

Deterministic Neutron Transport and Multiphysics Experimental Safety Analyses at the High Flux Isotope Reactor

A Dissertation Presented for the

Doctor of Philosophy

Degree

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DEDICATION

I would like to dedicate this work to my parents, Mike and Sharnell Hurt, who pushed me to work hard and push forward in all I've accomplished thus far, and to God, for blessing me with the many opportunities and doors that have been opened so that I can succeed in my life and career.

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ABSTRACT

The computational ability to accurately predict the conditions in an experiment under irradiation is a valuable tool in the operation of a research reactor whose scientific mission includes isotope production, materials irradiation, and neutron activation analysis. Understanding of different governing physics is required to ascertain satisfactory conditions within the experiment: the neutron transport behavior throughout the reactor and the coupled behavior of heat transfer, structural mechanics and fluid flow. Computational methods and tools were developed for robust numerical analysis of experiment behavior at the Oak Ridge National Laboratory (ORNL) High Flux Isotope Reactor (HFIR), including fully-coupled thermo-mechanics in three plutonium-238 (^{238}Pu) production targets. In addition, a new computational tool was developed that solves neutron transport using the discrete ordinates method on a finite element mesh and offers multiphysics coupling.

The thermo-mechanical models of the ^{238}Pu targets are solved using the COMSOL heat transfer and solid mechanics modules with irradiation behavior and thermophysical properties taken from measurements performed at ORNL. The experiments, placed in the permanent beryllium (PB) reflector, consist of neptunium dioxide/aluminum (NpO_2/Al) pellets in Al containment, the model taking advantage of axisymmetry in two-dimensional R-Z cylindrical geometry. At times, extended analysis was needed for incomplete data sets and time schedules; however, the thermal-structure models ensured progression through three project phases of target qualification.

The neutron transport equation was solved in COMSOL, using the discrete ordinates formulation in the weak form partial differential equation (PDE) interface. Validation studies were performed for the dimensions developed (one-, two- and three- dimensional Cartesian as well as two-dimensional R-Z cylindrical/axi-symmetric) and compared to external deterministic and stochastic codes. The method was then applied to a beginning-of-cycle (BOC) simplified HFIR core, with good comparison to other static

solutions of the HFIR, and a time-dependent extension to this tool was created and exhibited for a benchmark problem.

The research presented in this dissertation is the continued progress towards creating a comprehensive multiphysics methodology for studying the dynamic behavior of the HFIR core, and shows the capabilities of detailed space-time reactor physics studies and of multiphysics analyses for experiment qualification and safety analyses at a research reactor.

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1 Introduction

Chapter 1 provides a background for the research performed and introduces the key concepts behind it. Its subsections are the organization of this proposal, the purpose behind this research, and a literary review to establish the academic context of the research.

1.1 *Organization of Dissertation*

This dissertation is divided into several chapters based on their subject matter, including this introductory chapter. Chapter 1 provides a background for the research performed and introduces the key concepts behind the research. Its subsections are the organization of this dissertation, the purpose behind the research, a documentary review to establish the academic context of the research and a short background on nuclear engineering theory and nuclear energy. Chapter 2 introduces the ^{238}Pu production project and its project phases, as well as backgrounds on the project purpose, target fabrication, the HFIR safety review process, the targets within each phase, the project irradiation progress and HFIR experiment positions. Chapter 3 describes the computational tools used and the methodology behind the research.

Chapters 4 through 8 present the research of which this dissertation consists and are organized in an evolving scope of work. Chapters 4 through 6 shows coupled thermal-structural analyses of ^{238}Pu production target configurations irradiated at the HFIR, examined for their safety with relation to target integrity. Chapter 7 presents the development of the discrete ordinates methodology in COMSOL and its uses, and Chapter 8 presents an extension to time-dependent problems. Chapter 9 discusses the results and conclusions of the research in the previous five chapters, and introduces some potential future research avenues resulting from this work. Appendix A details supplemental neutron transport and depletion analysis of a rabbit target configuration.

Chapter 4 presents an account of the methodology used for thermo-mechanical analysis [1]-[10] of $^{237}\text{NpO}_2/\text{Al}$ cermet pellets in aluminum cladding, irradiated in the permanent beryllium (PB) reflector for the purposes of producing ^{238}Pu . Models for this project are developed in separate phases in accordance

with the target phases described in Chapter 2, however their methodologies overlap such that much of their implementation can be discussed in one segment. The models were created using COMSOL Multiphysics, using solid mechanics and heat transfer interfaces, with equations implemented for fission gases, gas gap conductance, contact conductance, and the input of pellet swelling/densification from current or projected data. The results presented are the sole work of this author, including the prototypical models discussed in Chapter 5 and production model in Chapter 6; however, the development of this methodology and modeling was done in consultation with colleague and mentor, Dr. J. D. Freels.

Chapter 5 presents the analyses of two prototypical targets [1]-[7], a partially loaded target (8 NpO_2/Al pellets) and a fully loaded target (~ 50 NpO_2/Al pellets) that encompass phases 2 and 3 of the ^{238}Pu production project, respectively, as described in Chapter 2. These targets were developed in 2-D R-Z geometries and analyzed at differing position and pellet fabrications and up to 2 cycles of irradiation at the HFIR. The safe irradiation of the targets was often dependent on post-irradiation examination (PIE) data incoming from previous phase target designs or from a lower number of irradiation operating cycles. Thus parameterized analysis was often needed for this complex problem in order to meet project schedules and adequately ensure safe irradiation within HFIR guidelines.

Chapter 6 presents analyses of a production target [1],[8],[9] containing 52 pellets in length, similar in geometry to the fully loaded target. Experience gained from previous models is incorporated into a more comprehensive production target model designed to qualify a target for 3 cycles of irradiation and illuminate potential in-reactor behavior of the target. New input data includes more irradiation data time steps (resulting in 30 time steps analyzed), more irradiation behavior data (including functions of dimensional swelling/densification), updated pellet material data (including temperature-dependent Young's modulus from stress-strain measurements), and input data at different target irradiation positions (eight pin location versus one to two previously). Fully coupled thermo-mechanical physics throughout the entire target domain allows the model to address structural integrity safety limits that were previously

analyzed in a less robust calculation. Further use and optimization of this model may be used to optimize the target design (a 2nd generation target to ensure greater axial clearance is being studied), the pellet fabrication (increased NpO₂ loading above 20% will allow greater product output), or inform other safety analyses (such as analyses on a 2nd generation target holder).

Chapter 7 describes the development (parts of this chapter are published in [11]) of the discrete ordinates equations in COMSOL, beginning with the static neutron transport equation and deriving the appropriate approximations until a PDE is available for input to the weak form PDE interface. An application is built using graphical user interface features of the application builder and underlying Java API programming, which allows the construction of discrete ordinates physics equations and boundary conditions for high numbers of angular quadrature and/or energy groups in a reasonable amount of time. The code is then validated for static benchmark problems including the Kobayashi benchmarks, a water-reflected sphere benchmark, arbitrary examples of high energy group problems with HFIR fuel material and finally a static clean HFIR reactor core model.

Chapter 8 introduces the development of the stationary neutron transport tool in Chapter 7 into a time-dependent solution of the neutron transport equation. A quasi-static implementation is described, which solves a shape function that is solved by the discrete ordinates method as described in Chapter 7 and an amplitude function solved by the point kinetics equations. This is implemented in sequential study steps within COMSOL for each shape function update that are automatically constructed as in Chapter 7. The time-dependent method is exhibited for a 1-D transient problem 16-A1 and compares well with benchmark results.

Appendix A presents neutronics analyses [12] of an LEU foil in nickel capsule irradiated in the hydraulic tube (HT) facility at 10-26 days for the purposes of producing ⁹⁹Mo. Nuclear heating rates at steady-state and transient conditions, as well as reactor feedback and nuclide inventories are analyzed using MCNP5 and SCALE6.1. MCNP5 is used for HFIR core eigenvalue and fixed source calculations, as well as target fixed source calculations for neutron, photon and electron transport. SCALE6.1's

ORIGEN-S and COUPLE modules are used to collapse cross sections from MCNP and calculate the depletion and activation of target materials, as well as target decay heat. Fabrication issues prevented the progress of this program and thus the targets were never irradiated.

1.2 Motivations and Goals

Under the sponsorship of the U. S. Department of Energy's (DOE), staff members at the Oak Ridge National Laboratory (ORNL) have been conducting studies to assess the feasibility and then demonstrate the production of ^{238}Pu using the existing domestic neptunium feedstock. Irradiations were performed at the High Flux Isotope Reactor (HFIR), however, the work is part of a multiple DOE facility effort to re-establish the domestic production of ^{238}Pu in support of ^{238}Pu -powered spacecraft utilized by the National Aeronautics and Space Administration (NASA).

The goals of the DOE ^{238}Pu supply project [13], [5] here at HFIR include:

1. Ensure that the ability of the reactor to perform its scientific missions is not significantly diminished.
2. Demonstrate the successful irradiation of NpO_2 pellets and subsequent chemical extraction of ^{238}Pu at the neighboring Radiochemical Engineering Development Center (REDC) on the ORNL site.
3. Collect pre- and post-irradiation material data on the as-yet unstudied NpO_2/Al cermet used in pellet production in the course of demonstration.
4. Ensure safe operation of the reactor as well as the structural integrity of the target cladding for different target designs and operating cycles.

Thus, in the course of this project, detailed experiment safety analyses are needed to assess the conditions in the target under irradiation, given the limited set of pre- and post-irradiation data on the target materials. The irradiation test program consists of four phases that provide an incremental

approach intended to reduce the risk of target failure during testing, the examination data from each phase being used to validate the previous analysis and enable analysis of the subsequent phase. As the limiting conditions for these targets have been under steady-state overpower conditions, the development of a fully-coupled thermal-structure model of the target has been crucial to project continuation.

Concurrently, ORNL staff members have been conducting studies under the sponsorship of the DOE's National Nuclear Security Administration (NNSA) to assess the safe conversion from high enriched uranium (HEU) fuel to low enriched uranium (LEU) fuel. The current HEU core was designed based on experiments, calculations, and expert opinions, while large-scale validation experiments are not a present option for re-design due to increased financial expenses in modern nuclear operations. Therefore, more advanced computational methods will be needed to fill this gap, including studies of reactor physics behavior. The motivation behind more versatile spatially-dependent reactor physics studies is then to remove assumptions and conservatisms in current methodology, while validating against measured behavior in the HEU design for subsequent use in LEU fuel environments.

The continuous development of and expertise in new methodologies and current computational tools is crucial in any scientific facility due to the common ailments of lack of maintenance, documentation, loss of expertise that often cause previous tools and methodologies to become incompatible with current standards. The deterministic studies presented here make use of finite element analysis codes, robust solvers and detailed 2-D R-Z or 3-D geometries. The stochastic studies presented here make use of Monte Carlo codes and detailed three-dimensional geometry. Discrete ordinates method-based physics are developed in this dissertation and are applied to some of the static problem sets because discrete ordinates offers direct multiphysics coupling and detailed, continuous flux distributions over Monte Carlo codes (where discrete detectors must be sampled) as well as the elimination of theoretical limitations with respect to other theories (diffusion theory, point kinetics). All of these tools are built to aid in detailed, accurate and efficient analysis of experiment and reactor operations in the unique reactor design of the HFIR.

COMSOL, a flexible finite element analysis software platform, has been implemented recently at HFIR for performing thermal-hydraulic analyses of the LEU and HEU fuel plates as well as a diffusion model for reactor transients. Three-dimensional models of HFIR fuel plates have been developed such that heat transfer in all three dimensions (across the width, axial length and thickness of the plate) is modeled, which is an improvement over current 1-D models of the fuel plates [14]. The successful implementation of this tool is another motivation behind the use of COMSOL for thermal, mechanical, and neutronics-based studies of reactor experiments. The diffusion theory model [15], which utilized the COMSOL PDE coefficient interfaces, was successfully applied to a simplified HFIR core and was thus the motivating principle behind Chapters 7 and 8 of this research.

1.3 Literature Review

The purpose of this section is to establish a satisfactory body of information and similar studies that serve to support and define the current work. In this section, the theoretical framework and methodology of previous related work will be discussed, as well as the new and original purpose of the current work within the context of the field. The following subsections are included with supporting documentation the subjects: 1) Codes of Discrete Ordinates 2) Discrete Ordinates Studies at HFIR, 3) Neutronics Modeling using COMSOL Multiphysics, and 4) Pellet Thermal-Structure Calculations.

1.3.1 Codes for Discrete Ordinates

Existing computer codes that solve the neutron transport problem using discrete ordinates, [16]-[25] , are often limited with respect to one or more of the following characteristics: Cartesian mesh, static modeling only, limited number of dimensions, and no availability of multiphysics coupling. An exception to these limitations exists [26]-[30]; however, it is used primarily for and developed for commercial power reactors with geometries, operating conditions, and purposes significantly different from the HFIR. HFIR is unique because of its compact core design (height = 2 ft, outer radius = 8.5 in), which is composed of 540 involute-shaped, HEU (93 % ^{235}U) inner and outer fuel plates that operates at

85 MW_{th}. In comparison, a typical commercial light water reactor is composed of approximately 50,000 fuel rods in bundles about 4 meters long and filled with uranium dioxide pellets enriched to ~5 percent in ²³⁵U.

1.3.2 Discrete Ordinates Studies at the HFIR

Studies of the HFIR reactor have previously been completed, the following is a short summary of the most recent [31]-[35]:

1. Radiation dose rate calculations in beam tube vessel walls using two- and three- dimensional discrete ordinates codes DORT and TORT.
2. Pressure-vessel flux calculations in three-dimensional discrete ordinates code TORT
3. A beam-tube flux calculation using the one- and two-dimensional code DOT4 and three-dimensional code TORT for discrete ordinates, with correction factors in final results.
4. The 1-D ANISN discrete ordinates code is used to aid in MCNP shielding calculation in HB-3.

The above efforts were all studies of the HFIR core and its components for the primary purposes of shielding calculations in the HFIR beam tubes, using finite-difference codes in a limited mesh not easily coupled to codes using other physics equations and no transient capabilities.

1.3.3 COMSOL Neutronics Modeling

Previous neutronics work in COMSOL has consisted of two static studies and two transient studies. The first two static studies [36]-[37] consisted of two-group diffusion theory models of LEU-fuel geometries. The first transient study consisted of a 3-group diffusion theory model [15] of the HFIR core for both static and transient conditions and the discrete ordinates development in this research is the programmatic extension of that effort. The fourth study was a point-kinetics multiphysics study of an aqueous uranyl nitrate solution [38], completed by the author. None of these studies utilized the more-

detailed and rigorous discrete ordinates method to solve the neutron transport equation. However, each of these studies did aid in establishing the framework for further neutron transport calculations in COMSOL.

1.3.4 HFIR Thermal-Structure Calculations

Modern thermo-mechanical analyses of experimental configurations at the HFIR primarily consist of fully coupled models in ANSYS that consider primarily the axial expansion and clearance of target materials under irradiation [39]-[42]. The irradiation of isotopes that undergo induced fission, as is observed in the ^{237}Np in the ^{238}Pu production target pellets, creates a variety of new and unique problem sets. Subsequently, the fully-coupled thermo-mechanical analysis of a fissionable NpO_2 material that includes: 1) 52 pellets under axial contact and a calculated clearance other target components, 2) strong contact occurring upon the cladding side wall for multiple pellets, and 2) burn-up dependent densification/swelling behavior included is entirely outside the normal realm of experiment target analyses at the HFIR.

This method is then best compared to reactor fuel-performance codes [43]-[47], most of which include a weak coupling between thermal and mechanical physics or alternatively, more detailed fully-coupled methodologies that have been released recently [48]-[51]. These codes however are designed and used primarily for commercial reactor UO_2 pellets in zircaloy cladding, which have a wealth of historical material correlations and measured experimental data to validate against and base assumptions and simulations upon. Examining less-validated materials in a unique environment therefore requires careful and creative modelling techniques and solution ranges.

2 Overview of the Plutonium-238 Supply Project

Plutonium-238 (^{238}Pu) oxide pellets fuel the radioisotope thermoelectric generators (RTGs) that are the established power sources for deep space missions where solar power is not viable. The Department of Energy (DOE) has been tasked to re-establish the domestic production of ^{238}Pu in support of ^{238}Pu -powered spacecraft utilized by the National Aeronautics and Space Administration (NASA).

