Application of the SHARP Toolkit to Sodium-Cooled Fast Reactor Challenge Problems

Nuclear Engineering Division

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EXECUTIVE ABSTRACT

The Simulation-based High-efficiency Advanced Reactor Prototyping (SHARP) toolkit is under development by the Nuclear Energy Advanced Modeling and Simulation (NEAMS) Campaign of the U.S. Department of Energy, Office of Nuclear Energy. To better understand and exploit the benefits of advanced modeling simulations, the NEAMS Campaign initiated the “Sodium-Cooled Fast Reactor (SFR) Challenge Problems” task, which include the assessment of hot channel factors (HCFs) and the demonstration of zooming capability using the SHARP toolkit. If both challenge problems are resolved through advanced modeling and simulation using the SHARP toolkit, the economic competitiveness of a SFR can be significantly improved.

The efforts in the first year of this project focused on the development of computational models, meshes, and coupling procedures for multi-physics calculations using the neutronics (PROTEUS) and thermal-hydraulic (Nek5000) components of the SHARP toolkit, as well as demonstration of the HCF calculation capability for the 100 MWe Advanced Fast Reactor (AFR-100) design. Testing the feasibility of the SHARP zooming capability is planned in FY 2018.

The HCFs developed for the earlier SFRs (FFTF, CRBR, and EBR-II) were reviewed, and a subset of these were identified as potential candidates for reduction or elimination through high-fidelity simulations. A one-way offline coupling method was used to evaluate the HCFs where the neutronics solver PROTEUS computes the power profile based on an assumed temperature, and the computational fluid dynamics solver Nek5000 evaluates the peak temperatures using the neutronics power profile. If the initial temperature profile used in the neutronics calculation is reasonably accurate, the one-way offline method is valid because the neutronics power profile has weak dependence on small temperature variation. In order to get more precise results, the proper temperature profile for initial neutronics calculations was obtained from the STAR-CCM+ calculations.

The HCFs of the peak temperatures at cladding outer surface, cladding inner wall surface, and fuel centerline induced by cladding manufacturing tolerance and uncertainties on the cladding, coolant, and fuel properties were evaluated for the AFR-100. Some assessment on the effect of wire wrap configuration and size of the bundle shows that it is practical to use the 7-pin bare rod bundle to calculate the HCFs. The resulting HCFs obtained from the high-fidelity SHARP calculations are generally smaller than those developed for the earlier SFRs because the most uncertainties involved in the modeling and simulations were disappeared. For completeness, additional investigations are planned in FY 2018, which will use random sampling techniques.

TABLE OF CONTENTS

Executive Abstract	i
Table of Contents	ii
List of Figures	iv
List of Tables.....	viii
Acknowledgments.....	x
1. Introduction	1
2. SFR Challenge Problems	3
2.1 Assessment of Hot Channel Factors	3
2.2 SHARP Zoom Capability.....	9
3. SFR Design Problems and Computational Tools.....	11
3.1 Advanced Fast Reactor as SFR Design Problem	11
3.2 Computational Tools and Resources.....	13
3.2.1 PROTEUS Neutronics Code	13
3.2.2 Nek5000 Thermal Hydraulics Code	14
3.2.3 Multiphysics Coupling Approach and Computational Resources.....	17
4. Assessment of Hot Channel Factors	20
4.1 Hot Channel Factors for Metallic Fuel SFRs	20
4.2 Strategy for Hot Channel Factor Assessments	21
4.3 Neutronics Results for Hot Channel Factor Calculations	25
4.3.1 Nominal Neutronics Results.....	25
4.3.2 Neutronics Results Associated with Uncertainties in Thermo-Physical Properties	30
4.3.3 Neutronics Results Associated with Uncertainties in Subchannel Flow Area ...	30
4.3.4 Neutronics Results Associated with Uncertainties in Fuel Pellet Fissile Content	33
4.4 Thermal-Hydraulic Results	34
4.4.1 Bare Rod Bundle Results.....	34
4.4.2 Wire Wrap Rod Bundle Results	47
4.5 Preliminary Estimation of Hot Channel Factors	51
5. Zoom Capability of SHARP Toolkit	53

5.1 Application of Zoom Capability to AFR-100 Peak Temperature Calculations.....	53
6. Activities in FY18.....	55
6.1 PROTEUS Plan in FY18.....	55
6.1.1 PROTEUS Plan for Hot Channel Factors.....	55
6.1.2 PROTEUS Plan for SHARP Zoom	55
6.2 Nek5000 Plan in FY18.....	56
6.2.1 Nek5000 Plan for Hot Channel Factors.....	56
6.2.2 Nek5000 Plan for SHARP Zoom	56
7. Conclusions.....	57
References.....	59
Appendix A. AFR-100.....	62
Appendix B. PROTEUS Sensitivity Studies.....	68
B.1 Multigroup Cross Section Generation	69
B.2 Mesh Preparation.....	70
B.3 Transport Solvers: PROTEUS-SN vs. PROTEUS-MOCEX	71
B.4 Mesh, Angle and Energy Convergence Studies	72
B.4.1 Axial Mesh Refinement.....	73
B.4.2 Energy Group Refinement.....	73
B.4.3 Radial Mesh Refinement	76
B.4.4 Angular Cubature Refinement.....	78
B.4.5 Convergence Study Conclusions.....	79
B.5 Discussion of PROTEUS-SN vs. PROTEUS-MOCEX Results	79
B.6 Discussion of Initial Temperature Condition	81
Appendix C. Nek5000 Sensitivity Study	87
C.1. Primary STAR-CCM+ calculations	87
C.2 Meshing Capability	102
Appendix D. Comparison of Hot Channel Factors	105

LIST OF FIGURES

Figure 2.1.1 Schematic of assessment of margin to fuel-cladding eutectic formation	3
Figure 2.1.2 SFRs operated or designed in the United States	5
Figure 2.1.3 Evolution of computational resources and codes	7
Figure 2.1.4 Peak cladding inner wall temperature depending on HCFs (artificial HCFs were hypothetically reduced from the CRBR HCFs)	8
Figure 2.2.1 Americium-bearing blanket (AmBB) concept.....	10
Figure 3.1.1 Core radial layout of AFR-100	11
Figure 3.1.2 Core axial layout and uranium enrichment distribution	12
Figure 3.2.2.1 Comparison of convergence behavior between Nek5000 and OpenFOAM [Sprague 2010]	16
Figure 3.2.2.2 Hierarchical structure of NEAMS TH tools	16
Figure 3.2.3.1 Schematic of online coupling using the SHARP toolkit	17
Figure 3.2.3.2 Schematic of offline coupling using components of the SHARP toolkit.	18
Figure 4.2.1 Depiction of fuel wrapped pin	21
Figure 4.2.2 Close-up mesh of 91-Pin fuel assembly (wire wrap (left) and varying sub-channel geometry in vicinity of wire wrap (3 right))	22
Figure 4.2.3 Nek5000 simulation for of 217-pin assembly with over 1 million grid points [Childs 2008].....	22
Figure 4.2.4 7-Pin (left) and 91-pin (right) configurations (not to scale)	23
Figure 4.3.1.1. MOCEX nominal condition axial power profile (7-pin)	26
Figure 4.3.1.2. MOCEX nominal condition axial power profile (91-pin)	26
Figure 4.3.1.3 Axial power profile comparison between DIF3D and MOCEX (7-pin)	28
Figure 4.3.1.4 Axial profiles for computed by 33g MOCEX simulation (7-pin)	29
Figure 4.3.1.5 Fission cross section for U-235 retrieved from National Nuclear Data Center website.....	29
Figure 4.3.3.1 Overlay of the initial and perturbed meshes to show cladding perturbation (- 0.05 mm change in cladding thickness).	31
Figure 4.3.3.2 MOCEX axial power profile for cladding thickness change (7-pin).....	32
Figure 4.3.3.3 MOCEX axial power profile for cladding thickness change (91-pin).....	32
Figure 4.3.4.1 Hypothetical peak pin power distribution based on random sampling	33
Figure 4.4.1.1 Transient outlet velocity distribution in 7-pin bare rod bundle	35
Figure 4.4.1.2 Transient gap region velocity distribution in 7-pin bare rod bundle	36

Figure 4.4.1.4 Averaged outlet velocity distribution in 7-pin bare rod bundle.....	37
Figure 4.4.1.5 Lateral velocity distribution in 7-pin bare rod bundle	37
Figure 4.4.1.6 Three axial power distributions applied to 7-pin bare rod bundle.....	38
Figure 4.4.1.7 Temperature distributions at different Elevations (4.0P, 4.2P, 4.4P, 4.6P, 4.8P, 5.0P) in 7-pin bare rod bundle using PROTEUS power distribution.....	39
Figure 4.4.1.8 Outlet temperature distributions with different axial power distribution in 7-pin bare rod bundle.....	40
Figure 4.4.1.9 Numbering scheme for sub-channels and rods in 7-pin bare rod bundle	41
Figure 4.4.1.10 Maximum temperature for different sub-channels and rods in 7-pin bare rod bundle.....	42
Figure 4.4.1.11 Outlet velocity and temperature distribution in 91-pin bare rod bundle	43
Figure 4.4.1.12 Sketch of 6 zones for volumetric heat flux calculation	44
Figure 4.4.1.13 Rod numbering scheme in 91-pin bare rod bundle.....	45
Figure 4.4.1.14 Maximum temperature for different rods in 91-pin bare rod bundle.....	46
Figure 4.4.2.1 Comparison of outlet velocity distribution between 7-pin bare rod bundle and 7-pin wire wrap rod bundle	47
Figure 4.4.2.2 Comparison of outlet temperature distribution between 7-pin bare rod bundle and 7-pin wire wrap rod bundle	49
Figure 4.4.2.3 Sub-channel maximum coolant temperature between 7-pin bare rod bundle and 7-pin wire wrap rod bundle	50
Figure 4.4.2.4 Maximum outer cladding temperature between 91-pin bare rod bundle and 91-pin wire wrap rod bundle	50
Figure 5.1.1 AFR-100 modeling for SHARP zoom calculation	54
Figure A.1 Core radial layout of AFR-100	63
Figure A.2 Core axial layout and uranium enrichment distribution	64
Figure A.3 Radial power distribution (MW per assembly in 1/3 Core).....	66
Figure A.4 Peak 2σ cladding inner wall temperatures ($^{\circ}\text{C}$).....	66
Figure A.5 Minimum 2σ margins to fuel melt ($^{\circ}\text{C}$).....	67
Figure B.1.1 Cross section generation procedure for heterogeneous 3D pin configurations ..	70
Figure B.1.2 General depiction of assembly into 1-D cylinder geometry (not to scale)	70
Figure B.2.1 Visualization of various neutronics meshes for the 7-pin configuration	71
Figure B.4.2.1 MOCEX axial power profile with varying group structure (7-pin).....	74
Figure B.4.2.2 MOCEX axial power profile for uniform enrichment problem (7-pin).....	75

Figure B.4.2.3 MOCEX axial power profile with varying group structure (91-pin).....	76
Figure B.4.2.4 MOCEX ring-wise axial power profiles with 33-groups (91-pin).....	76
Figure B.4.3.1 Converged 2D neutronics mesh (265 elements) for the 7-pin configuration...	77
Figure B.4.3.2 Converged 2D neutronics mesh (3061 elements) for the 91-pin configuration	78
Figure B.5.1 MOCEX vs. SN axial power profile comparison for uniform 300 K (91-pin)...	81
Figure B.6.2 MOCEX comparison of power profile at 300K and 800 K (91-pin).	83
Figure B.6.3 MOCEX and SN axial power distributions for different temperature initial conditions (91-pin)	85
Figure B.6.4 MOCEX and SN axial power distributions for different temperature initial conditions, zoomed in at upper 18.0% enriched core region to show detail (91-pin).....	86
Figure C.1.1 Snapshot of polyhedral mesh for wire wrap rod bundle	87
Figure C.1.2 Verifications with STAR-CCM+	89
Figure C.1.3 Boundary conditions for full length domain and 1 wire wrap pitch domain	90
Figure C.1.4 Mesh structure for wire wrap rod bundle with cladding and fuel	91
Figure C.1.5 Outlet temperature distributions of full length 91-pin wire wrap rod bundle with conjugate heat transfer	91
Figure C.1.6. Outlet velocity contour for full length and 1 pitch.....	92
Figure C.1.7 Detailed velocity distribution on the line between rods for full length and 1 pitch	92
Figure C.1.8 Minimum, average and maximum coolant temperature comparison on each elevation between full length and 1 pitch	93
Figure C.1.9 Normalized axial power distribution for BOC, MOC and EOC of AFR-100	94
Figure C.1.10 Maximum coolant temperature comparison at different elevations for full length and 1 Pitch models with BOC axial power distribution.....	95
Figure C.1.11 Lateral velocity distribution	96
Figure C.1.12 Asymmetric distribution feature of hot spots in wire wrap rod bundle	97
Figure C.1.13 Maximum coolant temperature with difference models in different sub-channels.....	99
Figure C.1.14 Sketch of fuel and cladding.....	99
Figure C.1.15 Temperature prediction with and without conjugate heat transfer	101
Figure C.1.16 Circumferential conduction in cladding and fuel.....	101
Figure C.1.17 Circumferential cladding temperature distribution of the center pin with different cladding thickness	102
Figure C.2.1 Hexahedral mesh generation for wire wrap rod bundle	103

Figure C.2.2 Mesh Generation for bare rod bundle with ICEM script	104
Figure C.2.3 Mesh generation for different physics codes	104

LIST OF TABLES

Table 2.1.1 Comparison of HCFs related to cladding mid-wall temperature	5
Table 3.1.1 Core performance parameters	12
Table 3.2.1.1 Strong spatial scalability of PROTEUS-SN on BlueGene/P (ANL)	14
Table 3.2.1.2. Weak angle scalability of PROTEUS-SN on BlueGene/P (ANL, JSC)	14
Table 4.1.1 Proposed hot channel factors for metallic fuel SFR	20
Table 4.2.1. Required high-fidelity calculations for HCF evaluations	24
Table 4.3.1.1. MOCEX nominal condition average pin power in each ring (91-pin)	27
Table 4.3.3.1 Cold cladding thickness perturbations and corresponding hot dimensions	30
Table 4.3.3.2 MOCEX eigenvalue results for cladding perturbation (7-pin)	31
Table 4.3.3.3 MOCEX eigenvalue results for cladding perturbation (91-pin)	31
Table 4.4.1.1 Volumetric heat flux in 6 zones	45
Table 4.5.1 Hot channel factors in bare rod bundle and wire wrap rod bundle	51
Table 4.5.2 Preliminary estimations of hot channel factors for selective uncertainties and manufacturing tolerance (7-pin)	52
Table 5.1.1 SHARP Zoom Milestones	54
Table A.1 Core performance parameters.	64
Table B.1 Hot radial dimensions for AFR-100 fuel assembly	68
Table B.2 Hot axial dimensions for AFR-100 fuel assembly	68
Table B.3.1 Comparison of PROTEUS-SN and PROTEUS-MOCEX neutronics solvers	72
Table B.4.1.1 MOCEX eigenvalues with varying degrees of axial refinement (7-pin)	73
Table B.4.2.1 MOCEX eigenvalues with varying group structures (7-pin)	74
Table B.4.2.2 MOCEX eigenvalue results with varying group structures (91-pin)	75
Table B.4.3.1 MOCEX eigenvalue results with varying azimuthal subdivisions (7-pin)	77
Table B.4.3.2 MOCEX eigenvalue results with varying radial subdivisions (7-pin)	77
Table B.4.3.3 MOCEX results with varying radial and azimuthal subdivisions (91-pin)	77
Table B.4.4.1 MOCEX eigenvalue results with varying angular cubature (7-pin)	78
Table B.4.4.2 MOCEX eigenvalue results with varying angular cubature (91-pin)	79
Table B.4.5.1 Recommended MOCEX discretization parameters	79
Table B.5.1 MOCEX vs. SN eigenvalue results for uniform 300 K temperature (91-pin)	80
Table B.6.1 MOCEX eigenvalue results at two uniform temperatures (7-pin)	82

Table B.6.2 MOCEX eigenvalue results at two uniform temperatures (91-pin)	82
Table B.6.3 MOCEX peak/average pin power in each ring at two uniform temperatures (91-pin)	83
Table B.6.3 Estimated temperature ranges for 7-pin and 91-pin configurations	84
Table B.6.4 MOCEX and SN peak / average axial power results for temperature profile initial condition (91 pin)	85
Table C.1.1 Maximum coolant temperature with difference models.....	98

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1. Introduction

The Simulation-based High-efficiency Advanced Reactor Prototyping (SHARP) toolkit [Mahadevan 2014], [Merzari 2015] is under development by the Nuclear Energy Advanced Modeling and Simulation (NEAMS) Campaign of the U.S. Department of Energy, Office of Nuclear Energy. The SHARP toolkit is a high-fidelity reactor simulation tool comprised of the neutronics module PROTEUS [Shemon 2014], thermal hydraulics module Nek5000 [Fischer 2008], and structural mechanics module Diablo, and therefore the toolkit can analyze multi-physics thermal-structural-neutronics phenomena of core configurations with complex geometric features.

After releasing the SHARP toolkit in 2016, the main focus of the Reactor Product Line (RPL) of the NEAMS Campaign was shifted toward testing, validation and verification of SHARP component codes. To better understand and exploit the benefits of advanced modeling simulations to improve fast reactor economics, the NEAMS Campaign initiated the “Sodium-Cooled Fast Reactor (SFR) Challenge Problems” task whose primary objective is to demonstrate the value of the SHARP toolkit to important problems relevant to SFRs.

The first challenge problem is the assessment of *hot channel factors* (HCFs) for SFR designs. The primary objective of this challenge problem is to demonstrate the reduction or elimination of uncertainties that are involved in the SFR designs, and assess the impact on fast reactor economics. For a particular design parameter such as fuel centerline temperature, the HCF is defined by the ratio of the maximum value of that parameter to the nominal value. It is noted that the difference between the maximum value and nominal values is due to uncertainties that are involved in the nominal value calculations: i.e., if a HCF is greater than unity for a particular parameter, the decimal part (i.e., HCF minus one) represents uncertainties.

In the United States, sets of HCFs have been developed for the Fast Flux Test Facility (FFTF), Clinch River Breeder Reactor (CRBR), and Experiment Breeder Reactor II (EBR-II), but additional attempts have not been made since the SFR development programs were canceled in the mid-1990s. Looking back at the earlier efforts on the HCF development for FFTF, CRBR, and EBR-II, limited computing power and approximations in modeling and simulation methods resulted in the prediction of neutronics and thermal-hydraulic parameters with relatively large uncertainties, where some uncertainties could only be quantified by expensive experiments. The high-fidelity and multi-physics capabilities of the SHARP toolkit, accompanied by remarkable progress in the computing technologies during the last few decades, now make it possible to calculate most design parameters without support of mockups or experiments and reduce uncertainties significantly compared to the uncertainties involved in the FFTF or CRBR designs. Reduction of the uncertainties (i.e., reduction of HCFs closer to unity) allows an increase in nominal parameters and safety margin, which in turn improves the economic competitiveness of the SFR. To demonstrate the economic benefits, the assessment of the HCFs using the SHARP toolkit was initiated in this study. However, it is also

recognized that the assessment of the HCFs are challenging because of significant computational resources requirements.

