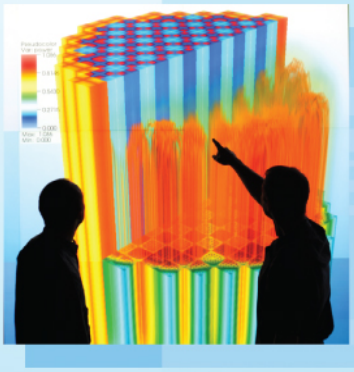
CASL-U-2013-0280-000

Power uprates
and plant life extension

Consortium for Advanced Simulation of LWRs



Engineering design
and analysis

L3:VRI.PSS.P7.03 Milestone Report

Coupled Single Assembly Solution with COBRA-TF/MPACT (Problem 6)

Science-enabling
high performance
computing

Brendan Kochunas
Dan Jabaay
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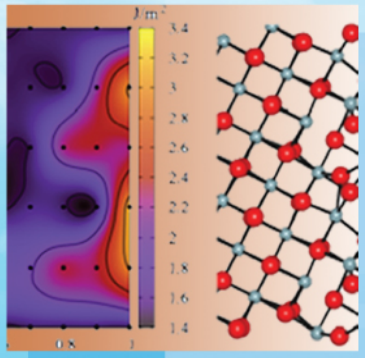
Thomas Downar
November 30, 2013



Fundamental science

Plant operational data

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

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REVISION LOG

Revision	Date	Affected Sections	Revision Description
0	11/30/2013	All	Initial version

EXECUTIVE SUMMARY

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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:VRI.PSS.P7.03– Coupled Single Assembly Solution with COBRA-TF/MPACT (Problem 6). The purpose of this milestone is to evaluate the modeling of a single PWR assembly 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.

In Section 2 of this report, a description is provided of the computer codes used in the coupling and Section 3 provides information on how the code coupling is performed. Section 4 contains a description of the test problem used in this Milestone and Section 5 provides MPACT results for the test problems and a comparison to the results previously submitted from the Insilico code. Finally, Section 6 provides conclusions and some recommendations.

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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) and 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 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 which is read directly by MPACT using readily-available XML libraries.

An example of a VERA common input file is shown in Appendix A – Input File.

2.2 COBRA-TF (CTF)

COBRA-TF (CTF) is a thermal-hydraulic simulation code designed for Light Water Reactor (LWR) analysis) [2]. CTF has a long lineage that goes back to the original COBRA computer 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 subsequent 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 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)

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 [3] and [4] contains a detailed description of the methods used in MPACT as a part of the VERA Core Simulator.

For work here MPACT's 2-D/1-D method is used to obtain the solution of the neutron flux. It also has available the 2-D and 3-D method of characteristics transport solvers. 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 for the axial direction. In the future this 1-D nodal diffusion method will be replaceable by higher order transport based 1-D methods when a higher degree of accuracy 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 two physics codes together to calculate the temperature, fission rate, and neutron flux distribution within a single PWR 17x17 fuel assembly. All neutronics aspects of the problem (cross-sections, neutron transport, and heat generation) 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 done 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 must be combined and compiled in a single executable. This is done by creating a top level LIME problem manager and refactoring CTF and MPACT so they are subroutines instead of standalone programs. 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 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 [6][9]. 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 [10]. 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) is an open source library [11] 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. The DTK website provides the following:

> *"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 [11].

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.

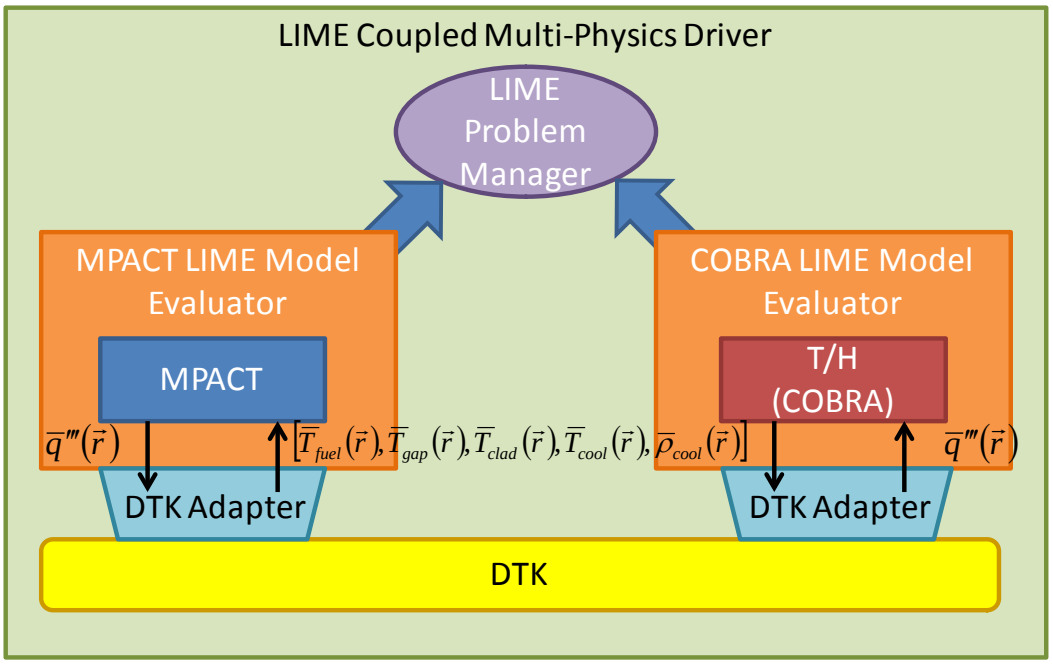


Figure 2-1 Key components of a coupled MPACT-CTF application created to solve the example problem.

