Extension and Demonstration of NEAMS Multiphysics Tools to Lead-Cooled, Sodium-Cooled, and Molten Salt Fast Reactor Applications

Nuclear Science and Engineering Division

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Extension and Demonstration of NEAMS Multiphysics Tools to Lead-Cooled, Sodium-Cooled, and Molten Salt Fast Reactor Applications

prepared by

Emily R. Shemon, Yiqi Yu, Yeon Sang Jung, Bo Feng, and Taek K. Kim
Nuclear Science and Engineering Division, Argonne National Laboratory

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EXECUTIVE ABSTRACT

The SHARP toolkit is a high-fidelity reactor simulation tool developed under the U.S. Department of Energy, Office of Nuclear Energy Advanced Modeling and Simulation (NEAMS) Campaign. SHARP toolkit is comprised of the neutronics module PROTEUS thermal hydraulics module Nek5000, and structural mechanics module Diablo. During FY17 and FY18, the PROTEUS and Nek5000 components of SHARP were applied to solve challenging sodium-cooled fast reactor (SFR) problems. In particular, selected hot channel factors (HCF) for a prototype metal-fueled SFR design (the AFR-100) were analyzed in high fidelity, and the “SHARP zooming capability” for SFRs was developed and demonstrated to reduce computational expense for full core problems in cases where detailed data is needed in selected fuel assemblies.

After the previous success applying SHARP to challenging SFR problems, the focus in FY19 expanded to additional fast reactor applications: lead cooled fast reactors (LFR), sodium cooled fast reactors (SFR), and fast molten salt reactors (MSR). The specific technical tasks were (1) assessment of hot channel factors for LFR, for which no data currently exists, (2) implementation of a gamma transport capability in the PROTEUS solvers to extend the zooming capability to non-fueled assemblies, (3) demonstration of zooming capability in assemblies of the Versatile Test Reactor (VTR), and (4) development of a new coupled capability for simulating fast MSRs, specifically modeling precursor transport inside and outside the core. The progress on tasks (1) and (3) are discussed primarily in this document. Tasks (2) and (4) are briefly mentioned in this document, and the interested reader is referred to separate reports for detailed information.

First-of-a-kind hot channel factor (HCF) estimation for LFR with high fidelity codes (PROTEUS/Nek5000) was successfully demonstrated in this study. Selected HCF were computed and compared with SFR data (AFR-100, EBR-II). The findings confirm that different reactor types, design parameters and uncertainties lead to different HCFs. Careful estimation of HCF for a specific design is necessary to obtain appropriate HCFs. In addition to improvement in HCF accuracy, high fidelity tools generate data to help the designer better understand the mechanism of the impact from these uncertainties. For example, the impact of cladding thickness manufacturing tolerance resulted in non-intuitive effects in the corner pins of the LFR assembly. This procedure of computing HCF using high fidelity models shows promise and flexibility for being repeated for any arbitrary reactor of choice, since these tools are targeted to solve many reactor types and geometries.

Progress was made towards extending the previously demonstrated SHARP zooming capability to non-fueled SFR assemblies. In particular, a gamma transport capability was implemented in both high fidelity PROTEUS solvers in order to accurately account for heat deposition caused by gamma particles, which accounts for ~10% of total core power. Neutronics verification cases were carried out for a candidate Versatile Test Reactor (VTR)

design using the new gamma transport capability in PROTEUS. Comparisons were made with continuous energy MCNP calculations and shown to agree well. The models for the full core design with heterogeneous control and fuel assemblies is in progress and will be completed in FY20.

In the fast molten salt reactor (MSR) domain, a new capability was developed to model the flow of neutron precursors both inside and outside of the core, which impacts the effective delayed neutron fraction of the system. The PROTEUS-SN and PROTEUS-NODAL solvers were coupled to Nek5000 in order to simulate precursor flow. The workflows were demonstrated on test problems. The fast MSR modeling capability was supported under two other work packages, and comprehensive details are included in a separate report.

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1. Introduction

The SHARP toolkit [Mahadevan 2014], [Merzari 2015] is a high-fidelity reactor simulation tool developed under the U.S. Department of Energy, Office of Nuclear Energy Advanced Modeling and Simulation (NEAMS) Campaign. SHARP toolkit is comprised of the neutronics module PROTEUS [Shemon 2014], thermal hydraulics module Nek5000 [Fischer 2008], and structural mechanics module Diablo.

During FY17 and FY18, SHARP was applied to solve challenging sodium-cooled fast reactor (SFR) problems [Shemon 2018]. In particular, selected hot channel factors (HCF) for a prototype metal-fueled SFR design (the AFR-100) [Grandy 2013][Kim 2012] were analyzed using the high fidelity codes PROTEUS and Nek5000. The SHARP-calculated hot channel factors were compared with legacy hot channel factors for the metal-fueled EBR-II reactor [Ku 1994] which were generated by a combination of low fidelity codes, empirical correlations, and mockup experiments. The findings of this study demonstrated that high fidelity modeling and simulation can offer a benefit in assessing hot channel factors for SFRs by (1) reducing modeling uncertainty due to the increased geometric and physics detail taken into account, and (2) eliminating the need for mockup experiments. Additionally, the “SHARP zooming capability” for SFRs was developed and demonstrated to reduce computational expense for full core problems in cases where detailed data is needed in only selected fuel assemblies. The zooming capability is enabled by a multi-resolution mesh in neutronics where high fidelity meshes are used only in the fuel assembly of interest. The power distribution is passed to the thermal fluids solver (Nek5000) which models only the assembly of interest due to sufficient isolation from neighboring assemblies by the duct walls.

After the success applying SHARP to challenging SFR problems in FY17 and FY18, the focus in FY19 expanded to demonstrating SHARP’s capability to target additional reactor types. In particular, the tasks performed in FY19 were: (1) Assessment of hot channel factors for a lead-cooled fast reactor (LFR) design, (2) Implementation of a gamma transport capability in the PROTEUS solvers to extend the zooming capability to non-fueled assemblies, (3) Demonstration of zooming capability in a fuel and control assembly of the Versatile Test Reactor (VTR), and (4) Technical guidance and support for developing a new coupled PROTEUS-Nek5000 capability for simulating molten salt reactors (MSR), specifically modeling precursor transport inside and outside the core. The progress on tasks (1) and (3) are discussed primarily in this document. Tasks (2) and (4) are briefly mentioned in this document, and the interested reader is referred to an additional FY19 companion report for detailed information on gamma transport [Jung 2019], or by contacting the authors of this report for more information on the MSR capability.

2. Assessment of Hot Channel Factors for a Lead-Cooled Fast Reactor Design

This chapter discusses the assessment of hot channel factors (HCF) for a Westinghouse Electric Company (WEC) lead-cooled fast reactor design using the NEAMS-developed SHARP tools PROTEUS and Nek5000. The ducted assemblies of this particular design make the simulation requirements of the LFR similar to conventional SFR designs. Additionally, there are no known published HCF datasets for LFRs, making the Westinghouse LFR an ideal candidate for this analysis. Application of SFR-based HCF dataset to an LFR design is questionable, and so HCF analysis of LFR is needed. This task demonstrates the ability of the SHARP tools to perform such an analysis by assessing a limited list of LFR HCFs which were prioritized by WEC.

2.1 Westinghouse Lead-Cooled Fast Reactor Design

Westinghouse Electric Company (WEC), together with an international team, is developing its next generation high capacity nuclear power plant (NPP) based on lead-cooled fast reactor (LFR) technology. WEC provided technical details of their LFR design (current as of late 2018) and helped prioritize the hot channel factors to assess during FY19. All design details contained within this report are openly available [Grasso 2019].

Key parameters of the WEC LFR design are listed in Table 2.1.1. This medium-size, simple, scalable and passively safe plant harnesses a liquid lead-cooled, fast neutron spectrum core operating at high temperatures in a pool configuration reactor. The power output is 950 MWth (~450 MWe). The core map is provided in Figure 2.1.1. The core consists of three concentric fuel assembly zones, two banks of control assemblies, safety, reflector and shield assemblies. In this work, hot channel factors are analyzed for the inner zone fuel assembly type only, a cross section of which is shown in Figure 2.1.2. As performed in conventional HCF calculations, the impact of neighboring assemblies is not accounted for in this analysis. The generated HCF are generic enough to be applied to specific pins or assemblies in a full core analysis to yield actual temperatures.

Table 2.1.1 Key parameters of Lead-Cooled Fast Reactor (LFR) model

<i>Parameter</i>	<i>Value</i>	<i>unit</i>
Thermal power	950	MW
Peak fuel pin burnup	200	MWd/kgHM
Active core height	105	cm
Number of fuel pins per assembly	127	-
Gap thickness	0.175	mm
Duct thickness	3.5	mm
Fuel pin diameter	10.7	mm
Fuel pin pitch	13.3	mm
P/D	1.24	-
Cladding thickness	0.9	mm

Fuel pellet outer diameter	8.55	mm
Fuel pellet inner diameter	4.0	mm
Reynolds number	5.1×10^4	-

Figure 2.1.1 LFR core map

Figure 2.1.2 LFR fuel assembly geometry

The fuel assembly pitch is 16.3 cm with a 4 mm lead-filled gap between assemblies and 3.5 cm thick duct wall. Each assembly contains 127 cladded fuel pins arranged in a triangular lattice with pitch 1.33 cm within a hexagonal wrapper (duct). Each fuel pin has a cold fuel inner/outer diameter of 4.00/8.55 mm respectively, a fuel-cladding gap of 0.175 mm and a cladding outer diameter of 10.7 mm with a cladding thickness of 0.90 mm, depicted in Figure 2.1.3. Helium gas is present in the empty regions. In order to minimize the flow speed and consequently mitigate corrosion issues, a relative wide lattice ($P/D=1.24$) design is adopted. Grid spacers are planned to maintain pin spacing, rather than the wire wrap used in conventional SFR designs. Annular MOX fuel (UPuO) is envisaged for countries with spent fuel management policies supporting reprocessing and reuse of plutonium. Annular fuel is very beneficial for fast reactors because of its availability for both high power and high burnup. Most of the annular pellets irradiated up to high burnup showed central-hole shrinkage due to deformation and restructuring during irradiation. This shrinkage has a great influence on power-to-melt, which is a main factor in deciding the maximum power in the fuel design [Ikusawa, 2017].

Figure 2.1.3 LFR annular fuel pin geometry

The MOX (UPuO) fuel composition in the inner fuel zone is specified as a mixture of depleted uranium (0.25 wt% U-235) and enriched plutonium (68.769 wt% Pu-239, 1.759 wt% Pu-241), with 23% $\text{PuO}_x / (\text{PuO}_x + \text{UO}_x)$. The cold fuel density is 10.423 g/cc. The wrapper (duct) and pin cladding are made of DS4 with density 7.970 g/cc. The coolant is lead with density 10.402 g/cc. The axial regions of the fuel assembly are described in Table 2.1.2. The lower gas plenum through upper gas plenum are represented explicitly in neutronics (except for homogenizing the spring and tube), and regions above and below these are modeled homogeneously. Thermal expansion factors are applied to generate hot condition dimensions (1.021% fuel, 0.937% DS4 wrapper, 1.005% DS4 cladding, and 0.715% AISI316).