The second challenge problem is the assessment of the impact of the “*SHARP Zoom*” capability, which is a hybrid core modeling and simulation scheme enabled by combining coarse-and-homogeneous meshes and fine-and-heterogeneous meshes: i.e., most assemblies are represented using conventional homogenized meshes, but few assemblies of interest are represented with pin-by-pin heterogeneous meshes in order to gain accurate local information. If the zoom capability is feasible and produces accurate results at selected local areas and integral quantities globally, the computational expense of using high fidelity SHARP toolkit will be significantly reduced, and improve the usability of SHARP toolkit. However, the implementation of the zoom capability is also challenging because the convergence of solutions and the resulting accuracy of the zooming calculations are dependent on the communication between the global coarse meshes and local fine meshes in multi-physics calculations.

The primary purpose of this study is to demonstrate the capability of the SHARP toolkit to resolve the two aforementioned challenge problems. For this study, the 100 MWe Advanced Sodium-cooled Fast Reactor (AFR-100) [Grandy 2013] was selected as a reference SFR for evaluating HCFs and testing the feasibility of the SHARP zoom capability.

In Section 2, the two SFR challenge problems are discussed in detail, including potential benefits from using high fidelity tools to solve the problems. Information on the AFR-100, the SHARP toolkit, and the computation resources used in this study are provided in Section 3. In Sections 4 and 5, the results of this study on the two SFR challenge problems are discussed, respectively. Finally, the conclusion of this study is in Section 6.

The majority of the first year efforts focused on development of the computational models, meshes, and coupling procedure for multi-physics analysis using the SHARP toolkit. Thus, various sensitivity calculations were performed in this study, and the results are presented in Appendices.

2. SFR Challenge Problems

In this chapter, we discuss the two types of problems targeted in this study as applications for the SHARP toolkit: hot channel factor (HCF) calculations, and the “SHARP Zoom” capability for a sodium-cooled fast reactor design (SFR).

2.1 Assessment of Hot Channel Factors

Various uncertainties are involved in the predictions of reactor design parameters, which include theoretical and experimental analysis uncertainties, instrumentation uncertainties, manufacturing tolerances, correlation uncertainties, and method and simulation uncertainties. In order to assure integrity of fuel elements and reactor structures and ultimately to protect the health and safety of the public and environment, the fuel, cladding, and coolant temperatures should not exceed the design limits with minimum margins to design limits. For instance, in order to assure cladding integrity of a metallic fuel SFR, the peak cladding inner-wall temperature is required to be below the fuel-cladding eutectic formation temperature as shown in Figure 2.1.1.

Figure 2.1.1 Schematic of assessment of margin to fuel-cladding eutectic formation

It is difficult to pin-point the exact eutectic formation temperature of a metallic fuel in an SFR because fuel-cladding eutectic formation is a complex phenomenon affected by fuel compositions, temperature, and irradiation histories. Thus, to account for theoretical and experimental uncertainties, the design limit of the eutectic formation temperature is lower than the value determined theoretically or by empirical corrections. On the other hand, the peak cladding temperature increases from the nominal calculation to account for the stochastic errors of cladding thickness and compositions from manufacturing tolerances and uncertainties from modeling and simulations. After considering all uncertainties, the difference between the design limit and the

peak cladding inner-wall temperature (gap between two red-lines in Figure 2.1.1) is defined as the minimum margin to limit.

In Figure 2.1.1, the gap from the nominal peak cladding inner-wall temperature to the eutectic formation temperature minus the minimum margin to limit denotes the uncertainties that are involved in the calculation of the design parameter, and in order to count the uncertainties in the reactor design, so-called *hot channel factor* (HCF) methods have been developed and utilized since the early days of civil nuclear plant development. The HCF for a particular design parameter is defined by the ratio of the maximum value of that parameter to the nominal value [Walter 1981]. It is noted that the difference between the maximum value and nominal values is due to the uncertainties that are involved in to calculate that parameter. If a HCF is greater than unity for a particular parameter, the decimal part (i.e., HCF minus one) represents direct or stochastic uncertainties in the parameter.

In the United States, the SFR HCFs have been developed under the various SFR development programs and the magnitudes of HCFs were strongly related to the status the modeling and simulations and computing power when the HCFs were developed. Figure 2.1.2 shows the SFR development, deployment, and operation history, including the activities on the HCFs development aiming at the specific SFRs. Four sets of HCFs have been developed under SFR programs in the United States. The first sets of HCFs were developed in 1976 for the FFTF, and the HCFs were updated in 1990. A significant effort on the development of HCFs has been conducted to support the licensing of Clinch River Breeder Reactor (CRBR) in 1980. The last set of HCFs were 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 FFTF were permanently shut down and SFR programs have been canceled in the mid-1990s, and therefore no additional efforts were made to develop HCFs since then except for reviews of existing HCF sets for new SFRs.

Figure 2.1.2 SFRs operated or designed in the United States

The HCFs of the CRBR [Carelli 1980] and EBR-II [Ku 1994] related to the cladding inner-wall temperature are compared in Table 2.1.1. The set of HCFs for the CRBR was developed in 1980, while the set for the EBR-II was developed in 1995. During the 15-year time-lag, number of HCFs was significantly reduced and the magnitudes of several HCFs were also changed. This trend informs that several uncertainties were eliminated or changed in the later design even though those uncertainties were involved in the earlier designs. The same trend is also observed when comparing two sets of HCFs for FFTF developed in 1976 and 1990.

Table 2.1.1 Comparison of HCFs related to cladding mid-wall temperature

	CRBR - 1980			EBR-II - 1995		
	cool	film	clad	cool	film	clad
Direct hot channel factor						
Power measurement	1.03	1.03	1.03	1.02	1.02	1.02
Inlet flow maldistribution	1.02	1.006				
Flow distribution calculated	1.03					
Assembly flow maldistribution	1.08					
Cladding circumferential temp.		1.7-2.1	0.8			
Pellet-cladding eccentricity		1.14	1.14			
Statistic hot channel factor (3-sigma)						
Reactor ΔT variation	~1.14	1.016				
Inlet flow maldistribution	1.059			1.079	1.025	
Wire Wrap orientation	1.01			1.01		
Sub-channel glow Area	1.019					
Film Heat Transfer Coefficient		1.12			1.20	

Pellet-cladding eccentricity		1.0 – 1.17	1.0-1.17			
Coolant Properties	1.017			1.06		
Fissile Maldistribution	1.058	1.005		1.06	1.06	1.06
Nuclear data				1.07	1.10	1.10
Cladding thickness and conductivity			1.12			1.085
Intra-assembly flow maldistribution	1.058	1.005		1.056	1.018	

The time evolution of available computing power (in particular, memory and computation speed) and modeling and simulation tools used for development of HCFs are shown in Figure 2.1.3. Early HCF development took place in the 1970's and 1980's. In the 1980's and 1990's, the computation codes currently used for SFR design were developed and refined. Post 2010, the SHARP toolkits that are under development in the NEAMS campaign are seen.

Looking back at the earlier efforts for the FFTF and CRBR during the 1970s and early 1980s, limited computing power and numerous approximations in modeling and simulation methods resulted in the prediction of neutronics and thermal-hydraulic parameters with relatively large uncertainties, where some uncertainties could only be quantified by expensive experiments. For instance, the neutronics codes (such as XSRES-W1DX, DOT(XY), W-2DB, etc.) used for HCFs developments solved few group, low-dimension (1D, 2D, or 1D/2D synthesis) diffusion equations in a homogeneous medium [Hardie 1969, Mynatt 1973, Little 1969], and in order to compensate for the simplifications and approximations, the resulting neutron fluxes and integral parameters (for instance, core multiplication factor, reactivity coefficients, kinetics parameters) were adjusted by mockups performed in zero power critical experiment reactors (ZPR, ZPPR). Similarly, other codes also solve simplified system equations using empirical correlations and approximations in simplified or approximated geometries. For instance, the thermal-hydraulic code such as the early version of COBRA and ENERGY solved single or multi-channel equations with approximated wire-wrap models, and the results were calibrated using the experiments [Yang 2005].

Figure 2.1.3 Evolution of computational resources and codes

During the last few decades, there were brilliant progresses in the computing power and computation code systems which enabled much more advanced and accurate modeling and simulation. For instance, the Mira BlueGene/Q supercomputer, one of the world's leading supercomputers, can do in one day what would take more than 1000 years using the IBM360 computer used in 1970s and 1980s, and today's high-fidelity multi-physics SHARP toolkit can solve the neutron transport and computational fluid dynamics equations without major physics approximations on the full geometry. Thus, the uncertainties associated with HCFs in the early SFR designs can be reduced or somehow eliminated using the high-fidelity multi-physics SHARP toolkit on high performance machines like Mira.

Based on the observations and lessons learned from the SFR development programs in the United States, following two questions related to the HCFs are raised as the motivations of this study:

1. Can the SHARP toolkits calculate hot channel factors without extra mockup or experiments?
2. Can uncertainties that have been involved in the earlier SFR designs be eliminated or reduced using the SHARP toolkit and current computation resources?

If the answers for both questions are "yes", there are great economic benefits to SFR development and deployment. The first question is related to the overall development cost of SFRs. As explained, mockups and experiments have been performed in the earlier SFR development programs to compensate for the simplifications and approximations involved in the reactor designs.

However, most legacy critical and experimental facilities have been decommissioned, and new construction of or recovering experimental facilities would be extraordinarily expensive or not allowed due to lack of fissile materials. Thus, if the SHARP toolkits can calculate HCFs reliably without mockups or experimental supports, overall development cost of future SFRs will be lowered significantly.

The second question is also related to reactor economic benefits and reliable operations because the reduction or elimination of uncertainties allows an increase in the peak cladding inner wall temperature, which ensure reliable operations with additional margin to design limits or/and permits extra increase in the reactor power rate. To emphasize the impact of HCFs reduction or elimination, the peak inner wall temperatures were evaluated using two sets of HCFs, and results are illustrated in Figure 2.1.4. The nominal values were arbitrarily selected from conventional SFR designs, the CRBR HCFs are obtained from Table 2.1.1, and the artificially improved HCFs were reduced by a factor of two from the CRBR HCFs.

Figure 2.1.4 Peak cladding inner wall temperature depending on HCFs (artificial HCFs were hypothetically reduced from the CRBR HCFs)

The peak cladding inner temperature increases to 623 °C from the nominal temperature of 581 °C when accounting for the uncertainties considered in the CRBR design. However, if the HCFs decreased by a factor of two, the peak cladding inner-wall temperature decreases to 602 °C. The reduction of cladding temperature of 21 °C would allow an increase in power rate: i.e., by assuming that other design parameters are also reduced with the same manner, the reactor power rate can be

increased by ~12%, which yields extra earnings of ~\$100M per year from a 1000 MWe fast reactor (based on current electricity cost of 12 cents per kWh).

Therefore, the reduction or elimination of uncertainties, and the calculations of HCFs without mockups or experimental supports will enhance the safety margins or/and improve the economic competitiveness of a SFR, and these benefits are the motivation of this study. As a tradeoff, however, the assessment of HCFs is challenging because high-fidelity computation tools (such as the SHARP toolkit) and high-performance computing power are required.

In this effort, the 100 MWe Advanced Sodium-cooled Fast Reactor (AFR-100) [Grandy 2013], DOE's non-water cooled small modular fast reactor, is selected as the reference fast reactor concept, and its neutron flux, power, and temperature distributions will be evaluated using the high-fidelity multiphysics tools PROTEUS (neutronics) and Nek5000 (CFD) codes which are physics modules in the DOE NEAMS SHARP Toolkit for multiphysics reactor analysis. Specifically, hot channel factors will be calculated for a variety of perturbations in the AFR-100 design.

2.2 SHARP Zoom Capability

The SHARP toolkit is under development to produce high-fidelity solutions on high-performance computing platforms for simulation of core configurations with complex geometric features. However, whole core, multi-physics calculations using the SHARP toolkit are still impractical for large size problems because of excessive computational resources and time required until the solutions are fully converged in the iterative multi-physics calculations between the sub-component modules of the SHARP toolkit. To address this concern, the "*SHARP Zoom*" concept was proposed.

The SHARP zoom concept is a hybrid core modeling and simulation scheme whereby 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.

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. Figure 2.2.1 shows the Americium-bearing blanket (AmBB) concept that is under development by CEA, France for minor actinide transmutation using a SFR. The recovered Americium from existing reactors and the external uranium are mixed together and loaded into radial blanket regions for burning minor actinides. For this case, by adopting the zooming concept (i.e., pin-by-pin modeling of AmBB assembly and

homogeneous modeling of other assemblies), the SHARP toolkits can provide detailed information (such as flux, temperature, burnup) that is needed for irradiation test of AmBB fuel pins.

Figure 2.2.1 Americium-bearing blanket (AmBB) concept

If the proposed SHARP zoom concept is shown to be accurate, the computational expense of using high fidelity SHARP toolkit will be significantly reduced, which would improve the usability of the SHARP toolkit. The convergence of solutions and the resulting accuracy of the SHARP zooming calculations are dependent on the communication between the global coarse meshes and local fine meshes. The feasibility of the SHARP zoom concept will be tested by comparing detailed pin-by-pin power and temperature distributions in the interested local areas with results obtained from conventional legacy code calculations.

3. SFR Design Problems and Computational Tools

In this study, the 100 MWe Advanced Fast Reactor (AFR-100) [Grandy 2013] was selected as the reference core to resolve the SFR challenge, and the PROTEUS and Nek5000 codes were selected as the neutronics and steady-state thermal-hydraulics analyses, respectively. In this section, information on AFR-100, the SHARP toolkit, and the available computational resources are described.

3.1 Advanced Fast Reactor as SFR Design Problem

The AFR-100 was developed to target emerging markets where a clean, secured and stable electricity resource is required but a large-scale plant is not accommodated. The AFR is aimed to be sized for local small grids, transportable from pre-licensed factories to the remote plant site for affordable supply, and able to operate for a long period without frequent refueling. To achieve these strategic goals, several design requirements have been proposed for the AFR core development; a power rating of 100 MWe which is equivalent to 250 MWth with the target thermal efficiency of 40%, a long refueling interval with small burnup reactivity swing, a core barrel diameter of less than 3.0 m, and an active core height of less than 1.5 m.

Detailed information on the AFR-100 is provided in Appendix A, including the computation methods. Figures 3.1.1 and 3.1.2 show the radial and axial core layouts of the AFR-100 core, respectively, and the major core performance parameters are summarized in Table 3.1.1.

Figure 3.1.1 Core radial layout of AFR-100

Figure 3.1.2 Core axial layout and uranium enrichment distribution

Table 3.1.1 Core performance parameters

Parameters	AFR-100
Thermal power, MWt	250
Refueling interval, year	30
Number of batches	1
Fuel form	U-Zr
Active core height, cm	110
Average power density, kW/l	64.3
Fuel pin overall length, cm	222
Initial heavy metal loading, t	23.9
Specific power density, MW/t	10.5
Average enrichment, %	13.7
Burnup reactivity swing, %Δk	1.1
Overall fissile breeding Ratio	0.80
Average discharge burnup, MWd/kg	101
Peak discharge burnup, MWd/kg	172
Peak fast fluence, 10^{23} n/cm ²	5.97
Linear heat rate (average/peak), kW/,	15.2 / 28.2

The AFR-100 core adopted an onion-type enrichment zoning concept that was developed for a long refueling scheme and flat radial power distribution. The active core is divided into three different enrichment zones radially, and each zone has multiple zones axially. The average uranium

enrichment is 11.97% for the inner core, 13.12% for the middle core, and 14.97% for the outer core. The core can maintain criticality for 30 years by employing the unique enrichment zoning strategy of the AFR-100 with low reactivity swing during the reactor life time. The average discharge burnup is 101 MWd/kg and the peak discharge burnup is 172 MWd/kg.

3.2 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, that were used to resolve the SFR challenge problems are briefly described, including the overall computation approach by coupling two component codes and computation resources.

3.2.1 PROTEUS Neutronics Code

PROTEUS has two neutronics solvers, PROTEUS-SN and PROTEUS-MOCES, and both solvers were used for this work. All published scaling studies were performed with the PROTEUS-SN code which we report below.

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 in this case.

Scaling data is provided for the BG/P architecture for a fast reactor problem in Tables 3.2.1.1 and 3.2.1.2 (all data accumulated at 1 MPI rank per core). Performance is very similar on the BlueGene/Q architecture provided the parallelization regime of >1500 spatial vertices/process and >1-2 angles per process is followed. The lower memory per core on BG/Q does not impact the simulations as long as parallelization in space and angle are maximized and the number of energy groups is less than 70. In cases with 70 or more energy groups, 8 MPI ranks per node or less are often required to fit the cross section data into memory.

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. While we do not have detailed scaling data to present for PROTEUS-MOCEX due to its recent development, it has performed well on both small, medium, and large clusters including the BlueGene/Q supercomputer. 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.

Table 3.2.1.1 Strong spatial scalability of PROTEUS-SN on BlueGene/P (ANL)

Total Cores	Vertices Per Process	Total Time (s)	Strong Scaling
8,192	7,324	2,402	100%
16,384	3,662	1,312	92%
24,576	2,441	873	92%
32,768	1,831	637	94%

Table 3.2.1.2. Weak angle scalability of PROTEUS-SN on BlueGene/P (ANL, JSC)

Total Cores	Angular Directions	Total Time (s)	Weak Scaling
32,768	32	579	100%
73,728	72	572	101%
131,072	128	581	100%
163,840	160	691	84%
294,912	288	763	76%

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.

3.2.2 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 3.2.2.1 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 3.2.2.2 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 SFR Grand Challenge program.

Figure 3.2.2.1 Comparison of convergence behavior between Nek5000 and OpenFOAM [Sprague 2010]

Figure 3.2.2.2 Hierarchical structure of NEAMS TH tools

3.2.3 Multiphysics Coupling Approach and Computational Resources

A schematic of the SHARP toolkit is shown in Figure 3.2.3.1. The PROTEUS neutronics solver and Nek5000 fluid computational dynamics code are individual physics modules of the SHARP toolkit developed at Argonne National Laboratory under the DOE NEAMS program and other (Nek5000) funding. PROTEUS calculates the detailed power density and flux distributions in a nuclear reactor. Nek5000 calculates the detailed velocity and temperature distributions in a nuclear reactor core. PROTEUS and Nek5000 are tightly coupled together within the SHARP Toolkit and information (temperature, power) can be seamlessly exchanged online during the simulation while iterating between the two physics. We do not discuss the Diablo structural mechanics code in this work as it is not relevant for our applications.