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:

- average fuel temperature, T_f
- average clad temperature, T_c
- average coolant temperature surrounding the rod, T
- average coolant density surrounding the rod, ρ

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.

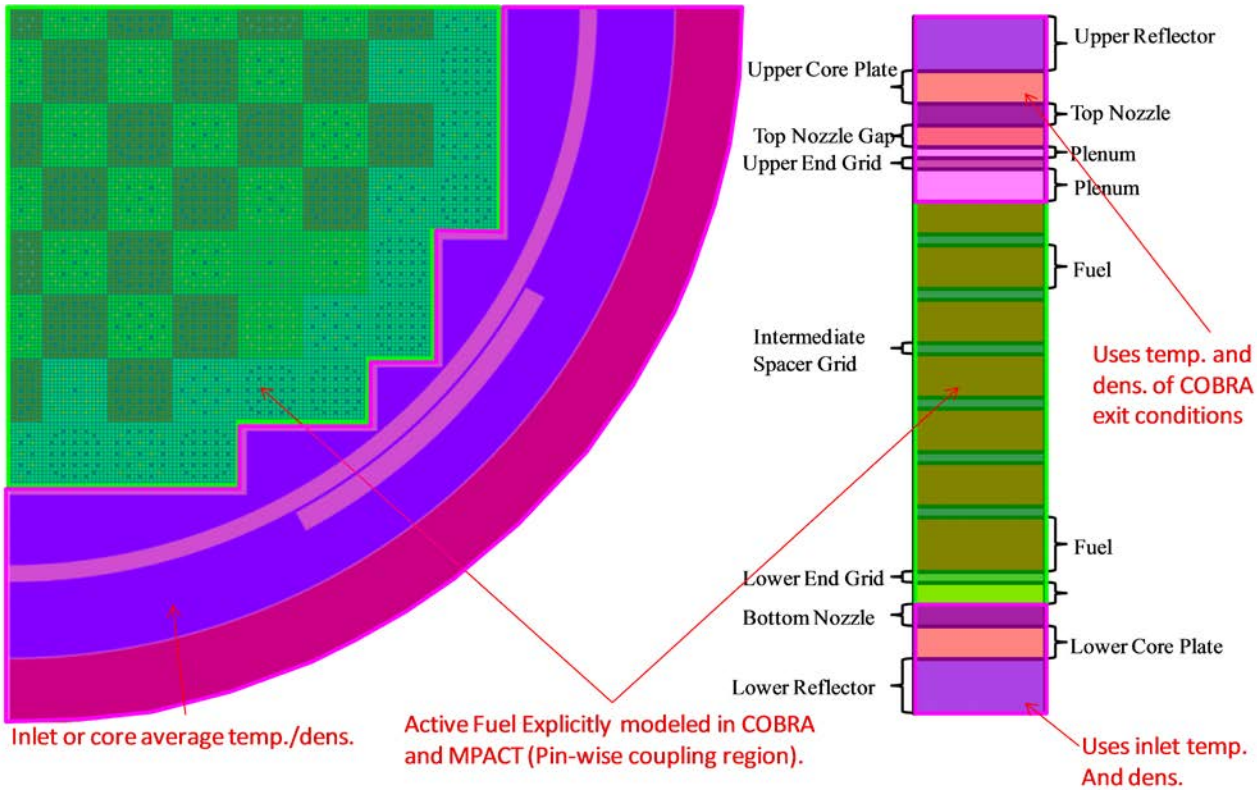


Figure 2-2 T/H Coupling of Core Regions in MPACT

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.