The technology demonstration activity supported by this research is focused on supporting future production capability; specifically, the target design, qualification and irradiation studies that have taken place to date at the HFIR and supporting ORNL facilities. The intended infrastructure for full-scale production includes multiple DOE facilities and target irradiation at research reactors at both ORNL (at the HFIR) and Idaho National Laboratory (at the Advanced Test Reactor) with chemical extraction taking place at REDC at ORNL. However, the focus of this research is on advanced multiphysics modeling to support target design, qualification and irradiation studies that have taken place at the HFIR that will enable and streamline full-scale activities throughout DOE facilities.

The neutron irradiation of ^{237}Np in a nuclear reactor yields ^{238}Pu as shown in the reaction and decay pathway in Figure 2.1 as well as other by-products including undesirable isotopes such as ^{236}Pu . It is anticipated that the HFIR at ORNL and the Advanced Test Reactor (ATR) at INL, together will irradiate sufficient NpO_2 to produce an estimated 1.5 kg of plutonium product per year.

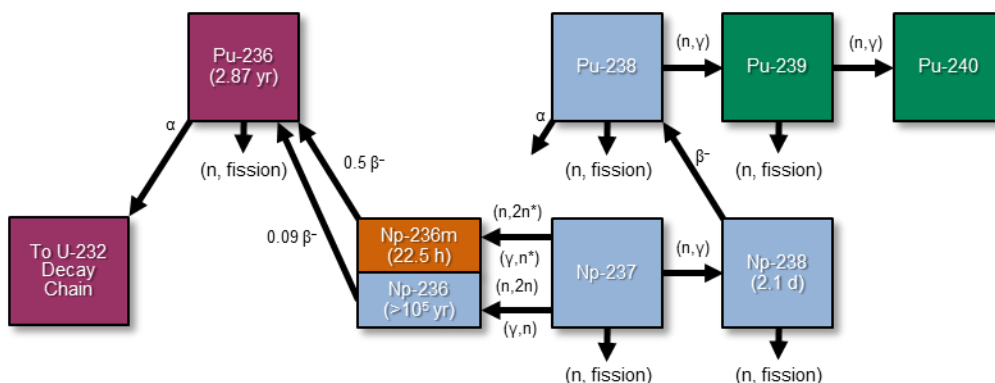


Figure 2.1: Important reaction and decay pathways in neutron irradiation of ^{237}Np .

The overview of the planned domestic supply chain is shown in Figure 2.2 [52], [53], where the irradiation efforts at HFIR are highlighted. The stored neptunium oxide is located at INL, from there it will be transferred to its fabrication location (ORNL), with some chemical processing to remove impurities before pellet pressing and target fabrication. Irradiations will then take place as previously discussed before chemical processing to extract the ^{238}Pu stock and remaining ^{237}Np feedstock for recycling before delivering the final product to Los Alamos National Laboratory, where it will be used in the powdered form of PuO_2 .

Before ^{238}Pu can be produced, a series of irradiation and processing tests are required to develop and validate the designs, procedures, process flow sheets, and specifications required during the production process.

Initial tests were conducted in the HFIR in order to expedite development of the knowledge base necessary for target design and are highlighted below. A series of target irradiations and post-irradiation examinations (PIEs) have provided a body of knowledge necessary to qualify prototypical, or production-style, targets. By the end of the project, production targets will be irradiated in HFIR. The use of existing hot cell facilities in the ORNL REDC to conduct chemical processing and recovery scale-up tests is not discussed in any detail here.

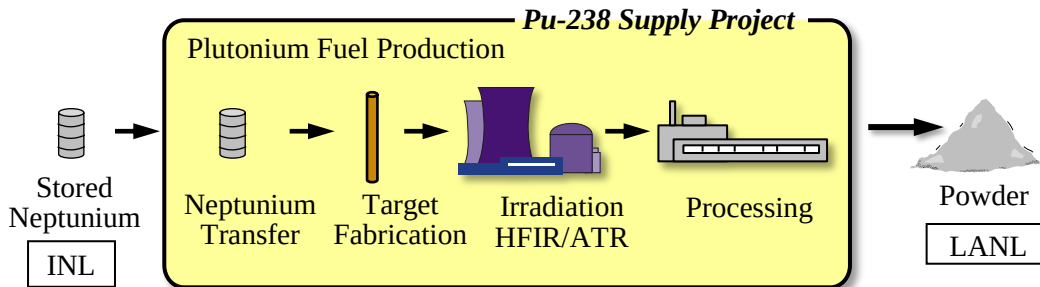


Figure 2.2: Overview graphic of the ^{238}Pu supply project.

2.1.1 Target Fabrication

Target fabrication requires several steps to prepare for irradiation:

- preparing neptunium feedstock for fabrication into pellet form, including the removal of ^{233}Pa , conversion to NpO_2 , and characterizing the resulting oxide powder to develop a material specification for NpO_2 ,
- blending the NpO_2 powder with aluminum powder, pressing them into pellets, verifying the composition through testing and analysis,
- loading the pressed pellets into an aluminum clad and then transferring the target to a welding glove box,
- seal-welding, leak testing, and radiographing the target, and
- hydrostatic compression of the target and radiographic inspection as necessary.

All of the above steps have been demonstrated on significant (~ 500 gm) quantities of NpO_2 . The current target design to be used consists of NpO_2/Al pellets ($\sim 1/4''$ diameter by $\sim 3/8''$ length) loaded into a sealed thin walled 6061 aluminum (Al-6061) containment housing tube [55]. The pellet loading from conversion and pressing yields volume fractions of approximately 70% Al, and 20% NpO_2 , and 10% void [54].

2.1.2 Target Qualification

The irradiation test program consists of four phases that provide an incremental approach intended to reduce the risk of target failure during testing. Additionally, PIE results from each phase serves as a hold point and is used to guide the course of the subsequent irradiations. The irradiation characteristics of ^{238}Pu production in the HFIR of particular interest are:

- pellet dimensional changes
- fission gas release fractions
- heat generation rates
- pellet clad interaction (PCI)
- ^{236}Pu production
- product yields

Figure 2.3 illustrates how several irradiation cycles have been used in the phased approach:

2.1.3 Experiment Safety Analysis Review

Experiment qualification at the HFIR requires that a safety review is completed to ensure that safe reactor operation is not impaired (via a large reactivity insertion, release of material into the reactor coolant, etc.) during nominal conditions as well as safety basis conditions from the HFIR Safety Analysis Report [56] that do not result in reactor fuel damage. In the case of this work, care is taken to ensure steady-state target cooling is maintained so that (1) maximum temperatures do not exceed melting ($\sim 650^\circ\text{C}$ for aluminum), (2) target surface temperatures do not exceed the reactor coolant saturation temperature (to avoid steam blanketing and potential burnout), and (3) internal spatial clearance is maintained or stress is not put on the containment past its material strength. The steady-state conditions analyzed include (1) nominal operating conditions, (2) 50% coolant flow, and (3) 130% overpower conditions including a raised inlet temperature. The principal failure mode of concern for the experiment designs during the initial three phases of the project (not including the production model in Chapter 6) has been the maximum target internal temperatures with respect to melting at 130% overpower conditions.

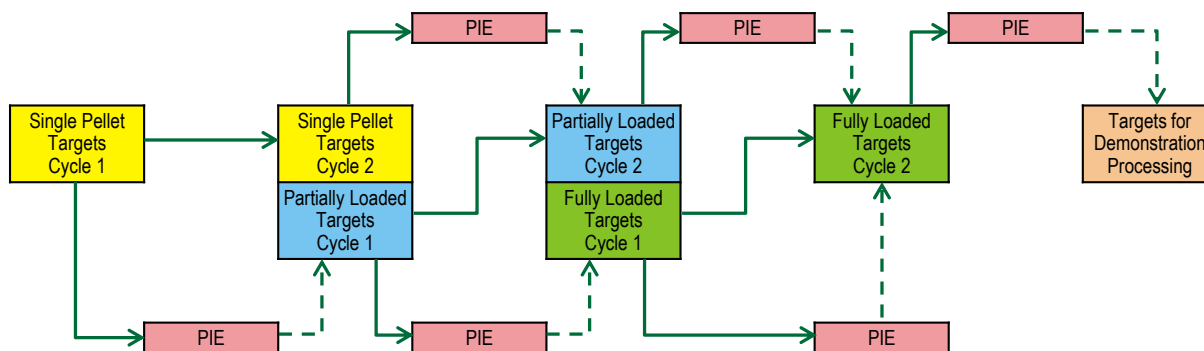


Figure 2.3: Phased target irradiation process.

The steady-state thermal-structure analyses presented are one part of the safety review required, where the target cooling calculations include both steady-state and transient heat transfer that is computed using nuclear safety software quality assurance (QA)-approved codes COMSOL Multiphysics and RELAP5 [57],[58], respectively. Separate calculations for neutron transport and material depletion [59], [60], [61] support these analyses (via heat generation rates, fission gas inventories, fission densities, etc.) as well as satisfy radionuclide inventory and reactivity requirements. However, a relevant transmutation characteristic to note is the linear build-in of fissile isotopes in the pellets (with some decay and build-in between cycles) that, along with increased flux in the reflector regions due to opening of the control plates, results in maximum heat generation rates at end-of-cycle (EOC) and therefore limiting thermal conditions are frequently observed at EOC.

Altogether these safety analyses support an experiment authorization basis document that presents the final target qualification with respect to the HFIR safety review. The safety review process for these experiments is shown in Figure 2.4, where the focus of the work presented in Chapters 4 through 6, steady-state thermal-structure analyses, is outlined in red

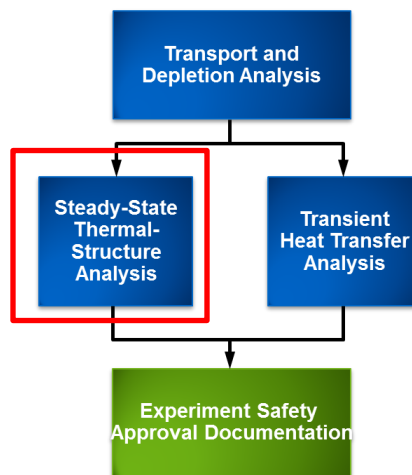


Figure 2.4: Simple diagram of the experiment safety review process at the HFIR.

2.1.3.1 Phase 1: Single Pellet Capsules

Three phase 1 target designs were qualified and irradiated in non-prototypical encapsulations that were specifically designed to prevent target failure due to the unknown pellet irradiation behavior (pellet swelling, fission gas release fractions, pellet-clad interaction (PCI)) while collecting needed PIE data for future phases.

The first target design, a single or bare pellet capsule, contained a single pellet of $\sim 1/4$ " diameter and $\sim 1/4$ " in length. The second target was a tensile specimen that was designed to confirm that chemical/mechanical reaction between the pellets and housing would not significantly weaken the housing tube wall. See Figure 2.5 for an image of the bare pellet capsule assembly and its parts.

The PIE results from the first cycle single pellet target irradiation revealed large densification or shrinkage of the pellet diameter that required a the third designed target, reduced-length pellet target, similar to the bare pellet target assembly except for a pellet of reduced length (from $\sim 1/4$ " to $\sim 1/8$ " in length).. The reduced-length pellet target was then irradiated for 1 and 2 cycles using NpO_2 powder heat-treated to temperatures of 800 °C, 900 °C, or 1200 °C. Pellet heat-treatments above 800 °C were conducted with the anticipation that pre-irradiation sintering at higher temperatures would reduce initial void volume and thus pellet diametrical shrinkage, as well as improve thermophysical properties.

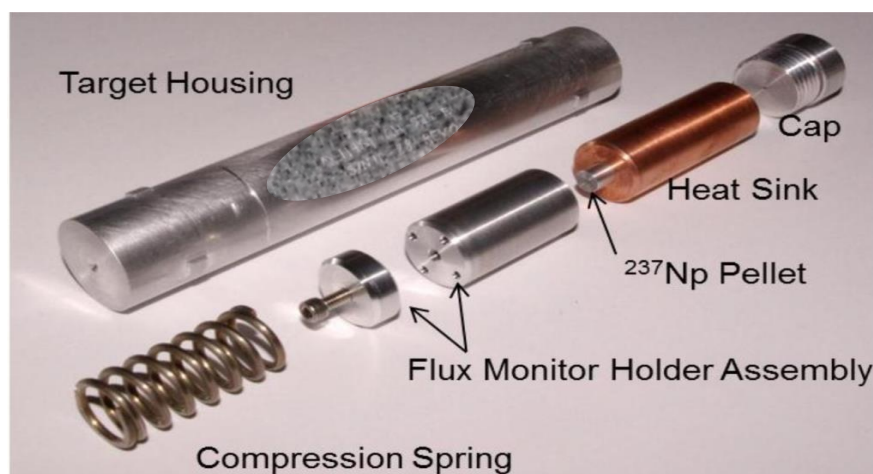


Figure 2.5: Single pellets target components.

2.1.3.2 Phase 2: Partially Loaded Targets

The phase 2 partially loaded target designs contained 8 NpO_2/Al pellets heat-treated at either 900 °C or 1200 °C in a prototypical target design. The targets were arranged in arrays of seven targets in specially designed holders.

The partially loaded targets were irradiated for both one cycle and two cycles. After each cycle, several targets were selected for PIE. During PIE, the targets were opened, pellets were retrieved, and post-irradiation dimensions were measured and compared to their pre-irradiation values, of particular interest being the pellet diameter. In addition, fission gas release fractions as well as other PIE data were collected. As a result of the thermal safety analyses, the 1200 °C heat-treated pellets were chosen for two cycles of irradiation due to their reduced impact of pellet diametrical shrinkage.

2.1.3.3 Phase 3: Fully loaded targets

The phase 3 fully loaded target designs contain 50-52 NpO_2/Al pellets all heat-treated at 1200 °C in a very similar encapsulation used in the partially loaded targets. The target irradiations have further confirmed irradiation behavior of the NpO_2/Al pellets as well as provide meaningful information on anticipated production yields. These targets are considered the first generation of design production targets. Figure 2.6 shows prototypical targets pins extending from the target holder used to hold seven targets during irradiation.



Figure 2.6: Prototypical targets in a target holder prior to irradiation.

The fully loaded targets were irradiated for both one cycle and two cycles. After each cycle, several targets were selected for post irradiation examination (PIE). During PIE, the targets were opened, pellets were retrieved, and dimensions were measured. Due to the large number of pellets per target, a large number of data points were added per target compared to previous phases. Currently, the final demonstration step of chemical processing of the fully loaded targets is underway.

2.1.3.4 Phase 4: Production and optimization of targets

Having completed the successful demonstration of irradiation for the first generation of design production targets in phase 3, optimization of the design and irradiation process is now an ongoing effort. As a part of that effort, an increased accuracy method for the neutronics calculation has demonstrated that the fully loaded production targets may be irradiated for three cycles within isotopic quality requirements [61]. A resulting part of the optimization is an increased accuracy thermo-mechanical model for the 3rd cycle safety review. Furthermore, optimization efforts in the design and fabrication of the target are currently being undertaken including the exploration of stainless steel housing tubing at the target ends and springs in place of expansion spacers. The target holder itself is also being redesigned to eliminate the individual coolant channels in order to simplify operations removal of the targets from the target holder after irradiation. Flow analyses of this new holder design as well as core flow diversion and beam tube flux impact analyses due to near-full loading of the HFIR PB are forthcoming [54].

2.1.4 Production Progress Overview

A summary of the current qualification efforts through cycle 456 (October 2014) is shown in Figure 2.7 as a function of HFIR operating cycle. Included are the number of target designs that have been irradiated and the increased throughput of estimated ²³⁸Pu production as the project approaches the final prototype phase and beginning of the production phase. The estimated ²³⁸Pu production is approximate, as some build-in is expected to occur during the first several days of decay time and it is important to note that chemical recovery will not be perfectly efficient. The fabrication effort of a variety of designs

between cycles was considerable, with qualification of increased neptunium loaded targets leading to increased ^{238}Pu production. An updated plot in Figure 2.8 shows the throughput until cycle 465 (February 2016) and indicates where production ramp-up has levelled off as fabrication and chemical processing portions of the ^{238}Pu supply project enter development before their ramp-up to production. An updated plot in Figure 2.9 shows the throughput until cycle 468 (September 2016) where increased ^{238}Pu production from 3rd cycle targets was enabled due to the studies described in Chapter 6 and the running total production is shown where a clear linear increase is observed after implementation of the fully loaded/production targets.