Table 2.1.2 Axial LFR zones and neutronics modeling information

Axial Zone	Neutronics Model Description	Upper Z (cm)	Neutronics XS Temp. (K)
Lower core plate	Homogenized mixture AISI316, DS4, Pb	10.0	693
Inlet wrapper	Homogenized mixture DS4, Pb	40.5	693
Lower bundle grid/pins plug	Homogenized mixture DS4, Pb	47.0	693
Lower gas plenum tube	Heterogeneous DS4 wrapper & cladding, Pb Homogenized DS4/He tube	132.0	693
Lower thermal insulator	Heterogeneous DS4, Pb, He, YSZ	133.5	693
Active core	Heterogeneous DS4, Pb, UPuO, He, Pb	238.5	808 (Wrapper, Pb) 843 (Cladding) 1300 (He, UPuO)
Upper thermal insulator	Heterogeneous DS4, Pb, He, YSZ	240.0	923
Upper gas plenum spring	Heterogeneous DS4 wrapper & cladding, Pb Homogenized DS4/He spring	252.0	923
Upper bundle grid/pins plug	Homogenized mixture DS4, Pb	257.0	923
Outlet wrapper	Homogenized mixture DS4, Pb	350.0	923

2.2 Selection of LFR Hot Channel Factors

A detailed background of hot channel factors in the nuclear design community can be found in the SFR applications report from FY18 [Shemon 2018]. A general overview is given here for brevity.

Various uncertainties are involved in the predictions of reactor design parameters, such as theoretical and experimental analysis uncertainties, instrumentation uncertainties, manufacturing tolerances, correlation uncertainties, and method and simulation uncertainties. These uncertainties impact the peak cladding, fuel and coolant temperatures in the system above those expected in the nominal condition (no uncertainties). The peak temperatures in the as-built system must be nevertheless be maintained at safe margins away from maximum temperatures that could compromise the integrity and performance of the materials. Therefore, the impact of uncertainties on the temperature predictions is typically accounted for through the assessment of “hot channel

factors”, which take into account the increase in temperature due to specific uncertainties. Figure 2.2.1 illustrates the nominal cladding temperature (lowest value), the impact of modeling and simulation uncertainties (raises to the peak value), and the design limit (a safe margin away from the physical eutectic formation temperature). The goal of this work is to reduce the size of the modeling and simulation (or other) uncertainties in order that the nominal peak cladding temperature can be raised, resulting in higher power and greater economic gains.

Figure 2.2.1 Schematic of assessment of margin to fuel-cladding eutectic formation

In the United States, four sets of HCFs have been developed under various SFR development programs, and the magnitudes of HCFs were strongly related to the status of modeling and simulation and computing power when the HCFs were developed. Figure 2.2.2 shows the SFR development, deployment, and operation history, including the activities on HCF development aimed at specific SFRs. A set of HCFs was developed for FFTF initially in 1976 and later updated in 1990. A significant effort to develop HCFs was conducted to support the licensing of Clinch River Breeder Reactor (CRBR) in 1980. The last set of HCFs was developed in 1995 under the Integral Fast Reactor (IFR) project to develop Mark-V metallic fuels in the EBR-II. However, the EBR-II and FFRF were permanently shut down, and SFR programs were canceled in the mid-1990s, and therefore no additional efforts were regarding HCFs since then, except for reviews of existing HCF sets for new SFRs. Therefore, the absence of any HCFs for LFR-based designs and questionable applicability of legacy SFR HCFs makes the LFR a good candidate for modern assessment of HCFs with the SHARP toolkit.

Figure 2.2.2 SFRs operated or designed in the United States

The following hot channel factors in Table 2.2.1 were considered during FY19, as prioritized by WEC given available computing time and code capabilities. WEC provided the associated tolerances and uncertainties. The modeling strategies and results for assessing each of the above uncertainties is discussed in individual sections.

Table 2.2.1 List of assessed LFR HCFs

LFR Hot Channel Factor	Description
Cladding thickness (subchannel flow area)	Assess impact of variances in cladding thickness due to manufacturing tolerance <i>Assumption: +/- 0.05 mm tolerance; change uniformly by maximum value in all pins due to meshing complexity</i>
Fissile fuel maldistribution	Assess impact of uncertainties in fissile content due to manufacturing tolerance <i>Assumption: +/-5% tolerance on Pu-239 enrichment; sample stochastically in all pins</i>
Coolant specific heat	Assess impact of uncertainties in lead coolant specific heat

	<i>Assumption: +/-5% uncertainty in lead specific heat</i>
Fuel thermal conductance across pellet-cladding gap	<p>In low conductivity fuels with no bond, uncertainty exists for the thermal conductance across the pellet cladding gap. Estimate the sensitivity of the fuel temperature to the gap by performing analysis at two bounding cases: assuming perfect eccentricity of the fuel at (1) fresh fuel with open gap (nominal condition), and (2) burned fuel with closed gap.</p> <p><i>Assumption: Detailed data on uncertainties in joint-oxide gain formation was not available, so the two bounding cases were analyzed. To assess the HCF, detailed fuel models and uncertainties are required which is outside the scope of the current SHARP toolkit and work scope.</i></p>

2.3 Computational Tools and Resources

The SHARP Toolkit is a DOE NEAMS software product that performs highly detailed multi-physics calculations with online data transfer. In this section, two sub-components of the SHARP toolkit, PROTEUS and Nek5000, used to assess the LFR HCFs are briefly described, including the overall computation approach by coupling two component codes and computation resources.

2.3.1 PROTEUS Neutronics Code

PROTEUS has two high fidelity neutronics solvers, PROTEUS-SN and PROTEUS-MOCES. The PROTEUS-MOCES solver was used for the HCF calculations. The PROTEUS-SN code was used for the VTR zooming calculations as well as for the MSR support so information is included here as well.

The PROTEUS-MOCES code solves the method of characteristics equations in the 2D plane for an unstructured mesh and solves the exact equations in the axial plane using the discontinuous Galerkin finite element method. The method is also known as “extruded MOC” as it relies on an extruded 2D mesh in the axial plane for geometry description. The method is more accurate than other extruded MOC methods such as DeCart and MPACT which rely on the 2D/1D synthesis method and can suffer from convergence and accuracy issues in certain core geometries. It is generally more memory intensive than the PROTEUS-SN code but uses less cores and less compute time, typically, to solve the same problem.

The PROTEUS-SN solver was a previous Gordon Bell Finalist for computational performance on the BlueGene/P (BG/P) architecture. It solves the second order, even parity form of the neutron transport equation using discrete ordinates approximation in angle, unstructured continuous finite

element method in space, and multigroup approximation in energy. The code relies on the PETSc linear solver package for performing large scale matrix solves of the underlying eigenvalue problem, the METIS package for online mesh partitioning, and the HDF5 package for detailed output. Parallelism is performed with MPI, and depending on the memory requirements for the cross section data, typically 1 MPI rank/core is optimal and reasonable. The code does not use multithreading at this point as threading is not particularly useful for the matrix operations.

Both PROTEUS-SN and PROTEUS-MOCEX have been studied for benchmark problems and compared well to Monte Carlo (MCNP or SERPENT) models as well as some limited validation data (ZPR, TREAT). However, the accuracy of high fidelity deterministic codes such as these is highly dependent on the accuracy of the multigroup constants fed into the codes as inputs. Significant research has been performed to assess the procedures for generating multigroup cross section data (an input parameter to deterministic neutronics codes like PROTEUS-SN and PROTEUS-MOCEX) for explicit pin-by-pin geometries [Hader 2014], [Jarrett 2016]. The techniques learned in the past few years have been implemented in this work.

2.3.2 *Nek5000 Thermal Hydraulics Code*

Nek5000 is an open source code designed to simulate unsteady incompressible Navier-Stokes flow, low Mach-number flows flow, heat transfer and species transport and incompressible magneto hydrodynamics (MHD). Nek5000 is a previous winner of the Gordon Bell Prize in high performance computing and continues to adapt to new architectures with its highly scalable algorithms. Its fast scalable multigrid solver can scale to more than 290,000 processors on the BG/P architecture using pure MPI with multiple ranks per core, and beyond 1M MPI ranks on BG/Q architecture at 60% efficiency with only 2000 DOFs/rank.

Nek5000 is based on a high-order spectral element method and achieves extremely rapid (exponential) convergence at low cost. Figure 2.3.1 shows the comparison of convergence behavior between Nek5000 and OpenFOAM (another well-known open source CFD code), where Nek5000 has a remarkable advantage on convergence behavior (fewer DOF are required for a desired accuracy). In addition to its high-order foundation, Nek5000 has several other features that make it ideally suited for large-scale parallel simulations. Temporal discretization is based on a high-order splitting that is third order accurate in time and reduces the coupled velocity-pressure Stokes problem to independent three Helmholtz and one elliptic solver per time step, i.e. for each velocity component and pressure, respectively. The velocity problems are diagonally dominant and thus easily solved by using Jacobi preconditioned conjugate gradient iteration. The pressure sub-step requires a Poisson solve at each step, which is performed through multigrid-preconditioned GMRES iteration coupled with temporal projection to find an optimal initial guess. Particularly important components of Nek5000 are its scalable coarse-grid solvers that are central to parallel multigrid. Nek5000 has been extensively tested for over 25 years.

More than 150 journal articles have been published by worldwide users of Nek5000. More than 400 tests have been performed to validate the models in the code in different research fields. The

user community includes over 400 scientists and engineers in academia, laboratories and industry. The Nek5000 has been used for numerous INCITE and ALCC awards at the ALCF in recent years. All required physics modules for this work are already included in Nek5000. Figure 2.3.2 shows a schematic representation of the full hierarchy of thermal hydraulic codes in NEAMS toolkit. Given the computational cost, we focus on RANS-based CFD simulations for this work.

Figure 2.3.1 Comparison of convergence behavior between Nek5000 and OpenFOAM [Sprague 2010]

Figure 2.3.2 Hierarchical structure of NEAMS TH tools

2.3.3 Multiphysics Coupling Approach and Computational Resources

PROTEUS calculates the detailed power density and flux distributions in a nuclear reactor core. Nek5000 calculates the detailed velocity and temperature distributions in a nuclear reactor core. In

FY16, a tightly coupled version of SHARP was released in which PROTEUS and Nek5000 transmit data (temperature, power) in memory via two-way iteration between the two physics on a fine grained (element-wise) basis. While in-memory coupling certainly provides very accurate transfer of data (element-wise basis), there are some limitations: (1) only one neutronics solver (PROTEUS-SN) and one CFD solver (older version of Nek5000) are currently connected to each other in the in-memory form of SHARP, (2) in the current in-memory form of SHARP, the codes must utilize the same number of compute processors during the simulation, and (3) parallelization in angle in PROTEUS within SHARP is prohibited, which means fewer cores total can be used and with a higher memory burden. These limitations can be untenable for larger simulation problems where parallelization in angle is needed, and where the two codes utilize very different numbers of compute processors.

The offline coupling scheme developed in FY17-FY18 for the SFR HCF assessment, shown in Figure 2.3.3, was again utilized for this work. The offline coupling scheme allows the PROTEUS-MOCEX solver (more efficient for the proposed single assembly calculations) to be used along with Nek5000 and also allows each code to choose its own optimal parallelization scheme, providing much greater computational flexibility and efficiency. The drawback of offline coupling is the coarser-grained data transfer as well as the manual interventions that are required between code iterations that preclude efficient 2-way coupling.

Figure 2.3.3 Schematic of offline coupling using components of the SHARP toolkit.