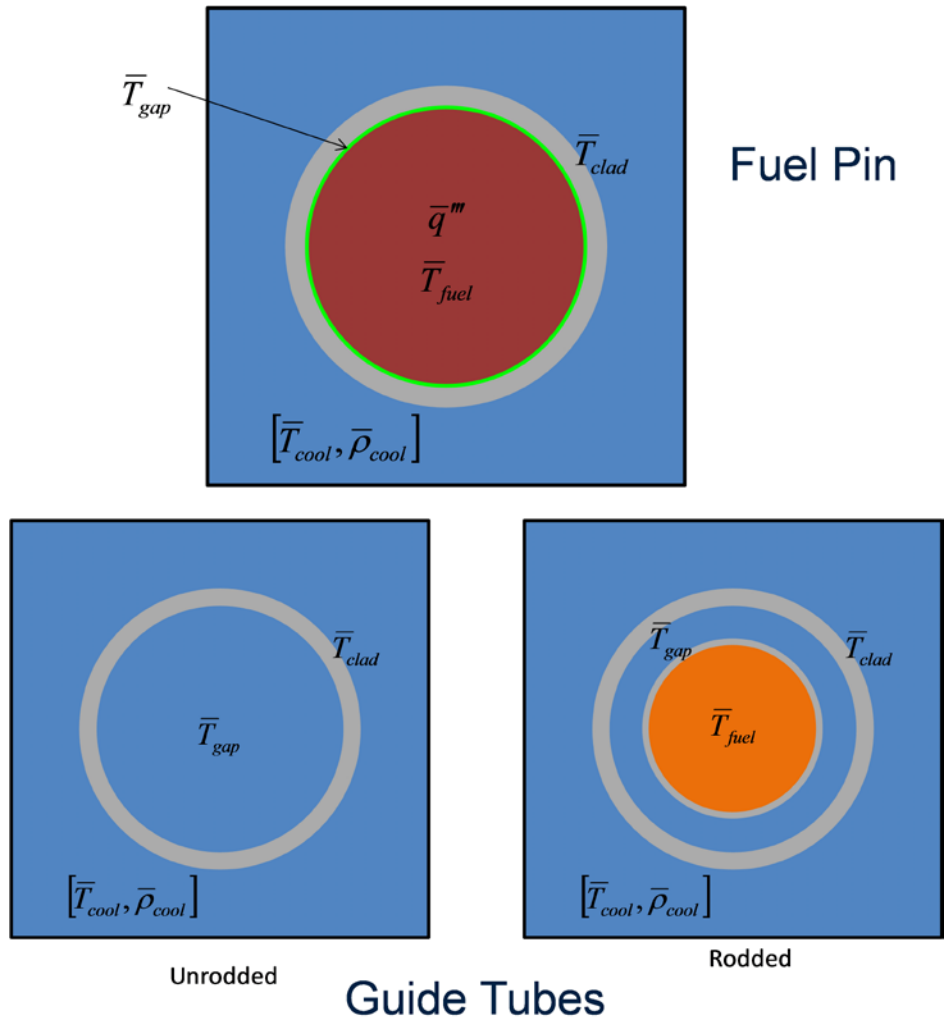


Figure 2-3 Pin Cell Coupling Models used in MPACT

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 needs 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 [9], 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

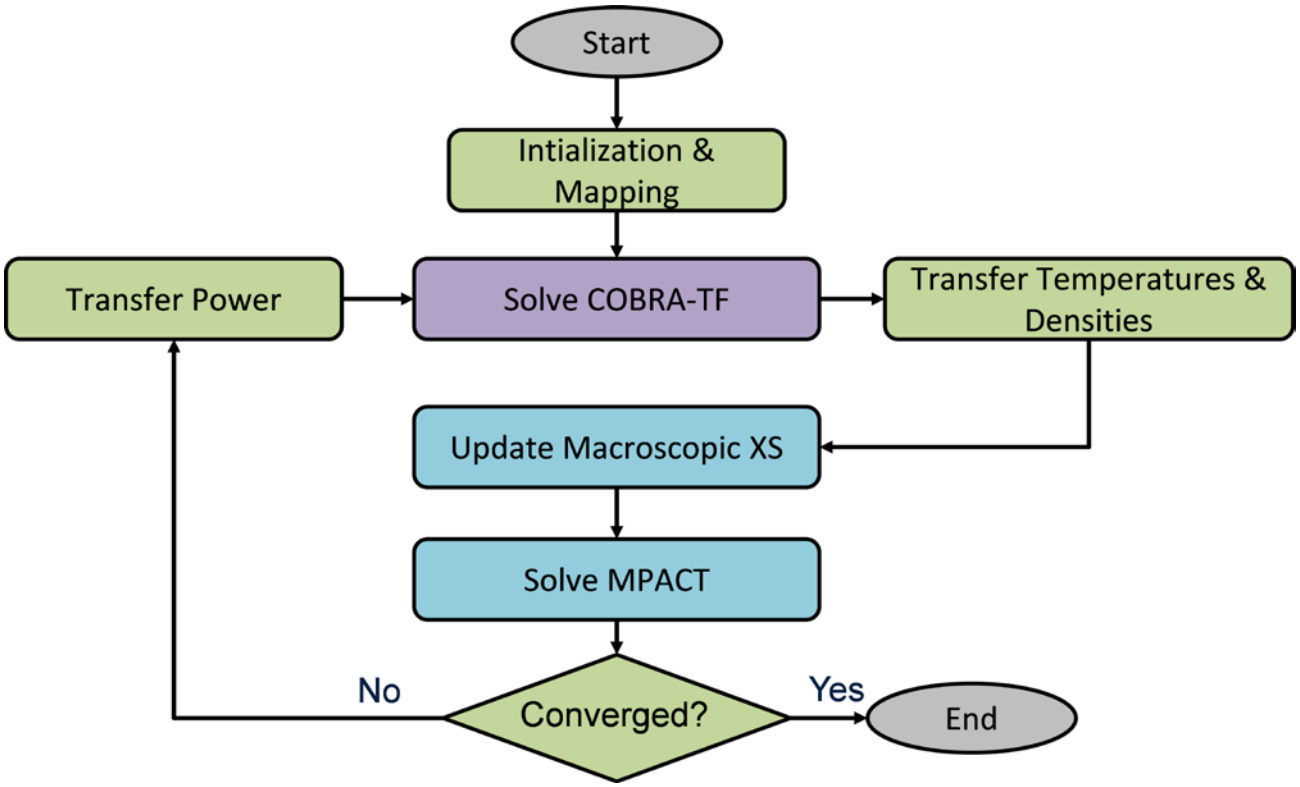


Figure 2-4 Simplified flow chart illustrating the coupled code fixed point algorithm