2.1.5 HFIR Experiment Positions

The HFIR provides a variety of in-core irradiation facilities as shown in Figure 2.10. Moving from the inner to outer regions of the core these regions include the target flux trap, removable beryllium facilities, control rod access plug facilities, the PB vertical experiment facilities (VXF) and slant engineering facilities. The VXF in the PB are where the ^{238}Pu target irradiations have taken and are intended to take place, chosen as they have a smaller impact on the power reactivity due to their distance from the core centerline. There are twenty-two VXF positions in the PB, sixteen small VXF and six large VXF. For now, target holders in the small VXF positions are considered and, more narrowly, those eleven inner small VXF positions closest to the core axial centerline. Specifically, for these studies, the analyses focus on the VXF-15 and VXF-3 positions, VXF-15 as the bounding highest flux inner small VXF position and VXF-3 as a lower flux option when PIE data is insufficient for qualification of irradiations at VXF-15. Moving towards production, a significant modeling effort is to ensure safe irradiation of targets in as many positions as possible in the PB, limitations including flux impact on the adjacent neutron scattering beam tubes and flow diversion from the core.

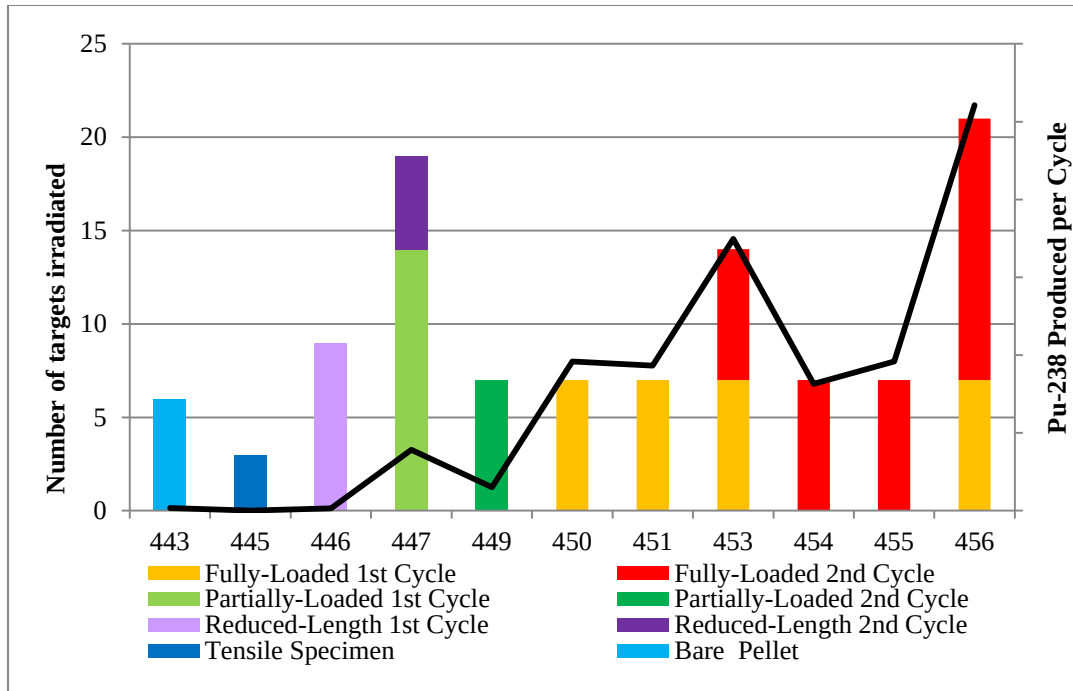


Figure 2.7: Irradiated target designs and ^{238}Pu production by HFIR operating cycle through cycle 456.

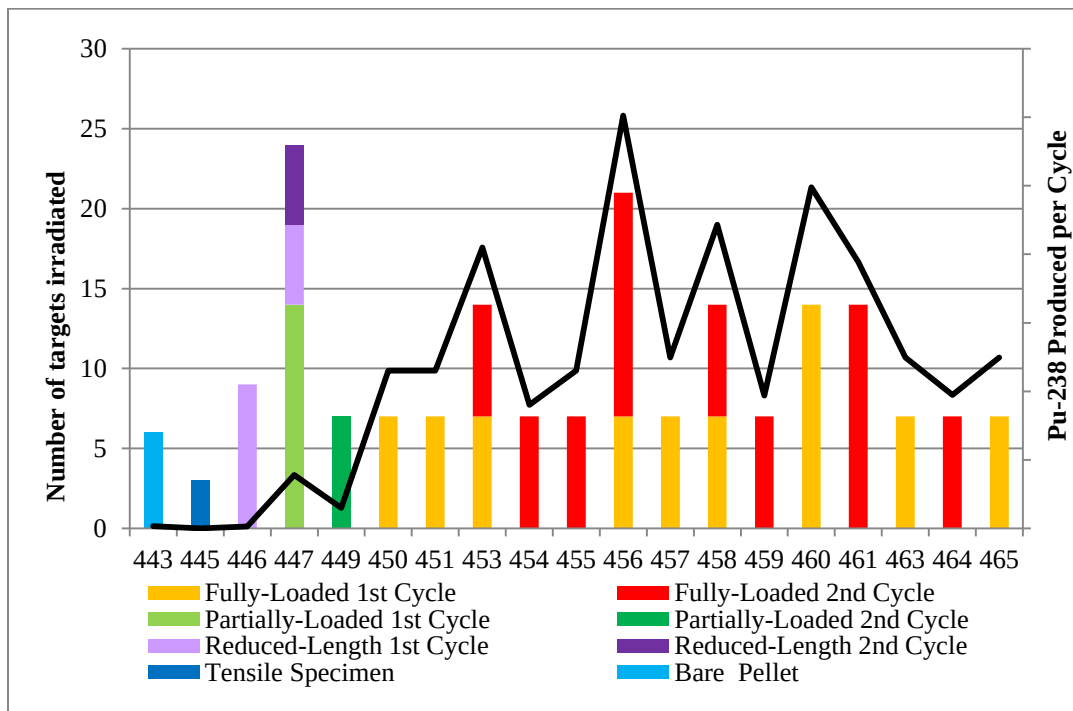


Figure 2.8: Irradiated target designs and ^{238}Pu production by HFIR operating cycle through cycle 465.

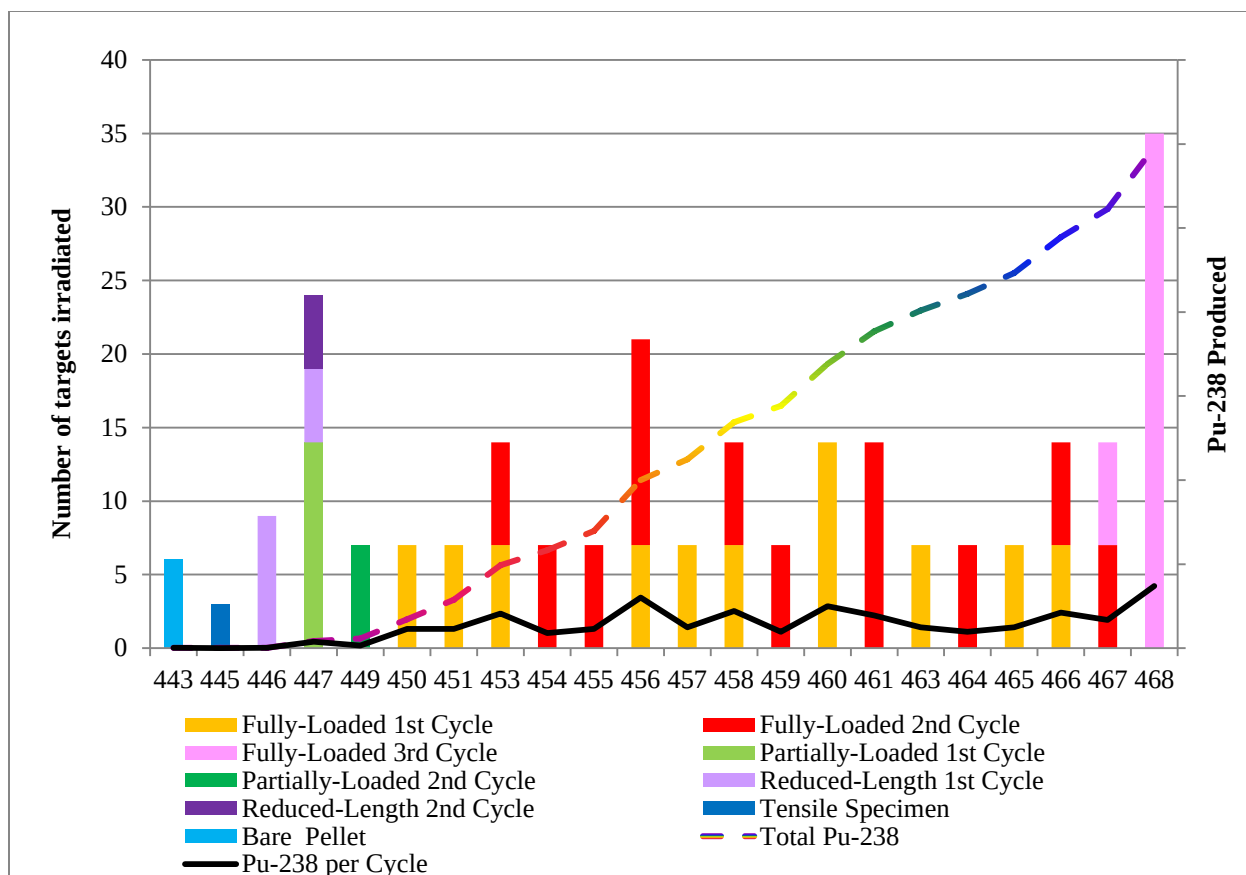


Figure 2.9: Irradiated target designs and ^{238}Pu production by HFIR operating cycle through cycle 468.

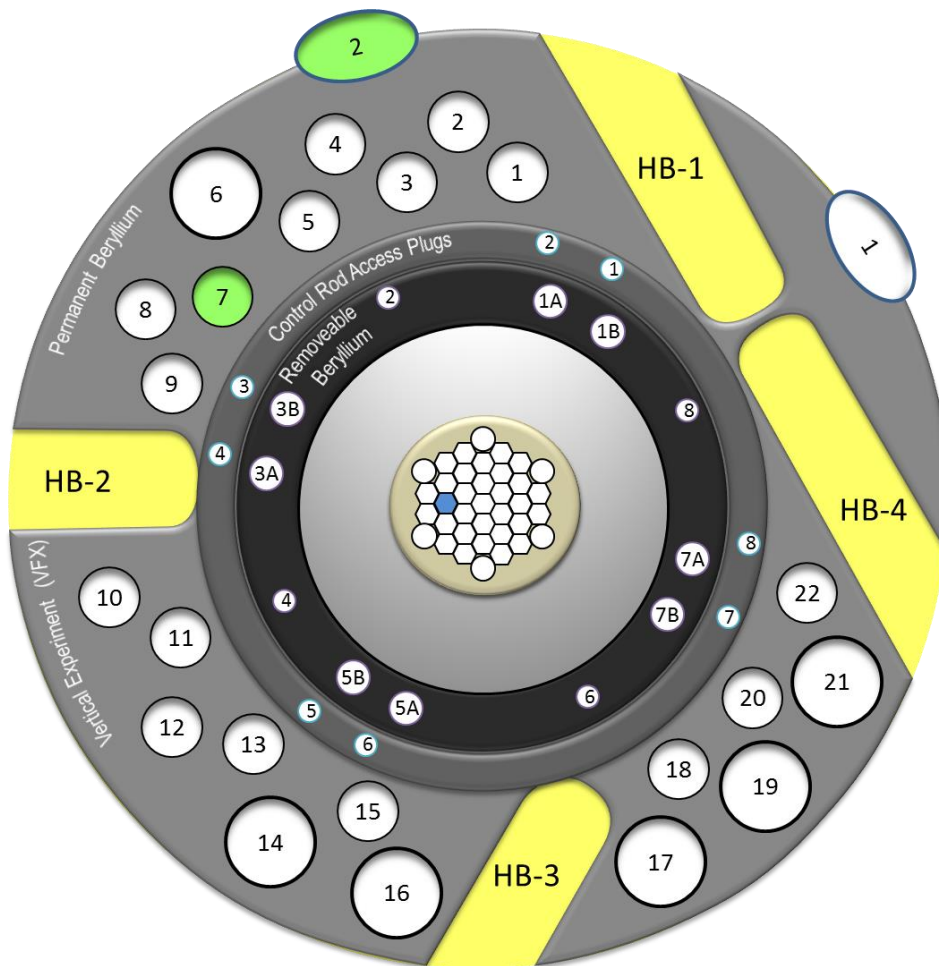


Figure 2.10: HFIR in-vessel target regions and beam tubes.

3 Description of Computer Codes

A variety of computational tools were used in the course of this research, the following subsections briefly describe these tools along with a short description of their utilization herein.

3.1 *COMSOL*

COMSOL Multiphysics is a general-purpose software platform, based on advanced numerical methods, for modeling and simulating physics-based problems. COMSOL Multiphysics is a flexible tool that typically uses finite element analysis in a variety of physics and engineering applications, especially coupled phenomena, or multiphysics. In addition to built-in physics-based interfaces, COMSOL also allows for entering coupled systems of partial differential equations (PDEs) using the weak formulation of finite element methods. The solid mechanics, heat transfer in solids built-in physics interfaces are utilized in Chapter 4, 5, and 6 of this research. In Chapter 7 the weak form PDE interface and Global ODE interface are utilized. Versions 4.3 [62], 5.0 [63], 5.1 [64], and 5.2 [65] of COMSOL are used in the course of this research.

3.2 *SCALE*

The Standardized Computer Analyses for Licensing Evaluation (SCALE) [66] modular code system was developed and is maintained at the Oak Ridge National Laboratory under an ongoing joint sponsorship with the U. S. Nuclear Regulatory Commission and the Department of Energy. The SCALE system consists of a suite of established nuclear engineering computer codes (also referred to as functional modules) and methods run within control sequences. The SCALE code is commonly utilized for criticality safety, reactor physics, radiation shielding, radioactive source term characterization, and sensitivity and uncertainty analysis. With over 89 computational modules, SCALE uses control modules to build and execute input decks for its various functional modules (or codes). The control modules and

functional modules in the SCALE 6.1 system, which is the version of SCALE used in these studies, used in the work are described in the following subsections.

3.2.1 CSAS

The Criticality Safety Analysis Sequences (CSAS) are control sequences in SCALE that automate problem-dependent cross-section processing and subsequent criticality calculation of the neutron multiplication factor. The two CSAS sequences used here include CSAS5 [67] and CSAS6 [68], which were developed for to utilize KENO V.a and KENO-VI, respectively.

CSAS utilizes several cross-section processing codes, or functional modules, in SCALE. BONAMI is used to correct for resonance self-shielding in the unresolved resonance range using the Bondarenko method. For the resolved resonance region, the functional module NITAWL can be used to calculate resonance self-shielding using the Nordheim Integral Treatment. Alternatively, the sequence of the WORKER, CENTRM and PMC modules are also used in the resolved resonance region: CENTRM computes a 1-D continuous-energy neutron spectra, PMC uses the neutron spectra from CENTRM as a weighting function on a pointwise nuclear data library to calculate multigroup self-shielded cross sections, and WORKER manages AMPX format cross section libraries for input to a criticality calculation sequence. While using NITAWL saves on computation time, the WORKER/CENTRM/PMC sequence is the default option, available for all ENDF libraries (NITAWL is restricted to ENDF/B-V and before), and the cross-section processing offered is higher fidelity as it accounts for resonance overlap for multiple absorbing isotopes. A third option of continuous energy cross section libraries is not applicable to this work.

After cross-section processing, the KENO sequences (described later) are used to calculate the neutron multiplication factor for 3-D system models.

3.2.2 TRITON

TRITON [69] is another control module of the SCALE code system that is used for transport, depletion, and sensitivity and uncertainty analysis. In this work, only its transport analysis capabilities are utilized, which provide for automated cross-section processing before a neutron transport calculation using either NEWT (a 2-D transport code) or XSDRN-PM (a 1-D transport code), which are both described later. The multigroup cross-section processing options are the two described for the CSAS modules as well as a full-spectrum BONAMI option, which serves as the fastest option yet is lower fidelity, and a heterogeneous option (not used).

