy_storage     0.02  !% 0.5e-3 default, should change to 0.5e-5 or less
!  mass_storage             0.05  !%

[COUPLING]
  epsk        5.0  ! pcm
  epsp        1.0e-4
```

```
rlx_power   0.6
rlx_tfuel   1.0
rlx_den     1.0
maxiter     15
```