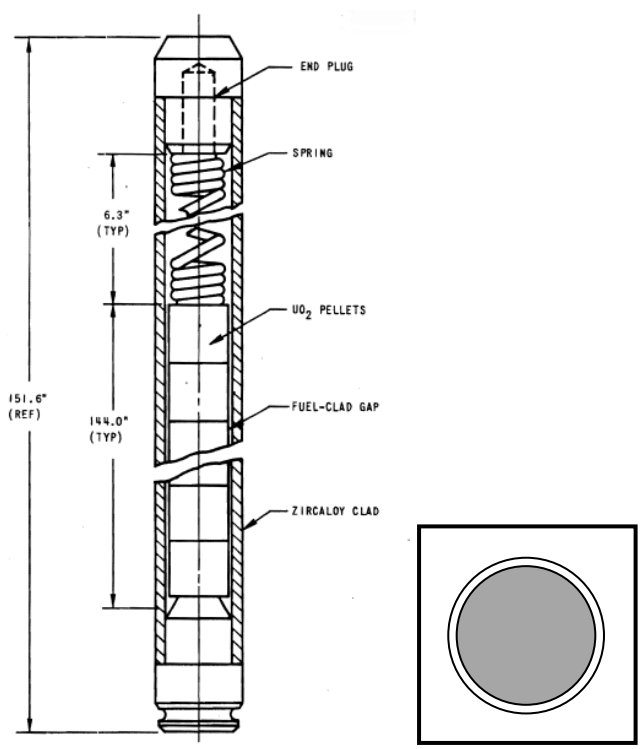
4. Problem Description

The example problem used in this Milestone is a PWR single assembly based on the dimensions and state conditions of Watts Bar Unit 1 Cycle 1. The dimensions for the assembly are identical to those in AMA Progression Benchmark 3 [1] Problems 3 and 6 are identical except that Problem 3 is at Hot Zero Power (HZP) and therefore has no T/H feedback, whereas Problem 6 is at Hot Full Power (HFP) and includes T/H feedback. (All dimensions are non-proprietary and are derived from the publically available Watts Bar Unit 1 FSAR [12].)

In addition to the boron and power levels specified in the benchmark specifications, additional test cases were run at different boron concentrations (600 and 1300 ppm) and power outputs (70% and 130% rated 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 [1]. The complete input listing for this problem is shown in Appendix A – 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	

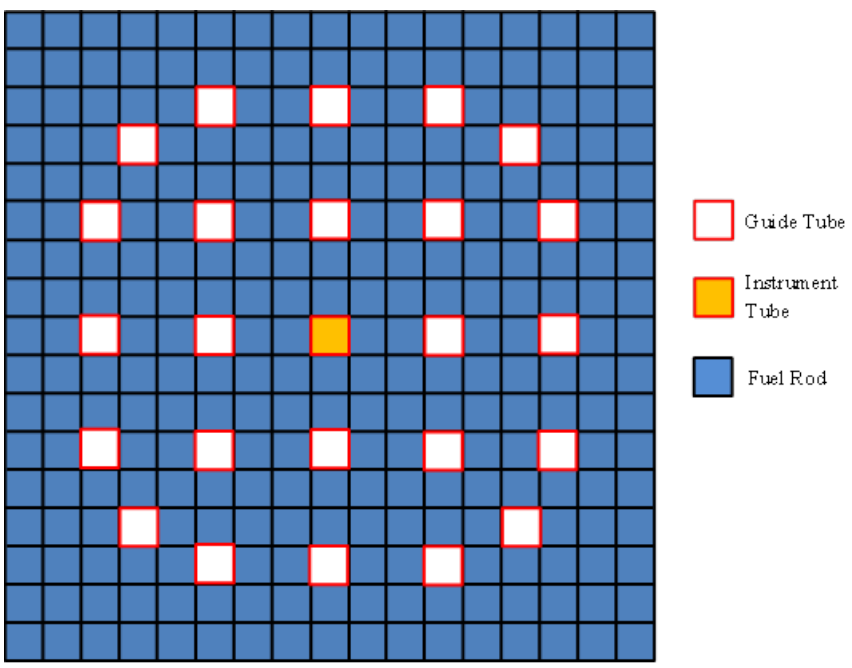


Figure 4-2 Assembly Layout Showing Guide Tubes (GT) and Instrument Tube (IT) placement.

Table 4-2 Assembly Specification

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 what differentiate Progression Problems 3 and 6.

Table 4-3 Nominal Thermal-Hydraulic Conditions

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

5. Test Problem 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). The ray spacing used was 0.05 cm. For the scattering source a "limited" transport corrected P0 approximation was used. This 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 only in 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 capture the axial leakage effects. The MOC meshing used for the radial domain is illustrated in the Figure 5-1 below.

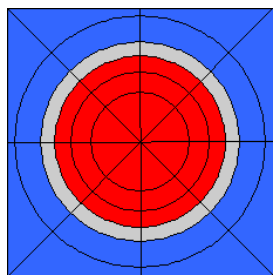


Figure 5-1 2-D MOC mesh for a fuel pin

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 heights, 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.

This problem uses the same discretization as that used for the reference AMA problem 3 results [14], so it is believed 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 Nominal 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 (K-iters) shows the number of MPACT eigenvalue 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 eight 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

Note that the convergence criterion for this problem is very tight. The eigenvalue convergence is set to 5 pcm ($1x10^{-5}$ delta-k). 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 5-2 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, not the density in each CTF channel. The calculation for this density is described in [13]. 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.

Average axial distributions for this problem are shown in Figures 5-4 and 5-5. Figure 5-4 includes the fuel temperature and Figure 5-5 does not include the fuel temperature so the coolant and clad temperature profiles are easier to see. Note the small “dips” in the axial fission rate and fuel temperature profiles. These dips are due to the presence of spacer grids. The spacer grids displace moderator in the coolant channels and decrease the neutron moderation around the grids. The decreased moderation causes a local depression in the flux and power.