Figure 3.2.3.1 Schematic of online coupling using the SHARP toolkit

While online coupling within the SHARP toolkit certainly provides very accurate transfer of data (element wise basis), there are some limitations: (1) only one neutronics solver and one CFD solver are currently hooked up, (2) in today's implementation of SHARP, the codes must utilize the same number of compute cores 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 may need a large amount of computational resources for certain types of problems. Therefore, an offline coupling scheme was introduced in this study as shown in Figure 3.2.3.2 which allows a different neutronics solver (more appropriate for the proposed work) 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 3.2.3.2 Schematic of offline coupling using components of the SHARP toolkit.

There were two motivations to use offline coupling for this work. First, the PROTEUS-MOCES solver was highly preferred due to performance issues of the PROTEUS-SN solver for the geometries chosen for the hot channel factor calculations. PROTEUS-MOCES is a neutronics solver using an extruded method of characteristics methodology which is highly accurate for heterogeneous geometries. However, since PROTEUS-MOCES is not hooked up with SHARP, it was necessary to perform coupling off-line. Secondly, the computational requirements of neutronics vs. T/H for this work are vastly different and would require artificially large meshes to be used in order to maintain good computational scaling.

The offline coupling was performed one-way: initial calculation with PROTEUS-MOCES, spatial distribution of power density given to Nek5000, and finally Nek5000 calculates temperature distribution. Ideally an iterative procedure would be implemented as shown in Figure 3.2.3.1, 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 fully necessary due to quick convergence. In this work, the initial temperature distribution was assumed to be uniform (standard assumption) for convergence studies as well as for the initial power profiles given to Nek5000. Additionally, a relatively cheap STAR-CCM+ [CD-Adapco 2009] calculation was tentatively used to provide a better temperature guess and comparisons are performed against the uniform temperature distribution.

The available computational resources for this work include small local clusters (debugging), medium-scale high performance clusters (smaller production runs), and large-scale supercomputing machines (large production runs). Due to the high computational resource demands of some of the proposed challenge problems, two competitive proposals were written to access time on leadership and high-performance machines.

The local machines and small clusters within the Nuclear Engineering Division are useful to perform pre-processing steps such as finite element mesh generation, multigroup cross section preparation, and testing of input files. No special proposals are needed to access these resources.

To perform more detailed testing, debugging, spatial and angular convergence studies, and small production runs for both PROTEUS and Nek5000, a pre-existing allocation at Argonne's Laboratory Computing Resource Center (LCRC) was utilized. Proposals are required for this resource and a proposal was submitted for FY18 in the amount of 450,000 core-hours. An existing allocation that was requested in FY16 was used for FY17 calculations. The LCRC is host to the Blues cluster which has roughly 350 Sandy Bridge Xeon and Haswell Xeon nodes which each have 16 cores and 64 GB memory per node. Roughly 150K-300K core hours are available per quarter, depending on user needs.

Finally, for the largest production simulations (in particular, PROTEUS heterogeneous neutronics simulations as well as Nek5000 wire wrap calculations), an Advanced Scientific Computing Research (ASCR) Leadership Computing Challenge (ALCC) proposal was written and awarded for 44 million core-hours of compute time at the Argonne Leadership Computing Facility (ALCF), host to the Mira BlueGene/Q supercomputer. ALCF's Mira has 49,152 IBM BG/Q nodes with 16 cores and 16 GB of RAM per node. The ALCC award runs from July 1, 2017 through June 30, 2018. It should be noted that ALCC proposals are always due at the end of January, and always begin in July. Therefore, the allocation did not begin until the last quarter of FY17, causing some delay in the large production simulations.

4. Assessment of Hot Channel Factors

The HCFs for the SFR were assessed and the results are presented in this Section. For this purpose, a literature review was performed and the HCFs that can be calculated with the SHARP toolkit were identified. A list of calculations to be performed as well as the neutronics and thermal hydraulics models and results for the hot channel factor calculations are discussed in this Section.

4.1 Hot Channel Factors for Metallic Fuel SFRs

The HCFs developed for the earlier SFRs have been reviewed in Appendix D, and the proposed set of HCFs for metallic fuel SFRs are listed in Table 4.1.1. In the last column, several HCFs are marked with “C” or “E” when the HCF can be calculated or eliminated by the SHARP toolkit, respectively. It is noted that two HCFs of “Intra-assembly flow maldistribution”, and “Physics Modeling” can be eliminated in the HCF list if the uncertainties on modeling and simulations with the SHARP toolkit are assumed to be negligibly small.

Table 4.1.1 Proposed hot channel factors for metallic fuel SFR

	Major source of uncertainties	Remark (C or E) ^{a)}
Direct Hot Channel Factors		
Power level measurement	Few percent overpower is assumed in reactor normal operation due to control rod dead-band	
Cladding circumferential temperature	Approximation in calculation of axial coolant velocity and azimuthal temperature distribution around a fuel pin. For instance, this HCF was evaluated with a simplified wire-wrap model using FATHOM-360 code and calibrated through ORNL-19 tests.	C
Control rod banking	Control rods are grouped (banking) in operation and there is manufacturing tolerance, which introduces asymmetric power because insertion depths are not identical.	
Statistical Hot Channel Factors		
Reactor ΔT and inlet temperature variation	Uncertainties of reactor ΔT due to deterioration of primary components.	
Inlet flow maldistribution	Uncertainties in inlet flow distribution due to flow maldistribution in lower plenum, manufacturing tolerances in internal structures and orifice, etc.	
Loop temperature imbalance	CRBR allows cold leg loop-to-loop temperature imbalance of 34 °F, which results in 4.9 °F (2-sigma) uncertainty in inlet temperature.	
Wire-wrap orientation	Analyzed by sub-channel code, COTEC, which is 1% uncertainty.	C

Sub-channel flow area	Uncertainties from clad fabrication tolerance, bowing, etc.	C
Film heat transfer coefficient	Uncertainties from correlations.	C
Cladding properties	Uncertainties from manufacturing tolerance and empirical correlations, etc.	C
Coolant properties	Uncertainties from material impurity and empirical correlations etc.	C
Intra-assembly flow maldistribution	Uncertainties of flow distribution within assembly, which are due to simplified model and applied empirical factors of sub-channel codes.	E
Physics Modeling	There are many sub-factors under this category such as nuclear data, flux solver approximation, 2D synthesis method, etc. In FFTF and CRBR, lumped uncertainties of power distribution were estimated using ZPR, ZPPR mockups.	E
Fissile fuel maldistribution	Manufacturing tolerance	C
Fuel thermal conductivity	Uncertainties due to fuel rod diameter, fresh and irradiated fuel conductivity, porosity of swollen fuel, redistribution, etc.	C
Power level measurement	Instrument uncertainties (flow rate, temperature, etc.) and control systems	

a) C or E indicates that the HCF can be calculated (C) or eliminated (E) using SHARP toolkit.

4.2 Strategy for Hot Channel Factor Assessments

In this section, we describe the planned hot channel factor calculations for the beginning of cycle (BOC) AFR-100 fast reactor design, described in Appendix A. The vented fuel concept shown in Figure 4.2.1 was chosen for this analysis due to its shorter axial height compared to the non-vented concept.

Figure 4.2.1 Depiction of fuel wrapped pin

Each AFR-100 fuel assembly contains 91 helically wire-wrapped, closely packed fuel pins. In this study, in order to obtain accurate solutions using available computation resources within reasonable computation time, a wide-range of sensitivity studies were conducted to determine the required mesh discretization and other parameters for the PROTEUS and Nek5000 (see Appendix B and C). Sample meshes of a single fuel assembly with wire-wrap are shown in Figures 4.2.2. One can observe the extraordinary mesh complexity in the wire wrapped case. The wire-wrap around each fuel pin is the main source of strong inter-channel cross flow which is a significant energy transport mechanism in SFR assemblies. The wires have global influences on the flow behavior, and high speed patches of turbulence due to vortex shedding downstream of the wire persist for about a quarter of the wire-wrap periodic length as shown in Figure 4.2.3. Part of this work will assess the hot channel factor in bare bundle vs wire-wrap modeling.

Figure 4.2.2 Close-up mesh of 91-Pin fuel assembly (wire wrap (left) and varying sub-channel geometry in vicinity of wire wrap (3 right))

Figure 4.2.3 Nek5000 simulation for of 217-pin assembly with over 1 million grid points [Childs 2008]

It is noted that single pin or 7-pin bundles were utilized to calculate HCFs in the earlier SFR programs because of limited computation resources and approximations in computation tools, but the SHARP toolkit can model the full assembly explicitly. Among the HCFs listed in Table 4.1.1, some HCFs, in particular if manufacturing tolerances are associated, need stochastic simulations using 91-pin full assembly model. For instance, the HCF of fissile content maldistribution related to peak cladding inner-wall temperature should be calculated by randomly distributing fissile contents over 91 pins based on the manufacturing tolerance. However, a simplified 7-pin bundle model is sufficient rather than 91-pin full assembly model for some HCFs (such as coolant density uncertainty) because the uncertainties are uniformly smeared in the assembly. Thus, in this study, both a 7-pin bundle configuration and 91-pin full assembly configuration, depicted in Figure 4.2.4, were used for evaluating HCFs. In addition, since it is expected that the wire-wrap effect is small in some HCFs, both 7- and 91-pin configurations were modeled with and without wire-wrap. The two configurations are summarized here:

1. The **7-pin configuration** is based on the AFR-100 inner fuel pin geometry (with and without wire wrap) surrounded by sodium coolant. Reflected boundary conditions are applied to the outer hex can.
2. The **91-pin single assembly configuration** is based on the AFR-100 inner fuel assembly geometry (with and without wire wrap) including assembly duct and inter-assembly sodium gap. Reflected boundary conditions are applied to the outer hex can. The 91-pin geometry includes duct wall effects present in the actual AFR-100 assembly, although the effect of neighboring assemblies in the core is not accounted for due to the reflected geometry conditions.

Figure 4.2.4 7-Pin (left) and 91-pin (right) configurations (not to scale)

The required high-fidelity calculations for the HCF evaluations are summarized in Table 4.2.1. The PROTEUS and Nek5000 references in this table indicates the required high-fidelity calculations by PROTEUS and Nek5000 codes, respectively, and the cells highlighted in yellow denote that the calculations were conducted in FY 2017. For completeness, additional calculations are planned in FY 2018.

Table 4.2.1. Required high-fidelity calculations for HCF evaluations

Hot channel factors	7-pin		91-pin	
	Bare bundle	With wire-wrap	Bare bundle	With wire-wrap
Nominal condition				
	PROTEUS Nek5000	Nek5000	PROTEUS Nek5000	Nek5000
Perturbed conditions				
Wire-wrap orientation				Nek5000
Cladding thickness ^{a)}	PROTEUS Nek5000			
Film heat transfer coefficient	Nek5000			
Cladding properties	Nek5000			
Coolant properties	Nek5000	Nek5000	Nek5000	Nek5000
Fissile maldistribution ^{b)}			PROTEUS Nek5000	Nek5000
Fuel thermal conductivity	Nek5000			

a) Sub-channel flow area.

b) Stochastic analysis based on random sampling is needed. About 30 simulations with PROTEUS and 1- 2 simulations with Nek5000 are expected.

Table 4.2.1 shows that PROTEUS calculations are needed in several spots, while Nek5000 calculations are needed at every spot. Generally, the PROTEUS calculations are not needed in most perturbed conditions because the impacts of the perturbed conditions on cladding, coolant, and wire-wrap orientation, etc. on neutronics characteristics (in particular, power distribution) are negligible. Thus, the power distributions at nominal condition without wire-wrap are sufficient to simulate the thermal-hydraulic perturbations. However, since the fissile maldistribution from manufacturing tolerance affects the neutronics characteristics, the PROTEUS calculations are needed to evaluate fissile maldistribution HCF. In this case, a stochastic analysis based on random sampling technique was suggested in this study because the distribution of the fissile content is statistically distributed in the assembly. The Nek5000 calculations are needed in every HCF because the change of thermo-physical properties may change the peak temperatures of cladding, coolant, and fuel. In Table 4.2.1, the calculations in most HCFs are focused on the 7-pin bare bundle configurations by assuming that the wire-wrap effect on those HCFs are small. The comparison of the bare bundle and wire-wrap bundle are discussed in Appendix C, and the difference between 7-pin bundle and 91-pin full assembly will be investigated in FY 2018.

4.3 Neutronics Results for Hot Channel Factor Calculations

For HCF calculations, iterations (i.e., data transferring and updating solutions) between PROTEUS neutronics calculations and Nek5000 thermal-hydraulics calculations are needed at both nominal condition and perturbed states which are associated with uncertainties. The Nek5000 code needs power distributions, and the PROTEUS code needs temperature distributions. The peak temperature values obtained from the Nek5000 calculations are sensitive to the neutronics results, while the neutronics results are less sensitive to the temperature variations because the variation from uncertainties is small (see the sensitivity studies in Appendix B). Thus, only one-way data transfer from PROTEUS to Nek5000 was considered, and the neutronics results at both nominal condition and perturbed status are discussed in this subsection. As discussed in Appendix B, the PROTEUS-MOCEX code was used for the neutronics analysis along with an offline coupling scheme to Nek5000.

4.3.1 Nominal Neutronics Results

Detailed convergence studies were performed to determine the sensitivity of the neutronics result on mesh, angle, and energy discretization. The full details are reported in Appendix B. Afterwards, axial power profiles for the nominal conditions of the 7-pin and 91-pin configurations were obtained with the discretization parameters listed in Section B.4.5 of Appendix B at a uniform 300 K temperature. To facilitate the data transfer to Nek5000, axial power profiles are normalized such that the power per unit length generated in the active core region has an average value of 1.0. The cost of the each simulation using the PROTEUS-MOCEX code is 8 core-hours (7-pin) and 61 core-hours (91-pin) on LCRC's Blues cluster.

The power profile for the 7-pin configuration is plotted in Figure 4.3.1.1. The peak/average power occurs at the top of the core with magnitude 1.9364, meaning that the power in this zone is 193% of the average axial power.

The power profile for the 91-pin configuration is plotted by ring in Figure 4.3.1.2. The peak/average power occurs at the top of the core with magnitude 1.7654 in the center pin, meaning that the power in this zone is 176% of the average axial power. The pins in other rings have nearly identical peak/average values, the largest deviation being pins in ring 6 which have 0.88% higher average/peak than the center pin. The average pin powers are reported in Table 4.3.1.1, which shows that both the pin power magnitudes and axial shapes are nearly identical in each ring.

Figure 4.3.1.1. MOCEX nominal condition axial power profile (7-pin)

Figure 4.3.1.2. MOCEX nominal condition axial power profile (91-pin)

Table 4.3.1.1. MOCEX nominal condition average pin power in each ring (91-pin)

Ring	Average Power per Pin (kW)	Peak/Average Axial Power per Pin
1 (center)	18.319	1.7654
2	18.310	1.7651
3	18.300	1.7649
4	18.302	1.7652
5	18.321	1.7673
6 (next to duct)	18.324	1.7810

As previously noted, the 7-pin and 91-pin axial power profiles do not follow a cosine shape along the axial dimension due to the unique enrichment pattern in the assembly, where the top and bottom regions are highly enriched (18.0%) compared to the middle region (8.8%). However, even more notably, the top-most region of the active fuel zone is the highest power zone in the pin. This power peaking happens to occur in the zone where the sodium coolant is also highest temperature and is likely to significantly impact the hot channel factor calculations. The peak/average axial power for the 7-pin calculation is 1.9364 and that of the 91-pin calculation is 1.7654. Therefore, the presence of the duct and inter-assembly gap decrease the overall power peaking along the axial dimension in the 91-pin configuration.

To further confirm and understand this behavior, a conventional 33-group DIF3D neutronics simulation using homogenized nodes on each axial plane was performed to reproduce the general behavior seen here (power peaking just below gas plenum). The detailed axial power distribution was reconstructed using a post-processing tool. The DIF3D simulation confirmed the general axial power shape, although the power peaking in the upper fuel zone (essentially just the top value in the figure which represents the power vs the axial average power) was calculated to be far less severe (1.6582 vs. 1.9364). The DIF3D simulation calculated the eigenvalue to be 1.12212 vs the “converged” MOCEX value of 1.12708 using the same 33g cross section sets. The differences are due to the high fidelity simulation capturing much more details effects particularly in the regions where the material changes. We note that a full detailed space-angle-mesh study was not performed by DIF3D here, but that DIF3D does have a limit on how finely detailed the axial mesh can be.

Figure 4.3.1.3 Axial power profile comparison between DIF3D and MOCEX (7-pin)

Once the power peaking was confirmed by conventional tools, the individual multigroup fluxes were examined to understand the origin of this behavior, which was somewhat unexpected and will impact the peak coolant temperature and subsequently the hot channel factors being calculated.

The power profile as well as multigroup fluxes from group 1 [10-14.190675 MeV], group 8 [301.97-497.87 keV], and group 25 [61.4-101.3 eV] are plotted in Figure 4.3.1.4 for the 33-group 7-pin calculation. Only the active core zones are shown for better visibility. The dramatic power peaking at the top of the fuel pins can be observed on the far left figure. The fast fluxes (groups 1 and 8) are *not* peaked in that axial zone, so fast fission is not the sole contributor of increased power in that zone.

However, peaks are seen in the group 25 flux (and subsequent thermal groups) as neutrons slow down and reflect back into the core from the sodium bond-filled gas plenum located directly above the active fuel. Since the fission cross section for U-235 is 1-3 orders of magnitude higher at epithermal and thermal energies as opposed to the fast energy groups (see Figure 4.3.1.5), the thermal fission is substantially increased in this zone. In fact, while the lower energy group flux in the power-peaked zone is two orders of magnitude lower than the fast flux (10^{10} vs 10^{12}), thermal fission contributes nearly as much energy in this zone as fast fission, leading to significantly higher total power production.

In conclusion, the nominal condition 7-pin and 91-pin configurations were generated successfully using the PROTEUS-MOCEX code. The center pin axial power distribution and magnitude accurately describes all of the pins, and thus is the only data needed for Nek5000.