The offline coupling was performed one-way: initial calculation with PROTEUS-MOCEX, spatial distribution of power density given to Nek5000, and finally Nek5000 calculates temperature distribution. Ideally an iterative procedure would be implemented where neutronics would update the material cross sections based on temperature, and produce a new power density for Nek5000,

but this would double the computational requirements and usually is not necessary due to only minor dependence of power distribution on temperature feedback for fast reactors.

Local machines and small clusters are used to perform pre-processing steps such as finite element mesh generation, multigroup cross section preparation, and testing of input files. To perform more detailed testing, debugging, convergence and sensitivity studies, as well as small production runs, an allocation at Argonne's Laboratory Computing Resource Center (LCRC) Bebop machine was utilized. The Bebop cluster has 664 Broadwall nodes with 36 cores/node and 128 GB/node, plus 352 Intel Xeon Phi (Knights Landing) nodes with 64 cores/node and 96 GB. Roughly 150K-300K core hours are available per quarter, depending on user needs.

While not needed in general for the HCF calculations (due to computational advancements in the Nek5000 single assembly model and lack of wire wrap), large production simulations are needed for the zooming calculations discussed later. An Advanced Scientific Computing Research (ASCR) Leadership Computing Challenge (ALCC) proposal was written and awarded 880,000 node-hours of compute time at the Argonne Leadership Computing Facility (ALCF) Theta machine. ALCF's Theta has 4,392 Intel Xeon Phi (Knights Landing) nodes with 64 cores and 16 GB of MCDRAM, and 192 GB DDR4 memory. The ALCC award runs from July 1, 2019 through June 30, 2020.

The required high-fidelity calculations for the HCF evaluations are summarized in Table 2.4.1. The PROTEUS and Nek5000 columns in this table indicate the required number of high-fidelity assembly calculations by PROTEUS and Nek5000 codes. A nominal condition calculation is required to understand the power and temperature distribution without accounting for any uncertainties. The peak temperatures obtained from each perturbed calculation is then compared with nominal condition temperatures to evaluate the hot channel factors.

Table 2.3.1. Required high-fidelity calculations for HCF evaluations

HCF	PROTEUS	Nek5000
Nominal Condition	1	1
Cladding Thickness	1	2
Fissile Maldistribution	30	30
Coolant Specific Heat	-	1
Gap Conductance (Bounding Case)	1	2

Only the fissile maldistribution case is analyzed using a stochastic sampling technique. Ideally the cladding thickness case would also have been treated this way, however, meshing stochastically variable pins is extremely time consuming, so instead the pins were changed uniformly by the maximum cladding tolerance value to decrease the cladding thickness to its thinnest size. In

Nek5000, both increased and decreased cladding thicknesses were analyzed to understand the dual impacts of changing subchannel flow area as well as changing cladding thickness. The coolant specific heat calculation is necessary only in Nek5000. The gap conductance bounding case is performed for burned fuel composition with a fully closed gap. Additional information on the formation of joint-oxide gain (JOG) is necessary to fully evaluate HCF for this case.

2.4 Neutronics Modeling Strategy

The PROTEUS-MOCEX transport solver was employed to solve each of the simulations shown in Table 2.4.1. Each simulation represents a single 3D LFR fuel assembly in fully heterogeneous detail, with reflective boundary conditions placed on the exterior radial boundaries and void boundary conditions placed on the top and bottom boundaries. PROTEUS-MOCEX was chosen due to its efficiency on relatively small but heterogeneous geometries, especially those including streaming effects in near-void regions (i.e. the annular fuel pellet). PROTEUS-MOCEX is based on a method of characteristics formulation in the radial (X-Y) plane and discontinuous Galerkin finite element formulation in the axial (Z) dimension.

2.4.1 Cross Section Generation

Multigroup cross sections were generated using the MC²-3 code [Lee 2012] which specializes in fast spectrum reactors. Heterogeneity effects were accounted for through a two-step procedure using MC²-3 in conjunction with TWODANT [Alcouffe 1984]. The workflow used for MC²-3/TWODANT is shown in Figure 2.4.1 and is based on previous experience generating multigroup cross sections for highly heterogeneous geometries [Hader 2014], [Jarrett 2016]. The assembly is converted into a 1-D geometry by homogenizing materials within each axial zone (active fuel, thermal insulator, etc). Each assembly axial zone is simulated as an infinite medium homogeneous mixture in MC²-3 to yield 1041-group cross sections. A 1041-group 1-D transport simulation is then performed in TWODANT to calculate the axial leakage in each axial zone. The resulting 1041-group region dependent fluxes are used to collapse the 1041-group cross sections for the non-fuel axial zones into broad group cross sections. For axial zones containing fuel, new 1041-group cross sections including pin radial heterogeneity effects were generated by converting the 127-pin geometry into 1-D cylindrical geometry in MC²-3 while preserving volume fractions of each material to model the explicit fuel, cladding and coolant materials. Such a conversion is depicted in Figure 2.4.2 (rings are not to scale or correct in number). The rings represent materials like fuel, cladding, coolant, etc. The resulting fuel zone 1041-group cross sections were then collapsed with the TWODANT 1041-group fluxes to yield broad group (33-group) cross sections with both local and global heterogeneity effects.

Figure 2.4.1 Cross section generation procedure for heterogeneous 3D pin configurations

Figure 2.4.2 Conversion of assembly into 1-D cylinder geometry (not to scale)

2.4.2 Mesh Generation

The PROTEUS MeshTools code was chosen to generate the PROTEUS meshes as it easily incorporates repeated pin cell features in a hexagonal geometry, as well as assembly ducts. Meshes of varying degrees of fidelity were generated in order to perform mesh convergence studies. The azimuthal intervals (A) and radial intervals (R) for the fuel pins can be varied independently of each other, and the number of axial planes can also be varied. Several 2D meshes for the 7-pin configuration are shown in Figure B.2.1 with variable azimuthal (A) and radial (R) intervals. For PROTEUS-MOCEX, a 2D finite element mesh is required, along with the axial plane discretization provided separately.

The nominal mesh is used for all simulations except the cladding thickness perturbation. The nominal cross section file is used for all simulations except the burned fuel simulation needed for the gap conductance study. While the material assignments change for the fissile maldistribution cases, they are based on the nominal cross section data.

2.4.3 Neutronics Discussion of Nominal Condition

Convergence studies in mesh and angular cubature were performed to ensure appropriate selection of discretization parameters in the neutronics model. The energy group structure was held

constant at 33 energy groups. The full assembly problem showed little to no dependence on mesh fidelity. A mesh with 10,980 elements in the X-Y plane and 48 axial planes was used in the final calculations (see Figure . The eigenvalue was strongly dependent on the angular cubature due to streaming regions in the annular fuel pellet. The cubature selected was Legendre-Tchebychev L7T17 (288 angles on the unit sphere) which exhibits a good balance of accuracy and computational cost. The 3D nominal condition fuel assembly eigenvalue was computed as 1.17701.

Figure 2.4.3 Top view of LFR neutronics mesh (left) and zoomed in (right)

Code-to-code verification of eigenvalues was performed for various LFR models to ensure the cross sections and geometry were generated correctly (Table 2.4.2). The MCNP6 continuous energy code was used for comparison to MC²-3 (when applicable) and PROTEUS-MOC. Three infinite medium cases were run (LFR MOX fuel, LFR pin cell, and LFR active fuel zone of assembly) and showed good agreement with both MC²-3 and PROTEUS-MOC eigenvalues. The 2D LFR pin cell also showed good agreement with both codes. Due to geometry limitations, geometrically complex cases are not performed in MC²-3. The 2D LFR assembly compared well to PROTEUS-MOC, and while the 3D LFR assembly (the case of relevance to the hot channel factors) showed larger errors, the agreement is still reasonable and could potentially be reduced with additional energy groups in PROTEUS-MOC. Notably, the pin power distribution in the LFR assembly center pin (pin 1) are compared in MCNP and PROTEUS-MOC and match within 1.5% error (see Figure 2.4.4). The pin power distribution is the only data transferred to Nek5000.

The LFR assembly model in MC²-3/PROTEUS therefore matches well against the completely independent model in continuous energy MCNP.

Table 2.4.2. Code-to-code eigenvalue verification of LFR-based problems

LFR Case	MCNP6 CE (pcm uncert.)	MC ² -3 1041g - MCNP (pcm)	PROTEUS-MOC 33g - MCNP (pcm)
Infinite medium (homogenized LFR MOX fuel)	1.65235 (15)	177	180
Infinite medium (homogenized LFR pin cell)	1.36242 (11)	77	184
Infinite medium (homogenized LFR active fuel zone of assembly)	1.28613 (11)	13	112
2D LFR pin cell	1.36625 (12)	65	188
2D LFR assembly (active core slice)	1.29446 (3)	-	214
3D LFR assembly ("nominal condition")	1.17288 (19)	-	413

Figure 2.4.4 Code-to-code verification of center pin power shape

The nominal condition calculation is simply the 3D LFR assembly case from Table 2.4.1. The power in the assembly was normalized to 3.7 MW. The pin power distribution for the center pin is shown in Figure 2.4.4. Three axial slices taken at the core bottom, middle, and top depict the radial power distribution in the assembly (Figure 2.4.5). The same color scale is used in all plots and shows that the power level is highest at mid-core, and slightly higher at the top of the core than at the bottom of the core (shifted cosine shape). This matches the pin power distribution in Figure 2.4.4. The pin powers exhibit a nearly flat radial power distribution at all axial levels. This is expected because of reflected boundary conditions placed on the exterior of the assembly. There is also a nearly constant axial shape and integrated pin power for all 127 pins. The maximum and minimum integrated fuel pin powers are 28.76 kW (outside corner pins) and 28.68 kW (inner rings), i.e. <0.2% difference. The maximum and minimum cladding powers are 100.6 W (outside corner pins) and 98.9 W (inner rings). The cladding power is negligible in the fuel assembly compared to the fission power generated in the fuel zones. However it is tallied separately for Nek5000 due to the fuel-cladding gap. No gamma transport was applied in these cases, so gamma particles are assumed to deposit heat at their source site. It should be noted that the total heat generation of the 127 fuel pins and cladding is 3.6577 MW, compared to 3.7 MW assembly power. The missing 1.1% of total assembly power is contained within duct walls or in regions outside the active core and is ignored in Nek5000. Power outside the active core is subsequently ignored in Nek5000 as it does not significantly contribute to the coolant, cladding, or fuel temperatures in the active core.

Figure 2.4.5 Left to right: Power distributions shown at bottom (z=135 cm), middle (z=187 cm) and top (z=240 cm) of core

Figure 2.4.6 Axial power shapes in fuel zone of pin 1 (center) and pin 122 (outside corner)

To summarize the nominal condition neutronics analysis, the pin and cladding power shapes are nearly identical. The same axial power shape can be used for both all fuel and cladding zones. A uniform power distribution across pins is also valid since the maximum and minimum integrated pin powers differs by only 0.2%. The nominal condition calculation requires 12 minutes of wall clock time on 96 Broadwell nodes (36 cores/node) or 691 core-hours. The MCNP verification calculation required 20 hours of wall clock time on 32 processors of Intel Xeon X5560 or 640 core-hours.

2.5 Thermal Fluid Modeling Strategy

In the Nek5000 CFD simulation, the cladding, fuel, helium gap and hollow are modeled explicitly. A new mesh script was developed to mesh these domains separately. Models for calculating the impact of the cladding thickness perturbation or other geometric perturbation can thus be easily built by taking advantage of the meshing script.