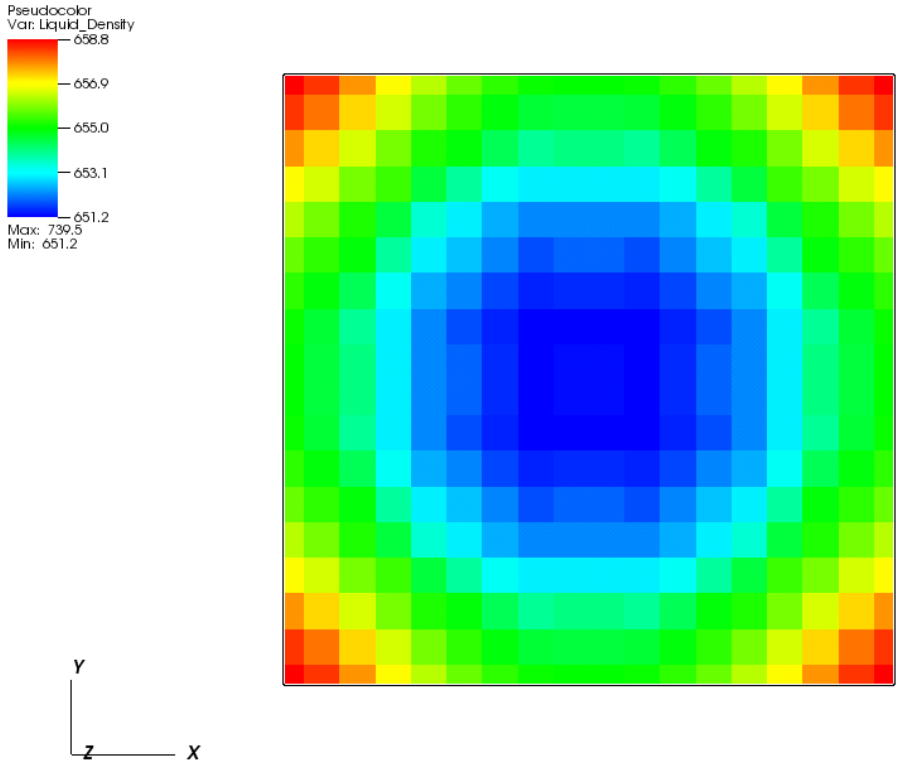


Figure 5-3 Exit Coolant Density (g/cc) at 600 ppm and 100% power

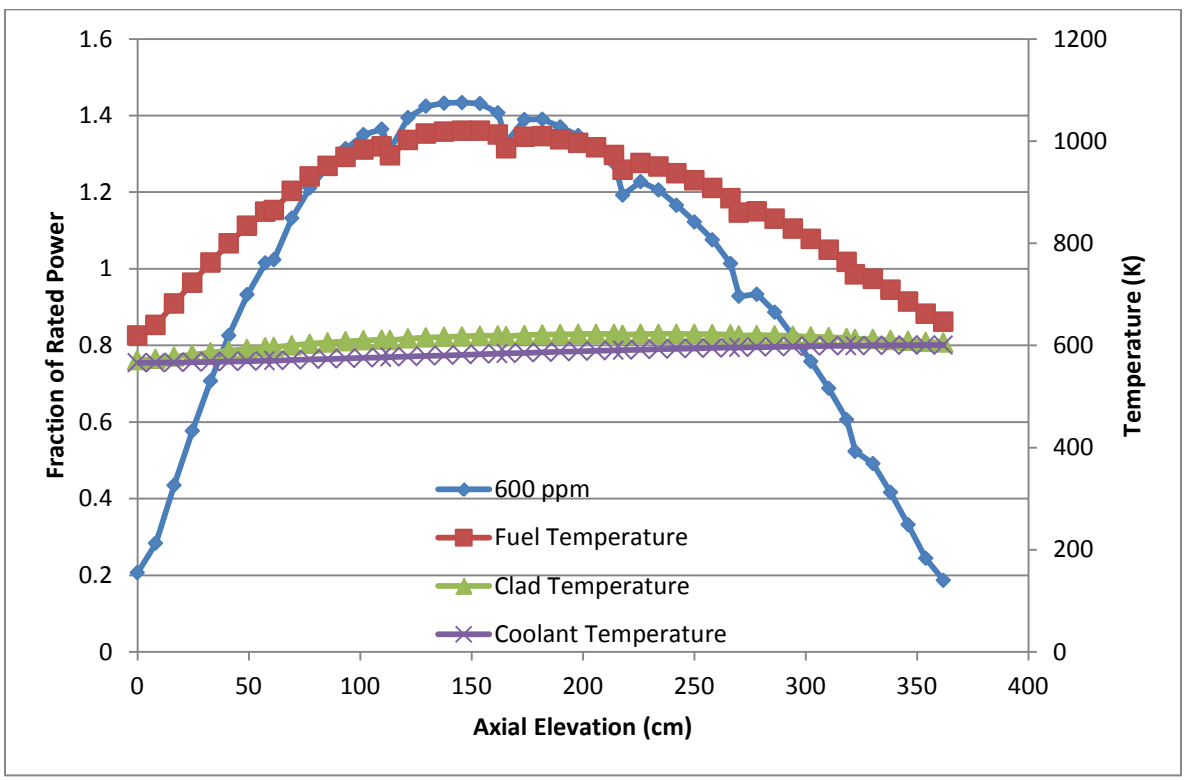


Figure 5-4 Axial Distributions at 600 ppm and 100% power (with fuel temperature shown)