3.2.3 KENO

KENO V.a [70] and KENO-VI [71] are 3-D codes or functional modules in the SCALE code system that calculate criticality transport for 3-D systems using the Monte Carlo method. In addition to calculating the neutron multiplication factor, the KENO codes calculate material and region-dependent absorptions, fissions, fluxes and fission densities, among other criticality parameters. KENO-VI offers improvements over KENO V.a, its predecessor, in terms of more exact geometry modeling by quadratic input as well as the ability to use continuous energy cross sections and calculate angular fluxes and flux moments. Both codes use a P_N scattering model in the cross sections.

The KENO sequences are used to create comparison models against the discrete ordinates method in COMSOL for multiple 3-D and 2-D R-Z configurations, including a simplified HFIR core model. The angular flux and flux moment data available in the KENO output is also used, as an option in the Application Builder GUI, to collapse cross-sections for input into few-group discrete ordinates problems in COMSOL.

3.2.4 ORIGEN-S

The Oak Ridge Isotope Generation (ORIGEN) code is the depletion and decay module in the SCALE code system and uses a matrix exponential expansion model to calculate time-dependent concentrations,

activities, and radiation source terms for a large number of isotopes due to fission, radioactive decay or neutron transmutation. The current version is ORIGEN-S [72], which acts as both a standalone code as well as having the ability to use multigroup cross-sections from transport evaluations. Neutron spectrums from other codes can be used to determine problem-dependent cross sections as an appropriate input to ORIGEN-S. This code, along with COUPLE and OPUS, are used to calculate time-dependent nuclide concentrations, decay heat times, and activities in ^{99}Mo production preliminary design and final safety studies.

3.2.5 COUPLE

The COUPLE code [73] is used to generate nuclear data libraries as input to the ORIGEN-S code, previously discussed. The COUPLE code calculates flux-weighted, problem-dependent neutron cross sections for ORIGEN and uses the most recent ENDF nuclear decay and fission product yield data (ENDF/B-VII was the most recent available at the time the work was completed).

3.2.6 OPUS

The OPUS utility code [74] is used for post-processing data from ORIGEN-S solutions into a condensed output format and/or plotting in the PlotOPUS graphics-plotting program.

3.2.7 NEWT

The NEWT (New ESC-based Weighting Transport) code [16] is a functional module in SCALE that calculates 2-D multigroup discrete-ordinates transport problems in complex geometric models (allowing for arbitrary polygon shapes). NEWT can be used for eigenvalue, critical-buckling, and fixed source calculations, as well as having the ability to prepare collapsed cross-sections. NEWT can be run as a standalone module or as part of the TRITON control module in several sequences, as part of transport, depletion, or sensitivity analysis studies. The NEWT module is used in this work to create comparison models against the discrete ordinates method in COMSOL for multiple 2-D configurations, comparing spatial flux and eigenvalue values.

3.2.8 XSDRNPM

The XSDRNPM code [17] is a functional module in the SCALE code system that is capable of 1-D discrete ordinates transport problems in slab, cylindrical, or spherical coordinates. XSDRNPM can be used for eigenvalue, criticality search, and fixed source calculations. XSDRNPM can be run as a standalone transport module or as part of the other code sequences in SCALE, as part of cross-section processing or collapsing, sensitivity analysis, or calculating bias factors.

3.3 MCNP5

The Monte Carlo N-Particle code (MCNP) is a three-dimensional particle transport code that was developed and is currently maintained by Los Alamos National Laboratory (LANL) [75]. MCNP uses the Monte Carlo method to statistically sample the phenomena of neutron streaming and thus solve the neutron transport equation stochastically, as opposed to deterministic methods. MCNP is commonly used to simulate neutron, photon, or coupled neutron/photon transport, as well as electron transport, or coupled neutron/photon/electron transport in many applications. The variety of variance reduction techniques to reduce its flux “tallies” and its versatile geometry features makes it a powerful tool in neutron transport. The latest version of MCNP, MCNP5, is used to solve coupled neutron/photon transport, photon transport and electron transport as described in Appendix A.

4 Plutonium-238 Production Studies: Methodology

In the following three chapters, safety studies are discussed that were performed to qualify the irradiation of neptunium-237 (^{237}Np) in neptunium dioxide aluminum cermet (NpO_2/Al) pellets in aluminum-clad targets throughout the HFIR permanent beryllium (PB) reflector in order to produce plutonium-238 (^{238}Pu). These studies were performed in order to facilitate four phases of the ^{238}Pu production supply project, which have been completed during the course of this research with design optimization being a continual effort. Although the author assisted in the initial single pellet phase modeling, the focus of this chapter is on the final three phases (as previously detailed in Chapter 2) and their models: the two prototypical targets (partially loaded and fully loaded) and the production target. The methodology for these models is discussed in this chapter, the prototypical target models and results are discussed in the next chapter and the production model and results are discussed in the Chapter 6.

This chapter focuses on the modeling methodologies in terms of model inputs, equations, and software utilization. Significant variation occurs between the methodologies for each model and where possible these variations are noted here, however the evolution of each model was a continuous process with some overlap in methods from each model that would require a needlessly complex explanation to fully detail. As models progressed, more accurate inputs and methods might allow a relaxation in conservatism or new unknowns might require an increase, however throughout the process it is always a priority to place the safe irradiation of the experiments before project schedule or cost.

4.1 *Use of Computational Software*

All documented calculations were performed on the betty.ornl.gov computation cluster using research reactors division (RRD) QA controlled software, with preliminary calculations run on other machines. The COMSOL Multiphysics software, versions 4.3 [62], 5.0 [63], 5.1 [64] and 5.2 [65] were utilized to model the thermo-mechanical behavior in the target and calculate parameters like maximum pellet temperature and target cladding stress. The COMSOL Java API was used to run sets of simulations that

were not amenable to parametric sweeps within the native COMSOL graphical user interface (GUI). In addition, supplementary calculation tools like the MATLAB R2015B Curve Fitting Toolbox and Microsoft Excel were used to process inputs and outputs to the COMSOL model.

4.2 *Material Properties*

The measurements and collection of material properties for target materials has been an ongoing effort that will continue past the publication of this dissertation. A full description of property measurements and their results is not within the scope of this report and would be better suited to its own separate publication, therefore only brief summaries of this effort and its relevance to the thermal safety analyses as inputs will be described here.

Primarily the material properties of the NpO_2/Al cermet pellet, a custom fabricated material for this project, have been important items of interest for this project. The important material properties (including thermal conductivity, thermal expansion, Young's modulus, etc.) and their variation with temperature and fabrication technique are discussed here. The COMSOL material library is used for non-pellet materials and either verified or modified using alternate established sources.

4.2.1 *Irradiation Behavior*

The possibility of significant densification and swelling in the neptunium oxide pellets was discussed prior to the Phase 1 irradiations, however the expectation was that for the production burn-up levels the observed densification of the pellets would be minor and swelling would be the more measurable factor. While swelling presents a safety consideration in possible breach or failure of the target housing, densification or negative swelling presents a safety consideration as it increases the gap between the pellets and target housing, hence, reducing radial heat transfer, and elevating pellet temperatures near melting.

The behavior of irradiated fuel oxides suspended in an aluminum mixture has been measured in previous experiments [76], [77], [78]. The experiment results exhibit the general characteristics of

densification and swelling as described in the equations and Figure 4.1 below. Fabrication void volumes experience a radiation-enhanced sintering which reduces the overall volume of the pellets for the early irradiation periods. Subsequently, the swelling due to fission gas and fission product release dominates the irradiation behavior as the reduction in void volume falls off.

$$\frac{\Delta V}{V_{swell.}} = \alpha * BU$$

Equation 4.1

$$\frac{\Delta V}{V_{dens.}} = P_0(e^{-\beta * BU} - 1)$$

Equation 4.2

The phase 2 and 3 partially and fully loaded target PIE measurements provide consistent data points, enabling the creation of a trend, as shown later for the 1200 °C heat-treated pellets. As shown in Figure 4.1, the irradiation behavior, as measured by the pellet dimensional changes in the PIE results, has mostly been observed in the time period after maximum volumetric densification. In this observable range swelling due to fission products is recovering the negative volume change – however a trend consistent with the theoretical curve in Figure 4.1 can be seen. The maxima densifications are observed early in the irradiation periods, which is consistent with previous oxide fuel studies at around less than 4,000 MWd/tHM [79], [77], [78].

The other crucial irradiation behavior with respect to thermal safety analyses in the targets has been the fission gas release fraction, which is typically assumed as a constant over one or more irradiation cycles that bounds previous results in the range of burnups expected [80]. Altogether these irradiation behaviors have a significant effect on the heat transfer in the gap between the pellets and housing tube, via either varying gap size or the gas thermal conductivity. As shown in the radial temperature profile in Figure 4.2, the temperature gradient in the gap can be very significant and is the primary driver behind maximum temperatures in the pellets.

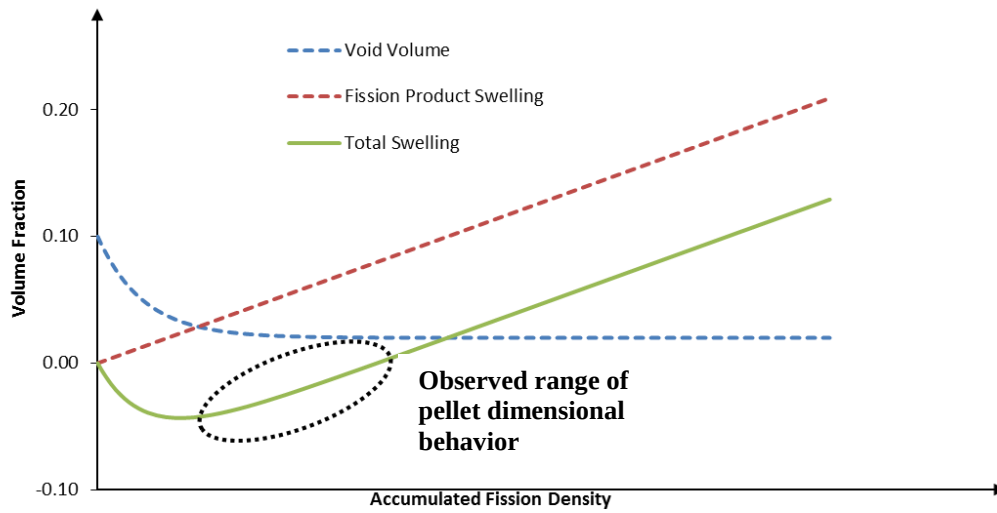


Figure 4.1: General trend and contributions to pellet dimensional irradiation behavior.

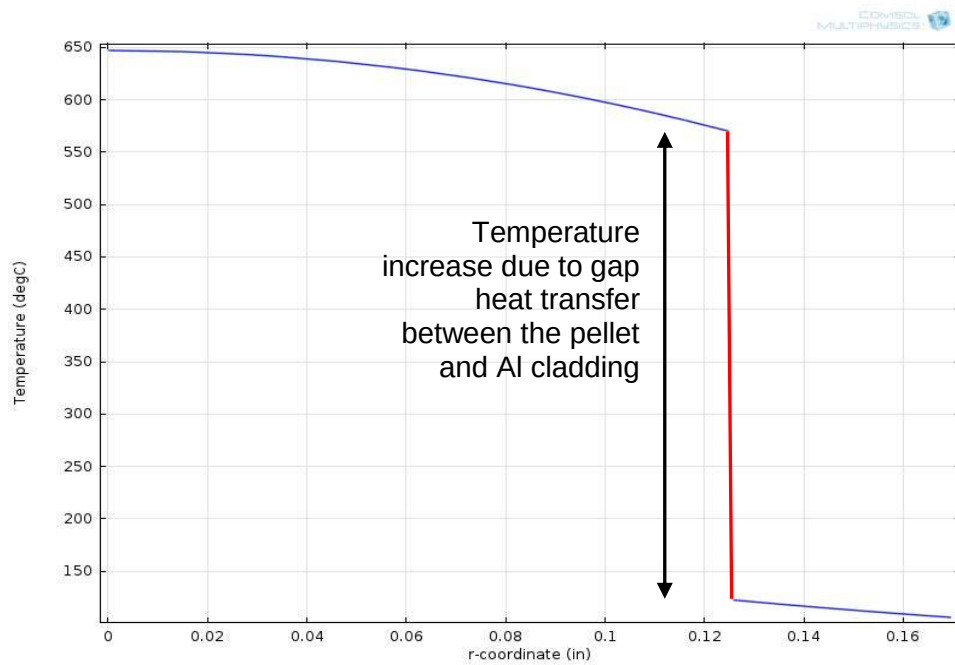


Figure 4.2: Example radial temperature profile taken from the fully loaded target model.

4.2.2 Pellet Properties

NpO₂/Al pellets are pressed from NpO₂ powder (which has been processed from Np feedstock by removal of ²³³Pa and oxide conversion) with aluminum (Al) powder, where an approximate volume composition is yielded of 70% Al, 20% NpO₂, and 10% void with an effective density of ~4.11 g/cm³.

4.2.2.1 Thermal Conductivity

The thermal conductivity of the pellet required initial measurements for the single pellet capsule irradiations, which showed for pellets heat-treated at around 590 °C that the thermal conductivity changed little with temperature and was around 50 W/m-K for the oxide+void packing in the measured pellets. The first prototypical encapsulation experiment for the partially loaded target used updated measurements for heat treatments at 800 °C, 900 °C, and 1200 °C where increasing thermal conductivity was seen for increasing heat-treatment temperature [81], adjusting for conservative bounds in the fabricated oxide+void volume percentage and a slight decrease with temperature [81], [57]. For the fully loaded targets, an updated conservative estimate for the 1200 °C heat-fired pellets was used, allowing for a narrower range of the oxide+void volume percentage given more extensive pellet fabrication experience.

4.2.2.2 Thermal Expansion

The initial thermal expansion measurements were performed at the same stage as the initial thermal conductivity measurements, showing a thermal expansion in proportion to that of pure aluminum according to its volume content in the pellets. A curve fit of this measurement was used as input for the thermal expansion coefficient. As with the thermal conductivity measurements, the partially loaded target model used updated measurements for heat treatments at 800 °C, 900 °C, and 1200 °C (see Figure 4.3) [82], where increasing thermal expansion was seen for increasing heat-treatment temperature.

4.2.2.3 *Young's Modulus and Poisson's Ratio*

The initial elastic or Young's modulus and Poisson's Ratio estimates were based on consensus expert opinion (taking into account measurements of a surrogate oxide material) in order to determine a conservative bounding estimate (with respect to maximum temperatures) of these values at 70 GPa and 0.1 (-)*, respectively. These values were used for the prototypical encapsulation target models, for the partially loaded and fully loaded target models in Chapter 5. The value of Poisson's ratio is between -1 and 0.5 for any stable, linear elastic material, but does not tend to vary significantly; indeed, the value of Poisson's ratio, $\nu(-)$, for constituent materials NpO_2 and Al are in the range from 0.3 to 0.4 (-) [83], [84], [85]. A value of 0.1(-) thus yields a likely low range value, where very little transverse expansion will be expected which is conservative with respect to target cooling as less gaps can be closed due to transverse strains.

However, as axial stresses due to aggregate pellet stack swelling became a concern during the transition to the "best-estimate" production model, updated measurements for the elastic modulus were taken at different pellet temperatures as shown in Figure 4.4 [86] [87]. What was observed was a strong dependence on temperature, where the modulus and ultimate strength of the pellet decreased with increasing temperature. Temperature-dependence of Young's modulus is thus derived as an interpolated table of the values derived from the measurements at 20, 200, 300, 400, and 500 °C. No Poisson's ratio measurements on the pellet material have been conducted, however a value between 0.1 and 0.35 is assumed, depending on which value is conservative for the assessment.

*Note that the text "(-)" or "-" is used to denote a dimensionless quantity or value for Poisson's Ratio.