Figure 4.3.1.4 Axial profiles for computed by 33g MOCEX simulation (7-pin)
((a) axial power profile in active core (b) group 1 flux, (c) group 8 flux, and (d) group 25 flux)

Figure 4.3.1.5 Fission cross section for U-235 retrieved from National Nuclear Data Center website

4.3.2 Neutronics Results Associated with Uncertainties in Thermo-Physical Properties

The HCF associated with the uncertainties in thermo-physical properties quantifies the effect of uncertainties in thermo-physical properties such as coolant heat transfer coefficient, coolant density, and cladding thermal conductivity. These properties are related solely to the thermal-hydraulics calculation, with the exception of coolant density, which may have a neutronics effect but is unlikely to change the normalized axial power profile if changed uniformly and in modest amounts. Therefore, the nominal condition power profile already calculated was provided to Nek5000 for these perturbation calculations.

4.3.3 Neutronics Results Associated with Uncertainties in Subchannel Flow Area

The focus of this HCF is to quantify the effect of uncertainties in subchannel flow area (area between pins) due to manufacturing tolerances in the fuel pin cladding. The manufacturing tolerance on the cladding thickness was obtained from the EBR-II MARK-V fuel fabrication, which is $\pm 3\%$ [Ku 1994]. In addition, based on the communications with the fuel experts who are currently involved in the SFR metallic fuel development, the manufacturing tolerance on the cladding thickness of ± 0.05 mm was also considered [Cheon 2017]. The cladding thickness of the *center pin only* was reduced for this study. With more compute time available and more time for meshing, the fuel pin cladding radius should be varied randomly according to a distribution. The presence of wire wrap with asymmetric fuel pin geometries causes severe meshing implications which are time consuming to resolve and to study.

Reducing the cold cladding thickness yields the new cladding dimensions in Table 4.3.3.1. The 0.05 mm reduction in thickness is a more dramatic scenario than reducing by 3% and results in a new cladding thickness of 0.473 mm (vs 0.508 mm). This small geometry perturbation is depicted in Figure 4.3.3.1 and is the only one considered for neutronics. As seen in the following tables, the effect on the power profile is negligible and the effect one eigenvalue is very small. Using the MARK-V perturbation would result in an even smaller effect.

Table 4.3.3.1 Cold cladding thickness perturbations and corresponding hot dimensions

	Cold Clad Thickness (cm)	Hot Inner Clad Radius (cm)	Hot Outer Clad Radius (Bare Bundle) (cm)	Hot Outer Clad Radius (w/ Smeared WW) (cm)	Hot Clad Thickness (w/ Smeared WW) (cm)
Unperturbed	0.0500	0.6993	0.7496	0.7516	0.0523
Thickness reduced by 3%	0.0485	0.6993	0.7481	0.7501	0.0508
Thickness reduced by 0.05 mm	0.0450	0.6993	0.7446	0.7466	0.0473

Figure 4.3.3.1 Overlay of the initial and perturbed meshes to show cladding perturbation (-0.05 mm change in cladding thickness).

Table 4.3.3.2 MOCEX eigenvalue results for cladding perturbation (7-pin)

Case	Energy Group	Eigenvalue	% of Total Power in Center Pin	Temp.	Angular Cubature	Mesh Elements (2D)	Mesh Refinement	Planes
Unperturbed	33	1.12708	16.657%	300K	L3T5	265	A1R1	78
Clad thickness reduced by 0.05 mm	33	1.12742	16.667%	300K	L3T5	265	A1R1	78

Table 4.3.3.3 MOCEX eigenvalue results for cladding perturbation (91-pin)

Case	Energy Group	Eigenvalue	% of Total Power in Center Pin	Temp.	Angular Cubature	Mesh Elements (2D)	Mesh Refinement	Planes
Unperturbed	33	1.10327	1.09856%	300K	L3T5	3061	A1R1	78
Clad thickness reduced by 0.05 mm	33	1.10330	1.09864%	300K	L3T5	3061	A1R1	78

The 7-pin configuration displayed a +34 pcm change in eigenvalue due to the 0.05 mm decrease in cladding thickness, but a negligible change in axial power profile or in the power distribution among pins. The 91-pin configuration displayed only a +3 pcm change in eigenvalue compared to the unperturbed case, and the axial power profile changed negligibly. This is reasonable because

the 91-pin configuration has 90 unperturbed pins and only 1 perturbed pin (only 1% of pins are perturbed) whereas the 7-pin configuration has 6 unperturbed pins and 1 perturbed pin (14% of pins are perturbed). The 7-pin and 91-pin axial power profiles are displayed in Figure 4.3.3.2 and Figure 4.3.3.3. The percent of total power in the center pin is reported in the previous tables.

In conclusion, the effect of the cladding perturbation in neutronics is negligible. The neutronics calculations were not repeated for the MARK-V cladding perturbation (3% reduction in cladding thickness) because the perturbation is even smaller. Using the unperturbed (nominal) condition power profiles in Nek5000 for the cladding perturbation hot channel factor calculation is therefore justified.

Figure 4.3.3.2 MOCES axial power profile for cladding thickness change (7-pin)

Figure 4.3.3.3 MOCES axial power profile for cladding thickness change (91-pin)

4.3.4 Neutronics Results Associated with Uncertainties in Fuel Pellet Fissile Content

Due to manufacturing tolerances, the fuel pellet fissile content can vary up $\pm 6\%$ from the target enrichment which affects the local pin power and temperature. Random sampling techniques will be used to simulate up approximately 30 cases in neutronics to develop axial power profiles for the 91-pin configuration and determine a distribution with bounding cases for thermal hydraulics. The plan for this work is laid out here, but will be completed in FY18.

Thirty neutronics datasets will be generated with randomly perturbed enrichments. To generate each of the 30 inputs, the following procedure will be performed.

1. Sample the number of pins having perturbed enrichment uniformly from 1 to 91 (N).
2. For perturbed pin 1 to N, sample the location of the perturbed pin uniformly from 1 to 91.
3. For perturbed pin 1 to N, sample the enrichment perturbation uniformly from the discrete set $\{\pm 6.0, \pm 5.0, \pm 4.0, \pm 3.0, \pm 2.0, \pm 1.0\}\%$. The top and bottom fuel enrichments are assumed to have the same enrichment in each pin, but the middle enrichment can vary independently. A discrete set is used in order to greatly simplify the definition of material compositions in neutronics.

The 30 simulations will be used to generate 30 pin-by-pin axial power profiles. The peak pin power from each simulation will be identified and plotted similar to Figure 4.3.4.1 to form a distribution. The peak pin power can be assumed to lie within the 2-sigma (95% confidence interval), and the power distribution from a case with peak power at 2-sigma above the mean will be simulated in Nek5000 to determine the resulting temperature distribution.

Figure 4.3.4.1 Hypothetical peak pin power distribution based on random sampling

The neutronics model for these simulations will rely on much of the existing work (including cross section generation and convergence studies), but also requires definition of many new compositions as well as unique pin-by-pin material mapping and output which was not previously required. This work will be performed in FY18.

4.4 Thermal-Hydraulic Results

Nek5000 calculations are computationally expensive due to the inclusion of high-fidelity features and also the significant manpower required to generate finite element meshes. So, before moving forward, detailed sensitivity studies were conducted to save computational resources and ensure the reliability of the calculations, which include the test of mesh generation schemes and performance comparison between bare rod bundle and rod bundle with wire-wrap with the commercial computational fluid dynamics code of STAR-CCM+. The full details are reported in Appendix C. When constructing a simulation for flow through a wire-wrapped fuel rod bundle, scientists may utilize a smaller bundle than design in order to minimize material or computational costs. The 7-pin rod bundle is the smallest bundle that can reasonably replicate the full assembly geometry. However, small bundles may not capture the required flow physics in larger bundles [Brockmeyer 2017]. Therefore, the simulation on the full-size rod bundle (91-pin) is also conducted. Hence, the hot channel factor calculations are performed for two geometry types: a 7-pin configuration based on AFR-100 with and without wire wrap and a 91-pin full AFR-100 fuel assembly with and without wire wrap.

4.4.1 Bare Rod Bundle Results

The pin pitch/diameter (P/D) ratio for AFR is about 1.08, which makes the assembly a tight lattice. The flow in tight rod bundles is characterized by long-term, large-scale coherent patterns in the stream-wise direction. Therefore, unsteady simulations are necessary if accuracy in the prediction of averaged statistics is needed. Since the Reynolds number in the AFR-100 assembly can reach 25,000, it is very expensive to perform the calculation with Large Eddy Simulation (LES) simulation. Some literatures ([Yu 2011], [Merzari 2008]) point out that Unsteady Reynolds-Averaged Navier–Stokes (URANS) simulation perform equally well, and solve for the transient solution at a fraction of the computational cost of large eddy simulation (LES). Therefore, URANS simulation with $k-\omega$ turbulence model are applied for this study. URANS simulations as performed in Nek5000 are more accurate than RANS simulations as performed in STAR-CCM+ because they capture the coherent structure in tight lattice, which is impossible to reproduce with RANS simulation.

Figure 4.4.1.1 shows the transient outlet velocity distribution in the 7-pin bare rod bundle at 0.5s time intervals. The asymmetric velocity distribution indicates strong flow oscillation. The flow oscillation develops gradually to a steady oscillation (i.e. the amplitude, shape and frequency of oscillation reaches a constant or quasi-constant value). That is why the contour shows some periodic feature of the velocity distribution. The flow is more obvious if we observed the velocity on cross section of the gap region (Figure 4.4.1.2). It can also be seen that the simulation reaches a steady oscillation since the wavelength of the oscillations is roughly the same. By capturing the flow oscillation well, URANS simulation from Nek5000 can reproduce the averaged velocity well. As shown in Figure 4.4.1.4, the time-averaged velocity from URANS has symmetric

features. Although qualitatively the velocity distribution may seem similar to what is predicted by RANS simulation, the magnitude of the velocity, especially near the gap region, can have more than 20% deviation from the prediction from RANS simulation.

The flow oscillation is caused by the coherent structure, as proposed by Jeong and Hussain [Jeong 1995]. The coherent structure appears in pairs on either side of the gap. The coherent structure will enhance the mixing between the adjacent sub-channels significant, which may also lead to strong heat transfer between sub-channels. As a consequence, the maximum lateral velocity can reach 22.5% of the average stream wise velocity (Figure 4.4.1.5).

Figure 4.4.1.1 Transient outlet velocity distribution in 7-pin bare rod bundle

Figure 4.4.1.2 Transient gap region velocity distribution in 7-pin bare rod bundle

Figure 4.4.1.4 Averaged outlet velocity distribution in 7-pin bare rod bundle

Figure 4.4.1.5 Lateral velocity distribution in 7-pin bare rod bundle

Three axial power distributions are applied to the 7-pin simulation: uniform power distribution, the core average BOC power distribution as estimated from initial design report [Grandy 2013], and the power distribution for the central fuel pin of the inner-core type fuel assembly calculated from PROTEUS. Uniform power distribution is the most common power distribution when performing CFD standalone calculations since neutronics information is either unnecessary or

unavailable. The axial power distribution from PROTEUS is a representative axial power profile of the AFR-100 assembly which may have peak temperatures based on the heterogeneous fissile distribution as shown in Figure 3.1.2, rather than the core average BOC power. These three power distributions are shown in Figure 4.4.1.6. The power distribution from PROTEUS deviates greatly from the uniform and core-average BOC power distributions, as explained in Section 4.3.1. The PROTEUS calculation also indicates that the deviation of the radial power distribution (power distribution from pin to pin) is negligibly small. Thus, the power distribution is considered radially uniform in the simulation.

Figure 4.4.1.6 Three axial power distributions applied to 7-pin bare rod bundle

Figure 4.4.1.7 shows the temperature distributions at different elevations within the last wire-wrap pitch (uppermost region of the active core) calculated using the power distribution from PROTEUS. The temperature is hotter in the center and cooler in the edge due to slightly increased amounts of coolant near the periphery of the 7-pin configuration. The magnitude of the temperature increases along the flow direction.

Figure 4.4.1.8 shows the outlet temperature with different axial power distribution. Without question, the maximum temperature appears in the fuel. The average coolant temperature stays the same in the three cases despite the very different power distributions. Since the power rate reaches maximum at outlet in PROTEUS's calculation while it reaches minimum in BOC power distribution, the maximum fuel temperature difference at outlet between these two cases is large. The maximum fuel temperature with power distribution from PROTEUS is 1010K while it is 896.1K for the BOC power distribution. Although the average outlet temperature is the same for three different axial power distributions, the higher power rate at the outlet can lead to higher

temperature gradients that cause higher maximum fuel temperature. In summary, without using a proper axial power profile from high fidelity tool calculation, the maximum fuel could be underestimated by more than 100K in this case. It also indicates that the maximum fuel temperature is quite sensitive to the power distribution, especially the value at the outlet.

Figure 4.4.1.7 Temperature distributions at different Elevations (4.0P, 4.2P, 4.4P, 4.6P, 4.8P, 5.0P) in 7-pin bare rod bundle using PROTEUS power distribution

a) Power distribution from PROTEUS

b) Uniform power distribution

c) Power distribution from core average power at BOC

Figure 4.4.1.8 Outlet temperature distributions with different axial power distribution in 7-pin bare rod bundle

It is beneficial to analyze the detailed maximum temperature in different sub-channels and rods according to the numbering scheme shown in Figure 4.4.1.9. Rod 1 is the center rod which is

surrounded by six sub-channels, labelled 1-6. Rod 2 through Rod 7 are located in the second ring of the assembly. Only sub-channels 1-6 as shown in the figure are analyzed because other sub-channels are located at the edge of the assembly and experience a sharp temperature drop.

The maximum temperature for the different sub-channels and rods are shown in 4.4.1.10. For the same axial power profile, the maximum temperatures in all the sub-channels are similar. The difference is within 2°C. The slight asymmetry of the maximum temperature is caused by the mixing introduced by the coherent structure in the fluid flow. The cladding and fuel maximum temperature of rod 1 is obviously higher than other rods that neighbor the edge sub-channels which are much cooler than the center sub-channels.

The case using the axial power distribution from PROTEUS has higher maximum temperature than the cases using the uniform or core average BOC power distributions. While the average bulk temperature in the core is the same for all power profiles (due to same average power production across the core), the higher power rate at the outlet in the PROTEUS distribution leads to higher heat flux at that location. The increased heat flux must be associated with an increased temperature gradient and therefore higher outlet temperature. However, the detailed maximum temperatures in different sub-channels and rods have similar trends despite the different axial power distributions. Therefore the axial power distribution only affects the magnitude of the maximum temperatures, and the overall trends are insensitive to the axial power shape.

Figure 4.4.1.9 Numbering scheme for sub-channels and rods in 7-pin bare rod bundle

a) Maximum Coolant Temperature in different Sub-channels

b) Maximum Cladding Temperature in Different Rods

c) Maximum Fuel Temperature in Different Rods

Figure 4.4.1.10 Maximum temperature for different sub-channels and rods in 7-pin bare rod bundle

a) Velocity Distribution

a) Temperature Distribution

Figure 4.4.1.11 Outlet velocity and temperature distribution in 91-pin bare rod bundle

The velocity and temperature distribution at the outlet in the 91-pin bare rod bundle are shown in Figure 4.4.1.11. The velocity in the edge sub-channels is obviously larger than that in other sub-channels due to larger hydraulic diameter. The temperature in the edge sub-channels is colder mainly because of two factors: increased velocity as shown, and lower volumetric heat flux in the edge zone.

In order to study the volumetric power distribution, the whole assembly is divided into 6 zones which follow a ring pattern as shown in Figure 4.4.1.12. Zone 1 is located at the peripheral layer of the assembly and Zone 6 is located at the center of the assembly. The other regions are located sequentially in between these two regions. The volumetric heat flux Q_v (W/m^3), in each region is calculated with the following formula:

$$Q_v = \frac{N_r \cdot S \cdot Q_s}{V}$$

where N_r is the number of rods in each region, S is the surface area of each rod (m^2), Q_s is the heat flux on the surface of each rod (W/m^2), and V is the volume of each zone. The flat-to-flat distance of the assembly is L . The height of the active core is H . The detailed volumetric heat flux in each zone is listed in Table 4.4.1.1. It is noted that the volumetric heat flux in zone 1 is different from that in other zone mainly due to fewer rods per unit of coolant mass in zone 1.

Figure 4.4.1.12 Sketch of 6 zones for volumetric heat flux calculation

Table 4.4.1.1 Volumetric heat flux in 6 zones

Zone	Number of rods	Volume (V)	Volumetric heat flux (Q_v)
Zone 1	16	$(\sqrt{3}L^2/2 - 75\sqrt{3}P^2/2)H$	$16Q_sS/(\sqrt{3}L^2/2 - 75\sqrt{3}P^2/2)H$
Zone 2	27	$27\sqrt{3}P^2H/2$	$2\sqrt{3}Q_sS/3P^2H$
Zone 3	21	$21\sqrt{3}P^2H/2$	$2\sqrt{3}Q_sS/3P^2H$
Zone 4	15	$15\sqrt{3}P^2H/2$	$2\sqrt{3}Q_sS/3P^2H$
Zone 5	9	$9\sqrt{3}P^2H/2$	$2\sqrt{3}Q_sS/3P^2H$
Zone 6	3	$3\sqrt{3}P^2H/2$	$2\sqrt{3}Q_sS/3P^2H$

Figure 4.4.1.13 Rod numbering scheme in 91-pin bare rod bundle

In order to better understand the temperature distribution in a 91-pin bare rod bundle, the maximum fuel and cladding temperature are analyzed. Based on the analysis of the 7-pin bare rod bundle, the temperature is quite homogeneous in each ring. Only 1/6th of 91-pin assembly will be examined. The numbering scheme of rods in 91-pin bare rod bundle is shown in Figure 4.4.1.13. Rod 1 is the center pin. Rod 9 and Rod 10 are located at the 5th ring of the assembly.

Figure 4.4.1.14 Maximum temperature for different rods in 91-pin bare rod bundle

Figure 4.4.1.14 shows the maximum temperature for different rods in 91-pin bare rod bundle. Given that only heat conduction plays a role between cladding and fuel, the trend of maximum temperature for fuel and cladding is similar. Within the 3rd ring of the assembly, the maximum

temperature is quite homogenous. The maximum temperature begins to drop at the 4th ring. At 5th ring, the maximum temperature drops significantly because it is right next to the peripheral layer of the assembly. For the first 3 rings, 4th and 5th ring act as an insulation from the coolest zone of the assembly. That reveals the mechanism of why the hot spots always appear within the first 3 rings (for AFR-100) of the assembly.

4.4.2 Wire Wrap Rod Bundle Results

The simulations on 7-pin and 91-pin wire wrap rod bundles are performed in Nek5000 to investigate the effect of the modeling the wire wrap explicitly as opposed to the bare bundle. The velocity distributions for both bare rod bundle and wire wrap rod bundle are shown in Figure 4.4.2.1. Obvious differences in the velocity distribution are observed due to the wire effect. Strong inter-channel mixing is introduced by the wire, which affects not only the lateral velocity but also the stream wise velocity.