2.5.1 Lateral Velocity Considerations

URANS simulations are performed with $k-\omega$ turbulence model for the LFR fuel assembly. Figure 2.5.1 shows the lateral velocity on different elevations. The simulation indicates there exists strong lateral velocity in the vicinity of the duct. The assembly has a relatively small gap between the outer ring of pins and the duct wall, which provides relatively strong shear stress. The flow near the duct swirls around the outmost layer pin when moving in the stream-wise direction. The magnitude of the strongest lateral velocity can reach 30% of the mean stream-wise velocity. It can also be observed that the lateral flow needs a certain distance to fully develop. On the first two

elevations near inlet, the lateral velocity is not very obvious. The lateral flow becomes fully developed after it flows past half of the domain. The strong lateral velocity only appears near the duct while it stays small in the center of the assembly.

Figure 2.5.1 Lateral velocity on different elevations of the LFR assembly

Figure 2.5.2 shows the transient lateral velocity near the corner of the LFR fuel assembly, i.e. how the lateral velocity changes over time. The fluid in the corner of the assembly oscillates in direction within the plane, which leads to similar time-averaged lateral velocity predicted from a RANS simulation. However, it is always preferable to capture these transient flow behaviors with a URANS model.

Figure 2.5.2 Transient lateral velocity near the corner of the LFR assembly

2.5.2 Turbulent Prandtl Number Consideration

Heavy metal fluid (lead) is different from sodium fluid. In general, the Prandtl number of heavy metal fluid is 2 order of magnitude lower than that of sodium fluid. Due to the low Prandtl number of lead, the thermal boundary layer in temperature field is much thicker than the viscous boundary layer in velocity field. Existing engineering turbulence models all use the Reynolds analogy for coupling temperature and velocity fields, which is not valid for Heavy Lead Metal (HLM) flow. Both experimental and theoretical studies [Reynolds 1975][Cheng 2004] available in the open

literature suggest a turbulent Prandtl number larger than 1.0 for liquid metal flows. Therefore, unlike for sodium flow, the selection of an appropriate turbulent Prandtl number is crucial for lead fluid simulation.

A sensitivity study is conducted for turbulent Prandtl number (Figure 2.5.3), which shows the temperature in the fluid on a line between two heated rods. The results shows that the temperature variation is sensitive to turbulent Prandtl number. Figure 2.5.4 shows the Nusselt number with the change of turbulent Prandtl number. A higher turbulent Prandtl number reduces the calculated Nusselt number by up to 18%.

Figure 2.5.3 Temperature distribution between rods with varying turbulent Prandtl number

Figure 2.5.4 Nusselt number with varying turbulent Prandtl number

Based on the results from open literatures [Myong 1989] [Cheng 2006], the following two correlations are proposed for calculating the heat transfer in LFR rod bundle assembly. The calculations shows consistent turbulent Prandtl number selection with $Pr_t^a = 1.5$ and $Pr_t^b = 1.455$. In the LFR simulations performed here, a turbulent Prandtl number of 1.5 is used. In the future, high fidelity LES simulations will be performed to help to select the best turbulent Prandtl number for this specific geometry.

$$Pr_t^a = \begin{cases} 1.5 & Pe \leq 2000 \\ 2.5 - 0.0005 & Pe \ 2000 \leq Pe \leq 3000 \\ 1.0 & Pe \geq 3000 \end{cases}$$

$$Pr_t^b = 0.75 + \frac{1.63}{\ln(1 + Pr/0.0015)}$$

Figure 2.5.5 Turbulent Prandtl number correlations from open literature

2.6 HCF Associated with Uncertainties in Cladding Thickness

The cladding material is assume to be double-stabilized austenitic stainless steel (DS4) with a manufacturing tolerance of ± 0.05 mm. While the variations in cladding thickness should ideally be modeled stochastically for each pin, this requires an extraordinary amount of mesh preprocessing effort and different number of cases. Therefore, the two bounding cases were modeled (-0.05 mm cladding thickness in all pins and +0.05 mm cladding thickness in all pins) in Nek5000. Only the reduction in cladding thickness case was modeled in neutronics as it was found to have no impact on the power distribution. The hot cladding dimensions are summarized in Table 2.6.1.

Table 2.6.1. Cladding perturbation parameters

Case	Cold Clad Thickness (mm)	Hot Clad Thickness (mm)	Hot Inner Clad Radius (mm)	Hot Outer Clad Radius (mm)
Nominal	0.900	0.909	4.495	5.404
Perturbed (-0.05 mm thickness)	0.850	0.859	4.495	5.354
Perturbed (+0.05 mm thickness)	0.905	0.914	4.495	5.409

2.6.1 Neutronics Discussion

The neutronics results determined that the cladding thickness reduction has a negligible impact on both power shape and magnitude. The nominal and perturbed power shapes in a corner pin (pin 122) are compared in Figure 2.6.1 and shown to be identical. The eigenvalue for the perturbed case did increase from 1.17701 (nominal case) to 1.18121 (perturbed case) but the power details were unaffected given that the power was normalized to the same level as the nominal condition case.

Figure 2.6.1 Nominal and perturbed axial power shapes in pin 122 (outside corner)

A tiny fraction of power was shifted from the outside corner pin fuel and cladding zones to the inner rings, essentially flattening out the power distribution even more than it already was in the

nominal condition. The axially integrated (along active fuel zone) fuel and cladding powers are shown in Figure 2.6.2 and 2.6.3. Pin 1 is the center pin, and pins 2-7 are in ring 2, and so forth. Pin 122 is one of the 6 corner pins in the fuel assembly.

The maximum pin power difference occurs in the outer corner pins (-9 W reduction in fuel power, <1 W reduction in cladding power). This is negligible compared to the total integrated fuel power of the pin itself (28.76 kW per pin). Therefore the neutronics impact of the cladding perturbation can be completely ignored in terms of power shape and power magnitude in each pin. Since reduction of the cladding thickness did not impact the neutronics solution, the increased cladding thickness case was not performed.

Figure 2.6.2 Nominal and perturbed integrated fuel powers (all pins)

Figure 2.6.3 Nominal and perturbed integrated cladding powers (all pins)

The nominal condition power profile was used in the Nek5000 analysis for the cladding perturbation case. Both the cladding thickness increase and decrease were modeled because the combined effect of the changing coolant subchannel flow area as well as the decreased cladding thickness for heat transfer have undetermined effects.

2.6.2 Thermal Hydraulics Discussion

As a reminder, the uncertainty of the cladding thickness is $\pm 0.05\text{mm}$. The uncertainty is applied to all pins. In conventional HCF estimation, the uncertainty of the cladding thickness is taken as an independent factor and is calculated as an analytical solution. In actuality, the change of cladding thickness will have impact on power distribution, flow area, velocity distribution and thermal conduction. All of these effects are coupled together to influence the temperature. Therefore, the temperature change depends on which effects dominate in a specific location. In the high fidelity simulations performed here, these sub-factors are taken into account simultaneously. The resulting HCF calculated will be certainly more accurate than an analytical solution.

Figure 2.6.4 Numbering scheme of fuel assembly

Figure 2.6.5 Maximum coolant temperature responding to the uncertainty of cladding thickness

Figure 2.6.4 shows the pin numbering in the LFR fuel assembly. Figure 2.6.5 shows the maximum coolant temperature (outer cladding temperature) with maximum cladding thickness uncertainty. In the inner rings (pins 1-91), the maximum coolant temperature responds to the cladding thickness uncertainty in an intuitive way. The larger cladding thickness leads to smaller flow region and thus smaller bulk velocity and *higher* coolant temperature.

In the outermost ring (pins 92-127), the maximum coolant temperature for most of the pins respond to the cladding thickness uncertainty in the same way whereas the corner pins respond differently. For the corner pin, a larger cladding thickness leads to *lower* maximum coolant temperature. The heat transfer mechanism in the corner region is dominated by different factors. In

the corner, the flow is surrounded by two duct walls, which makes the total shear stress greater than that in other regions. The flow velocity is quite small in that region. Further decreasing the flow here will have a smaller impact on the maximum coolant temperature than it does in other regions. However, increasing the cladding thickness increases the distance for heat conduction through the cladding, which will lead to coolant temperature drop. In other word, the heat transfer mechanism in the corner pin regions is different from that in other regions. The maximum coolant temperature for the corner pin respond to the uncertainty of the cladding thickness counterintuitively. Through the high fidelity coupled simulation, not only the hot channel factor but also the supporting data is obtained. The data can be used to study the physics mechanisms at play. Each hot channel factor is no longer taken as an independent factor and can be studied comprehensively for results that are more reliable.

2.7 HCF Associated with Uncertainties in Fuel Pellet Fissile Content

The MOX fuel is specified to be 23% $\text{PuO}_x/(\text{PuO}_x+\text{UO}_x)$. The uranium is depleted (0.25 wt% U-235), and the Pu is enriched (68.769 wt% Pu-239, 1.759 wt% Pu-241). Due to manufacturing uncertainty, the Pu-239 content has a manufacturing tolerance of $\pm 5\%$ (3-sigma normal distribution) from the target enrichment. This variability in enrichment can causes changes in local pin power and temperature.

2.7.1 Neutronics Discussion

A stochastic (random sampling) technique was used to assess the impact of fissile content uncertainty. To obtain meaningful stochastic distributions, thirty independent neutronics inputs were randomly selected as follows:

1. The fissile content in each pin is sampled individually and not affected by neighboring pins.
2. A normal distribution is used to sample each enrichment perturbation, with mean=0% and 1-sigma = 1.67% (3-sigma = 5%). In such a distribution, more than 99% of fuel pins will have enrichments within 5% of the target manufacturing value.
3. The sampled enrichment perturbations are rounded to the nearest integer in the discrete set $\{\pm 6, \pm 5, \pm 4, \pm 3, \pm 2, \pm 1, 0\}\%$. Limiting the enrichment perturbations to integers simplifies the definition of material compositions in neutronics.
4. The density of the fuel for each pin was assumed constant by modifying Pu-240 content to compensate for changing Pu-239 content.
5. The fuel assembly power was held constant at 3.7 MW for each independent simulation.

The eigenvalues from the thirty simulations (B1-B30) were binned in a histogram chart (Figure 2.7.1) and generally follow a normal distribution. The eigenvalue histogram uses bin widths of 66 pcm (0.00066). The average k-eff is 1.7699 which is within 2 pcm of the nominal condition calculation (1.7701).

Figure 2.7.1 Distribution of eigenvalues across 30 random samples

Of the thirty independent simulations, Simulation “2” yielded the pin with the highest local power, 29.80 kW in Pin 81. This value is 1.04 kW higher (3.6% higher), and in a different pin location, than the expected maximum pin power of 28.76 kW in the nominal condition which occurs in corner pins such as Pin 92. A mid-core slice showing the power distribution for the nominal condition and Simulation 2 is shown in Figure 2.7.2. The nominal case assumes all pins are manufactured with the targeted Pu-239 content. Simulation 2 contains pins with randomized fissile content perturbations according to the normal distribution described in this section. The color scale is identical in the two figures. The uniform pin powers in the nominal condition are in stark contrast to the highly variable powers in the stochastic simulation.

Figure 2.7.2 Power distribution at core mid-plane in nominal condition (left) and randomized fissile content bounding case in Simulation 2 (right).

In Simulation 2, Pin 81 was stochastically assigned an enrichment perturbation of +6% which is outside the 3-sigma range of the distribution (99.73% confidence interval). However, given the 3,810 enrichment perturbation sampled (127 pins/sample*30 samples), about 1% or 10 samples are expected to lie outside this interval.