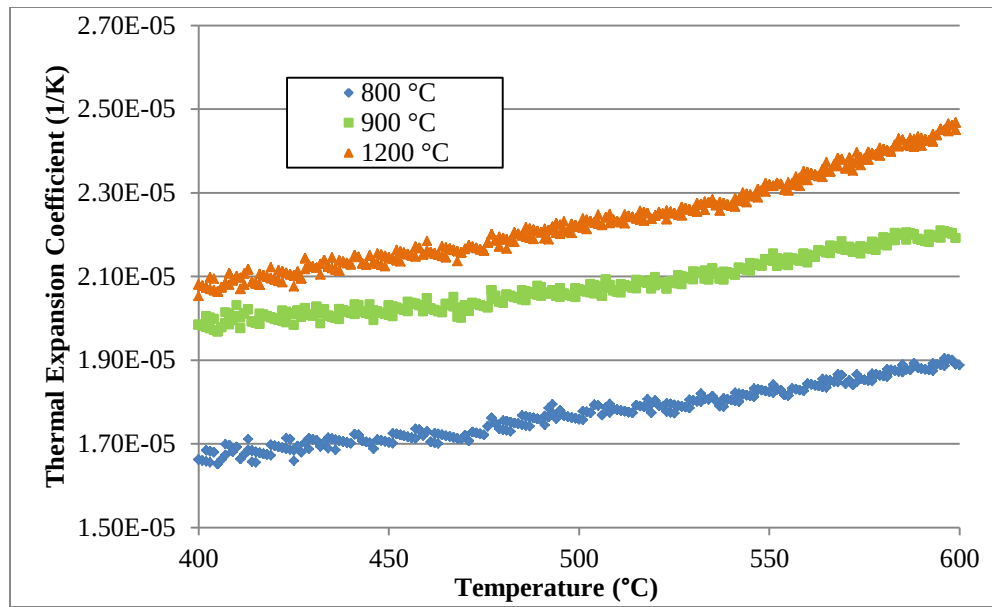


Figure 4.3: Pellet thermal expansion for varying heat-treatment temperatures as a function of temperature.

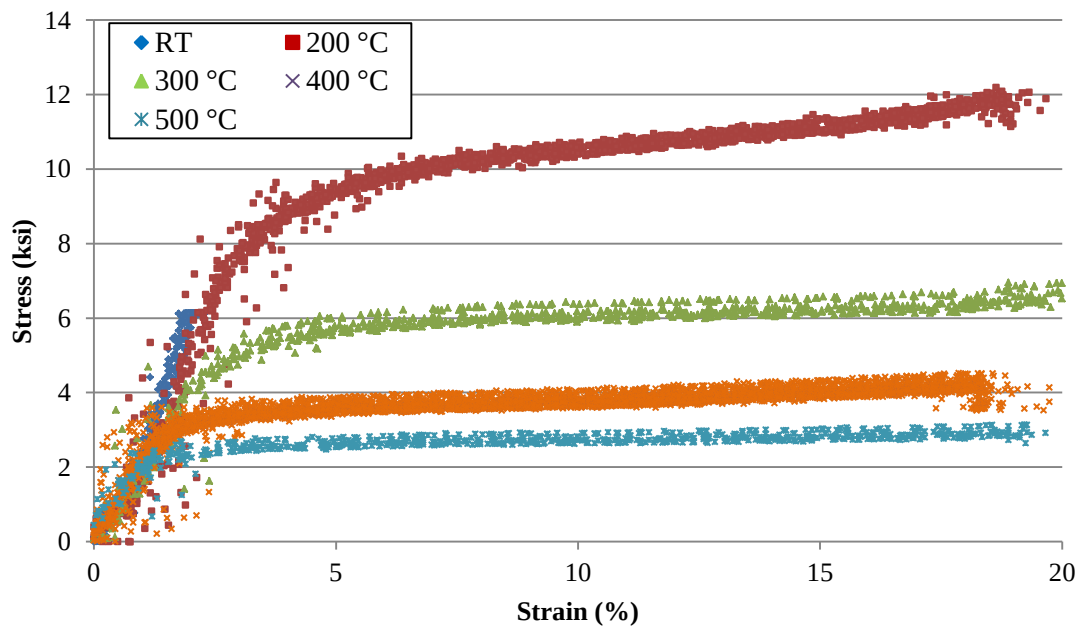


Figure 4.4: Measured pellet stress-strain curves at varying temperatures.

4.2.2.4 Pellet-clad interaction

A tensile specimen irradiation experiment was conducted in order to examine the interaction between the NpO_2/Al material and the 6061 aluminum cladding material, a commonly measured effect in commercial reactors known as pellet clad interaction (PCI). The results, from 3 test capsules of 4 specimens each, concluded that a negligible effect on the cladding strength occurred compared to irradiated cladding material not in contact with the pellet powder [55]. A greater loss in ductility occurred for cladding specimens in contact with NpO_2 , yet this greater loss in ductility (approximately 10%) remained above a 5% elongation at failure.

4.2.2.5 Density, Heat Capacity, Melting Temperature

The pellet material density is typically taken directly or derived from pellet fabrication reports, in conjunction with conservative estimates of volume percentages of components. The current production model uses the same estimated density used in the input heat generation calculations as an initial density and adjusts with respect to thermal and irradiation dimensional changes.

Since the analyses in this report are steady-state and the heat capacity only affects the time derivative of the heat equation, an accurate estimate of the heat capacity is not needed. However, it is input as the heat capacity of aluminum in COMSOL.

The melting temperature of the pellet components NpO_2 and Al are $\sim 2,800^\circ\text{C}$ [88] and 660°C [89], with potential NpO_2 and Al reactants melting by a eutectic reaction above 649°C [90], making the utilized melting temperature of 650°C the safety limit estimate.

4.3 Plutonium-238 Model Governing Physics

The models' governing equations are briefly described below and in the following subsections the inputs, pellet dimensional behavior and gas gap/contact conductance is discussed in greater detail. The models take advantage of the symmetry about the axial centerline of the targets to utilize two-dimensional

(2-D) R-Z or axisymmetric geometry, thus heat transfer and mechanical loads are invariant of the rotation angle.

4.3.1 Heat Transfer

The built-in Heat Transfer physics interface is used, which is governed by the domain equation given in Equation 4.3, where ρ , C_p , and k are the material density (kg/m^3), heat capacity at constant pressure (J/kg-K) and thermal conductivity (W/m-K), respectively. T and u are the field variables, temperature ($^{\circ}\text{C}$) and velocity (m/s), respectively, while t is the time (seconds) and Q is a volumetric heat source (W/m^3). For this problem, the transient heat and convection terms are eliminated as the analysis is for steady-state conditions in a solid medium (excluding fission gas regions).

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{u} \cdot \vec{\nabla} T + \vec{\nabla} \cdot (-k \vec{\nabla} T) = Q$$

Equation 4.3

4.3.1.1 Power Production

Heat source specifications in COMSOL take the form shown in Equation 4.4 below:

$$Q_i = f_{\text{power}} \rho_i \dot{q}_m$$

Equation 4.4

where the subscript i denotes the target component domain, f_{power} denotes the power factor (1.0 for nominal reactor conditions), ρ_i denotes the component material density (kg/m^3), and $\dot{q}_m$ is the component mass-specific heating rate (W/g). The mass-specific heating rates are taken from input neutronics calculations [59], [60], previously discussed. For non-pellet components, the domain-averaged heating rate is commonly given, with an exception for prototypical target components with heights on the order of the target length (the housing/cladding tube, coolant volume, and target holder).

The pellet input heating data takes the form of individual pellet heating rates for the single pellet capsule, with end-of-cycle (EOC) pellet heat loads on the order of ~ 0.3 to 0.5 kW, and partially loaded

target models (total EOC pellet heat loads ~3 to 4 kW). In the fully loaded target model (total EOC pellet heat loads ~12.5 to 16 kW), which contains 52 pellets, heating in “material regions” from the reference calculation is used to generate a mass-specific heating function that is axial position-dependent. The pellet mass-specific heating rate is therefore defined as a 5-degree polynomial and as displayed for the 1st cycle of irradiation for the fully loaded target in Figure 4.5. The radial power production profile was not provided at the time of these analyses; subsequent preliminary estimates put the flux variation from the reactor-facing side to the shielded side in the range of 20% at EOC-2.

Total non-pellet heat loads are highest for the partially loaded target (~1.1 kW), largely due to high neutron absorption material (tantalum) dummy pellets at the end of the 8-pellet stack, followed by single pellet capsules (~0.85 kW) and fully loaded targets (~0.3 kW) which have smaller volumes of non-Al components outside the pellet stack.

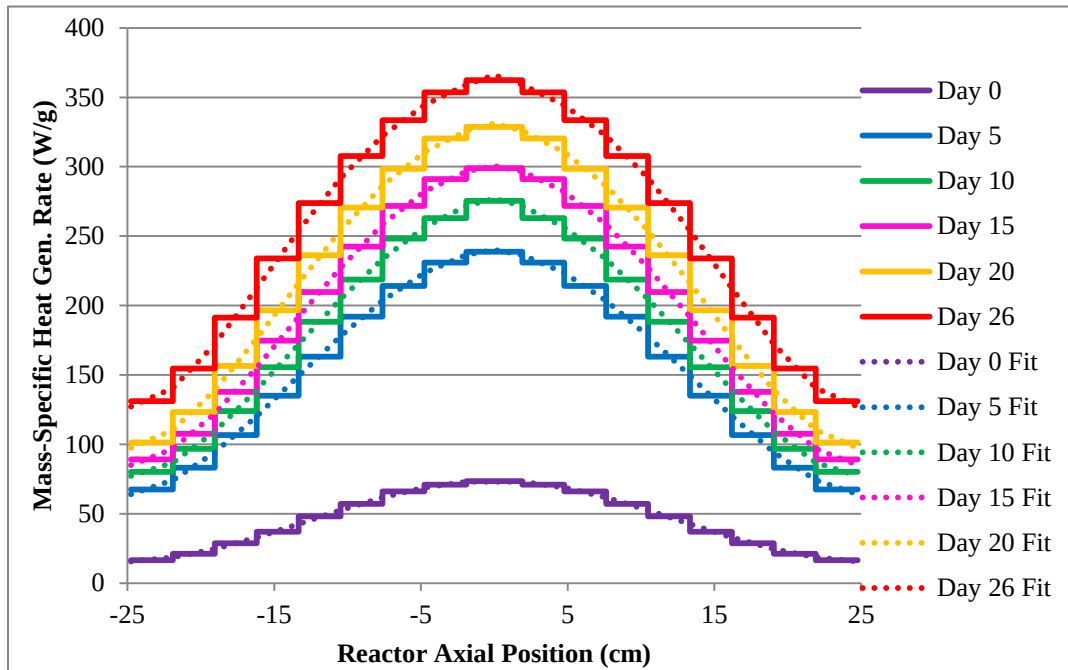


Figure 4.5: Pellet heating rate vs. axial position for the polynomial fits and input data at 0, 5, 10, 15, 20, and 26 days into the 1st cycle.

4.3.2 Solid Mechanics

The solid mechanics interface is designed for structural mechanics in R-Z geometries to solve the dependent variables u, v, and w for displacement. The contact pair conditions and gravity body force are defined under this interface. This physics interface is applied to only the pellet(s) and surrounding components (i.e. housing/cladding tube or heat sinks) in these preliminary models. In addition, the temperature field from the heat transfer interface is used to determine all temperature-dependent properties, serving as a coupling between the two physics.

The interface is governed by the domain equations, Equation 4.5 through Equation 4.7. Equation 4.5 is the equation of motion. where F_V is the volumetric body force or load (N/m³) – gravity is one such body force - and σ is the stress (Pa) in the target:

$$\vec{\nabla}\sigma + F_V = 0$$

Equation 4.5

The strain tensor, ε (-), is given in terms of the displacement field variable, u (m), in Equation 4.6 and the stress tensor, σ (Pa), is related to the strain tensor via Hooke's law in Equation 4.7, where C is the fourth-order elasticity tensor (Pa), the subscript 0 denotes initial stresses and strains, and ε_{th} is the strain due to thermal expansion (-).

$$\varepsilon = \frac{1}{2} \left((\vec{\nabla}u)^T + \vec{\nabla}u + (\vec{\nabla}u)^T \vec{\nabla}u \right)$$

Equation 4.6

$$\sigma = \sigma_0 + C(\varepsilon - \varepsilon_0 - \varepsilon_{th})$$

Equation 4.7

The bottom of the target is fixed in the z-direction to denote the fixed position of the target while sitting in the VXF position. The axial symmetry node applies only to the boundaries at r=0 and represents symmetry in the loads and geometry. These are the only external constraints on the geometry.

All models previous to the production model used the penalty factor method for contact pairs, while the newest production model makes use of a new feature called augmented Lagrangian, considered to be more robust and accurate.

4.3.2.1 Thermal Expansion

The thermal expansion strain (-) is defined as $\epsilon_{th} = \alpha(T - T_{ref})$, where the reference temperature is T_{ref} (~20 °C) and the coefficient of thermal expansion is α (1/K). For all solid domains which are not the NpO_2/Al pellets the coefficient of thermal expansion is retrieved from the built-in material properties in COMSOL, while the pellet thermal expansion property is user-input in the previous section. For the newest production model, the coefficient of thermal expansion is modified to include the irradiation swelling as shown in Equation 4.8.

$$\alpha_{modifiedL} = \alpha_L(T) + \frac{1}{3} \frac{dV}{V} (FD(z, t)) \frac{1}{(T - T_{ref})}$$

Equation 4.8

The first term is simply the material property of the NpO_2/Al pellets, and the second term includes the pellet swelling behavior under irradiation, where dV/V is the pellet volumetric swelling strain (-) as a function of FD, which is the pellet fission density (fissions/cm³) function, that is itself a function of z, the axial position (m), and the irradiation time, t. The pellet swelling behavior is thus included as the pellet volumetric swelling strain divided by the temperature difference term and a factor of three to convert to linear strain (from volumetric) for isotropic materials.

4.3.3 Boundary Conditions

The bottom of the target is fixed in the z-direction to denote the fixed position of the target while sitting in its vertical experiment facility (VXF) position. The axial symmetry node applies only to the boundaries at $r=0$ and represents symmetry in the loads and geometry. Thermally, insulation is assumed at the top and bottom ends of the target. The outside walls of the target experience internal forced

convection from the reactor coolant where the bulk temperature is conservatively calculated and a thermally resistant oxide layer modifies the heat transfer coefficient for the prototypical models, as explained in greater detail in section 4.3.7. These are the only external constraints on the geometry.

Concerning internal boundaries, continuity (in heat transfer and structural) was assumed between components far away from the pellet(s). Conduction in small gas regions between solid components were not modelled to save on meshing and computation time, where either thermal insulation or 1-D heat transfer in the form of thermally resistive layers is conservatively assumed. In models with multiple pellets, the axial heat transfer within a pellet stack is conservatively neglected (i.e. thermal insulation is assumed on NpO_2/Al pellet tops and bottoms) – however, the equations to model this effect are setup to test and confirm that heat transfer is predominantly in the radial direction. The radial heat transfer between pellets and the surrounding components (the lower heat sink or cladding/housing tube) is coupled to the contact pair gap distance in equations explained section 4.3.6.

Contact pairs are applied to internal components that may come into contact or where the gap distance needs to be calculated, where possible, in particular for axial contact between pellets in a pellet stack and between pellet(s) and radially adjacent components. The prototypical models in Chapter 5 used the penalty factor method for contact pairs, while a modified version of the penalty method, augmented Lagrangian, which is better at preventing penetration, was used for the production model in Chapter 6.

4.3.4 Contact Conductance

This section describes the local definitions that are used to calculate the “solid spot” or contact conductance between the pellet sides and housing tube, which is a function of the contact pressure and material properties. In addition, some other material properties are defined under this variable grouping.

For the purpose of the contact conductance calculation, the following defined properties of the contacting surfaces are solved: the harmonic mean of the thermal conductivity, k , the effective or reduced elastic modulus, E' , and the effective combined surface roughness, σ , as shown in Equation 4.9 through

Equation 4.11. In equation form, these definitions are obtained from Equation 3.3 on page 23 and the example on page 40 from Madhusudana [91].

$$k_m = \frac{2 k_1 k_2}{k_1 + k_2},$$

Equation 4.9

$$E' = 2 \left[\left\{ (1 - \nu_1^2) / E_1 \right\} + \left\{ (1 - \nu_2^2) / E_2 \right\} \right]^{-1},$$

Equation 4.10

$$\sigma = (\sigma_1^2 + \sigma_2^2)^{0.5}$$

Equation 4.11

where the indices 1 and 2 in the equation above denote the two adjacent materials meeting at the gap and k, E, ν , and σ denote the thermal conductivity (W/m-K), Young's elastic modulus (Pa), Poisson's ratio (-), and surface roughness (m), respectively. For the side gaps, the materials are Al-6061 T4 temper (-t4) and the NpO_2/Al pellet.

The mean absolute slope of the asperities, m (-), representing the unevenness or ruggedness of a surface of the side pellet gap, is defined here. This quantity is purely a function of the surface roughness, and is also often written as “ $\tan \Theta$ ”, and is found in [92] in equation form as shown in Equation 4.12.

$$m = 5253 \sigma^{0.743}$$

Equation 4.12

A sensitivity study is conducted on this parameter to ensure use of the above correlation is accurate, where other correlations by Lambert [93] and Antonetti [94] are used to form a bounding estimate given the significant range shown in measurements [95], [96].