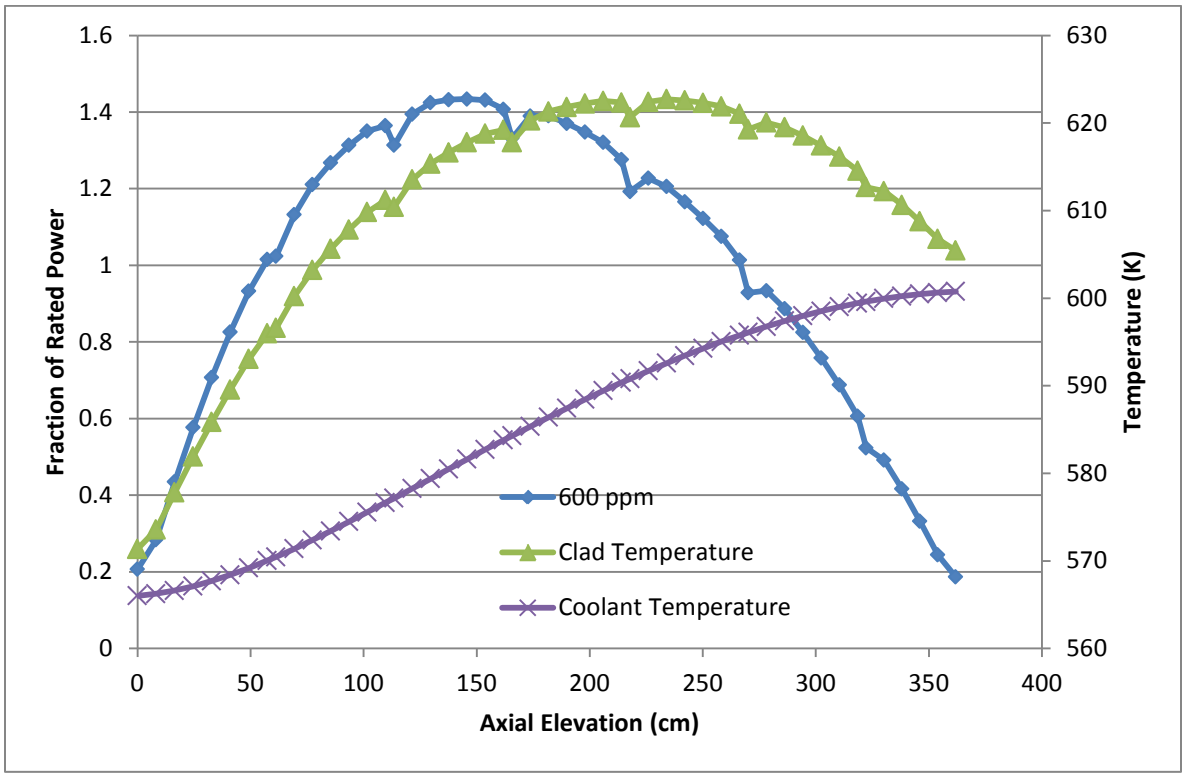


Figure 5-5 Axial Distributions at 600 ppm and 100% power (without fuel temperature)

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	Total K_{eff} Iterations
0 ppm	1.32907	4:50:24	8	140
600 ppm	1.24710	4:39:58	9	129
1300 ppm	1.16467	5:04:01	10	129

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 you would see 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.