Figure 4.4.2.1 Comparison of outlet velocity distribution between 7-pin bare rod bundle and 7-pin wire wrap rod bundle

Although the velocity difference is obvious as expected between wire wrap rod bundle and bare rod bundle, the maximum coolant temperatures between the two cases are very close, within 0.2°C deviation (Figure 4.4.2.2). We point out that the initial STAR-CCM+ simulation calculates a 7°C maximum coolant temperature difference between wire wrap and bare rod bundle. This discrepancy occurs because STAR-CCM+ use RANS model which cannot reproduce the lateral velocity caused by the coherent structures. Nek5000 uses URANS to better capture the flow oscillation in the bare rod bundle to get a more precise temperature distribution.

The maximum coolant temperature in different sub-channels is shown in Figure 4.4.2.3. Due to stronger inter-channel mixing in the wire wrap rod bundle, the deviation of the maximum coolant temperature in different sub-channel is larger. However, the hottest sub-channel has similar maximum coolant temperature in both the bare and wire wrap rod bundles. This finding reveals that modeling the wire wrap has a limited effect on HCF calculations. Bare rod bundle simulation can accurately capture the maximum temperature in spite of missing the precise local temperature distribution. Given that the bare rod bundle calculation is much cheaper, the bare rod bundle model is a more practical and efficient model for such calculations. In addition, the wire wrap model can introduce extra error due to simplifying the contact point between the wire and the rod, without taking into account the conjugate heat transfer and by using the periodic boundary condition. The analysis performed on 91-pin wire wrap rod bundle confirm these findings. Figure 4.4.2.4 shows the maximum outer cladding temperature in the 91-pin bare rod and wire wrap bundles. The maximum outer cladding temperature deviation between bare rod bundle and wire wrap rod bundle is about 2°C. In addition, the outer cladding maximum temperature appears on Rod 3 and Rod 5 in the wire wrap rod bundle, which is well captured by bare rod bundle model.

a) wire wrap rod bundle

b) bare rod bundle

Figure 4.4.2.2 Comparison of outlet temperature distribution between 7-pin bare rod bundle and 7-pin wire wrap rod bundle

Figure 4.4.2.3 Sub-channel maximum coolant temperature between 7-pin bare rod bundle and 7-pin wire wrap rod bundle

Figure 4.4.2.4 Maximum outer cladding temperature between 91-pin bare rod bundle and 91-pin wire wrap rod bundle

4.5 Preliminary Estimation of Hot Channel Factors

The previous sections describe the models for the nominal condition. Since the perturbation is usually not big enough to change the flow and heat transfer behavior significantly, the study associated with the uncertainties is investigated based on the model built for the nominal condition.

The HCFs due to perturbed coolant density and coolant specific heat are calculated in both the bare rod bundle and the wire wrap rod bundle. The results listed in Table 4.5.1 show that the calculated hot channel factors of the peak cladding temperature induced by the uncertainties in the coolant properties are not sensitive to the number of pins in the bundle configurations, and the results from the bare rod bundle configuration are more conservative than those from wire-wrap rod bundle configuration. Thus, the 7-pin bare bundle configurations were utilized tentatively to calculate HCFs in this study.

Table 4.5.1 Hot channel factors in bare rod bundle and wire wrap rod bundle

	Uncertainties	7-pin		91-pin	
		Bare rod bundle	Wire wrap rod bundle	Bare rod bundle	Wire wrap rod bundle
Coolant density	$\pm 0.5\%$	1.001	1.0002	1.001	1.0002
Coolant specific heat	$\pm 3\%$	1.002	1.002	1.002	1.002

Based on the results of neutronics and thermal-hydraulics calculations using the SHARP toolkit, some perturbed cases (due to some physical uncertainty, manufacturing tolerance, or modeling approximation) are investigated in 7-pin bare rod bundle and assessed the increase in the peak temperatures due to a given perturbation/uncertainty. The results are listed in Table 4.5.2. The uncertainties or manufacturing tolerances and HCFs for EBR-II were obtained from Ref. [Ku 1994], which was developed for Mark-V fuels. Compared to the HCFs for EBR-II Mark-V fuel, the newly estimated HCFs using the SHARP toolkit are smaller generally due to the reductions of uncertainties in modeling and simulations. For instance, in the EBR-II, the uncertainty of fuel thermal conductivity was considered as the HCF of fuel centerline temperature by assuming that the fuel centerline temperature is proportional to the fuel thermal conductivity. However, the calculated variation of the peak fuel centerline temperature was slightly smaller than the uncertainty of fuel thermal conductivity because there is non-linear correlation between them while the circumferential heat conduction is taken into account.

Table 4.5.2 Preliminary estimations of hot channel factors for selective uncertainties and manufacturing tolerance (7-pin)

Temperature Location	HCF Estimate	Cladding thickness of the center rod	Cladding thermal conductivity	Fuel thermal conductivity	Coolant density
Uncertainties (3 sigma), %		± 3	± 7	± 25	± 0.5
Cladding Outer Wall	EBR-II	-	-	-	1.016
	SHARP Tool	-	-	-	1.001
Cladding Inner Wall	EBR-II	1.03 ~ 1.05	1.088	-	-
	SHARP Tool	1.018	1.043	-	-
Fuel Centerline	EBR-II	-	-	1.25	
	SHARP Tool	-	-	1.226	-

5. Zoom Capability of SHARP Toolkit

The feasibility and accuracy of the SHARP zoom capability, where only local domains of interest are represented with high fidelity and the other parts of the domain are represented with conventional homogenized geometry, are discussed in this section. If the SHARP zoom capability is feasible and can produce accurate results at selected local areas, the computational expense of using high fidelity SHARP toolkit will be significantly reduced, and improve the usability of SHARP toolkit.

The convergence of solutions and the resulting accuracy of the zooming capability are dependent on the communication between the global coarse meshes and local fine meshes. In particular, at the interface surface between the homogeneous assembly and the pin-by-pin heterogeneous assembly, the flux of homogeneous assembly should be re-distributed to fit the pin-by-pin heterogeneous assembly meshes. In addition, in order to minimize the propagation of homogeneous assembly mesh effect, the local pin-by-pin assembly of interest should be surrounded by extra fine-meshed assemblies.

Since the feasibility and accuracy of the zooming capability are strongly dependent on the modeling of the local assembly of interest and neighboring assemblies, the major activities in FY 17 for zooming calculations were focused on the modeling of local assembly of interest and its neighboring assemblies.

5.1 Application of Zoom Capability to AFR-100 Peak Temperature Calculations

Two high-fidelity multi-physics calculations are proposed using the full core AFR-100 design (no wire wrap will be modeled for this work) with SHARP tools. In the first calculation, a selected “assembly of interest” will be modeled with pin-by-pin explicit geometry in both neutronics and thermal hydraulics, and the other assemblies will be modeled with a conventional homogenized assembly approach. In the second calculation, the assembly of interest will be modeled pin-by-pin, as well as the surrounding ring of six assemblies.

The AFR-100 assembly with peak cladding temperature was selected as the zone of interest of the zooming calculations. In Figure 5.1.1 (left), the peak cladding temperature is 693 K, which occurs at the outer core fuel assembly at beginning of cycle (BOC). Thus, the core will be modeled explicitly in neutronics as shown in Figure 5.1.1 (middle and right). At this moment, it is unclear how many neighboring assemblies are needed to be explicitly modeled to obtain the correct flux distribution in the focal assembly. For sensitivity analysis, two zooming cases are considered in this study. Only the focal assembly is explicitly modeled in the first case (single-heterogeneous assembly model), and the focal assembly and surrounding six assemblies (seven-heterogeneous assembly model) were explicitly modeled. The single assembly modeling is depicted in Figure 5.1.1.

Figure 5.1.1 AFR-100 modeling for SHARP zoom calculation

Results will be compared to conventional modeling with pin power reconstruction using DIF3D/RCT/SE2-ANL tools [Yang 1995] to assess the value and benefits of using SHARP Zoom. The proposed calculations (not yet performed) are defined in Table 5.1.1. Considering the neutron diffusion length is typically shorter than the assembly pitch in a SFR, it is expected that the results from seven-heterogeneous assembly model would be accurate. If the single-heterogeneous assembly model yields similar results to the seven-heterogeneous assembly model, the SHARP Zoom concept is promising as it indicates that local distributions are not sensitive to modeling approximations outside the assembly of interest.

Table 5.1.1 SHARP Zoom Milestones

Mile-stone	Geometry	Details	Simulations
A. Assess “SHARP Zoom” Concept (Full Core) Perform two full core simulations with 1 and 7, respectively, high-fidelity fuel assemblies. Assess the difference in power and temperature distributions to determine whether the “zoom” capability yields accurate answers.			
A.1	Full Core Bare Bundle	Nominal Condition (One heterogeneous assembly)	PROTEUS Nek5000
A.2	Full Core Bare Bundle	Nominal Condition (Seven heterogeneous assemblies)	PROTEUS Nek5000
A.3	Full Core Bare Bundle	Nominal Condition (All homogeneous assemblies)	PROTEUS DIF3D/RCT/SE2-ANL

6. Activities in FY18

6.1 *PROTEUS Plan in FY18*

6.1.1 *PROTEUS Plan for Hot Channel Factors*

The remaining hot channel factor calculations to be performed for PROTEUS are the fuel pellet fissile content maldistribution studies detailed in Section 4.3.4. These calculations require pin-by-pin mesh and material assignments due to the random nature of the distribution. Initial work has already been performed to set up these problems. A workflow for analysis of the 30 distributions will be developed.

Additionally, as discussed in Appendix B, Sections B.5 and B.6, various neutronics solutions were generated depending on the solver (MOCEX vs SN) and the temperature distribution (uniform 300 K, uniform 800 K, and temperature gradient using linear interpolation) which differed slightly in their axial power distributions. While the resulting axial distribution differences were small, the effect on Nek5000 temperature should be quantified for further confidence in the Nek5000 solution when using a one-way coupling scheme.

6.1.2 *PROTEUS Plan for SHARP Zoom*

The bulk of the SHARP Zoom analysis will be performed in FY 18. Significant input still needs to be generated for the full core neutronics problem: generation of appropriate multigroup constants including local and global heterogeneity effects, as well as an automated material mapping procedure. It has not yet been determined whether the PROTEUS-MOCEX or PROTEUS-SN solver is more appropriate for this problem. The number of trajectories required to ray-trace the entire 3D core may be too expensive in MOCEX, so PROTEUS-SN solver may be used especially since the bulk of the model is homogeneous in all cases. The compute time to perform these calculations has already been awarded at the Argonne Leadership Computing Facility (ALCF) and will last through June 2018.

The full core AFR-100 problem with heterogeneous assemblies is likely too large in terms of degrees of freedom to run within the SHARP toolkit, due to parallelization issues in the current implementation of SHARP. Therefore, offline coupling will be required even if the PROTEUS-SN solver is used. The information of interest will again be the normalized axial power profiles, which will be transferred to Nek5000 on a pin-by-pin, block-wise basis. This is a much more complicated data transfer than performed for the hot channel factor simulations, which required only one pin's data due to symmetry and near identical pin powers in each ring. Techniques will be developed to make the data transfer more seamless.

Some time will be devoted to learn how to set up the homogeneous problem using the legacy technique as the SE2-ANL code is not well documented.

6.2 Nek5000 Plan in FY18

6.2.1 Nek5000 Plan for Hot Channel Factors

In FY 18, additional modeling on wire wrap rod bundles will be performed to investigate the effect of the manufacturing uncertainties and uncertainties in various thermo-physical properties. Since the approach is still too computationally expensive to use for routine design purposes, simplification on the model will be investigated to save computational cost. HCF calculations on additional uncertainties or tolerances will be carried out.. Additionally, studies will be performed to understand the differences between the 7-pin and 91-pin models and whether a 7-pin model can accurately compute the HCF for the AFR-100.

6.2.2 Nek5000 Plan for SHARP Zoom

The SHARP zoom thermal hydraulic calculations will be carried out in FY 18. Mature Nek5000 models built for HCF calculations will enable the SHARP zoom calculations to commence quickly once the power distributions are available from PROTEUS. The detailed temperature distribution in the focal assembly of the core will be calculated and assessments will be made about the accuracy for different numbers of heterogeneous assemblies.

7. Conclusions

The Simulation-based High-efficiency Advanced Reactor Prototyping (SHARP) toolkit is under development by the Nuclear Energy Advanced Modeling and Simulation (NEAMS) Campaign of the U.S. Department of Energy, Office of Nuclear Energy. After releasing the SHARP toolkit in 2016, the main focus of the Reactor Product Line (RPL) of the NEAMS Campaign was shifted toward testing, validation and verification of SHARP component codes. To better understand and exploit the benefits of advanced modeling simulations, the NEAMS Campaign initiated the “Sodium-Cooled Fast Reactor (SFR) Challenge Problems” multi-year task.

The SFR challenge problems include the assessment of hot channel factors (HCFs) and the demonstration of a zooming capability on the 100 MWe Advanced Fast Reactor (AFR-100) using the SHARP toolkit. The primary objective of the first challenge problem is to reduce or/and eliminate HCFs using the high-fidelity SHARP toolkit and eventually improve the SFR economics. The HCF is a quantified uncertainty that is involved in nominal calculation of a design parameter. The second challenge problem is the demonstration of the SHARP zooming capability, which is a hybrid core modeling and simulation scheme enabled by combining coarse-and-homogeneous meshes and fine-and-heterogeneous meshes. If both challenge problems are resolved using this SHARP toolkit, the economic competitiveness of a SFR is significantly improved by saving computation costs and enhancement of safety margins.

The efforts in the first year have focused on the development of the computational models, mesh capabilities, and coupling procedures for multi-physics calculations using the neutronics (PROTEUS) and thermal-hydraulic (Nek5000) component codes of the SHARP toolkit, and demonstration of the HCF calculation capability. This report summarizes the progresses achieved in the first year, and further work is planned in FY 2018 to demonstrate the feasibility of the SHARP zooming capability.

Several hot channel factors for metal fueled SFRs were identified through literature review as potential candidates for reduction or elimination through high-fidelity simulations. In this study, a one-way offline coupling method was tentatively used to evaluate the HCFs where the neutronics solver PROTEUS computes the power profile, and the thermal hydraulics solver Nek5000 evaluates the peak temperature using the neutronics power profile. It is noted that the temperature feedback to neutronics code for updating the power profile was not considered in order to save computation time and resources. If the initial temperature profile used in the neutronics calculation is reasonably accurate, the one-way offline method used in this study is valid because the neutronics power profile has relatively weak dependence on small temperature variation. In order to get more precise results, the proper temperature profile for initial neutronics calculations was obtained from the STAR-CCM+ calculations in this study, although it can also be well obtained by some simple analytic calculation.

The HCFs of the peak temperatures at cladding outer surface, cladding inner wall surface, and fuel centerline induced by cladding manufacturing tolerance and uncertainties on the material thermo-physical properties were evaluated. The HCFs calculations in the bare rod bundle and wire wrap rod bundle indicate that the HCF is not sensitive to the rod number. The prediction from bare rod bundle is more conservative than that from wire wrap rod bundle. On the other hand, due to the complexity of the wire wrap configuration, it is extremely computationally expensive to perform explicit wire-wrap modeling in Nek5000. In addition, with the wire wrap configuration, the conjugate heat transfer in the fuel pin has to be neglected due to the difficulty of meshing. Thus, some extra error will be introduced owing to neglecting the circumferential heat conduction. Another profit from the model with bare rod bundle configuration is that we can afford the computational cost by using random sampling techniques with some simplification. Based on the assessment mentioned above, this study demonstrated the capability to calculate the HCFs using bare bundle configurations. As expected, the resulting HCFs obtained from the high-fidelity SHARP calculations are generally smaller than those developed for the earlier SFRs because the most uncertainties involved in the modeling and simulations were disappeared. In FY18, additional investigations are planned to calculate HCFs with random sampling techniques and for other sub factors.

Finally, full core AFR-100 simulations to test the feasibility of SHARP zooming capability is planned in FY 2018. Several bounding design parameters (i.e., peak temperatures at cladding inner wall surface and fuel centerline) and integral and average parameters (i.e., core multiplication factor, and assembly-average power distribution, etc.) will be evaluated and compared with the results obtained from calculations using legacy codes.

In summary, the PROTEUS and Nek5000 high fidelity tools developed under NEAMS can deliver more precise power distribution and thermal hydraulic results than previous tools. Not only can the HCFs can be obtained but also the information around hot spot regions can be explicitly analyzed. The results obtained this year with the SHARP toolkit has already demonstrated the potential reduction in calculated HCFs compared to legacy techniques.

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APPENDIX A. AFR-100

The AFR-100 was developed to target emerging markets where a clean, secured and stable electricity resource is required but a large-scale plant is not accommodated. The AFR is aimed to be sized for local small grids, transportable from pre-licensed factories to the remote plant site for affordable supply, and able to operate for a long period without frequent refueling. To achieve these strategic goals, several design requirements have been proposed for the AFR core development; a power rating of 100 MWe which is equivalent to 250 MWth with the target thermal efficiency of 40%, a long refueling interval with small burnup reactivity swing, a core barrel diameter of less than 3.0 m, and an active core height of less than 1.5 m.

The ANL suite of fast reactor analysis code system was used for the neutronics design. Fuel cycle analysis was performed with the DIF3D/REBUS-3 code system [Palmiotti 1995, Toppel 1983]. Region-dependent 21-group neutron cross section sets generated for a typical metallic fueled sodium-cooled fast reactor under the USDOE Integral Fast Reactor (IFR) program were utilized in this study. Using three-dimensional hexagonal-z geometry model, fuel cycle analyses were performed. Material thermal expansion at operating condition is modeled by adjusting the hexagonal pitch, axial meshes, and the fuel and structure volume fractions appropriately. The radial and axial thermal expansions were assumed to be the same as SS-316 (0.615%) and HT-9 (0.731%).

The U-10Zr binary metallic fuel was used as the primary fuel form of the AFR-100 because of its potential inherent safety features, favorable behavior for a long refueling interval, and because it is rapidly deployable. For accommodating the irradiation induced swelling, the binary metallic fuel has smeared density fuel of 75%, and the swelling was modeled by a uniform axial growth of 8% in the core design.

Reactivity feedback coefficients and reactor kinetics parameters are calculated by positioning the primary control assemblies at the critical location. The coolant, fuel, and structural material density coefficients and the sodium void worth are determined using the VARI3D perturbation code [Adams 1975]. The first-order perturbation theory option is used for density coefficients, while the exact perturbation theory option is employed for the coolant void worth. The effective delayed neutron fraction and prompt neutron lifetime are also calculated using the VARI3D code. The radial and axial expansion coefficients and the control assembly worth are determined by the direct differences in the eigenvalues for the base and perturbed conditions using the DIF3D code.