The Garimella reference [92] is originally used in the prototypical models. However, it is bounded by the Antonetti correlation over all surface roughness values and the Lambert correlation provides a bounding value for these two correlations for larger surface roughness values. The conservative

estimation of the mean absolute slope of asperities, used in the production model, is thus the minimum of all three correlations as shown in Equation 4.13:

$$m = \min \left\{ \begin{array}{ll} \textit{Garimella} & 5253 \sigma [1/m]^{0.743} \\ \textit{Lambert} & 0.076 \sigma [1/\mu m]^{0.52} \\ \textit{Antonetti} & 0.124 \sigma [1/\mu m]^{0.743} \end{array} \right\}$$

Equation 4.13

The solid spot conductance for elastic deformation, h_e , for the contacting surfaces is defined here. This portion of the total gap conductance represents that portion due to the pressure forces acting on the two touching solid surfaces. Note that the quantity $\tan \Theta$ also is written here as the variable m which denotes the mean absolute slope of the asperities. In equation form the elastic solid spot conductance, h_e (W/m²-K), is written as Equation 4.14 [91], [92]:

$$h_e = 1.55 \left(k_m m / \sigma \right) \left(P \sqrt{2} / E' m \right)^{0.94}$$

Equation 4.14

where the variable P denotes the surface pressure (Pa) acting on the surface. The pellet side surface receives pressure that results from the forces computed by the side gas-gap closure due to the thermal expansion and irradiation swelling of the pellet into the target housing. A separate variable is defined for this side contact pressure which requires utilization of a COMSOL feature which maps the surface pressure from the housing to the adjacent surface on the pellets. This variable must be maximized against a minimum pressure, chosen as 1 Pascal, in order to prevent zero divides.

The solid spot conductance for plastic deformation of the contacting surfaces, h_p (W/m²-K), is defined in Equation 4.15 [91].

$$h_p = 1.13 \left(k_m m / \sigma \right) (P/H)^{0.94}$$

Equation 4.15

where H is the hardness (Pa) of the softer surface material or minimum hardness of the two mating surfaces. It has been observed that the solid spot conductance under elastic deformation gives a conservatively lower value than the plastic deformation definition, and commonly this is used for all model versions except the production model. However, a plasticity index, $\psi(-)$, as defined in Equation 4.16 [91] may be used to determine the type of deformation:

$$\psi = m \frac{E'}{H}$$

Equation 4.16

where a value above 1.0 has been observed to exhibit plastic deformation even at light loads and a value below 0.7 exhibits elastic deformation even under heavy loads. A linear interpolation of the two conductance values for a plasticity index range between 0.7 and 1.0 is then utilized (only in the production model) to complete the continuous function of contact conductance, h_s (W/m²-K), as a function of plasticity, as shown in Equation 4.17:

$$h_s(\psi) = \begin{cases} \psi < 0.7 & h_e \\ 1.0 > \psi > 0.7 & \frac{1.0 - \psi}{0.3} (h_p - h_e) \\ \psi > 1.0 & h_p \end{cases}$$

Equation 4.17

The “mean separation between the surfaces” of two surfaces under conforming contact as provided by Equation 4.18 [91] represents a mean minimum gap distance (m), δ_{mean} , as input to the gap conductance defined in a later section, or alternatively the combined surface roughness may be used for significant pressures.

$$\delta_{mean} = 1.53 \sigma (P/H)^{-0.097}$$

Equation 4.18

where P/H is the ratio of applied surface pressure and the surface hardness. The hardness is set to be the minimum of the hardness of the two mating surfaces. The applied surface pressure is assumed constant at

the pressure created by the spring force at both the top and bottom surfaces. This feature is generally only used for axial conduction between pellets, however since this is insignificant for the prototypical designs it is neglected by the conservative assumption that no axial conduction occurs between pellets.

4.3.5 Fission Gas

The definitions in this section are used to ultimately calculate the effect of fission gas release on the heat transfer in the gas gap, via a reduction factor to the gas thermal conductivity, weighting factors used to calculate each gas's contribution to the “thermal jump” effect explained later, as well as mass fractions used to calculate gas mixture material properties.

The initial number of moles of helium is estimated by the following equation based on the ideal gas law (see Equation 4.19) , where n is the number of moles, P is pressure (Pa), V is volume (m^3), R is the ideal gas constant $0.0821 \text{ atm-L}/(\text{mol-K})$, and T_{ref} is the reference temperature (K) at fabrication:

$$n_{He0} = \frac{P_{He} * V_{He}}{R * T_{ref}}$$

Equation 4.19

The number of moles, n , of helium, xenon, and krypton gas can be calculated by the following equations Equation 4.20 and Equation 4.21:

$$n_{He} = f_{He} * n_{HeFiss} + n_{He0}$$

Equation 4.20

$$n_i = f_i * n_{iFiss}$$

Equation 4.21

where the subscript i denotes the fission gas element xenon or krypton, f is the fission gas release fraction, and n_{iFiss} is the fission gas inventory of element i in moles.

The mole fractions, x , of helium, xenon, and krypton are calculated in Equation 4.22, where the subscript i denotes the fission gas element:

$$x_i = \frac{n_i}{n_{He} + n_{Xe} + n_{Kr}}$$

Equation 4.22

The mass of helium, xenon, and krypton gas can be calculated by Equation 4.23, where m is mass, M is molar mass or atomic weight (in grams), and the subscript i denotes the fission gas element:

$$m_i = n_i * M_i$$

Equation 4.23

The mass fractions, mf_i , are then simply the ratio of the mass of the gas of interest to the total of the three fission gas masses as shown in Equation 4.24, using the definitions from Equation 4.23.

$$mf_i = \frac{m_i}{m_{He} + m_{Xe} + m_{Kr}}$$

Equation 4.24

An intermediate dimensionless variable, C_i , used to calculate a gas weighting factor for helium, xenon, and krypton gas, can be calculated by Equation 4.25. Where following, a gas weighting factor, w_i , for helium, xenon, and krypton, which is used in Equation 4.36, is finally calculated in Equation 4.26.

$$C_i = \frac{mf_i}{(M_i)^{\frac{1}{2}}}$$

Equation 4.25

$$w_i = \frac{\frac{mf_i}{(M_i)^{\frac{1}{2}}}}{\sum_{j=1}^3 \frac{mf_j}{(M_j)^{\frac{1}{2}}}} = \frac{C_i}{\sum_{j=1}^3 C_j}$$

Equation 4.26

The thermal conductivity of the resulting gas mixture within the capsule is approximated by a reduction factor in the thermal conductivity of the pure helium gas, f_{kHe} . This can be estimated by a

curve fit, f_{kNASA} , of the xenon-gas mole fraction and is derived from a NASA reference set of measurements [97] as Equation 4.27. In addition, two conservative curve fits are derived from data that is found in the TPMD [98] – for a thin-hot wire (see Equation 4.28), $f_{kthinwire}$, and thick-hot wire (see Equation 4.29), $f_{kthickwire}$, method of measuring the thermal conductivity. These curve fits conservatively include the sum of the krypton and xenon mole fractions in place of the xenon mole fraction. The reduction in helium thermal conductivity is therefore the average of these three fits as shown in Equation 4.30.

$$f_{kNASA} = -1.7299 * (x_{Xe} + x_{Kr})^5 + 5.6988 * (x_{Xe} + x_{Kr})^4 - 7.7342 * (x_{Xe} + x_{Kr})^3 + 5.9074 * (x_{Xe} + x_{Kr})^2 - 3.1041 * (x_{Xe} + x_{Kr}) + 1$$

Equation 4.27

$$f_{kthinwire} = -0.5372 * (x_{Xe} + x_{Kr})^5 + 2.6203 * (x_{Xe} + x_{Kr})^4 - 4.9526 * (x_{Xe} + x_{Kr})^3 + 4.9348 * (x_{Xe} + x_{Kr})^2 - 3.0198 * (x_{Xe} + x_{Kr}) + 1$$

Equation 4.28

$$f_{kthickwire} = 2.9406 * (x_{Xe} + x_{Kr})^6 - 10.5127 * (x_{Xe} + x_{Kr})^5 + 15.6983 * (x_{Xe} + x_{Kr})^4 - 13.4061 * (x_{Xe} + x_{Kr})^3 + 7.7818 * (x_{Xe} + x_{Kr})^2 - 3.4658 * (x_{Xe} + x_{Kr}) + 0.9999$$

Equation 4.29

$$f_{kHe} = \frac{(f_{kNASA} + f_{kthinwire} + f_{kthickwire})}{3}$$

Equation 4.30

Generally, the thin-hot wire method results and NASA results agree fairly well, while the thick-hot wire is usually more conservative (has a greater reduction in helium thermal conductivity) than the other two. The initial single pellet models used the NASA fit with only the xenon mole fraction as a fit

parameter, later the other fits and krypton mole fraction were added in the prototypical models for greater conservatism.

4.3.6 Thermal Gap Jump

The definitions in this grouping are used to calculate the thermal or gap “jump” effect described in [91]: an artificial addition to the gap separation distance between two metal surfaces used to account for the ineffectiveness of gas-to-solid heat transfer. The gap jump distance is calculated at three locations across the gap: at the pellet outer surface, the housing inner surface, and the center or average gap. As an improvement to previous models, the gap distance contributions to both sides are added to arrive at a more accurate total gap jump distance ([91], Equation 4.6), rather than using an average value. This is found to be conservative with respect to the average gas gap approximation.

In order to calculate these gap jump distances separately, all of the parameters contained herein are calculated using the gas/surface temperatures at the appropriate locations. The pellet surface temperature, T_p , and inside housing temperature, T_h , are calculated using surface coupling operators, while the average gap temperature, T_g , is the average of the two. All subsequent definitions related to the gap jump calculation (as shown below) are then recreated with subscript **p**, **h**, or **g** to denote their values at the pellet side, housing side, and average gap locations, respectively. These definitions without subscripts are evaluated at their local values in the model.

The data available for the accommodation coefficient of gases, a dimensionless variable that characterizes the energy transfer efficiency between surface atoms and a colliding gas molecule, is specific to metal types and its surface cleanness. Therefore, the specific gas-metal accommodation coefficient is difficult to find for this application and relations for UO_2 were generally preferred.

The accommodation coefficient for helium gas, α_{He} , was taken from page 51 of [91], based on experimental results of UO_2 and stainless steel surfaces, and is represented as a variable to be as shown in Equation 4.31, where the temperature T is in units of Kelvin. The accommodation coefficient function

for xenon gas (see Equation 4.32), α_{Xe} , was taken from measurements by Ullman et al. [99] for UO_2 and stainless steel surfaces correlated by Thomas and Loyalka [100]. An interpolation based on atomic or molecular weight between the two correlations for xenon and helium gas was used for krypton's accommodation coefficient, α_{Kr} , as shown in Equation 4.33. This krypton accommodation coefficient was found to be bounded, on the high side, by the suggested value of 0.8 ± 0.1 from Hall and Martin for UO_2 surfaces [101], which is conservative in the context of the final thermal jump definition, later defined.

$$\alpha_{He} = 0.425 - 2.3 \times 10^{-4}T$$

Equation 4.31

$$\alpha_{Xe} = 0.749 - 2.5 \times 10^{-4}T$$

Equation 4.32

$$\alpha_{Kr} = \alpha_{He} + (M_{Kr} - M_{He}) * \frac{\alpha_{Xe} - \alpha_{He}}{M_{Xe} - M_{He}}$$

Equation 4.33

These variables represent the mean free path of the respective gases. An equation for the mean free path of a gas is readily available (for example, from [102], page 9-2, equation 2) as Equation 4.34:

$$\lambda_{gas} = \left[\frac{1}{\sqrt{2}\pi n d^2} \right] = \left[\frac{k_B T}{\sqrt{2}\pi d^2 p_{gas}} \right]$$

Equation 4.34

where:

n = the number of gas molecules per unit volume (molecules/m³),

k_B = Boltzmann's constant = $1.38060504 \times 10^{-23}$ J/K,

T = the temperature of the gas which is a solved field in the COMSOL model (K),

d = the collision diameter of the gas molecule (m), and

p_{gas} = the pressure of the gas which is an input to the COMSOL model (Pa).

The mean free path for the fission-product gases Xe and Kr were previously calculated using ratios to helium at constant temperature [103], however their mean free path is now calculated using the equation above and their molecular or collisional diameters. While the solution is not very sensitive to this parameter, the gas collision or molecule diameter is derived as the average from three different methods of characterization: Van der Waals radii [104], [105], viscosity [105], and second virial coefficients [106]. The helium pressure is assumed to be constant at the pressure during the capsule assembly at 1 atm.

These variables represent the “temperature jump distance” and are specific to individual gases as provided by Equation 4.35[91] and repeated here

$$g = \frac{(2 - \alpha)}{\alpha} \frac{2}{(\gamma + 1)} \frac{k_g}{(\mu C_v)} \lambda = \frac{(2 - \alpha)}{\alpha} \frac{2\gamma}{(\gamma + 1)} \frac{k_g}{(\mu C_p)} \lambda$$

Equation 4.35

where

α = accommodation coefficient (-),

γ = ratio of specific heats = C_p/C_v (-),

k_g = thermal conductivity of the gas (W/m-K),

μ = dynamic viscosity of the gas (Pa-s),

C_p, C_v = gas heat capacity (J/kg-K) at constant pressure and volume, respectively, and

λ = mean free path of gas molecules (m).

The gas jump for a mixture of gases on a single surface is then a combination of each calculated gas jump as shown by Equation 4.36[91] and simplified by the weighting factors from Equation 4.26.

$$g_m = \frac{\sum (x_i g_i / M_i^{0.5})}{\sum (x_i / M_i^{0.5})} = \sum_{i=1}^3 w_i g_i$$

Equation 4.36

where

x_i = mass fraction of constituent gas i (-),

M_i = molecular mass of constituent gas i (g), and

g_i = temperature jump distance of constituent gas i (m).

The definitions from this section lead to the definition of the gas gap conductance in Equation 4.37, calculated as the one-dimensional (1-D) conductance relation of thermal conductivity of the fill gas helium, k_{gHe} (W/m-K), over gap distance, δ (m), with the modifications of (1) a thermal conductivity reduction factor, f_{kHe} (-), from Equation 4.29 due to fission gas release, and (2) thermal “jump” distances, g_i (m), from Equation 4.36 for each surface that are used to account for inefficient gas-to-solid heat transfer particular to that surface/gas combination.

$$h_g = \frac{f_{kHe} k_{gHe}}{\delta + g_1 + g_2}$$

Equation 4.37

where δ is the physical gas-gap size between the two surfaces.

The total thermal conductance, h (shown in Equation 4.38), between two surfaces (the pellet and cladding/housing here) is then the sum of the gap conductance and contact conductance (defined previously), where radiation conductance, h_r , is conservatively considered negligible due to the low absolute temperatures in the target.

$$h = h_c + h_g + h_r = h_c + h_g = h_c + \frac{k_g}{\delta + g_1 + g_2}$$

Equation 4.38

In COMSOL, the total gap resistance heat transfer, h_s , is input, according to the above and previous sections' definitions as shown in Equation 4.39.

$$h_g = k_s/d_s = h_c + \frac{f_{kHe} k_{He}(T)}{\max(\sigma, \delta) + g_1 + g_2}$$

Equation 4.39

4.3.7 Target Surface: Heat Transfer Coefficient, Bulk Temperature, and Oxide Layer

The target surface cooling for the single pellet models was calculated using a different heat transfer coefficient and no inclusion of bulk temperature or oxide layer effects, therefore the methodology discussed here is for the prototypical and later target models.

The average heat transfer coefficient, h , is used for internal forced convection as a convection-cooling boundary in COMSOL and is obtained from Incropera [107]. The functional form used is shown in Equation 4.40. The calculated heat transfer coefficient is alternatively compared to external forced convection correlations [107] and Dittus-Boelter, with the finding that differing calculations of the heat transfer coefficient have negligible impact on the final solution.

$$\begin{aligned} Re_D \leq 2500 \quad h &= 3.66 \frac{k}{D} \\ Re_D > 2500 \quad h &= 0.027 \frac{k}{L} Re_D^{4/5} Pr^n \left(\frac{\mu}{\mu(T)} \right)^{0.14} \end{aligned}$$

Equation 4.40

where:

Pr = the Prandtl number, $\mu C_p / k$,

Re = the Reynolds number, $\rho UL / \mu$,

D = the hydraulic diameter,

μ = the dynamic viscosity of water,

C_p = the heat capacity of water,

ρ = the density of water, and

U = the coolant velocity, given by a calculated 5.0 gallons per minute (gpm) volumetric flow and maximum channel dimensions.

n = 0.4 if $T < T_{\text{bulk}}$ and 0.4 if $T \geq T_{\text{bulk}}$.