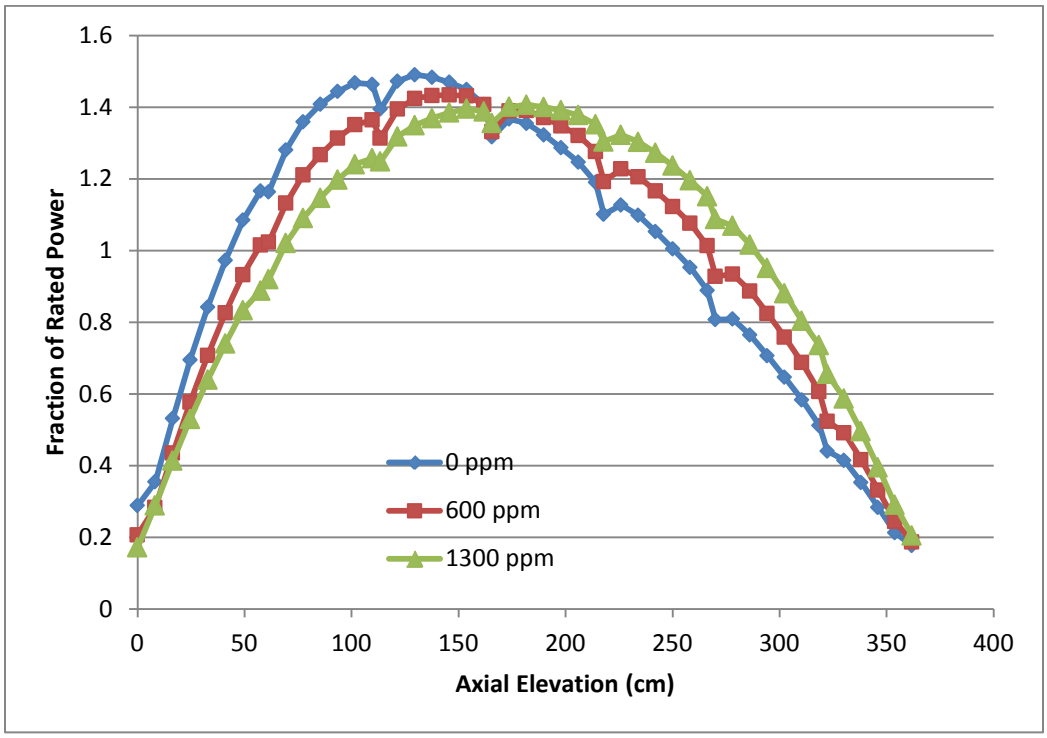


Figure 5-6 Axial Plot of Fission Rates at Different Boron Concentrations

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.)

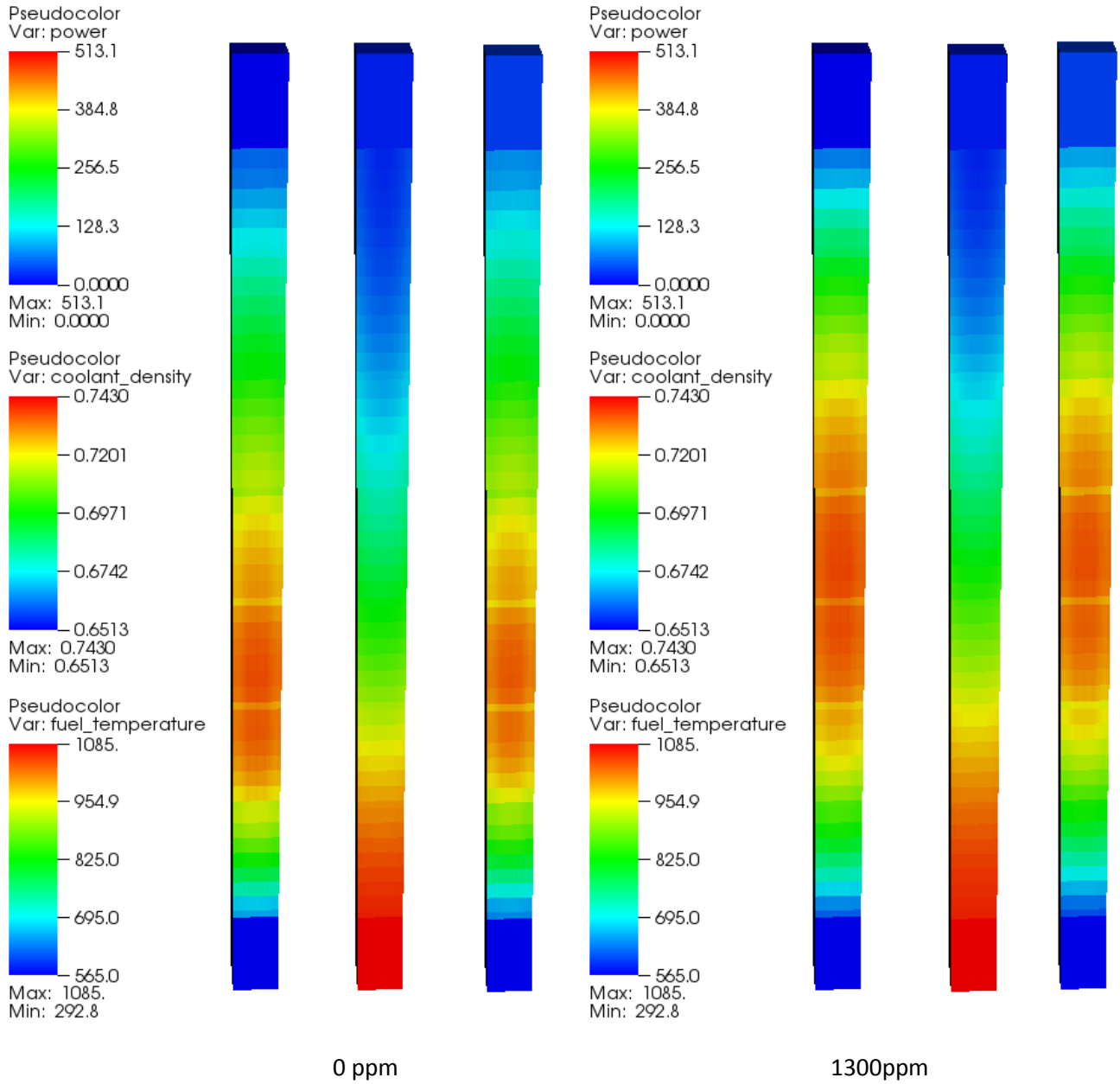


Figure 5-7 Graphical Output of the Fission Rate, Coolant Density, and Fuel Temperatures at 0 and 1300 ppm Boron

5.4 Power Perturbations

In order to see 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

Boron Concentration	Eigenvalue	Wall Time (HH:MM:SS)	Coupled Iterations	Total K_{eff} Itertions
70%	1.25301	4:35:52	9	125
100%	1.24710	4:39:58	9	129
130%	1.24080	5:20:52	10	143

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.