Reactor orifice zoning and flow allocation were determined through steady-state thermal-hydraulic analyses. Heating rates for thermal-hydraulic calculations were determined by coupled neutron and gamma heating calculations. Region-dependent 9-group neutron cross section set and 21-group gamma cross section set were used along with a gamma production matrix generated with NJOY and SDX codes in 9 neutron groups and 21 gamma groups. Neutron and gamma flux calculations were performed using the triangular-z finite difference option of the DIF3D code. Following the neutron flux calculation, the gamma source distribution was determined with the

GAMSOR [Adams 1987] code. Using this gamma source distribution, the gamma flux calculation was performed as a fixed source problem. The neutron heating distribution was determined by multiplying the neutron flux by the neutron KERMA factors, and the gamma heating distribution is determined by multiplying the gamma flux by the gamma KERMA factors. The total heating rate was appropriately normalized to the reactor power.

The sub-channel analysis code SE2-ANL was employed for whole core temperature calculations. SE2-ANL is a modified version of the SUPERENERGY-2 [Beitel 1984] thermal-hydraulic code interfaced with Argonne heating calculations. The SUPERENERGY-2 code is a multi-assembly, steady-state sub-channel analysis code designed specifically to perform efficient calculations of the detailed core-wide coolant temperature profiles in sodium cooled fast reactor core geometries. At Argonne, reactor hot spot analysis methods as well as fuel and cladding temperature calculation models have been added to the original version of SUPERENERGY-2. Both nominal and 2σ temperatures are calculated for the fuel and cladding. The nominal fuel and cladding temperatures are obtained by solving a steady-state one-dimensional conduction equation. The 2σ temperatures are calculated using the semi-statistical method.

Figures A.1 and A.2 show the radial and axial core layouts of the AFR-100 core, respectively, and detailed design parameters are provided in Ref. [Grandy 2013].

Figure A.1 Core radial layout of AFR-100

Figure A.2 Core axial layout and uranium enrichment distribution

The AFR-100 core adopted an onion-type enrichment zoning concept that was developed for a long refueling scheme and flat radial power distribution. The active core is divided into three different enrichment zones radially, and each zone has multiple zones axially. The average uranium enrichment is 11.97% for the inner core, 13.12% for the middle core, and 14.97% for the outer core.

Table A.1 provides the major core performance parameters of the AFR-100. The core can maintain criticality for 30 years by employing the unique enrichment zoning strategy of the AFR-100 with low reactivity swing during the reactor life time. The average discharge burnup is 101 MWd/kg and the peak discharge burnup is 172 MWd/kg.

Table A.1 Core performance parameters.

Parameters	AFR-100
Thermal power, MWt	250
Refueling interval, year	30
Number of batches	1
Fuel form	U-Zr
Active core height, cm	110

Average power density, kW/l	64.3
Fuel pin overall length, cm	222
Initial heavy metal loading, t	23.9
Specific power density, MW/t	10.5
Average enrichment, %	13.7
Burnup reactivity swing, % Δk	1.1
Overall fissile breeding Ratio	0.80
Average discharge burnup, MWd/kg	101
Peak discharge burnup, MWd/kg	172
Peak fast fluence, 10^{23}n/cm^2	5.97
Linear heat rate (average/peak), kW/,	15.2 / 28.2

Figure A.3 shows the power distribution in MW per each assembly at BOC and EOC. The peak radial power at BOC occurs in the sixth row, which is in the outer core zone, but the location moves to the second row, which is in the inner core. Figures A.4 and A.5 show the peak cladding inner wall temperatures and the minimum margins to fuel melt, respectively, with 2σ hot channel factors that were employed in the CRBR core design. In the AFR-100, the flow rate of each assembly was determined to have flat coolant exit temperatures, and the calculated cladding and fuel temperatures were affected by the flow rates. The overall peak 2σ cladding inner wall temperature is 693°C. The overall minimum margin to fuel melt is higher than 420 °C.

It is noted that all design parameters were calculated using the ANL legacy tools, and significant reductions of the peak cladding and fuel temperatures are expected when the parameters are re-evaluated using the SHARP toolkits and newly developed HCFs in this study.

Figure A.3 Radial power distribution (MW per assembly in 1/3 Core).

Figure A.4 Peak 2σ cladding inner wall temperatures ($^{\circ}\text{C}$).

Figure A.5 Minimum 2σ margins to fuel melt ($^{\circ}\text{C}$)

APPENDIX B. PROTEUS SENSITIVITY STUDIES

Before performing multi-physics calculations with the Nek5000 code, a series of neutronics sensitivity studies were performed to identify optimal discretization parameters to ensure accuracy and efficiency. The PROTEUS neutronics approach, models, and results are discussed in this section.

Unlike computational fluid dynamics simulations, heterogeneous neutronics simulations require a comprehensive description of material compositions, densities, and interaction cross sections in addition to the detailed geometry input. Significant time was spent developing the detailed material densities for the hot configuration (assuming 0.615% SS316 and 0.731% HT9 thermal expansion factors, 8% fuel axial swelling, fuel radial swelling contacts hot inner cladding radius, displaced sodium bond to 27 cm above active core, B₄C swelling ignored in lower shield). Specific neutronics approximations include replacement of fission gas in plenum with helium, geometrical homogenization of helium into cladding, and smearing the wire wrap into the cladding. The hot radial and axial dimensions are summarized in Table B.1 and Table B.2.

Table B.1 Hot radial dimensions for AFR-100 fuel assembly

Assembly Parameter	Value at Hot Condition
Assembly Pitch	16.6176 cm
Duct Flat-Flat	16.2996 cm (outer) 15.6959 cm (inner)
Pin Pitch	1.6121 cm
Clad Radii	0.7516 cm (outer w/ smeared WW) 0.7496 cm (outer bare bundle) 0.6993 cm (inner)
Elevation	292.9491 cm (total) 96.6198 to 216.1504 cm (active core)
Pin Power	18.315 kW/pin

Table B.2 Hot axial dimensions for AFR-100 fuel assembly

Axial Zone	Lower Z (cm)
Lower Structure	0.0
Lower Shield	30.2139
Lower Reflector	63.4169
Inner Bottom Core	96.6198
Inner Middle Core	120.4933
Inner Top Core	196.2649

Vented Gas Plenum with Displaced Sodium Bond	216.1504
Vented Gas Plenum with Fission Gas	243.3153
Upper Structure	262.7352

B.1 Multigroup Cross Section Generation

Multigroup cross section generation is the first step in performing any deterministic neutronics simulation. This step involves condensing the material interaction cross section data (a highly complex function of energy for each isotope and reaction type) into constants associated with broad energy group ranges that can be input to the deterministic transport solver. This is done by weighting the continuous energy data with the expected neutron flux in the energy group to preserving the total reaction rate in the energy group. The presence of heterogeneous geometry features (pin-by-pin representation, assembly duct, etc) increases the difficulty of generating accurate multigroup cross sections because the local neutron flux in each spatial region is difficult to accurately determine without advanced tools.

In this work, the MC²-3 advanced cross section generation code [Lee 2012] in conjunction with TWODANT [Alcouffe 1984] was used to generate multigroup constants due to its ability to account for heterogeneity effects. Prior to running these codes, the material compositions were determined for hot conditions by taking the manufactured compositions, converting natural elements into isotopics (needed by MC²-3), and smearing the composition over the expanded hot volumes. Then, homogenized compositions for each axial segment (needed only for cross section generation procedures) were calculated based on the hot volume fractions.

The workflow used for MC²-3/TWODANT is shown in Figure B.1.1 and is based on previous experience generating multigroup cross sections for highly heterogeneous geometries [Hader 2014], [Jarrett 2016]. An infinite medium homogeneous mixture for each axial composition was simulated in MC²-3 to yield 1041-group cross sections. These compositions were then used in a TWODANT R-Z radially-homogenized model (either 7-pin or 91-pin) to capture the axial leakage effect in 3D. The resulting 1041-group region dependent fluxes were used to collapse the 1041-group cross sections for the non-fuel axial zones to obtain heterogeneous cross sections. For axial zones containing active fuel, new 1041-group cross sections including pin radial heterogeneity effects were generated by converting the 7-pin or 91-pin geometry into 1-D cylindrical geometry in MC²-3 while preserving volume fractions of each material to model the explicit fuel, cladding and sodium materials. Such a conversion is depicted in Figure B.1.2 (rings are not to scale or correct in number). The resulting fuel zone 1041-group cross sections were then collapsed with the TWODANT 1041-group fluxes.

Figure B.1.1 Cross section generation procedure for heterogeneous 3D pin configurations

Figure B.1.2 General depiction of assembly into 1-D cylinder geometry (not to scale)

Broad group (4-group, 9-group, 33-group, 70-group) cross sections configurations were generated including assembly duct, inter-assembly sodium gap, and 6 rings of pins for the 91-pin assembly calculations at two temperatures (300K and 1000K) with specific naming conventions according to the PROTEUS temperature interpolation requirements.

B.2 Mesh Preparation

When preparing meshes for coupled calculations using the SHARP toolkit, the H5M (MOAB) mesh format is required for all physics modules. The offline coupling method used in this work removes this restriction, so each physics module can use its own mesh generator and mesh format. The UFMesh format from the PROTEUS MeshTools suite 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 for both the 7-pin and 91-pin configurations 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-SN, a 3D finite element mesh is required. For PROTEUS-MOCEX, a 2D finite element mesh is required, along with the axial plane discretization provided separately.

Figure B.2.1 Visualization of various neutronics meshes for the 7-pin configuration

B.3 Transport Solvers: PROTEUS-SN vs. PROTEUS-MOCEX

The original intention of this analysis was to use the PROTEUS-SN solver so that the offline coupling method could be compared to online coupling method using the SHARP toolkit. However, the 7-pin configuration studied in this work presented serious challenges for the PROTEUS-SN solver. Slow performance with reflective boundary conditions is a known problem with PROTEUS-SN because the preconditioner used in PETSc cannot properly precondition the reflective boundary condition part of the matrix. For larger domains such as the 91-pin configuration, the relative burden of the reflected boundary conditions becomes smaller, but the 7-pin case is quite small and thus, ironically, the effect is more severe. To understand this from a physics perspective, numerous angles are coupled together on the reflected boundary surface which require the definition of a preconditioner that handles the full angular connections (this was attempted in the past, but failed to scale in parallel). Without a proper preconditioner (acceleration), the time required to converge the angular boundary conditions is prohibitive. DIF3D-VARIANT, for example, also shows poor convergence behavior for optically thin, infinite Cartesian problems. Most first order discrete ordinates (SN) codes have serious problems with this issue and some actually forbid it by only allowing 3 reflected boundary conditions. It should be noted that while thermal hydraulics codes like Nek5000 can compute the result to this infinite problem by ignoring the connection to all other assemblies, PROTEUS-SN cannot ignore these connections and was not built to run efficiently on infinitely large problems.

Therefore, the PROTEUS-MOCEX neutronics solver was chosen to solve both the 7-pin and 91-pin configurations because it does not suffer from convergence issues due to reflective boundary conditions. Additionally, for highly heterogeneous geometry, the PROTEUS-MOCEX solver is expected to yield a more accurate solution than PROTEUS-SN due to its different methodology (discontinuous Galerkin/MOC vs. continuous FEM). A limited number of PROTEUS-SN calculations are performed for the 91-pin configuration in order to draw comparisons to the PROTEUS-MOCEX solver. The two solvers are briefly summarized in Table B.3.1.

Table B.3.1 Comparison of PROTEUS-SN and PROTEUS-MOCEX neutronics solvers

Features	PROTEUS-SN	PROTEUS-MOCEX
Formulation	2 nd order even parity formulation with continuous finite elements	2D method of characteristics + discontinuous Galerkin finite elements in Z dimension
Multiphysics	SHARP coupling, deformation, temperature and density feedback	T/H module in progress, temperature interpolation possible with input file manipulation
Mesh Discretization	3D unstructured finite element	2D unstructured finite element extruded in the 3 rd dimension
Angle Discretization	Discrete ordinates	Discrete ordinates
Energy Discretization	Multigroup	Multigroup
Performance on Heterogeneous Problems	Better for homogeneous and partially heterogeneous systems (explicit duct wall, but not explicit pins)	Ideal for fully heterogeneous systems
Performance with Reflected Boundary Conditions	Severe convergence issues for optically thin domains	No convergence issues

B.4 Mesh, Angle and Energy Convergence Studies

A series of mesh, angular, and energy convergence studies was performed in the following section. This step is always necessary in deterministic neutronics simulations, and especially worthwhile to guarantee the accuracy of the 7-pin bare bundle and 91-pin bare bundle nominal condition simulations for hot channel factor, which will be re-used to provide power profiles to Nek5000. A uniform 300 K temperature distribution was used for the convergence studies.

B.4.1 Axial Mesh Refinement

The 7-pin and 91-pin configurations have identical fuel pin axial geometry as listed in Table B.2. The only difference between the two configurations, axially, is the extra duct and inter-assembly sodium gap present in the 91-pin configuration which extend the entire axial length.

Axial refinement studies were performed for the 7-pin geometry. The axial active fuel zones (inner bottom, inner middle, and inner top core) were subdivided into <5 cm axial intervals already in order to apply different temperatures in future calculations. Several calculations with MOCEX were performed with different axial subdivisions among non-fuel zones as well as further refinement of the fuel zone (156 plane case) as specified in axial division as specified in Table B.4.1.1. The group structure, temperature, cubature, and 2D mesh were held constant to isolate the axial discretization effects. It was determined at 78 axial subdivisions were optimal based on eigenvalue convergence. The same axial refinement can be assumed to apply for the 91-pin configuration.

Table B.4.1.1 MOCEX eigenvalues with varying degrees of axial refinement (7-pin)

Energy Group	Eigenvalue	Temperature	Angular Cubature	Mesh Elements (2D)	Mesh Refinement	Number of Planes
4	1.13044	300K	L3T5	3061	A1R1	36
4	1.12976	300K	L3T5	3061	A1R1	54
4	1.12980	300K	L3T5	3061	A1R1	78
4	1.12980	300K	L3T5	3061	A1R1	156

B.4.2 Energy Group Refinement

Energy group refinement studies were performed using 4-, 9-, 33-, and 70-group cross section data sets generated with the MC²-3/TWODANT procedure defined in Section B.1. The temperature, cubature, 2D mesh, and axial discretizations were held constant to isolate the energy group discretization effects.

Table B.4.2.1 presents the 7-pin eigenvalues as a function of energy groups. A minimum of 33 energy groups is necessary. The 70-group cross section set changes the eigenvalue by -59 pcm, but, as shown in Figure 4.3.4.2.1 the normalized axial power does not significantly differ between the 33-group and 70-group calculations. This is reflected in the similar peak/average axial power reported in the table for the 2 calculations (differ by less than 1%). Heterogeneous fast reactor problems typically do require the use of 33 or more energy groups.

Table B.4.2.1 MOCEX eigenvalues with varying group structures (7-pin)

Energy Group	Eigenvalue	Peak/ Average Axial Power	Temperature	Angular Cubature	Mesh Elements (2D)	Mesh Refinement	Planes
4	1.12976	1.7982	300K	L3T5	3061	A1R1	78
9	1.12902	1.9410	300K	L3T5	3061	A1R1	78
33	1.12708	1.9364	300K	L3T5	3061	A1R1	78
70	1.12649	1.9298	300K	L3T5	3061	A1R1	78

Since the 70-group calculation significantly increases the computational requirements and has nearly the same peak/average power axially, the 33-group cross section set is satisfactory for future calculations. Note, only the power from the first ring was plotted in Figure B.4.2.1 because the power in both rings are nearly identical.

Figure B.4.2.1 MOCEX axial power profile with varying group structure (7-pin)

The axial power profile in Figure B.4.2.1 is unusual due to the onion-type enrichment pattern of the inner fuel (18.0% enriched at the top and bottom zones and 8.8% in the middle zone) also described in Figure 3.1.2. A quick test was performed to give confidence in the model by assigning to the entire active fuel region a uniform 18.0% enrichment. The expected cosine shape for the uniform enrichment case is clearly seen in Figure B.4.3.2 using a 4-group model and confirms the material and geometry mapping. The power peaking seen in the upper core region (close to 216 cm axial height) is discussed in the main body of this report in Section 4.3.1. For now, we note that that the peak axial power is in the axial center of the core in the uniform enrichment case (roughly

125% of average axial power), whereas it is located at the top of the core in the actual AFR-100 design (193% of average axial power). This has significant impact on the outlet temperature distribution as will be seen in the Nek5000 calculation section.

Figure B.4.2.2 MOCEX axial power profile for uniform enrichment problem (7-pin)

Energy group convergence studies were similarly performed for the 91-pin configuration. In this case, the difference in eigenvalue between 33-group and 70-group simulations is only 7 pcm. Inspection of Figure B.4.2.3 indicates the 33-group and 70-group power profiles (for the center pin) are almost identical. Thus, 33-group cross sections are sufficient for the 91-pin configuration. The difference in ring-wise power profiles is negligible as shown in Figure B.4.2.4. Therefore, the center-pin (Ring 1) profile is representative of all pins in the 91-pin geometry.

Table B.4.2.2 MOCEX eigenvalue results with varying group structures (91-pin)

Energy Group	Eigenvalue	Temperature	Angular Cubature	Mesh elements (2D)	Mesh Refinement	Planes
4	1.09641	300K	L3T5	3061	A1R1	78
33	1.10327	300K	L3T5	3061	A1R1	78
70	1.10320	300K	L3T5	3061	A1R1	78

Figure B.4.2.3 MOCEX axial power profile with varying group structure (91-pin)

Figure B.4.2.4 MOCEX ring-wise axial power profiles with 33-groups (91-pin)

B.4.3 Radial Mesh Refinement

Radial mesh refinements studies were performed for the 7-pin configuration. The starting 2D mesh (denoted A1R1, indicating azimuthal order 1 and radial order 1) was refined by first increasing the azimuthal order while maintaining a constant value for the radial division of the fuel sections. The calculation was extremely insensitive to varying either the azimuthal order or increasing the number of radial subdivisions. We note that the results in the following tables used

the coarse 4-group cross section set for quick throughput of calculations; however, the same trends typically apply for finer cross section sets so do not need to be repeated for the 33-group set. The converged radial mesh is depicted in Figure B.4.3.1.