The distribution of enrichment perturbations for Simulation 2 is depicted in Figure 2.7.3 as a histogram. Most of the samples are clustered within $[-3, +3]$, which makes sense because the range $[-3.33, +3.33]$ represents the 2-sigma interval (95.45% confidence level). Therefore, the distribution looks qualitatively valid. Figure 2.7.4 depicts the distribution of pin powers in Simulation 2. The peak pin power in pin 81 is clearly identified.

Figure 2.7.3 Distribution of enrichment perturbations for pins in Simulation 2 (simulation with maximum pin power)

Figure 2.7.4 Distribution of pin powers in Simulation 2 (simulation with maximum pin power)

The normalized axial power distribution for each pin needed for Nek5000 is plotted in Figure 2.7.5. The selected pins have the following enrichments perturbations and locations: Pin 1 (-2%, ring 1), Pin 42 (-4%, ring 4), Pin 81 (+6%, ring 6), Pin 106 (+0%, ring 7). The figure demonstrates that the axial power shape is not significantly impacted by the local enrichment perturbations or by pin location. Therefore, the same axial power shape can be used for all of the pins in Nek5000, where the scaling factor (pin power) is unique.

Figure 2.7.5. Normalized axial power distribution for selected pins within Simulation 2

A follow-on calculation (C) was carried out to identify the impact of directly changing the corner pin (Pin 92)’s Pu-239 content by +5%. This could be considered a “direct” rather than “statistical” calculation of the same hot channel factor. In the direct calculation, the maximum power was calculated to be 29.68 kW in Pin 92. This value is lower than the pin power observed from the stochastic simulations, therefore it is less conservative.

Table 2.7.1. Summary of fissile maldistribution impact on peak pin power

Case	Location	Peak Pin Power (kW)
(A) Nominal	Pin 92 (ring 7)	28.76
(B1-B30) Stochastic; all pins perturbed according to normal distribution with 3-sigma = 5%	Pin 81 (ring 6)	29.80
(C) Direct; Pin 92 perturbed by 5%	Pin 92 (ring 7)	29.68

2.7.2 Thermal Hydraulics Discussion

In the past, due to the lack of computational resource, only the neutronics simulation with the maximum peak pin power was conservatively chosen to transfer power to Nek5000. Development of Nek5000 during FY19 enabled improved computational efficiency, and consequently, all thirty cases were simulated in Nek5000. Due to the relatively small number of samples (30), the simulation with the maximum peak temperature was chosen to estimate hot channel factor. A normal distribution would be more likely to occur with more random sampling and the simulation with a peak pin power lying in the 95% confidence interval (2-sigma) could be selected as shown in Figure 2.7.6.

The observed distribution of peak power and maximum cladding temperature is shown in Figure 2.7.7. A more standard normal distribution is expected if more samples are used. The maximum coolant temperature, cladding temperature, fuel temperature and peak power for all 30 cases are presented in Figure 2.7.8 – 2.7.10. The benefit of performing 30 Nek5000 simulations is well explained in these figures. The maximum peak power occurs in neutronics Simulation 2, corresponding to T/H Case 2. However, the maximum temperature in coolant, cladding and fuel does *not* all occur in Case 2. The maximum coolant temperature occurs in Case 13 rather than Case 2. This is because the maximum temperature depends on not only the magnitude of the peak power but also the position of the peak power. Although the results show that the maximum cladding

temperature and fuel temperature still shows in Case 2 (red frame in Figure 2.7.9), they also demonstrate that higher peak power does not automatically lead to higher maximum temperature (green frame in Figure 2.7.9 showing a high cladding temperature despite the lower peak pin powers compared to the rest of the simulations). Table 3 that lists the rank of peak power and maximum coolant, cladding and fuel temperature rise for all 30 cases can further demonstrate that in detail. Similar results are observed in Figure 2.7.8 and Figure 2.7.10 as well.

Figure 2.7.6 Hypothetical peak pin power distribution based on random sampling with a very large number of samples.

Figure 2.7.7 Distribution of peak power and maximum cladding temperature

Figure 2.7.8 Maximum coolant temperature and peak power for all 30 cases

Figure 2.7.9 Maximum cladding temperature and peak power for all 30 cases

Figure 2.7.10 Maximum fuel temperature rise and peak power for all 30 cases

Table 2.7.2 Rank of peak power, coolant, cladding and fuel temperature rise for all 30 cases

case number	Peak Power x1000	Peak Power Rank	Maximum Coolant ΔT Rank	Maximum Cladding ΔT Rank	Maximum Fuel ΔT Rank
1	29.80	30	8	8	9
2	29.65	1	6	1	1
3	29.44	5	21	9	6
4	29.51	17	17	25	24
5	29.40	11	29	21	11
6	29.29	25	13	27	27
7	29.42	28	25	29	29
8	29.55	21	14	13	18
9	29.52	9	3	10	10
10	29.34	10	2	15	16
11	29.43	27	11	30	28
12	29.68	19	12	26	21
13	29.39	4	1	7	4
14	29.43	26	19	16	26
15	29.73	20	22	18	19
16	29.63	3	27	3	3
17	29.42	6	5	4	5
18	29.58	22	16	14	22
19	28.70	8	18	5	8
20	29.40	24	26	19	23
21	29.29	29	30	28	30
22	29.50	13	15	17	12
23	29.59	7	10	6	7
24	29.49	14	7	20	17
25	29.78	2	28	2	2
26	29.43	18	9	22	20
27	29.48	16	24	12	13
28	29.48	15	20	11	15
29	29.50	12	4	23	14
30	29.42	23	23	24	25

Figure 2.7.11 Location of maximum coolant temperature for Case 2

Figure 2.7.12 Location of maximum cladding temperature for Case 2

Figure 2.7.13 Location of maximum fuel temperature for Case 2

A detailed simulation for HCF estimation produces a large amount of data for critical parameters of the target reactor. The simulation data can be used for mechanism studies to help the designer better understand the impact of the uncertainty. Moreover, in the process of the HCF calculation, some improvement or optimization may be found to be necessary. For instance, the locations of maximum coolant, cladding and fuel temperature for Case 2 (which has the maximum peak power among all 30 cases) is shown in Figures 2.7.11 – 2.7.13. The maximum coolant temperature does not show up in the center of the assembly as per the usual case. It shows up in the corner of the assembly. It is not easy to predict that before conducting the simulation. However, in this LFR design, the gap between pins and duct is relatively small, which results in small bulk velocity in the corner of the assembly. The heat transfer is thus reduced, which leads to higher coolant temperature. In the fuel pellet, the peak power and circumferential conduction take its role. The maximum fuel temperature appears in Pin 81 which has peak power. The precise location of the hot spot for cladding (Pin 104) and fuel (Pin 81) are obtained from the simulation. This information can be of interest to industry to optimize their design.

2.8 HCF Associated with Uncertainties in Coolant Specific Heat

No neutronics simulations were necessary to examine the impact of uncertainties in coolant specific heat since this is purely thermal hydraulic parameters. Therefore, the nominal condition power solution was used for the thermal hydraulic analysis of this hot channel factor. The HCF for coolant properties due to the uncertainties from material impurity or empirical correlations is important in thermal hydraulic aspect. The lead coolant is assumed to have a specific heat value of 144 J/kg·K with physical uncertainty of -5%. Lower specific heat value can cause less heat carried by the coolant, which leads to higher maximum coolant temperature. To assess the HCF due to uncertainties in material properties, the coolant specific heat was modified directly in the code performing the calculations; by doing so, the effects of uncertainties are properly taken into account.

2.9 HCF Associated with Uncertainties in Gap Conductance

At the initial fresh fuel condition, there is a sizable helium gap between the fuel pellet and cladding. This gap allows for fuel expansion due to thermal and irradiation-induced swelling. As the fuel burns up (around 8%) [Rineiskii 1999], fission products are generated in the fuel and some of these byproducts migrate preferentially towards the fuel pellet edge due to high volatility and strong temperature gradient [Smith 2017]. The fission products form compounds that accumulate in the space between the fuel and cladding called “joint oxide gain (JOG)”, shown in the gap region of Figure 2.9.1. The JOG formation does not smoothly contact the cladding in reality but has jagged edges. The conductance of the joint oxide gain vs. the gap is a subject of interest when computing the fuel temperature.

JOG grows regularly with increasing burn-up. JOG contains mainly Mo, Cs, O with frequent presence of Ba, Te, Pd [Melis, 1993]. The thermal conductivity of the JOG material is of particular

interest since it is the main input parameter in any fuel-clad gap conductance calculation. Moreover, the clear understanding on the impact of the JOG layer is of potential importance to fuel behavior at high burn-up. Its presence may result in a stabilization or even lowering of fuel temperatures and provide a joint with beneficial plastic properties which could ease fuel-clad mechanical interaction effects. JOG also has the effect of decreasing the fuel swelling and improving the gap conductance due to decomposition of solid fission products. The gap conductance, mainly in the case of cladding swelling, is dependent not only on fission gas conductance, but also on the fission product conductivity and JOG size. The JOG size depends on many factors such as temperature, pressure, burn-up and fission gas release.

Figure 2.9.1 JOG formation in pellet-cladding gap

Given limited information on the formation of joint oxide gain (JOG), the two bounding conditions are compared: (1) nominal condition, where fuel is fresh and there is a fully open fuel-cladding gap with no JOG formation, and (2) perturbed condition, where fuel is burned and the fuel-cladding gap is assumed to be completely closed due to JOG formation.

2.9.1 Neutronics Discussion

In neutronics, simulation of the perturbed condition requires the burned fuel composition, which was provided by Westinghouse at 41 MWd/kgU burnup. The true gap size is unknown at this burnup, but assumed to be closed. In the neutronics model, the neutron physics is similar whether the gap is open or closed provided the fuel mass is preserved. Therefore the original mesh with open gap was used to simulate this burned case, and a burned fuel density resembling the original density was used. The effect of the depleted fuel composition on the power shape and magnitudes was observed compared to the nominal condition.

The eigenvalue for the burned case is 1.10391 compared to the fresh fuel case of 1.17697. Figure 2.9.2 shows the nominal and burned axial power profiles in the center pin of the LFR fuel assembly.

Increased power (+6%) is observed at the top and bottom of the active core which changes the profile slightly from the nominal condition. The middle of the core power is slightly suppressed (-1.7%). The maximum pin power in the burned case is 28.80 kW (+40 W from nominal condition), located in the same corner pins as the nominal condition. Therefore the burned power distribution does exhibit differences compared to the nominal condition.

Figure 2.9.2 Nominal and burned axial power profile (center pin)

The burned power distribution from PROTEUS is used in Nek5000 for simulation of the closed gap condition.

2.9.2 Thermal Hydraulics Discussion

In order to investigate the thermal conductance of the gap, two literature correlations are referenced. Since the major composition of JOG is Cs_2MoO_4 , one reference [Ikusawa 2017] assumes that the thermal conductivity of JOG is established by that of Cs_2MoO_4 as in the following equation:

$$K_{JOG} = \frac{1-1.848 \cdot P}{0.895} \times \left(\frac{132.56}{T_{gap}} + 0.03 + 3.2 \times 10^{-10} \cdot T_{gap}^3 \right) \quad \text{Eq. (2.9.1)}$$

K_{JOG} = thermal conductivity of JOG

P = porosity of JOG

T_{gap} = gap temperature

The JOG shown in the gap region of Figure 2.9.1 shows cracks but visible porosity. Since the cracking usually takes place during cooling down, JOG without any porosity is expected to have filled the fuel-cladding gap during irradiation. Eq. 2.9.1 is a simplified expression to compute the conductance of a specific type of JOG compound.