In COMSOL, several variables define the total heating for discrete target components as a function of axial position along the coolant flow direction, where they have a minimal value of zero at the top of the target and maximum at the bottom of the target. These variables are most simply described as the local mass-specific heating multiplied by the local density, cross-sectional area and axial position of the component(s).

The bulk temperature is a function of axial centerline position and it makes use of the above variables. The equation to determine it is a simple heat balance, where all heat generated in the target is removed to the coolant flow, assuming no other heat sinks, as shown in Equation 4.41:

$$T_{\text{bulk}}(z) = pf \frac{z \sum H_i \rho_i A_i}{\dot{V}_w \rho_w C_{pw}} + T_{\text{inlet}}$$

Equation 4.41

where:

T_{bulk} = bulk coolant temperature,

pf = the power factor fraction (1.0 or 1.3),

z = the axial position along the coolant flow,

H_i = the mass-specific heating rate of component i ,

ρ_i = the density of component i ,

A_i = the cross-sectional area of component i ,

$\dot{V}_w$ = the coolant volumetric flow rate, 5 gpm, and

T_{inlet} = the inlet temperature (at the top of the target).

The following definitions are used to calculate the thickness of an oxide layer on the aluminum target surface. Per the HFIR SAR, Chapter 4, corrosion is expected on the fuel plates and oxide buildup correlations are used based on measurements with aluminum. These correlations are conservatively applied here although there is reason to expect that at the much lower heat fluxes this buildup would be considerably less or negligible (target fluxes are $\sim 3 \times 10^3$ Btu/(h-ft²) compared to the experimental range of 1.0 to 2.0×10^6 Btu/h/ft²). The oxide buildup correlation from the HFIR Safety Analysis Report [56] (developed for the HFIR aluminum fuel plates as detailed in [108]) is conservative for estimating the thickness of oxide buildup on the target housing.

The oxide thickness is given by the correlations referenced previously and is shown in Equation 4.42. And the buildup terms, ψ_{k-1} , are used to include the effect of buildup from previous cycles, as shown in Equation 4.43.

$$X_k = 443(\psi_{k-1} + t)^{0.778} e^{\frac{-8290}{T_{Sk}}}$$

Equation 4.42

where:

X_k = the oxide layer thickness for cycle k (mils),

t = the time in the kth operating cycle (hours), and

T_{Sk} = the surface temperature of the target for cycle k (°R).

$$\psi_{k-1} = (\psi_{k-2} + \Delta t) e^{10,656 \frac{T_{Sk-1} - T_{Sk}}{T_{Sk-1} T_{Sk}}}$$

Equation 4.43

where:

ψ_k = the buildup term for cycle k (hours), and

Δt = the 26-day operating cycle time (hours).

The oxide layer is modeled by using the computed oxide layer thickness to provide additional heat transfer resistance between the plate surface and the coolant bulk temperature. This is equivalent to utilizing a COMSOL “thin film resistance” and is implemented by coupling this boundary condition to the convective cooling boundary condition by the adjustment to the heat transfer coefficient shown in Equation 4.44.

$$h_{modified} = h \frac{1}{1 + \delta_{oxide} \left(X_{oxide} * \frac{h}{k_{oxide}} \right)}$$

Equation 4.44

where:

δ_{oxide} = an “on/off switch” for the oxide buildup that has a value of 0 or 1,

h = the convective cooling heat transfer coefficient, and

k_{oxide} = the thermal conductivity of the oxide, boehmite, 1.3 Btu/(h-ft-degF) [108].

4.4 Solver Methodologies

Two solution methods were used: 1) direct fully-coupled solver was the preferred setting for the solver for all models, solving all equations in one step, and 2) a segregated solver using a lumped fully coupled step of the temperature and displacement field variables, followed by a second solution step of the contact pair variable(s). The former method was primarily used and preferred, although it uses greater computational resources and poses greater convergence issues, due to its more robust and accurate solutions.

A steady-state solution is sought and obtained for all solutions shown in this report to the default residual value of 1e-3. A smaller residual, .e.g., 1.0e-6, will typically add several iterations, but no

significant change in the temperature field, the maximum of which, is usually what is being examined for this type of simulation.

The initial guess for the solution is important to convergence, sometimes requiring manual scaling of the field variables in order to improve stability or speed. The difficulty in model convergence, particularly for those cases with strong contact between the pellet side and inside containment housing tube surface, has commonly required approaching solutions with an increased load, either increasing the power factor, irradiation day, or other parameter in increasing steps, while using the previous solution as an initial guess.

The finite-element basis function that is used for the variable interpolation between node points of the model observed some variation for each model, where its increase, along with the solution mesh, considerably increases both the computation resources and accuracy of the solution. Linear, quadratic, and cubic linear basis function were used, with commonly either quadratic or cubic basis solutions used for the final solution. In addition, mesh refinements were commonly performed to ensure adequate solution convergence, with variations in memory usage between a few GB to around 25 GB.

5 Plutonium-238 Production Studies: Prototypical Target Models

The prototypical targets included the partially loaded and fully loaded targets, both of which were qualified for two cycles. During model development, careful awareness of the qualifying PIE data (typically not yet available) was needed in order to ensure that the calculation scope would adequately ensure the safe irradiation of the targets. This often required parametric approaches, including solutions sweeping and solution searching methods, which would provide outputs within the anticipated range of qualifying PIE data.

The prototypical models shared common features including both being modeled in 2-D R-Z cylindrical or axisymmetric geometries, which offered improvement on computation memory and time over a 3-D geometry. With increasing number of pellets and pellet side surfaces (8 or 52) however, the need to solve the structural mechanics equations over a larger domain and the highly non-linear contact heat transfer over a larger surface area created challenges in assuring model accuracy and convergence.

5.1 *Prototypical Target Geometries*

As opposed to a top-down approach of geometry building by importing CAD geometries into COMSOL, a bottom-up approach was taken for the prototypical target geometries, building the geometries entirely from global parameters defined in COMSOL. This was done in order to gain easier control of the model geometry, for purposes of adjusting to conservative design tolerances and to be able to execute parametric sweeps to examine the effects of geometry changes, among other reasons.

The partially loaded target (see Figure 5.1) was the first of the prototypical target designs, all around 33" in length, with many features that hold over for the fully loaded target and production target designs. The Al-4047 top end cap (TEC) and bottom end cap (BEC) both contained plenums for increased helium volume and the TEC had a threaded top for HFIR operations removal of the target. A TIG weld at the BEC and an E-beam weld at the TEC connect the end caps to the housing tube. Two stainless steel grade 316 (SST316) spacer tubes are at either end of the target, a lower spacer tube (LST) and an upper spacer

tube (UST), with thin walls to accommodate a greater plenum volume. The pellet stack contains eight (8) NpO_2/Al pellets, around $\sim 0.25''$ diameter and $\sim 0.375''$ in length, with a tantalum (Ta) dummy pellet at either end, which is placed to dampen end flux peaking with its high neutron absorption cross section. A ~ 35 mil thick Al-6061-t4 housing tube encapsulates the internal components, containing six outer fins designed to stabilize the target in its holder (to prevent excess vibration) and to better mix flow.

The fully loaded target geometry (see Figure 5.2) shares several common features with the partially loaded target, including a TEC with a threaded top and helium plenum. However, the end caps are Al-6061-t6 and the welds are switched to an E-beam weld at the TEC and TIG weld at the BEC, which has no plenum and uses an additional swage joint, to complete the target encapsulation. Due primarily to a large increase in the pellet stack, the lengths of the spacer tubes significantly decrease. A weld backing/support tube (WBT) is added below the UST to support the E-beam weld. The dummy pellet material is now Al-6061-t6, as damping pellet end fluxes is no longer a major concern for the large pellet stack, with aluminum weld wires at their center. The major difference is a 50-52 NpO_2/Al pellet stack that increases the stack length from $\sim 3''$ to $\sim 19.5''$. The housing tube is of similar design using ~ 35 mil thick Al-6061-t4.

5.1.1 Target Holder Geometry

The target holder geometry for the prototypical models (as well as the production model in chapter 6) is the same, made of an aluminum alloy consistent with other HFIR holders. Seven prototypical target pins are held in seven bolt holes that act as coolant channels to each pin or target. One pin is located in the center of the holder, with six outer pins rotated 60° around the holder. By convention, “Pin 1” is denoted as the pin facing the reactor core with the other pins named sequentially in the clockwise direction and pin 7 as the center pin. Pin 1, being closest to the reactor core, experiences the highest heat generation rates and therefore receives the greatest degree of examination by these safety calculations.

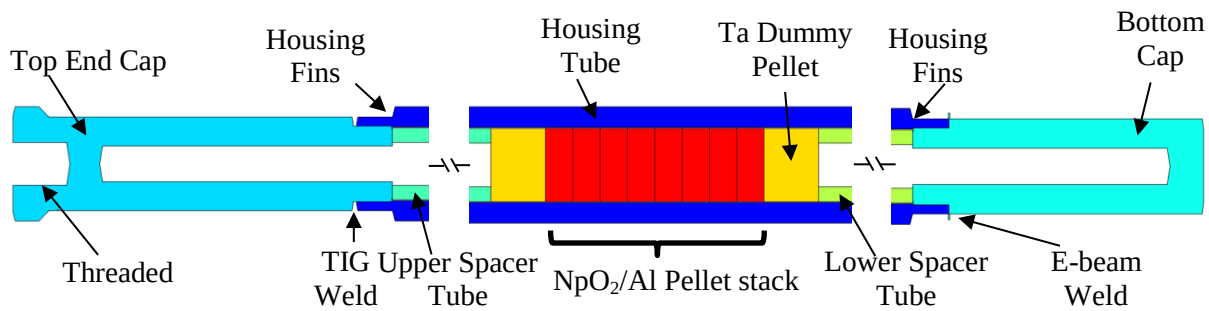


Figure 5.1: Representation of partially loaded model target pin components.

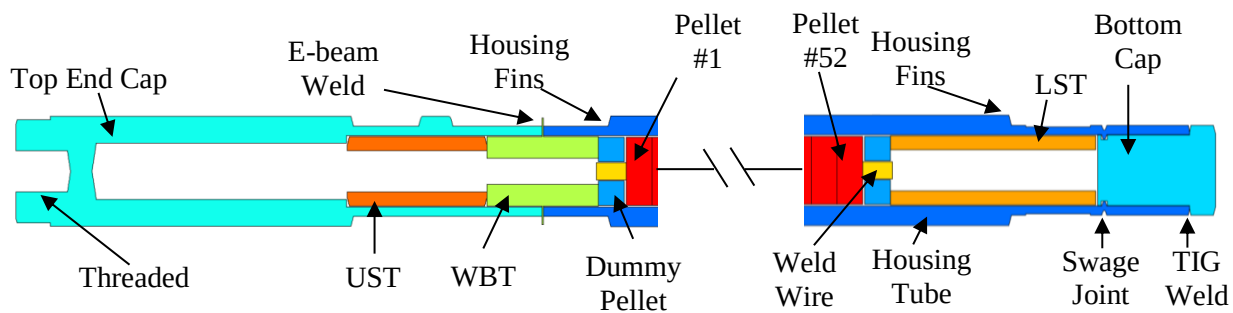


Figure 5.2: Representation of fully loaded model target pin components.

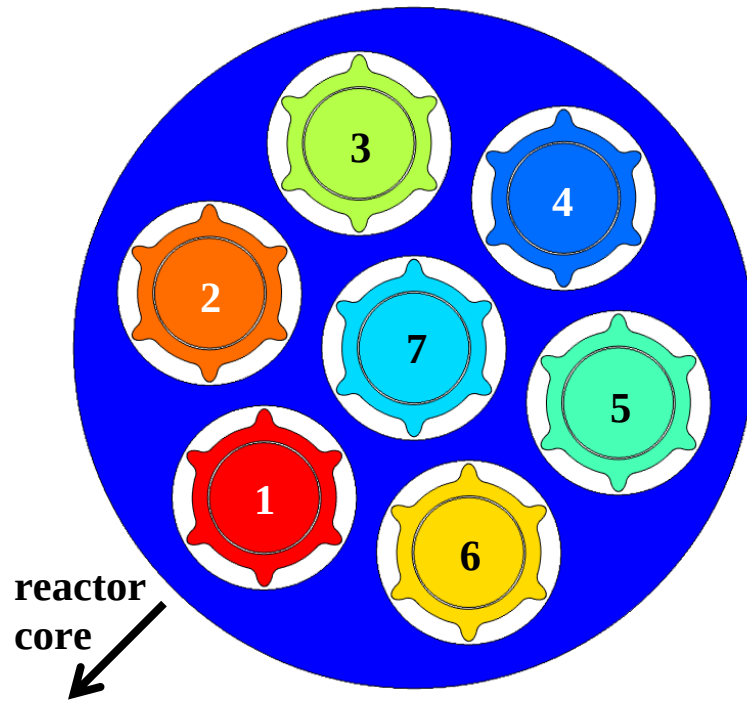


Figure 5.3: Radial cut-view of prototypical target holder with seven prototypical target “pins”.

5.2 *Prototypical Mesh*

A total of five mesh sizes were employed to analyze these models. These 5 mesh sizes, in order of increasing detail, are designated: (1) extremely-coarse, (2) extra-coarse, (3) coarse, (4) normal, and (5) fine. Each mesh case is characterized by a free mesh size name that corresponds to the mesh case names (extremely-coarse, extra-coarse, coarse, normal, and fine). Four mesh cases were analyzed for the partially loaded target and fully loaded target models as listed in Table 5.1. It is worth noting that COMSOL offers nine increasingly detailed default free mesh levels (only some of which are used here) in order: (1) extremely-coarse, (2) extra-coarse, (3) coarser, (4) coarse, (5) normal, (6) fine, (7) finer, (8) extra-fine, and (9) extremely-fine.

The mesh is designed so that the pellet mesh is the dominate control feature of the mesh design. This was done after preliminary analysis revealed that the predominate temperature change in the problem occurs in and around the pellet, with all other temperature features extending out beyond the pellet requiring less detail than within the pellet.

An extensive mesh-density evaluation of this problem was performed early in the study and revealed that the mesh case 1 (extremely coarse for the fully loaded target model and extra coarse for the partially loaded target model) was sufficient to analyze this problem provided that a quadratic finite-element basis function was also exercised with the fine-mesh to confirm that the quadratic-basis function at the first (1st) mesh level was sufficiently accurate. Therefore, the results corresponding to mesh cases 2, 3, and 4 are not the utilized results, only the 1st mesh case results will be examined in this section excluding mesh refinement efforts.

The primarily used mesh cases for each target model (extremely-coarse and extra-coarse for the fully loaded and partially loaded target, respectively) are shown in the pellet domain in Figure 5.4. Higher mesh levels (coarse, normal, and fine) are shown for the pellet domain in Figure 5.5. The extremely-coarse, extra-coarse and fine mesh in the pellet and housing-adjacent domains are shown in Figure 5.6.

Table 5.1: Mesh cases for partially and fully loaded target analyses.

Mesh Case	Mesh Size	
	Partially Loaded Targets	Fully Loaded Targets
1	extra-coarse	extremely-coarse
2	coarse	extra-coarse
3	normal	normal
4	fine	fine

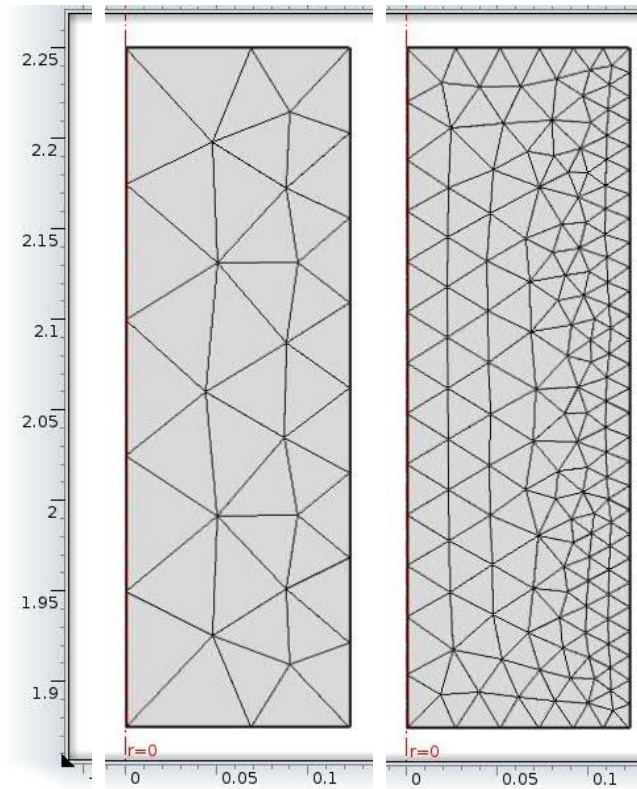


Figure 5.4: Extremely-coarse and extra-coarse mesh at the pellet domain that serve as the primary mesh for the fully and partially loaded targets, respectively.