Table B.4.3.1 MOCEX eigenvalue results with varying azimuthal subdivisions (7-pin)

Energy Group	Eigenvalue	Temperature	Angular Cubature	Mesh Elements (2D)	Mesh Refinement	Planes
4	1.12980	300K	L3T5	265	A1R1	78
4	1.12977	300K	L3T5	529	A2R1	78
4	1.12977	300K	L3T5	1057	A4R1	78
4	1.12977	300K	L3T5	1585	A6R1	78

Table B.4.3.2 MOCEX eigenvalue results with varying radial subdivisions (7-pin)

Energy Group	Eigenvalue	Temperature	Angular Cubature	Mesh Elements (2D)	Mesh Refinement	Planes
4	1.12980	300K	L3T5	265	A1R1	78
4	1.12980	300K	L3T5	529	A1R2	78
4	1.12978	300K	L3T5	1057	A1R4	78

The 91-pin configuration displayed similar insensitivity to the radial mesh, as shown in Table B.4.3.3, despite the addition of the duct and inter-assembly sodium gap. The A1R1 mesh, depicted in Figure B.2.1, produces sufficiently converged results.

Table B.4.3.3 MOCEX results with varying radial and azimuthal subdivisions (91-pin)

Energy Group	Eigenvalue	Temperature	Angular Cubature	Mesh Elements (2D)	Mesh Refinement	Planes
33	1.10327	300K	L3T5	3061	A1R1	78
33	1.10323	300K	L3T5	6121	A2R1	78
33	1.10324	300K	L3T5	16609	A4R2	78

Figure B.4.3.1 Converged 2D neutronics mesh (265 elements) for the 7-pin configuration

Figure B.4.3.2 Converged 2D neutronics mesh (3061 elements) for the 91-pin configuration

B.4.4 Angular Cubature Refinement

Angular cubature refinement studies are necessary for all deterministic codes using the discrete ordinate approximation. For this (and most) analysis the Legendre-Tchebychev product cubature is preferred because it allows the number of axial angular directions to be varied independently of the radial angular directions. The Legendre (L) order dictates the number of axial planes at which collections of Tchebychev angles are placed on the sphere. When reflected boundary conditions are applied, only certain sets of angular cubature are permitted which preserve the angular reflection off the planes present in the geometry. The L3T5, L7T11, and L7T17 cubatures meet these requirements (among others).

The MOCEX eigenvalue was not dependent on the cubature for the 7-pin case at all and therefore cubature order L3T5 is sufficient for this problem.

Table B.4.4.1 MOCEX eigenvalue results with varying angular cubature (7-pin)

Energy Group	Eigenvalue	Temperature	Angular Cubature	Mesh Elements (2D)	Mesh Refinement	Planes
4	1.12980	300K	L3T5	265	A1R1	78
4	1.12980	300K	L7T11	265	A1R1	78
4	1.12980	300K	L7T17	265	A1R1	78

The 91-pin configuration was slightly more sensitive to cubature than the 7-pin configuration. Increasing the cubature from L3T5 to L7T11 yielded +17 pcm, and another +4 pcm when increasing to L7T17. However, since the axial profile was nearly identical in all three cases, the dramatic increase in computational resources (61 core-hours for L3T5 vs. 252 core-hours for L7T17) was not justified, and L3T5 is recommended.

Table B.4.4.2 MOCEX eigenvalue results with varying angular cubature (91-pin)

Energy Group	Eigenvalue	Temperature	Angular Cubature	Mesh Elements (2D)	Mesh Refinement	Planes
33	1.10327	300K	L3T5	3061	A1R1	78
33	1.10344	300K	L7T11	3061	A1R1	78
33	1.10348	300K	L7T17	3061	A1R1	78

B.4.5 Convergence Study Conclusions

In summary, the PROTEUS-MOCEX calculation for both 7-pin and 91-pin configurations was insensitive to spatial resolution and angular cubature. A minimum of 33 energy groups should be used along with axial mesh subdivisions less than or equal to 5 cm. Based on these observations, the energy, angle, and mesh discretization parameters listed in Table B.4.5.1 are recommended to obtain converged axial power profiles in subsequent hot channel factor calculations.

Table B.4.5.1 Recommended MOCEX discretization parameters

Configuration	Energy Group	Angular Cubature	Mesh Elements (2D)	Mesh Refinement	Axial Planes
7-Pin	33	L3T5	265	A1R1	78
91-Pin	33	L3T5	3061	A1R1	78

For a uniform 300 K temperature distribution, the axial power distribution and relative power magnitude across pins is nearly identical in the 7-pin configuration and also in the 91-pin configuration, meaning the center pin power axial distribution is representative of all pins in each configuration. This simplifies the amount of data required to be transferred to Nek5000 as the same power profile can be applied to all pins.

B.5 Discussion of PROTEUS-SN vs. PROTEUS-MOCEX Results

The PROTEUS-SN code was not used for the 7-pin configuration due to convergence issues related to the boundary conditions. However, it was used to solve a limited number of test cases for the 91-pin configuration. The code performance was much slower than PROTEUS-MOCEX, by a

factor of 100-1000x the computational cost, most likely due to the reflective boundary conditions. While we assess is not practical to use the PROTEUS-SN code for this geometry, we present some results for comparison, since this is the solver within SHARP.

Table B.5.1 displays several eigenvalue results using both codes with varying levels of mesh and angular refinement. It is well known that the SN code (based on the continuous finite element method) requires many more finite elements than the MOCEX code for similar accuracy due to the inability to capture steep spatial gradients with a coarse mesh. The results show a discrepancy of about 210 pcm between the most refined SN and MOCEX calculations which we have not been able to resolve. It may be an inherent issue with one of the methodologies for reflected boundary conditions. Regardless, the MOCEX result is more trustworthy for this calculation due to its underlying methodology being accurate for heterogeneous calculations.

Table B.5.1 MOCEX vs. SN eigenvalue results for uniform 300 K temperature (91-pin)

Code	Options A=Azimuthal mesh fidelity R=Radial mesh fidelity Z=Axial mesh fidelity	Eigenvalue	Computational Cost
MOCEX	33g L3T5 A1R1Z2 (3540 ele/plane, 78 planes)	1.10327	62 core-hours (1.3 hr on 48 Blues cores)
MOCEX	33g L3T5 A2R1Z2 (7080 ele/plane, 78 planes)	1.10323	139 core-hours (2.9 hr on 48 Blues cores)
MOCEX	33g L3T5 A4R2Z2 (18528 vert/plane, 78 planes)	1.10324	298 core-hours (3.1 hr on 96 Blues cores)
MOCEX	33g L7T11 A1R1Z3 (3540 ele/plane, 90 planes)	1.10340	206 core-hours (4.3 hr on 48 Blues cores)
SN	33g L3T5 A2R1Z1 (7080 ele/plane, 55 planes)	1.09995	1536 core-hours (1.5 hr on 1024 Blues cores)
SN	33g L3T5 A4R2Z1 (18528 ele/plane, 55 planes)	1.10090	7782 core-hours (3.8 hr on 2048 Blues cores)
SN	33g L7T11 A2R1Z1 (7080 ele/plane, 55 planes)	1.10042	8806 core-hours (4.3 hr on 2048 Blues cores)
SN	33g L7T11 A2R2Z3 (9264 ele/plane, 90 planes)	1.10119	109773 core-hours 6.7 hr on 16384 BGQ cores

Figure B.5.1 MOCEX vs. SN axial power profile comparison for uniform 300 K (91-pin)

Figure B.5.1 shows the normalized axial power profiles between the most converged MOCEX and SN solutions available. There are inherent differences: the power appears to be shifted towards the top of the core in the SN solution, yielding a higher peak/average axial value (1.8256) vs the MOCEX value (1.7654). This is a difference of +3.4%. The SN solution should be simulated in Nek5000 to determine the sensitivity of Nek5000 on this difference.

In summary, while the PROTEUS-SN code can be used to solve the 91-pin configuration, it is not recommended at this point due to unexplained differences from the PROTEUS-MOCEX simulation which we believe to be more accurate for this geometry. It is also much more computationally expensive for this problem. Nonetheless, if the discrepancy cannot be resolved, the SN power profile should be simulated in Nek5000 to determine the effect on the hot channel factor, if any.

B.6 Discussion of Initial Temperature Condition

The previous neutronics calculations assumed a uniform 300 K temperature (room temperature), since there is no temperature interpolation capability in PROTEUS-MOCEX, and the PROTEUS-SN temperature interpolation capability was limited to SHARP coupled problems (called from SHARP driver). This is valid because the power shape does not usually have a strong dependence

on temperature. Since the average core temperature is actually closer to 800K, a uniform 800K simulation was tested to assess any differences in the axial power profile.

Between the uniform 300 K and 800 K temperature simulations, the 7-pin 800 K simulation eigenvalue was lower by 653 pcm as shown in Table B.6.1. However, the normalized power profiles for 300 K and 800 K, shown in Figure B.6.1, did not exhibit significant difference in terms of shape or magnitude. The peak axial power differed by only 0.6% in the two cases. Additionally, the fuel pins in each ring did not show significant differences in their reported power.

Table B.6.1 MOCEX eigenvalue results at two uniform temperatures (7-pin)

Energy Group	Eigenvalue	Peak / Average Power	Temperature	Angular Cubature	Mesh Elements (2D)	Mesh Refinement	Planes
70	1.12649	1.9364	300K	L3T5	265	A1R1	78
70	1.11996	1.9250	800K	L3T5	265	A1R1	78

Figure B.6.1 MOCEX comparison of power profile at 300K and 800 K (7-pin).

The 91-pin 800 K simulation eigenvalue was 874 pcm lower than the 300 K value, shown in Table B.6.2. The peak/average axial pin powers are listed in Table B.6.3 by ring number. One can see that the higher 800 K uniform temperature elevates the peak/average power at the top of the active core by

Table B.6.2 MOCEX eigenvalue results at two uniform temperatures (91-pin)

Energy Group	Eigenvalue	Temperature	Angular Cubature	Mesh Elements (2D)	Mesh Refinement	Planes
33	1.10327	300K	L3T5	3061	A1R1	78
33	1.09453	800K	L3T5	3061	A1R1	78

Table B.6.3 MOCEX peak/average pin power in each ring at two uniform temperatures (91-pin)

Ring	Peak/Average Axial Power per Pin (300 K)	Peak/Average Axial Power per Pin (800 K)	% Increase in peak/average pin power at 800 K
1 (center)	1.7654	1.7972	+1.8%
2	1.7651	1.7962	+1.8%
3	1.7649	1.8009	+2.0%
4	1.7652	1.8077	+2.4%
5	1.7673	1.8225	+3.1%
6 (next to duct)	1.7810	1.8726	+5.1%

Figure B.6.2 MOCEX comparison of power profile at 300K and 800 K (91-pin).

However, uniform temperature profiles are not representative of the true temperature condition in the reactor which varies along the axial dimension due to the power shape. The temperature

range in the fuel, cladding, and sodium coolant were estimated by quick STAR-CCM+ calculations and shown in Table B.6.3.

Table B.6.3 Estimated temperature ranges for 7-pin and 91-pin configurations

Zone	7-Pin Temperature Range	91-Pin Temperature Range
Fuel	718 – 854 K	668 – 948 K
Cladding	672 – 808 K	668 – 863 K
Sodium Coolant	668 – 784 K	668 – 873 K

In order to use a non-uniform temperature profile as the initial condition, code development was needed. First, automatic temperature interpolation was enabled in standalone PROTEUS-SN. This feature was previously enabled from the SHARP driver using Nek5000 temperature feedback to drive the cross section interpolation, so enabling temperature feedback in initial condition neutronics calculations required only modest code changes due to the existing infrastructure. For PROTEUS-MOCEX, a script was developed to define linear combinations of materials at different temperatures to simulate temperature interpolation via the input file.

The lower temperature bound in Table B.6.3 was assigned to the bottom of the active fuel zone, and the upper temperature bound was assigned to the top of the active fuel zone. The middle of the active fuel zone was assigned temperatures based on linear interpolation of the lower and upper bounds. Materials above and below the active core were assigned a constant value according to the lower or upper range. Using these temperatures for an initial condition in neutronics should yield a good estimate of the coupled SHARP result that iterates back and forth between neutronics and T/H.

The results of the temperature gradient study are shown in the following table and figures. Applying the temperature gradient impacted the axial power profile by suppressing the power in the upper-most zones of the active fuel, lowering the peak / average power of the axial power profile. This behavior was observed in both the MOCEX and SN, although the impact was greater in the MOCEX calculations. The difference between the SN and MOCEX results is relatively significant, as mentioned in the preceding section. For the temperature gradient calculations, the power peaking is 1.7045 in MOCEX vs 1.7926 in SN. This could cause a large effect on the thermal hydraulics calculation of temperature. This will be investigated in FY18.

Table B.6.4 MOCEX and SN peak / average axial power results for temperature profile initial condition (91 pin)

Code	Temperature	Discretization	Peak/Avg Axial Power
MOCEX	Uniform 300 K	33g L3T5 R1A1 78 planes	1.7654
MOCEX	Temp. Profile	33g L3T5 R1A1 78 planes	1.7045
SN	Uniform 300 K	33g L7T11 R2A2 90 planes	1.8256
SN	Temp. Profile	33g L7T11 R2A2 90 planes	1.7926

Figure B.6.3 MOCEX and SN axial power distributions for different temperature initial conditions (91-pin)

Figure B.6.4 MOCEX and SN axial power distributions for different temperature initial conditions, zoomed in at upper 18.0% enriched core region to show detail (91-pin)

APPENDIX C. NEK5000 SENSITIVITY STUDY

C.1. Primary STAR-CCM+ calculations

Nek5000 is generally computationally expensive due to its high fidelity features and requires more manpower resources than other commercial CFD tools. In the early stages of investigation, it is necessary to perform some preliminary calculations to obtain basic information on the problem such as the temperature range, the sensitivity to the mesh and the model. We use STAR-CCM+ for these preliminary calculation and sensitivity studies at the early stages due its relatively low computational requirements.

STAR-CCM+ is a commercial CFD code which is developed by CD-Adapco (Computational Dynamics-Analysis & Design Application Company Ltd), a multinational computer software company that authors and distributes applications used for computer-aided engineering. STAR-CCM+ included the world's first commercially available polyhedral meshing algorithm. The use of a polyhedral mesh has proven to be more accurate for fluid-flow problems than a hexahedral or tetrahedral mesh of a similar size (number of cells), but is considerably more difficult to create. Due to the complexity of the geometric feature of wire wrap rod bundle, meshing the model is very challenging. As so, the automatic polyhedral meshing technology built in STAR-CCM+ is very useful. The polyhedral mesh snapshot for wire wrap rod bundle is shown in Figure C.1.1. The prismatic cell layers generated can help capture the boundary layer, turbulence effects, and heat transfer near the wall boundaries.

Figure C.1.1 Snapshot of polyhedral mesh for wire wrap rod bundle

The objects of the primary calculation with the commercial CFD code STAR-CCM+ are as follow:

- Justify the simplification: The AFR drive assembly has 91 fuel rods. The height of the active core is about 5 wire wrap pitches. If we choose to perform the calculation for the wire wrap rod bundle of full length (5 wire wrap pitches), the cell number of the simulation could easily reach 1~2 billion. Those simulations become either too costly or unnecessary. Preliminary calculations can help us to find and justify reasonable simplifications which have a tradeoff between fidelity and computational cost.
- Provide references and initial conditions: Preliminary simulations can provide the basic information on velocity and temperature distribution within the assembly. The information can be applied to initial conditions preparation, mesh generation and code-to-code comparison for further Nek5000 calculation.

In order to achieve the goals mentioned above, several sensitivity studies and preliminary calculations with STAR-CCM+ are performed as listed:

- Full length vs 1 wire wrap pitch: The wire wrap rod bundle shows the periodic geometric feature. It is reasonable to assume that the flow behavior is periodic so that we can only model the domain of 1 wire wrap pitch to capture the flow behavior in the interested area.
- Power distribution of BOC vs uniform power distribution: The axial power distribution can bring in some error if we only use 1 wire wrap pitch domain. The calculation can help us to quantify the error.
- Bare rod bundle+ Momentum source term vs Wire wrap rod bundle: The wire wrap rod bundle has more complex geometry than bare rod bundle. We can introduce the wire effect in bare rod bundle geometry by implanting some momentum source term. The calculation can test the flexibility of this approach.
- Bare rod bundle vs Wire wrap rod bundle: The wire wrap rod bundle is usually simplified as bare rod bundle because that can reduce the difficulty of meshing and the computational cost by an order of magnitude. The calculation can estimate the effect of the wire.
- With Conjugate Heat Transfer vs Without Conjugate Heat Transfer: The effect of the heat transfer between the fluid domain and the solid domain are assessed through the calculation.
- Perturbed cladding thickness: The calculation can help us understand the effect of the cladding thickness on the Hot Channel Factor which will be further modeled in Nek5000.

Some verification studies on mesh and turbulence model are performed to make sure that the model can be properly used for the analysis. Based on the verification studies shown in Figure C.1.2, the mesh cell size of 1mm (corresponding to 2.5 million cell number since the cell number will be different for different domain size) with aspect ratio 1:4 and realizable k- ϵ turbulence model are chosen to be the practical combination.

Figure C.1.2 Verifications with STAR-CCM+

A full length wire wrap rod bundle with conjugate heat transfer is modeled for reference. The velocity inlet and pressure outlet are adopted as the boundary conditions for the full length domain (Figure C.1.3). The total cell number reaches 13,794,629. The mesh structure is shown in Figure C.1.4. The cell size in the solid domain is relatively larger than that in the fluid domain since only heat conduction is solved in the solid domain. The temperature distributions at outlet shown in Figure C.1.5 indicate that in the center region the fluid is always hotter which leads to hotter cladding and fuel temperature. Therefore, the hot spots always appear in the center region of last pitch where the blue frame is in Figure C.1.3. Since the area of interest is only within the last pitch of the domain, a domain of 1 wire wrap pitch (Figure C.1.3) with periodic boundary condition can be adopted for predicting the flow behavior within the interested area.

Figure C.1.3 Boundary conditions for full length domain and 1-wire wrap pitch domain

Figure C.1.4 Mesh structure for wire wrap rod bundle with cladding and fuel

a) ALL

b) Fluid

c) Cladding

d) Fuel

Figure C.1.5 Outlet temperature distributions of full length 91-pin wire wrap rod bundle with conjugate heat transfer

For convenience, in this report “*Full length*” represents the domain of 5 wire wrap pitch with velocity inlet and pressure outlet boundary condition and “*1 pitch*” represents the domain of 1 wire wrap pitch with periodic boundary condition in the stream-wise direction. Figure C.1.6 shows the comparison of outlet velocity distribution between Full length and 1 pitch. The contours look almost identical with only 8.9×10^{-3} m/s maximum velocity deviation. The qualitative comparison shows a global agreement of velocity distribution between Full length and 1pitch. The local velocity distribution comparison is also very necessary. Figure C.1.7 shows the detailed velocity distribution on the line between two rods for Full Length and 1 Pitch. The good agreements indicate that the domain of 1 wire wrap pitch with periodic boundary condition in the stream-wise direction can significantly simplify the model and give the same velocity prediction as the full length model can.