The second database is from an experimental study of thermal gap and contact conductance between depleted uranium dioxide (UO₂) and Zircaloy-4 (Zr4) [Garnier 1979]. The experimental data shows that analytical expressions for ideal gap conductance (such as Eq. 2.9.1) seems to underestimate the value. As shown in Figure 2.9.3, JOG growth is non-uniform in the axial direction which can causes the gap to be non-uniformly closed (zigzag shape).

Figure 2.9.3 The effect of irradiation on the fuel-clad gap (top) and CFD model (bottom)

In CFD modeling, the shape of the gap is simplified as a centrosymmetric cylinder. The gap thickness can change from zero (fully closed) to fully open. The gap conductance depends not only on the fission gas conductance but also on the JOG size (Figure 2.9.4).

Figure 2.9.4 Outline of thermal computation in the pellet-cladding gap with JOG

When the gap is fractionally filled with JOG, the gap conductance can be calculated from the following equation:

$$H_{GAP} = \frac{h_{GAPi} \cdot h_{JOG}}{h_{GAPi} + h_{JOG}} \quad \text{Eq. (2.9.2)}$$

H_{GAP} = gap conductance with an effect of JOG

h_{GAPi} = gap conductance of mixed gas in a gap of size GAP'

h_{JOG} = gap conductance of JOG

Two correlations were applied to calculate the gap conductance improvement due to the JOG formation in Figure 2.9.5. The “Gap conductance improvement_coefficient” series results from Eq. 2.9.1 and 2.9.2. The “Gap conductance improvement_experiment” series is from the experimental reference [Garnier 1979].

Figure 2.9.5 Gap conductance improvement due to the JOG formation

In Figure 2.9.5, the relative improvement in gap conductance (compared to a case with no JOG formation) is plotted against the relative JOG thickness within the gap. When the gap is half filled with JOG (relative JOG thickness of the initial gap size=50%), the expression and the experimental data leads to similar gap conductance improvement (around 1.5-1.9). When the gap is fully filled with JOG (relative JOG thickness of the initial gap size=100%), the two correlations show large differences. The expression [Eq 2.9.1] predicts a 4-fold improvement in gap conductance while the experimental data obtains 40-fold gap conductance improvement compared to the no-JOG case. This trend is consistent with the conclusion from the experimental research [Garnier 1979] that the expression usually underestimate the actual gap conductance. First, the JOG fully filling the gap is an ideal situation, so the deviation between the expression and the experimental data usually is much smaller since the JOG formation does not cover the entire gap. For instance, if we look into the case with relative JOG thickness of the initial gap size=90%, the deviation between expression and experiment drops dramatically. Secondly, the experimental data covered a wide range of conditions and showed up to 18-fold factor difference in gap conductance. The gap conductance is highly dependent on different pressure, temperature and gas composition. Estimation of an accurate gap conductance is necessary through experimental research and/or advanced fuels modeling.

Table 2.9.1 shows the temperature rise with different gap conductance from expression and experiment for a “fully closed” gap with JOG. The JOG formation improves the gap conductance, which is beneficial for reactor design in terms of fuel temperature reduction. In term of coolant temperature and cladding temperature, the impact of gap conductance is slight.

Table 2.9.1 Temperature rise with different gap conductance

Gap Conductance	$\Delta T_{\text{Coolant}}$	$\Delta T_{\text{Cladding}}$	ΔT_{Fuel}
Nominal (gap fully open)	279.00	28.62	1175.36
Perturbed expression (gap fully closed)	279.00	28.61	955.99
Perturbed experiment (gap fully closed)	277.30	28.47	749.65

2.10 HCF Evaluation and Summary

First-of-a-kind high fidelity hot channel factor calculations were carried out for a lea-cooled fast reactor design. Specifically, HCFs for perturbed coolant properties and manufacturing tolerances were evaluated for Westinghouse’s LFR design (inner zone assembly) with the SHARP toolkit (PROTEUS/Nek5000). The results are listed in Table 2.10.1 along with the HCF estimation for

AFR-100 computed by SHARP in FY18 and the legacy HCF data for EBR-II. The uncertainty in LFR parameters were taken from SFR data (cladding thickness) and from discussion with Westinghouse. Code to code comparison, sensitivity studies, and model selection were performed to improve the reliability of the results. No attempt is made to fit the data to EBR-II data since most HCF data for EBR-II comes from low fidelity model or lump parameter method.

The cladding thickness calculation was based on direct calculations where the cladding thickness was changed in all pins by the maximal and minimal amounts. The high fidelity simulation accounts simultaneously for the impact of cladding thickness on heat transfer in the cladding as well as the flow area around each pin. Localized temperature impacts were found that were non-intuitive. Due to different pin and assembly dimensions and materials, the impact of cladding thickness manufacturing tolerance has a much larger impact on the peak cladding temperature for the LFR design than for the AFR-100.

The coolant specific heat calculation was based on a direct calculation where the coolant specific heat property was perturbed by -5%. No neutronics calculations were necessary. The larger uncertainty in lead specific heat caused a larger hot channel factor for LFR than seen in the SFR designs.

The hot channel factor from manufacturing fissile mal-distribution was evaluated based on a stochastic technique. Thirty fuel assembly models were randomly generated according assuming a normal distribution in pin Pu-239 content. The models were simulated in PROTEUS, and the resulting power distributions were provided to Nek5000 for temperature calculations. The manufacturing tolerance and fuel type was different in the LFR design (MOX fuel vs metallic fuel in EBR-II and AFR-100). Such differences make it difficult to compare and apply hot channel factors across reactor types, however, the LFR HCF was in the (somewhat wide) range of those observed for SFRs.

The study on gap conductance consisted of simulations at fresh condition (open gap, fresh fuel) and at burned condition (closed gap, burned fuel) to estimate the bounding cases. Literature correlations were referenced to compare gap conductance models. The formation of JOG was shown to be beneficial for reactor design in term of fuel temperature reduction. If more information on JOG formation is available, HCFs can be evaluated.

Table 2.10.1 demonstrates the usefulness of performing detailed HCF analysis for different reactor designs. First, the uncertainties are different for different reactor. Second, the impact of these uncertainties are different as well. For instance, the HCF of coolant specific heat for LFR are higher than that for SFR because the density of lead is almost 10 times higher than that of sodium, and because the uncertainty is higher for lead. It is not recommend to use HCF from a different reactor type since the data may not be conservative. This procedure of computing HCF using high fidelity models shows promise for being repeated for any arbitrary reactor of choice, since these tools are targeted to solve many reactor types and geometries.

Table 2.10.1 HCF Estimation for EBR-II, AFR-100, and LFR

HCF	Uncertainties (3 σ) %			Coolant HCF (A)			Cladding HCF (B)			Fuel HCF (C)		
	EBR-II	AFR-100	LFR	EBR-II	AFR-100	LFR	EBR-II	AFR-100	LFR	EBR-II	AFR-100	LFR
Cladding Thickness (mm)	±0.05	±0.05	±0.05				1.03~1.05	1.02	1.05			
Coolant Specific Heat	±3%	±3%	±5%	1.017	1.016	1.04						
Fissile Mal-distribution	±6%	±6%	±5%				1.06	1.04	1.04	1.06	1.02	1.04

Table 2.10.2 Evaluation of LFR temperature rises (degrees K) in hot channels

HCF	Uncertainties (3s)	Coolant HCF (A)		Cladding HCF (B)		Fuel HCF (C)	
		ΔT_N	ΔT_P	ΔT_N	ΔT_P	ΔT_N	ΔT_P
Cladding Thickness	±0.05 mm			28.62	29.93		
Coolant Specific Heat	±5%	278.79	289.94				
Fissile Maldistribution	±5%			28.62	29.73	1305.6	1357.3

N: Nominal P: Perturbed

Table 2.10.3 Equations to compute coolant, cladding, and fuel hot channel factors

Coolant HCF (A)	$HCF_A = (T_{max_coolant} - T_{inlet_coolant})_{perturbed} / (T_{max_coolant} - T_{inlet_coolant})_{nominal}$
Cladding HCF (B)	$HCF_B = (T_{cladding_innerwall} - T_{cladding_outerwall})_{perturbed} / (T_{cladding_innerwall} - T_{cladding_outerwall})_{nominal}$
Fuel HCF (C)	$HCF_C = (T_{fuel_centerline} - T_{fuel_outerwall})_{perturbed} / (T_{fuel_centerline} - T_{fuel_outerwall})_{nominal}$

3. Implementation of Gamma Transport Capability in PROTEUS

During FY19, the transport of gamma particles and their associated heat deposition was implemented into both the PROTEUS-SN and PROTEUS-MOC solvers. While neutron fission reactions contribute the majority of heating in a fast nuclear reactor system, gamma particles produced by various neutron interactions contribute ~10% of the overall heating. For non-fueled assemblies where the fission reactions are zero, heating is dominated by gamma particles. In the existing version of PROTEUS, gamma heating was accounted for by assuming the heat was deposited exactly where the reaction took place. However, in reality, gamma particles are transport through various materials and deposit their heat some distance away from their initial generation site. In order to correctly assess the heating distribution in non-fueled assemblies (i.e. control assembly), coupled neutron-gamma transport should be taken into account. Therefore, implementation of a gamma transport capability was a prerequisite to performing the full core Versatile Test Reactor (VTR) problems with a focus on control assemblies (discussed in Chapter 4).

Therefore, in order to support multiphysics applications of NEAMS tools, the gamma transport capability was implemented in the high fidelity solvers of PROTEUS to perform coupled neutron and gamma transport calculations. Through the coupled calculations, the detailed gamma distribution can be obtained, and the energy released from the neutron-gamma reaction can be accurately accounted for in the total heating distribution. The coupled neutron and gamma transport capability of PROTEUS will allow a more accurate estimation of heating and power distribution.

Since both neutron and gamma transport solvers solve the identical form of the Boltzmann transport equation, the gamma transport capability could be realized in the framework of the SN and MOC solvers of PROTEUS by extending the existing transport solvers. As summarized in Figure 3.1, new functions required for the gamma transport calculation were implemented and coordinated with associated routines such as the fixed source solver. Additionally, the heating capability of PROTEUS was updated to compute the neutron and gamma contributions explicitly using the KERMA factor available in the gamma interaction data. The output processing routines were also updated to include the mesh-wise neutron and gamma heating data in the main output file.

Figure 3.1 Workflow of the Gamma Transport Calculation in PROTEUS

Verification tests for the gamma transport capability was performed using a 2D SFR core problem which is composed of 4 rings of homogeneous fuel assemblies surrounded by 2 rings of reflectors. The neutron and gamma heating distributions of the test problem produced from PROTEUS and VARIANT-GAMSOR calculations matched well as shown in Figure 3.2, indicating that the gamma capability were correctly implemented in the PROTEUS code.

Figure 3.2 Neutron and Gamma Heating Solutions of PROTEUS for the 2D SFR Test Problem

A comprehensive description of the gamma transport capabilities in PROTEUS and their verification is included in a separate topical report focused on PROTEUS code development and applications [Jung 2019].