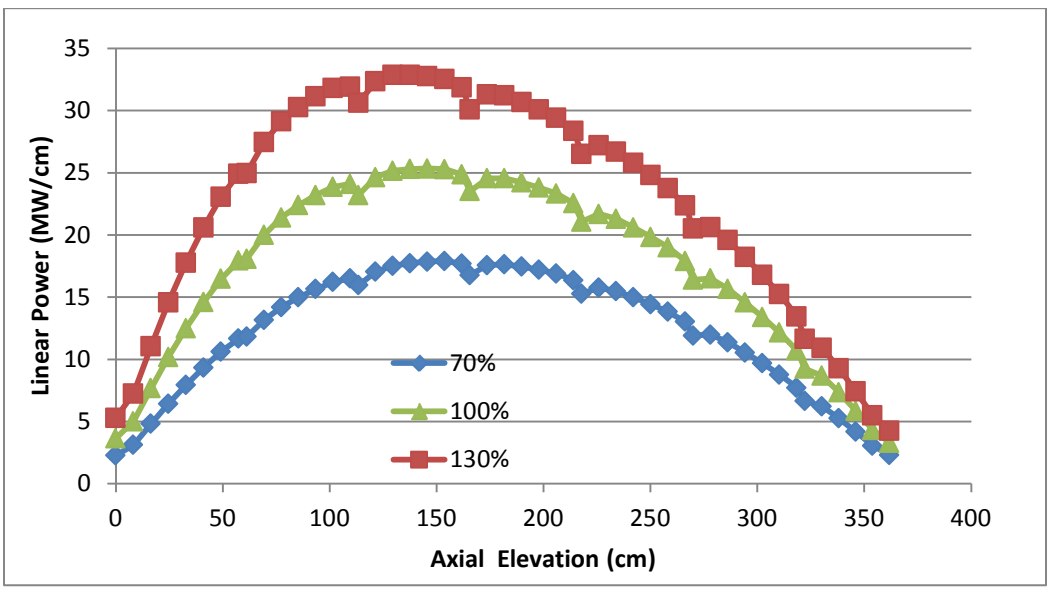


Figure 5-8 Axial Plot of Fission Rates at Different Power Levels

6. Conclusion and Recommendations

This objective of this milestone was to demonstrate the successful multiphysics coupling of the MPACT neutronics code to the CTF thermal hydraulics code. The codes were coupled using the LIME and parallel data transfer was performed with the DTK library. Several cases were performed to demonstrate that the coupling was working properly. Cases were run at three different boron concentrations. The successful coupling of MPACT and CTF for AMA 6 provides the framework to extend the coupling from a single assembly problem to a PWR full-core Problem 7 which will combine the full-core capabilities developed in Problem 5 [5] with the thermal-hydraulic feedback capabilities developed in Problem 6. The result will be the capability to model a full-core problem with thermal-hydraulic feedback at the beginning of life (BOL).

6.1 Recommendations

While this Milestone successfully meets all the objectives of coupling multiphysics codes together, there are still some areas that require further study and/or improvements. The following recommendations are provided:

- A convergence study should be performed with CTF to determine the optimum code options for coupled calculations. This includes values for the number of rings in the fuel rod conduction model and the number of axial mesh.
- Implement the capability for the coupled code system to run in parallel with MPACT using angle and spatial parallel domain decomposition.
- The current iteration strategy using in this code coupling should be studied and improved. Some suggestions include:
    - Implement dynamic convergence criteria in the neutronics solution that changes with iteration number. Current industry nodal codes have had success using dynamic criteria that sets the neutronics convergence at each coupled iteration to 0.01 times the current convergence observed in the coupled solution. These criteria may reduce the number of neutronics iterations needed at the beginning of the calculation.
    - Investigation into the sensitivity of the equivalence cross section computed by the subgroup calculation to the T/H feedback. Presently, the subgroup calculation is performed every fixed point outer which represents a significant run-time burden so this presents an opportunity to significantly reduce run times.
    - Determine root cause of why so many 2-D/1-D iterations are needed by MPACT when the coupled solution is very near “convergence”.
- Standardize output for visualization and for comparisons.
- Detailed comparisons and analysis to results produced by coupled COBRA-Insilico and some other reference methodology.

- Implement restart or checkpoint files for MPACT and the coupled code system so that extremely long computations can be run as multiple jobs.
- The current code coupling only provides for the use of rod-averaged values at each axial elevation. Additional work should be performed to extend this to intra-rod distributions.

7. References

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

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

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

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

[5] J. C. Gehin, et al., "Operational Reactor Model Demonstration with VERA: Watts Bar Unit 1 Cycle 1 Zero Power Physics Tests," CASL-U-2013-0105-000, June 7, 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] R. Pawlowski, R. Bartlett, N. Belcourt, R. Hooper, R. Schmidt, A Theory Manual for Multiphysics Code Coupling in LIME Version 1.0, Sandia National Laboratories, SAND2011-2195, March 2011.

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

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

[12] Watts Bar Unit 2 Final Safety Analysis Report (FSAR), Amendment 93, Section 4, ML091400651, April 30, 2009. http://adamswebsearch2.nrc.gov/idmws/ViewDocByAccession.asp?AccessionNumber=ML091400651

[13] L3.AMA.VDT.P6.03_report, S. Palmtag, "Coupled Single Assembly Solution with VERA (Problem 6), July 25, 2013.

[14] B. Collins, S. Stimpson, B. Kochunas, and T. Downar. "Application of MPACT 2D/1D to AMA Benchmark Problem 5," CASL-U-2013-0273-000, 2013.

Appendix A – Input File

This appendix contains the input listing for a PWR assembly. All of the input for CTF, Insilico, 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
```