Figure C.1.6. Outlet velocity contour for full length and 1 pitch

Figure C.1.7 Detailed velocity distribution on the line between rods for full length and 1 pitch

Figure C.1.8 Minimum, average and maximum coolant temperature comparison on each elevation between full length and 1 pitch

Temperature prediction is very critical in HCF calculations. Figure C.1.8 compares the minimum, average and maximum coolant temperature on elevation 4P, 4.2P, 4.4P, 4.6P, 4.8P and 5P between Full length and 1 pitch. All the data are almost identical, further justifying the use of the 1 pitch model with periodic boundary conditions to save computational resources.

The axial power distribution in a nuclear reactor is not uniform. Figure C.1.9 shows the normalized axial power distributions in AFR-100 [Kim 2012]. The axial power distribution of the AFR-100 is different from a chopped cosine shape, which is typical power shape in a sodium cooled

fast reactor. The Begin of Cycle (BOC) power peaks at the core bottom because of the high uranium enrichment and lower reflector. However, the high neutron leakage through the upper structure decreases the power at the core top although the enrichment is the same as the core bottom. The power skews to the core central zone as the burnup increases because the burning zone moves into the core center. As a result, the axial power shape becomes a chopped cosine shape at End of Cycle (EOC). However, it could bring in some error if the power distribution is not uniform in CFD model. As shown in Figure C.1.10, no influence on maximum coolant temperature prediction is observed by applying BOC axial power distribution. The report will use BOC as the axial power distribution for the latter primary calculation.

Figure C.1.9 Normalized axial power distribution for BOC, MOC and EOC of AFR-100

The wire wrap can introduce strong lateral mixing between sub-channels, which cannot be captured if we simplify the model to bare rod bundle. Figure C.1.11 shows the lateral velocity distribution in both wire wrap and bare rod bundle. The maximum lateral velocity in wire wrap rod bundle can reach about 50% of the averaged stream wise velocity while that in bare rod bundle can only reach 2% in RANS simulation. In order to improve the hydraulic modeling of wire-wrap spacers in a rod bundle, Argonne developed a three-dimensional momentum source model (MSM) [Hu 2013] to model the anisotropic flow without the need to resolve the geometric details of the wire-wraps. Computing resources can be saved with the MSM since it can be used on a much coarser computational mesh. The lateral velocity distribution predicted by bare rod bundle with

momentum source is also shown in Figure C.1.11. As can be seen, the magnitude of the lateral velocity is improved by the MSM model although it still fails to capture some detailed velocity distribution to some extent. Figure C.1.12 shows the hotspots distribution on each elevation at last pitch of the assembly. The hot spots are defined as the locations where the temperature is within the range 99% ~100% of the maximum temperature. It reconfirms that the hottest area should appear in the center of the assembly. In addition, it is easy to see some asymmetric distribution feature of hot spots which is due to the wire wrap effect.

However, it is very significant to estimate how much effect the wire wrap can bring in on predicting the HCF, in other word, the maximum temperature. Although strong lateral mixing is introduced by the wire wrap, the temperature distribution does not necessarily respond to that effect intensively because the radial power distribution is identical which leads to similar average sub-channel temperature. Table C.1.1 lists the maximum coolant temperature with different model. The bare rod bundle model has about 7°C deviations of maximum coolant temperature prediction from wire wrap rod bundle model. It indicates the lateral velocity does enhance the mixing between the sub-channels which reduce the maximum coolant temperature. The MSM model only has 1.237°C deviations since it captures the lateral velocity better.

Figure C.1.10 Maximum coolant temperature comparison at different elevations for full length and 1 Pitch models with BOC axial power distribution

Figure C.1.11 Lateral velocity distribution

a) hot spots on each elevations

b) Overlap of the hot spots on each elevations from top view

Figure C.1.12 Asymmetric distribution feature of hot spots in wire wrap rod bundle

Table C.1.1 Maximum coolant temperature with difference models

Case	Maximum Coolant Temperature, °C	Deviation, °C
Wire wrap rod bundle	578.61	-
Bare rod bundle	585.56	6.95
Bare rod bundle + Momentum Source	579.84	-1.23

Figure C.1.13 shows the non-dimensional maximum coolant temperature in the sub-channel around the center pin. For bare rod bundle, the maximum coolant temperature in different sub-channel is quite uniform. As for wire wrap rod bundle, the deviation of the maximum temperature in different sub-channel is bigger. Although the MSM model capture the magnitude of the maximum temperature well, it fails to capture the wire effect on the local temperature distribution. For instance, the maximum temperature is higher than that in other sub-channel in MSM model while it is the total opposite in wire wrap model. From some mesh sensitivity test, the results from the MSM model become suspect when the mesh is coarser than some critical point. Since the MSM cannot save as much computational resource as we expect and it also required extra coding efforts to implant the model into Nek5000, we will not use the model for further Nek5000 simulation. However, the MSM model still has the potential use to model rod bundle with different wire wrap orientation in which case the direct meshing becomes impractical.

b) Sub-channel Maximum Coolant Temperature

Figure C.1.13 Maximum coolant temperature with difference models in different sub-channels

Figure C.1.14 Sketch of fuel and cladding

Conjugate Heat Transfer (CHT) is used for applications that involve simultaneous heat transfer in both solid and fluid domain. In our case, if the solid domains are not modeled simultaneously, we can get the analytic temperature solution within the solid domain through the law of heat conduction, also known as Fourier's law. According to Fourier's law, we can obtain the maximum cladding and fuel temperature derived from the following equations:

$$T_{cladding_max} = T_{cladding_max} + \frac{Q_s \times R_c \times \ln(R_c/R_f)}{k_{cladding}}$$

$$T_{fuel_max} = T_{cladding_max} + \frac{Q_v \times R_f^2}{4 \times k_{fuel}}$$

Where Q_s is surface heat flux, Q_v is volumetric heat flux, R_c is cladding outer radius and R_f is fuel radius (Figure C.1.14). Figure C.1.15 shows the temperature prediction with and without conjugate heat transfer. As shown, the maximum coolant temperature is insensitive to the conjugate heat transfer model. The model with and without conjugate heat transfer predict the same maximum temperature. Because the thermal conduction of sodium is about 100 times larger than water, the circumferential heat conduction in sodium is much stronger. It does not leave room for claddings to further homogenize the circumferential temperature since the circumferential heat transfer through sodium is already strong. Given that the thickness of the cladding is only 0.5mm, the maximum temperature in the cladding is also not obvious between the conjugate heat transfer calculation and the theoretical derivation based on Fourier's law. The maximum fuel temperature is over estimated by Fourier's law due to Fourier's law's one dimensional heat conduction assumption. No circumferential heat conduction is taken into account by the theoretical derivation. From the temperature contour of fuel and cladding shown in Figure C.1.16, the isolines in either cladding or fuel are not absolute concentric circles, which indicates the circumferential heat conduction. The CHT further homogenize the circumferential temperature distribution. That's why the maximum fuel temperature is 4.12°C lower.

a) Maximum Coolant Temperature

b) Maximum Cladding Temperature

c) Maximum Fuel Temperature

Figure C.1.15 Temperature prediction with and without conjugate heat transfer

Figure C.1.16 Circumferential conduction in cladding and fuel

It's worthwhile mentioning that the CHT modeling in the fuel is impractical for Nek5000 calculation due to the difficulty in meshing for the wire wrap rod bundle. According to the primary calculation with STAR-CCM+, the bare rod bundle model can overestimate the coolant temperature by 6.95°C while the wire wrap rod bundle model without CHT can overestimate the fuel temperature by 4.12 °C. Thus, the deviation of maximum fuel temperature prediction between the bare rod bundle with CHT model and the wire wrap rod bundle without CHT model can be only 2.83 °C.

Some primary simulations with different cladding thickness are performed to investigate the effect of the cladding thickness on HCF (Figure C.1.17). The thickness of the cladding does not influence the maximum cladding temperature but the deviation of the circumferential cladding

temperature. Smaller cladding thickness leads to larger circumferential cladding temperature deviation. These primary simulations may help us to understand the effect of the cladding thickness. The information is very useful for both meshing and calculation with Nek5000.

Figure C.1.17 Circumferential cladding temperature distribution of the center pin with different cladding thickness

Some conclusions can be drawn based on the STAR-CCM+ simulation introduced in this section.

- Full length domain can be simplified to 1 wire pitch domain with proper boundary conditions to reproduce the velocity and temperature distribution in the interested area.
- Conjugate Heat Transfer (CHT) does not have an obvious effect on coolant temperature prediction.
- Bare rod bundle model with CHT can be used to calculate the HCF with less than 3°C deviation of maximum fuel temperature prediction from that predicted by the wire wrap rod bundle model without CHT.

C.2 Meshing Capability

Advanced meshing capabilities are required for both bare rod bundle and wire wrap rod bundle with a variety of perturbations due to physical uncertainty, manufacturing tolerance, or modeling approximation. Nek5000 requires a hexahedral mesh, which needs to be taken into account before developing the meshing capability. In order to achieve that goal, two sets of meshing capabilities are developed for this purpose. The first one is a Matlab script for meshing wire wrap rod bundles. Another one is an ICEM script for meshing bare rod bundles.

For wire wrap rod bundles, the wires rotate circumferentially along the stream wise direction (Figure C.2.1). The basic meshing strategy is to generate surface mesh on each elevation and connect them. It has minimum layer requirements in stream wise to represent the wire wrap. Otherwise, the mesh quality can be too poor to use. Therefore, a minimum number of elements are typically required for wire wrap rod bundles. For instance, 91-pin wire wrap rod bundle of 1 pitch usually require at least 2 million elements. In general, the wire wrap rod bundle calculation is at least 10 times more computationally expensive than bare rod bundle calculation.

As for the bare rod bundle meshing capability, the following basic requirements on the script need to be satisfied for this project:

- The mesh should only consist of hexahedral quadratic elements which is adaptive to both PROTEUS and Nek5000.
- The scale of critical parameters such as rod diameter, cladding thickness and fuel diameter are adaptable
- The mesh density should be easy to control in different regions.
- The scripts should be able to provide the mesh with any naming scheme for PROTEUS.

Figure C.2.2 shows the meshes generated by ICEM script for the assemblies of different pin number. The script also provides the flexibility to adjust the mesh density locally, include the duct region and export the mesh with different format. As shown in Figure C.2.3, ICEM script can export hex27 for Nek5000 and hex20 for PROTEUS. In addition, it creates boundary layer for Nek5000 near the wall and adds more layers in the cladding for PROTEUS.

Figure C.2.1 Hexahedral mesh generation for wire wrap rod bundle

a) 7-pin

b) 19-pin

c) 91-pin

Figure C.2.2 Mesh Generation for bare rod bundle with ICEM script

a) Nek5000 (Hex27)

b) PROTEUS (Hex20)

Figure C.2.3 Mesh generation for different physics codes

Appendix D. Comparison of Hot Channel Factors

The hot channel factors (HCFs) developed for CRBR, FFTF, and EBR-II have been reviewed and the recommended sets of HCFs for metallic fuel SFRs are proposed in this study. Since the HCF naming is inconsistent between three sets of HCFs, all HCF sets were lined up based on the source of uncertainties and a representative name is proposed in the recommendation. In addition, several direct hot channel factors were reclassified into statistical hot channel factors because statistical uncertainties are involved in calculations.

CRBR	FFTF	EBR-II	Recommendation
Direct factor			
Power level measurement and control system dead band <ul style="list-style-type: none"> “Power level measurement” and “control rod dead band” are considered simultaneously as a direct factor. This HCF concept is equivalent to “Control rod dead band” of the FFTF HCF [Friedland 1980]. 	Control dead band <ul style="list-style-type: none"> “Control dead band” is dependent on the max. power allowance without control rod moving Control rod dead band is defined in “Operation Tech Spec.” 	Power level measurement <ul style="list-style-type: none"> Calibration error in power measurement based mainly on water flow rate and feed water temperature measurement uncertainties in the steam cycle. 	Control rod dead band. <ul style="list-style-type: none"> Power level measurement was reclassified into statistic factors because major uncertainties in measurements of flow rate, temperature, and control systems are statistical errors or manufacturing tolerance of instruments.
Inlet Flow Maldistribution <ul style="list-style-type: none"> Uncertainties in the assembly flow distribution due to flow maldistribution in the lower plenum, manufacturing tolerances in internal structures and orifice, etc. Direct factor of 1.02 was determined based on engineering judgment. 	(Equivalent HCF concept is Inlet Flow Maldistribution , but this uncertainty was treated as a statistical factor)	(Equivalent HCF concept is Precision in total coolant flow rate through an assembly , but this uncertainty was treated as a statistical factor)	<ul style="list-style-type: none"> Reclassify this hot channel factor into statistic factor as like FFTF and EBR-II.
Flow Distribution Uncertainty <ul style="list-style-type: none"> Uncertainties of flow distribution within assembly. Uncertainties are mainly due to the simplified model and applied empirical factors of sub-channel codes. 	(Equivalent HCF concept is Intra-subassembly flow distribution , but this uncertainty was treated as a statistical factor)	(Equivalent HCF concept is Precision in total coolant flow rate within an assembly , but this uncertainty was treated as a statistical factor)	Intra-subassembly flow maldistribution <ul style="list-style-type: none"> Reclassify this hot channel factor into statistic factor

Cladding Circumferential Temp. Variation <ul style="list-style-type: none"> Axial coolant velocity and cladding temperature around a fuel pin have strongly azimuthal dependence due to wire-wrap. This HCF was measured at ORNL 7 and -19 pins tests and firstly evaluated by FATHOM-360 code (NSE. 64, 1977). 	Wire-wrap Peak HCF name is different, but the concept is the same to the CRBR's Cladding Circumferential Temperature Variation.	(This uncertainty was not considered)	Cladding Circumferential Temp. Variation <ul style="list-style-type: none"> Called differently in CRBR and FFTF, but the concept is the same.
Pellet-Cladding Eccentricity <ul style="list-style-type: none"> In CRBR, it was conservatively calculated by assuming that the fresh fuel contact to cladding. This uncertainty impacts on cladding and film temperatures. 	(This uncertainty was not considered)	(This uncertainty was not considered)	<ul style="list-style-type: none"> This HCF is not applicable to metallic fuel For oxide fuel, eccentricity uncertainty is importance due to a poor thermal conductivity of gap.
Physics Modeling <ul style="list-style-type: none"> There are many sub-factors under this category such as flux solver approximation, 2D synthesis method), etc. In CRBR, the lumped uncertainty of the power distribution was estimated using the ZPPR mockup of CRBRP (the C/E error is about +-2% except for specific locations). 	Considered as statistic factor (see Nuclear Power Distribution).	(Equivalent HCF concept is Precision in neutron and gamma flux distribution)	<ul style="list-style-type: none"> Reclassify this hot channel factor into statistic factor For FFTF and EBR-II, this HCF was considered as statistic factor because the total power is normalized to 100% in calculation (so, not directly impact on the temperature) and uncertainties are mainly due to the experimental (statistical) errors.
Control Rod Banking <ul style="list-style-type: none"> Control rods are grouped and there is manufacturing tolerance (i.e., insertion depth is not identical), which introduces asymmetric power. 	(This uncertainty was not considered)	(This uncertainty was not considered)	Control Rod Banking <ul style="list-style-type: none"> This is a direct factor because peak temperature increases as much as bank asymmetric uncertainty. This is dependent on design requirement. For CRBR, tolerance is +- 1.5 inches,

			which affects about 2%.
Statistical factors			
Reactor delta-T and inlet temperature variation <ul style="list-style-type: none"> Uncertainties of reactor delta-T due to deterioration of primary components. This HCF was formulated in terms of inlet temperature, reactor delta-T and outlet temperature. 	Primary Sodium Temperature Measurement	(This uncertainty was not considered)	Reactor delta-T and inlet temperature variation
Inlet Flow Maldistribution <ul style="list-style-type: none"> Uncertainties of pressure measurement, manufacturing tolerance, orifice flow rate, assembly flow rate, etc. 	Inlet Flow Maldistribution	Precision in total coolant flow rate through assemblies	Inlet Flow Maldistribution <ul style="list-style-type: none"> Consistently count this uncertainty in three reactors with comparable HCF values.
Loop Temperature Imbalance <ul style="list-style-type: none"> Loop temperature imbalance affects inlet temperature distribution. CRBR allows cold leg loop-to-loop temperature imbalance, which results in uncertainty in inlet temperature. 	(This uncertainty was not considered)	(This uncertainty was not considered)	Loop Temperature Imbalance
Wire-wrap Orientation <ul style="list-style-type: none"> Analyzed by subchannel code, COTEC, which is 1% uncertainty. 	(This uncertainty was not considered)	Wire-wrap Orientation	Wire-wrap Orientation
Subchannel Flow Area <ul style="list-style-type: none"> Uncertainties of rod dimension tolerance, bow, etc. 	Rod Diameter, Pitch and Bow	(This uncertainty was partially counted in fuel thermal conductivity HCF)	Subchannel Flow Area
Film Heat Transfer Coefficient <ul style="list-style-type: none"> Uncertainties of correlation, etc. 	Film Coefficient	Film Heat Transfer Coefficient	Film Heat Transfer Coefficient
Pellet-Cladding Eccentricity	(This uncertainty was not considered)	(This uncertainty was not considered)	<ul style="list-style-type: none"> For oxide fuel, it may be importance due to a poor thermal

<ul style="list-style-type: none"> In CRBR, it was conservatively calculated by assuming that the fresh fuel contact to cladding. This uncertainty impacts on cladding and film temperatures. 			conductivity of gap, but this HCF is not applicable to metallic fuel.
Cladding Thickness and Conductivity		Cladding thermal conductivity and thickness manufacturing deviation	Cladding properties
Coolant Properties	(This uncertainty was not considered)	Coolant Properties	Coolant Properties
Flow Distribution Calculation <ul style="list-style-type: none"> The flow and temperature distributions were calculated using subchannel code of COBRA, COTEC, and THI-3D. 	Intra-assembly Flow Maldistribution Calculation	Precision in Coolant Flow Profile within an Assembly	Intra-assembly Flow Maldistribution Calculation <ul style="list-style-type: none"> Magnitude of uncertainty is dependent on the code performance.
Nuclear Data	Nuclear Power Distribution	Neutron and gamma flux distribution	Physics modeling <ul style="list-style-type: none"> Modeling and simulation uncertainties.
Fissile fuel maldistribution <ul style="list-style-type: none"> Due to manufacturing tolerance. 	Fissile maldistribution	Fissile content	Fissile maldistribution
		Fuel Thermal Conductivity <ul style="list-style-type: none"> Uncertainties due to pellet diameter, fresh and irradiated fuel conductivity, porosity of swollen fuel, redistribution, etc. 	Fuel Thermal Conductivity

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