4. Zooming Capability for the Versatile Test Reactor

Disclaimer: All references to VTR design in this report are based on preliminary information provided by the VTR core design team. Several elements of the design such as the control assembly had not been finalized or have changed since this work was initiated. For up-to-date information on the VTR design, please contact the VTR program.

This chapter describes the progress made on demonstrating the SHARP zooming capability for the Versatile Test Reactor (VTR). This work will continue in FY20 under carryover funding. The individual physics models have been almost completed this FY19 but the full core simulations are deferred to FY20 due to computational time availability and pre-requisite of gamma transport capability, both of which were available only recently in July 2019.

4.1 Review of Zooming Capability

During FY17-FY18, the SHARP zooming capability was developed and demonstrated for sodium-cooled fast reactor (SFR) applications. The SHARP zooming concept is a multi-resolution modeling scheme which allows significant reduction in computational cost for full-core simulations which provide local information. This zooming concept is useful to produce bounding values that are needed for development of licensing documents or a specific fuel development. For instance, in order to assure the integrity of fuel elements, the bounding values such as peak cladding inner-wall temperature, peak fuel centerline temperature, peak discharge burnup, peak linear power density, etc., are needed rather than the integral or average values. For development of a specific fuel concept, local irradiation information is needed rather than the integral information.

In neutronics (PROTEUS), coarse-and-homogeneous meshes and fine-and-heterogeneous meshes are combined: i.e., most assemblies are represented using the conventional homogenized meshes, but a few assemblies of interest are represented with pin-by-pin heterogeneous meshes in order to gain accurate local information. The detailed information from the heterogeneous focal region is post-processed and transferred to the thermal hydraulics code (Nek5000) which simulates a single assembly in explicit detail. Surrounding assemblies can be ignored due to sufficient insulation of individual assemblies by the assembly duct structures. This zooming procedure was demonstrated in FY18 on a fuel assembly in the AFR-100 SFR core (Figure 4.1.1) for calculating temperature distributions in a selected fuel assembly. The zooming capability was able to identify the hot spot location within the focal assembly.

Key benefits of the zooming calculation are the ability to build the neutronics model once provided each focal assembly is explicitly represented, and then the execution of T/H simulations on multiple assemblies in parallel on a smaller geometry domain. This method enabled calculations requiring full-core neutronics to be computationally feasible in multiphysics.

Figure 4.1.1 AFR-100 neutronics modeling for SHARP zoom calculation

4.2 Description of VTR Zooming Objectives

The focus in FY19 was the application of the multi-physics coupling and zooming capabilities developed in FY18 to the Versatile Test Reactor (VTR) SFR design. In particular, a control assembly will be modeled and simulated by extending the previously demonstrated capabilities to a non-fueled assembly. The objective of the zooming calculations is to provide accurate control rod worth, power (gamma heating), and temperature distribution in the control assembly because the legacy tools used in the VTR design overestimate control rod worth. While the VTR control assembly design is still evolving, VTR designers were consulted to select a single preliminary design for this analysis.

Development of the gamma transport capability (discussed in Chapter 3) was a pre-requisite to initiating this work to yield the correct heating distribution in a non-fueled assembly. Physics models will also be developed to calculate accurate detailed power distributions in a fuel assembly. Global and local spectrum effects are taken into account via the full core simulation with localized geometry heterogeneity as well as heterogeneous cross section treatment. Detailed power distributions (based on the full core model with zooming method) are transferred to T/H in order to compute the detailed temperature distributions. Gamma heating distributions within the control assembly will be compared with a verification calculation (either MCNP or DIF3D/GAMSOR).

4.3 VTR Model Description (see disclaimer at beginning of chapter)

The VTR model used in this work was based on preliminary information provided by the VTR core design team. Several elements of the design such as the control assembly had not been finalized, but a reasonable choice was selected so that the analysis could proceed.

The VTR is a sodium-cooled fast reactor design optimized for flexible experimental control in the numerous test locations denoted in Figure 4.3.1. Due to the large number of test assembly locations (which can be empty or hold various materials to be irradiated), only 6 assembly positions are reserved for control rods. The design of the control assembly is being selected to optimize performance from several aspects. First, the control rod worth should be maximized since there are fewer positions available to insert control material. In order to maximize control rod worth, more control material should be packed into the assembly (closer pin pitch) yet these rods expand and

swell under irradiation conditions, which can interfere with vertical motion of the inner duct within the stationary outer duct. Finally, the materials must be maintained within temperature limits.

Figure 4.3.1 VTR core map

Figure 4.3.2 VTR core map showing focal assembly locations and meshes

The control assemblies are all in the 5th hexagonal ring of the core, so no individual control assembly is significantly “hotter” than the others. The primary control assemblies are surrounded by 6 fuel assemblies, while the secondary (safety) assemblies have 5 fuel assemblies and 1 reflector assembly as neighbors. The primary control rods probably see a slightly higher neutron and gamma flux. Additionally, the primary rods are inserted in the core during operation. The primary rods will be modeled in the zooming calculation. The 6 control rods are effectively in equivalent positions around the core, so it does not matter which one is chosen for modeling, unless the flux is tilted due to asymmetric control rod positioning or material loading in the test assemblies.

Table 4.3.1 VTR control assembly parameters

Parameter	Cold Value	Units
Assembly pitch	12.0	cm
Inter-assembly gap	0.3	cm
Outer duct outside flat-flat	11.7	cm
Outer duct inside flat-flat	11.1	cm
Outer duct thickness	0.3	cm
Inter-duct sodium gap thickness	0.3	cm
Inner duct outside flat-flat	10.5	cm
Inner duct inside flat-flat	9.9	cm
Inner duct thickness	0.3	cm
# Rods	37	-
P/D	1.02231	-
Cladding outer radius	0.7398	cm
Cladding thickness	0.0825	cm
Helium bond thickness	0.0514	cm
B4C absorber radius	0.6060	cm
Wire wrap	Yes	-

Figure 4.3.3 VTR control assembly neutronics mesh (slice)

Table 4.3.2 VTR fuel assembly parameters

Parameter	Cold Value	Units
Assembly pitch	12.0	cm
Duct flat-flat	11.7	cm
Duct thickness	0.3	cm
# Rods	217	-
P/D	1.18	-
Cladding outer radius	0.3125	cm
Cladding thickness	0.0435	cm
Sodium bond thickness	0.0360	cm
Fuel slug radius	0.2330	cm
Wire wrap	Yes	-
Active fuel length	80	cm
Fuel	U-20Pu-10Zr	-

Figure 4.3.4 VTR fuel assembly neutronics mesh (slice)

The control rods are parked 5 cm above the top of the active core in the “withdrawn / out” position. The control rods are parked 5 cm below the bottom of the active core in the “inserted / in” position. The safety rods shown in the core map are always in the “withdrawn” position.

Axial dimensions, materials, and details of the other assemblies are left out for brevity as they are not vital to the results shown here.

4.4 Neutronics Calculations

PROTEUS-SN was selected as the neutronics solver for the zooming calculations because it offers significant computational advantages over PROTEUS-MOCES for large core problems with significant homogenization. This section describes the details of the neutronics calculations.

The neutronics objectives are to calculate (1) control rod worth, (2) power distribution in control assembly (control rods inserted), and (3) power distribution in fuel assembly (control rods withdrawn). The power from (2) and (3) will be transferred to Nek5000 for computation of temperature fields.

Due to the focus on control assembly physics, development of a gamma transport capability was first required. Unlike fuel assemblies where fission energy dominates the power distribution, in non-fueled assemblies, absorption reactions and other gamma producing reactions dominate the power distribution. These gamma particles transport from one region to another until they deposit heat in the medium. Gamma transport capability accounts for this movement correctly. The

previous version of PROTEUS made a simplifying assumption that gamma heating is deposited at the source generation site (no transport), which properly preserves the heating amount, but not the correct distribution. Gamma transport was fully implemented in both PROTEUS-SN and PROTEUS-MOC as of June 2019, as discussed briefly in Chapter 3. Since the detailed PROTEUS calculations were delayed until July 2019 due to gamma transport prerequisite as well as availability of computational time, several MCNP calculations were set up and run as verification calculations. Full core calculations with homogeneous assemblies were completed in both MCNP (including gamma transport) and PROTEUS-SN. Progress on the full core calculations with heterogeneous assemblies is also reported.

4.4.1 Neutronics Verification Calculations

Verification calculations were set up to compare the eigenvalues and flux distributions in PROTEUS-SN with those in MCNP6. Several cases were performed ranging from a 2D slice of the heterogeneous fuel assembly, the 3D core in a fully homogenized configuration (control rods in and out), and the 3D core with a heterogeneous control assembly (control rods in and out). All of the desired MCNP6 calculations were completed, however the full core heterogeneous neutronics calculations with PROTEUS are postponed to FY20. This is due to two reasons: (1) the gamma transport capability was completed in June 2019 which is a pre-requisite for all of the calculations involving analysis of a control assembly and (2) the competitive ALCC award received for computer time was received starting in July 2019. Therefore the full core cases could not be initiated until July-August 2019. The homogeneous models were completed in FY19 but the heterogeneous cases are more complex and compute-intensive and will be in FY20.

The results of the verification studies in Table 4.4.1 show excellent agreement between continuous energy Monte Carlo (MCNP) and PROTEUS-SN with 33 energy groups. The differences are less than 125 pcm for the full core homogeneous cases and the heterogeneous 2D fuel assembly slice. The estimated control rod worth for the homogeneous case is 6072 pcm, but this does not include the heterogeneity effects under investigation in this work. As seen from the MCNP calculation, the heterogeneous control rod worth is 251 pcm. We expect similar results in PROTEUS-SN.

Table 4.4.1 Eigenvalue verification for VTR cases

VTR Case	MCNP (pcm uncertainty)	PROTEUS-SN 33g (pcm diff from MCNP)
<i>2D het fuel assembly</i>	<i>1.74035 (7)</i>	<i>1.74160 (125)</i>
3D homogeneous core – control in	1.02761 (6)	1.02646 (-115)
3D homogeneous core – control out	1.08826 (6)	1.08718 (-108)
Control worth in pcm (homogeneous core)	6065 (9)	6072 (7)
3D het control assembly core – control in	1.03044 (5)	In progress – FY20
3D het control assembly core – control out	1.08858 (6)	In progress – FY20
<i>Control worth in pcm (het control assembly core)</i>	<i>5814 (8)</i>	In progress – FY20

The axial power distributions in the focal fuel and control assemblies from the homogeneous full core calculations with gamma transport (MCNP and PROTEUS-SN) were compared in Figure 4.4.1 and Figure 4.4.2. The MCNP active core profile was normalized to the same power level as PROTEUS-SN since MCNP does not use a set power level. The power shapes in the fuel and control assemblies show excellent agreement for the homogenous (control in) cases.

Figure 4.4.1 Verification of axial power profile in fuel assembly (homogeneous full core, control inserted)

Figure 4.4.2 Verification of axial power profile in control assembly (homogeneous full core, control inserted)

Additionally, the PROTEUS-SN and MCNP radial power profiles near the core-midplane $Z=(128.9, 132.8)$ cm was plotted in Figure 4.4.3 (control inserted) and Figure 4.4.4 (control withdrawn). The relative errors for the control inserted case and control withdrawn case for this axial zone are plotted in Figures 4.4.5 and 4.4.6, respectively. The control inserted case shows around a -5% error in control assembly power compared to MCNP. The control withdrawn case shows less than 0.5% error in all assemblies.

Figure 4.4.3 PROTEUS-SN and MCNP radial power profiles (homogeneous full core, control inserted)

Figure 4.4.4 PROTEUS-SN and MCNP radial power profiles (homogeneous full core, control withdrawn)

Figure 4.4.5 Relative error in radial power profile in core (homogeneous full core, control inserted)

Figure 4.4.6 Relative error in radial power profile in core (homogeneous full core, control withdrawn)

4.4.2 Progress on Heterogeneous Assembly Calculations

The full core VTR calculations with heterogeneous assemblies are in the process of being set up, debugged, and executed on high performance machines. So far, the full core cross sections were generated for both control in and control out configurations, using a two-step procedure in MC2-3/TWODANT as described in Chapter 2, Figure 2.4.1.

For debugging reasons, the simulations for heterogeneous fuel assembly and heterogeneous control assembly have been separated into two cases. The full core with heterogeneous fuel assembly mesh (top-view) is depicted in Figure 4.4.7 and Figure 4.4.8 (zoomed in to see details of fuel assembly). The full core with heterogeneous control assemblies mesh (top-view) is depicted in Figure 4.4.9 and Figure 4.4.10 (zoomed in to see details of fuel assembly). Note the propagation of mesh refinement into neighboring assemblies due to the conformal mesh requirements of PROTEUS.

Figure 4.4.7 Full core mesh with detailed fuel assembly

Figure 4.4.8 Full core mesh with detailed fuel assembly (zoomed on fuel assembly)

Figure 4.4.9 Full core mesh with detailed control assemblies

Figure 4.4.10 Full core mesh with detailed control assembly (zoomed on control assembly)

The full core jobs with heterogeneous assemblies will be analyzed in FY20. The power distributions in a fuel and control assembly will be processed and sent to Nek5000 for simulation of the temperature fields.

4.5 Thermal Hydraulic Calculations

The Nek5000 calculations for the temperature field are dependent on the PROTEUS power solution as input and require significant computational time. These will be performed in FY20. However, some key aspects of the model are briefly discussed.

In the Nek5000 CFD model, the B₄C absorber, cladding, gap and two ducts are modelled explicitly as shown in the top view of the CFD mesh in Figure 4.5.1. As opposed to the neutronics calculations, only the control assembly itself needs to be modeled. The assembly ducts sufficiently insulate the interior of the assembly from the temperature and flow of neighboring assemblies. Adiabatic boundary conditions are places on the exterior boundaries. The URANS solver is used for this configuration.

The predicted temperature distribution of the control assembly are shown in Figure 4.5.2 using the power distribution obtained from MCNP (since PROTEUS results were not yet available). The

temperature bias due to the power tilt is observed. The control rods closer closest to the center of the core are hotter than the rods closer to the exterior of the core.

Figure 4.5.1 Thermal hydraulics mesh for control assembly (top view)

Figure 4.5.2 Temperature distribution of top-most control assembly based on MCNP power distribution

Figure 4.5.3 Pin numbering in control assembly

Figure 4.5.4 Maximum cladding temperatures in control assembly (MCNP power)

Figure 4.5.5 Maximum absorber temperatures in control assembly (MCNP power)

The control pin numbering is shown in Figure 4.5.3. Detailed information on the peak cladding and B4C absorber temperatures of each pin are shown in Figure 4.5.4 and 4.5.5. Nek5000 predicts

both the magnitude and location of the peak cladding and B4C temperatures. The temperature shows bilateral symmetry due to the geometric symmetry of the core. The peak temperature prediction with the high fidelity Nek5000 tool ought to be more accurate than results from sub-channel code or other legacy code that is previously used for peak temperature estimation. The information obtained in this study can be used to inform the control rod design in the VTR program.

4.6 Summary and Future Work

Verification cases have been performed to test the cross sections and meshes for homogeneous full core cases in neutronics as well as a heterogeneous fuel configuration. Additional verification cases are necessary for the heterogeneous control configurations. Excellent agreement of the eigenvalue calculation was observed between MCNP and PROTEUS for the cases performed. The axial and radial power profiles for the control assembly also compared favorable for the homogeneous core case, showing that the gamma transport capability is implemented correctly.

Debugging and setup of the full core neutronics cases with heterogeneous assemblies will be performed in FY20. The control rod will be computed from the cases with control rods in and control rods out. The power distribution from the control rods in case will be transferred to Nek5000 for the control assembly for temperature calculation (and can be compared with the existing results). The power distribution from the control rods out case will be transferred to Nek5000 for the fuel assembly. The competitive computer allocation on ALCF's Theta machine, which started in July 2019 and runs through June 2020 will be utilized for the calculations.

5. Development of a Fast Molten Salt Reactor (MSR) Code Capability

A multi-discipline collaboration across several teams (PROTEUS development, Nek5000 development, and MSR analysts) was undertaken to solve a major challenge problem inspired by industry: develop and apply the capability of a coupled neutronics/thermal-hydraulics solution to solve the delayed neutron precursor distribution in fast spectrum MSRs.

Specifically, this capability is important for designs with flowing fuel salt that leaves the core region because the loss of these precursors from the core reduces the β_{eff} (effective delayed neutron fraction) of the system and can potentially impact safety performance. A computational fluid dynamics code like Nek5000 was used for this coupled calculation to account for the potentially complex fuel salt cross flow inside a fast spectrum MSR core (or tank) which typically does not include channels or moderators. In terms of the neutronics code, several flux solver options were considered at the onset of this work: PROTEUS-NODAL, PROTEUS-SN, and PROTEUS-MOC. Their distinguishing characteristics in terms of MSR modeling are summarized below:

PROTEUS-NODAL

- Includes a recently-added precursor drift model for MSRs
- Models only axially-extruded geometries (no axially non-uniform geometries)
- Light computational requirements (homogeneous lattice, diffusion)

PROTEUS-SN

- No built-in precursor drift model for MSRs
- Can model as-built 3D geometries including axially non-uniform geometries
- Finite element mesh with corresponding computational requirements

PROTEUS-MOC

- No built-in precursor drift model for MSRs
- Models only axially-extruded 3D geometries (no axially non-uniform geometries)
- Ideal for heterogeneous problems with steep flux gradients
- Finite element mesh with corresponding computational requirements

Given these characteristics, and to maximize the chances for successful coupling, two approaches for the coupling development were pursued simultaneously: PROTEUS-NODAL/Nek5000 and PROTEUS-SN/Nek5000. The PROTEUS-NODAL option already has the complex precursor drift model built-in and has a light computational burden that is preferred by industry, so it was a good choice to couple with Nek5000, with the understanding that some mesh interpolation would be required. However, it is limited to diffusion and simpler regular geometries (no finite element mesh) so PROTEUS-SN was also chosen for coupling to offer an option with transport and as-built 3D geometries. PROTEUS-MOC was not selected given that it offers only transport without the ability to model axially-varying geometries.

Due to the complexity of the task of coupling two high-fidelity codes for this specific purpose, for the first year, a few approximations were made to obtain a working model for a few test cases:

- No cross section updates with new temperature distributions; this will be performed in future work)
- No impact of delayed neutrons on flux and power distributions; the impact was tested for typical fast MSR systems and it was found to be negligible)

Figure 5.1 shows a schematic for the PROTEUS-NODAL/Nek5000 coupled solution approach. Initially, PROTEUS-NODAL is used to solve the steady-state power distribution and passes this information via script to Nek5000. Nek5000 then calculates the velocity field of the fuel salt for the entire core and passes it back to PROTEUS-NODAL. PROTEUS-NODAL then uses this velocity field as input in its precursor drift model and neutronics solver to iteratively calculate the precursor distribution and initial precursor source distribution until convergence. After convergence, the updated power distribution can then be sent back to Nek5000 to confirm convergence.

Figure 5.2 shows the PROTEUS-SN/Nek5000 approach which uses PROTEUS-SN to solve for the initial power distribution and initial precursor source distribution under steady-state conditions. This information is then based into Nek5000 which performs not only the heat transfer and fluid dynamics calculations but also the precursor tracking. For this approach, the precursor distribution calculated by Nek5000 is the final answer because feeding this information back to PROTEUS-SN to recalculate the flux (rigorous solution) would require significant code development. Hence, the assumption was that the impact of any updated precursor distributions would not impact the flux or power distributions.

The capabilities to use both of these coupled approaches were successfully developed and tested on simple single channel models as well as more complex 2D and 3D MSR representations, which should be encouraging results to share with our industry partners. Additional details of the results are available upon request.

Figure 5.1 PROTEUS-NODAL/NEK5000 coupled solution approach for delayed neutron precursors in fast MSR

Figure 5.2 PROTEUS-SN/NEK5000 coupled solution approach for delayed neutron precursors in fast MSR

6. Conclusions

This document summarizes the extension and application of SHARP tools for various fast reactor types (LFR, SFR, and MSR) during fiscal year 2019. The multiphysics coupling methods developed for SFRs in FY17-FY18 were employed in this work for LFR and SFR, and new coupling methods were developed for MSR calculations.

In the lead-cooled fast reactor (LFR) domain, first-of-a-kind hot channel factor (HCF) estimation with high fidelity codes (PROTEUS/Nek5000) was successfully demonstrated in this study. Selected HCF were computed and compared with SFR data (AFR-100, EBR-II). The findings confirm that different reactor types, design parameters and uncertainties lead to different HCFs. Careful estimation of HCF for a specific design is necessary. In addition to improvement in HCF accuracy, high fidelity tools generate substantial data to both support the HCF calculation and help the designer better understand the mechanism of the impact from these uncertainties. For example, the impact of cladding thickness manufacturing tolerance resulted in non-intuitive effects in the corner pins of the LFR assembly. To restate, during the process of the HCF calculation, the reactor design is analyzed carefully with a high fidelity model. Some improvement or optimization may be found to be necessary. This procedure of computing HCF using high fidelity models shows promise and flexibility for being repeated for any arbitrary reactor of choice, since these tools are targeted to solve many reactor types and geometries.

In the sodium-cooled fast reactor (SFR) domain, progress was made towards extending the previously demonstrated SHARP zooming capability to non-fueled assemblies. In particular, a gamma transport capability was implemented in high fidelity PROTEUS solvers in order to accurately account for heat deposition caused by gamma particles, which accounts for ~10% of total core power. The SHARP zooming capability demonstration in FY18 showed that ducted assemblies such as those in a conventional SFR design can be modeled as isolated assemblies in thermal hydraulics to the insulation provided by the ducts. This year, neutronics verification cases were carried out for a candidate Versatile Test Reactor (VTR) design using the new gamma transport capability in PROTEUS. Comparisons were made with continuous energy MCNP calculations and shown to agree well. The models for the full core design with heterogeneous control and fuel assemblies is in progress and will be completed in FY20.

In the fast molten salt reactor (MSR) domain, a new capability was developed to model the flow of neutron precursors both inside and outside of the core, which impacts the effective delayed neutron fraction of the system. The PROTEUS-SN and PROTEUS-NODAL solvers were coupled to Nek5000 in order to simulate precursor flow. These two workflows were chosen due to benefits and drawbacks in each one. The workflows were demonstrated on test problems. The fast MSR modeling capability was supported under two other work packages, and comprehensive details are included in a separate report.

Future work in FY20 is planned to compute additional HCF for the LFR design and continue the zooming calculation for the VTR. Continuation of applications to the MSR community is planned as well.

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Nuclear Science and Engineering Division

Argonne National Laboratory
9700 South Cass Avenue, Bldg. 208
Argonne, IL 60439

www.anl.gov

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