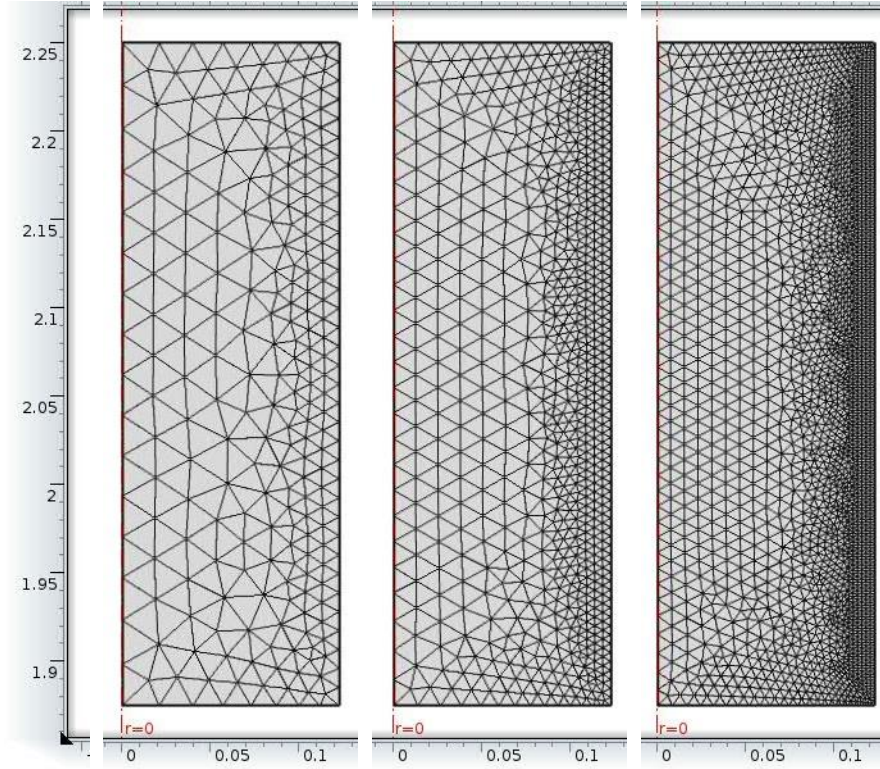


Figure 5.5: Coarse, normal, and fine mesh at the pellet domain.

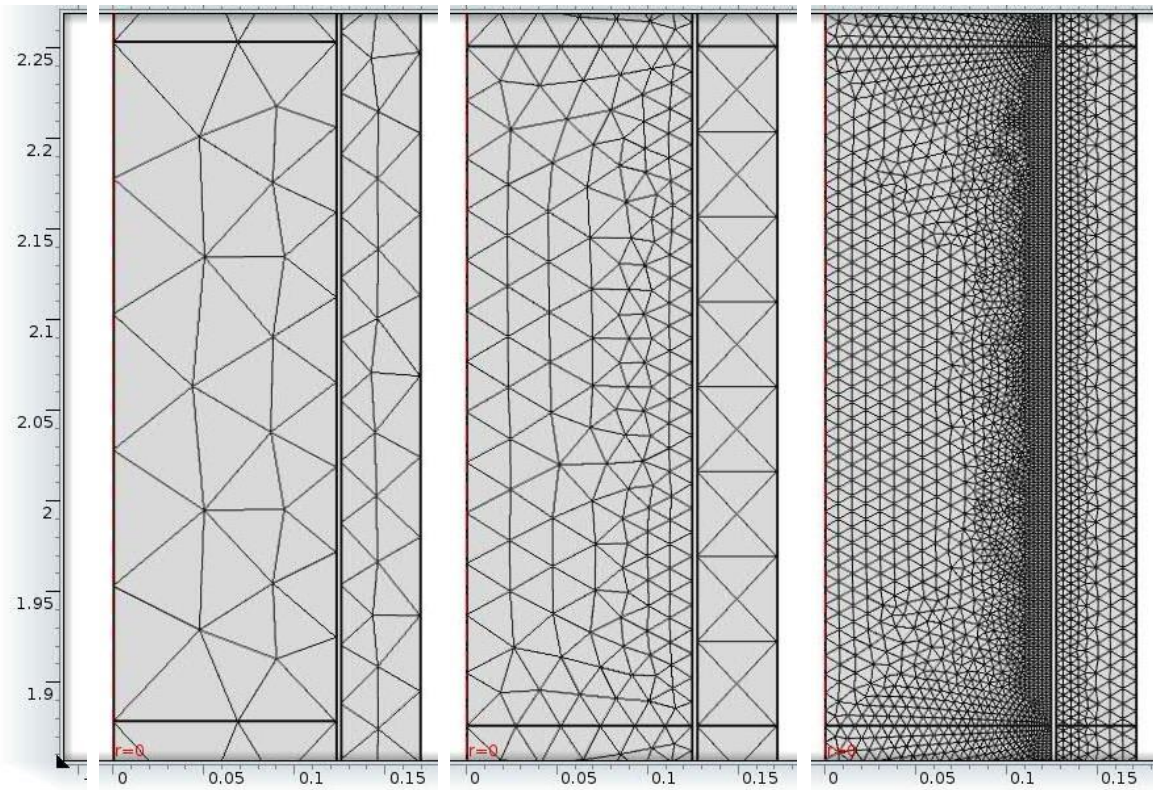


Figure 5.6: Extremely-coarse, extra-coarse, and fine mesh at the pellet and housing adjacent domains.

The extra-coarse mesh in the domain of the TEC and BEC welds is shown in Figure 5.7 and Figure 5.8, respectively, for both the partially loaded and fully loaded target models.

5.3 *Partially Loaded Target Model*

The partially loaded target model, containing eight (8) NpO_2/Al pellets, marked a significant diversion from previous target designs as well as in the modeling methodology from the single pellet capsules. The target consists of a prototypical design including a pellet stack inside an aluminum tubing cladding, with end caps welded to the “housing tube” cladding. Internal components include spacer tubes and tantalum dummy pellets at the ends of each stack in order to decrease flux peaking at the pellet stack ends. After target fabrication, the housing tube is hydrostatically collapsed onto the internal components, in order to minimize the radial gas gap, and helium-leak checked to ensure integrity of the welds.

The target model uses a 2-D R-Z geometry, in order to take advantage of the axial symmetry of the target and decrease computational resource demands that would otherwise prove significant given the increase in pellet loading. In addition, many of the equations and inputs, particularly for the fission gas inventories, are updated and improved for improved accuracy and/or to identify areas requiring greater conservatism.

5.3.1 Partially Loaded Model Analysis

The partially loaded model was analyzed at both EOC-1 and EOC-2 in order to qualify irradiations of the partially loaded target for 2 cycles in position VXF-15. At this time, two heat treatments during pellet fabrication were under consideration, at higher temperatures of 900 °C and 1200 °C in order to reduce the void density and thus increase advantageous thermophysical pellet properties like its thermal conductivity and thermal expansion.

In addition to the added solution space of different pellet types, there was a considerable unknown in the size of the cold radial side gap, small variations of which significantly increase pellet temperatures. Due to schedule limitations, the dimensional PIE data from reduced-length pellet capsule irradiations and

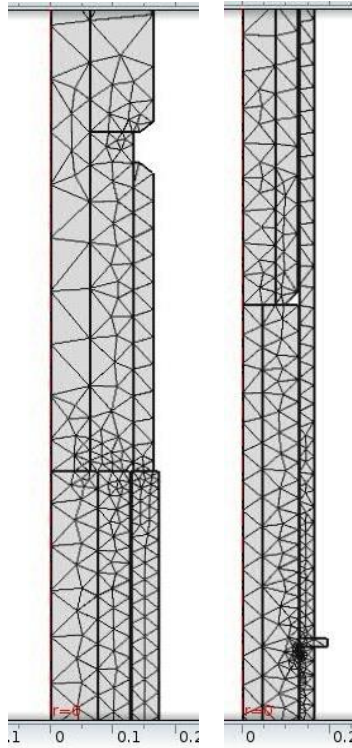


Figure 5.7: Extra-coarse mesh at the TEC/UST/housing and TEC/UST/WBT/housing domains for the partially loaded and fully loaded target models, respectively.

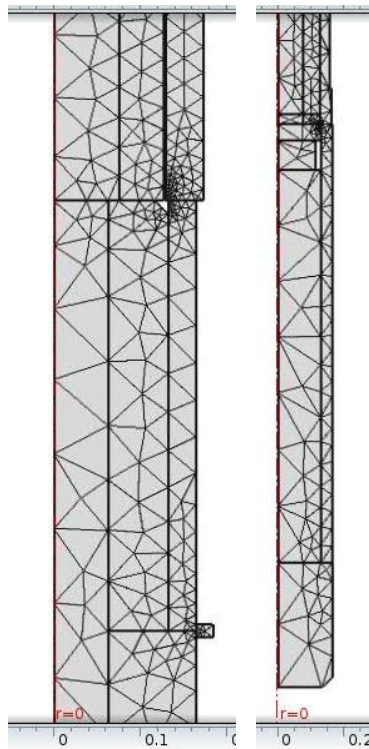


Figure 5.8: Extra-coarse mesh at the BEC/LST/housing domains for the partially loaded and fully loaded target models.

the target fabrication experience to estimate a maximum radial fabrication gap were not expected to be available in time to perform the safety analysis, so instead the thermal analysis was set up as a parametric study to allow for satisfactory qualification of the targets once data was available. The dimensional PIE data was expected to be available as discrete data points, not sufficient for fitting as a function of pellet burnup, and the radial fabrication gap would be available as a bounding value. The parametric analysis was then completed to find the allowable pellet diametrical shrinkage and its corresponding radial fabrication gap that yielding maximum temperatures just below the melting temperature for the SB condition. This parametric analysis was completed for both pellet heat-treatments for EOC-1 and EOC-2 as shown in Figure 5.9 and Figure 5.10, respectively. There is a significant difference between the allowable diametrical shrinkages for the two heat-treatments (around 0.5 mils) and significant decrease in these values from the first to second cycle (~1.5 mils). As can be seen, this also confirmed that the net allowable radial gap size (radial densification/shrinkage and fabrication gap) did not vary with changing diametrical shrinkage (i.e. the increased heating density due to densification is negligible).

The partially loaded target 3-D rotated temperature profile in the the pellet stack and its surrounding components region can be seen in Figure 5.11, where temperatures drop off precipitously outside the pellet stack. A zoomed-in view of the pellet side gap temperature profile in Figure 5.12 with deformation due to thermal expansion enabled and a distorted view shows the characteristic hourglass shape also shown in UO_2 pellets. The axial temperature profile along the axial centerline is shown in Figure 5.13 where the maximum temperature in the pellet third from the bottom of the pellet stack can again be seen.

Figure 5.14 shows the result of six PIE measurements of the diametrical pellet shrinkage from the reduced-length pellets, three for the 900 °C heat-treatment pellets and two for the 1200 °C pellets, with bounding lines determined using the corresponding fabrication gap from Figure 5.10. The figure shows the 1200 °C pellets fall within their bounding tolerance of ~3.6 mils while the 900 °C pellets have a data point that is outside their tolerance. For this reason, only 1200 °C heat-fired pellets were irradiated for the partially loaded targets.

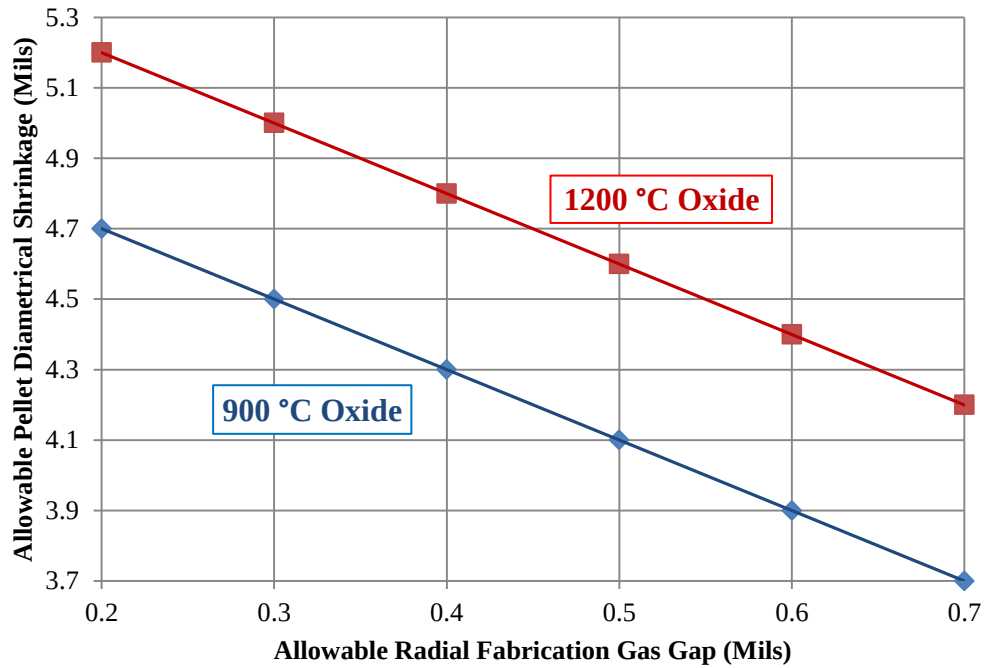


Figure 5.9: Allowable pellet shrinkage vs. fabrication gas gap for safety-basis of a 1 Cycle Irradiation.

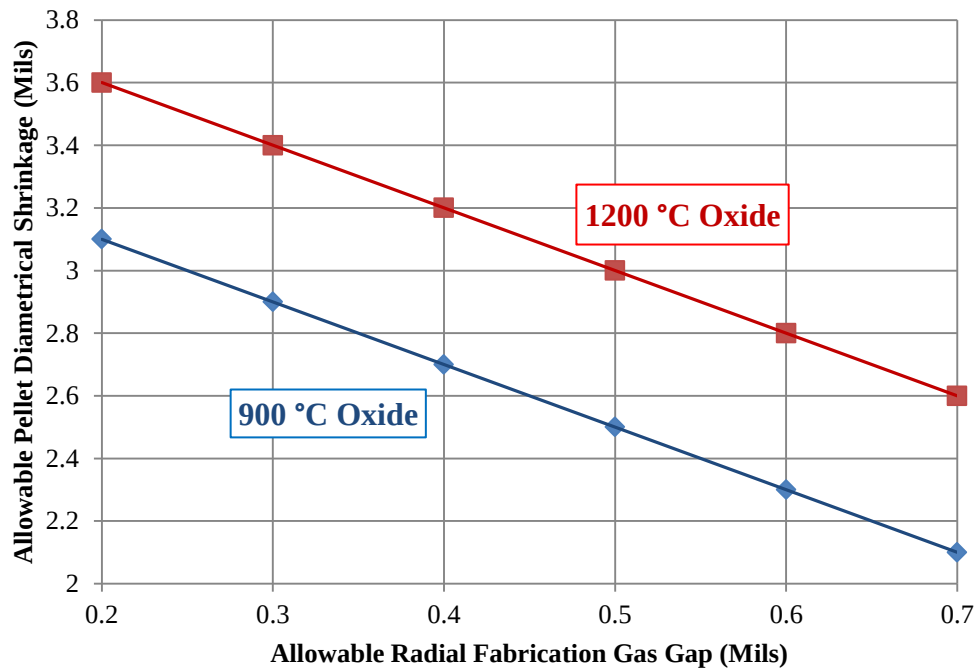


Figure 5.10: Allowable pellet shrinkage vs. fabrication gas gap for safety-basis of a 2 Cycle Irradiation.

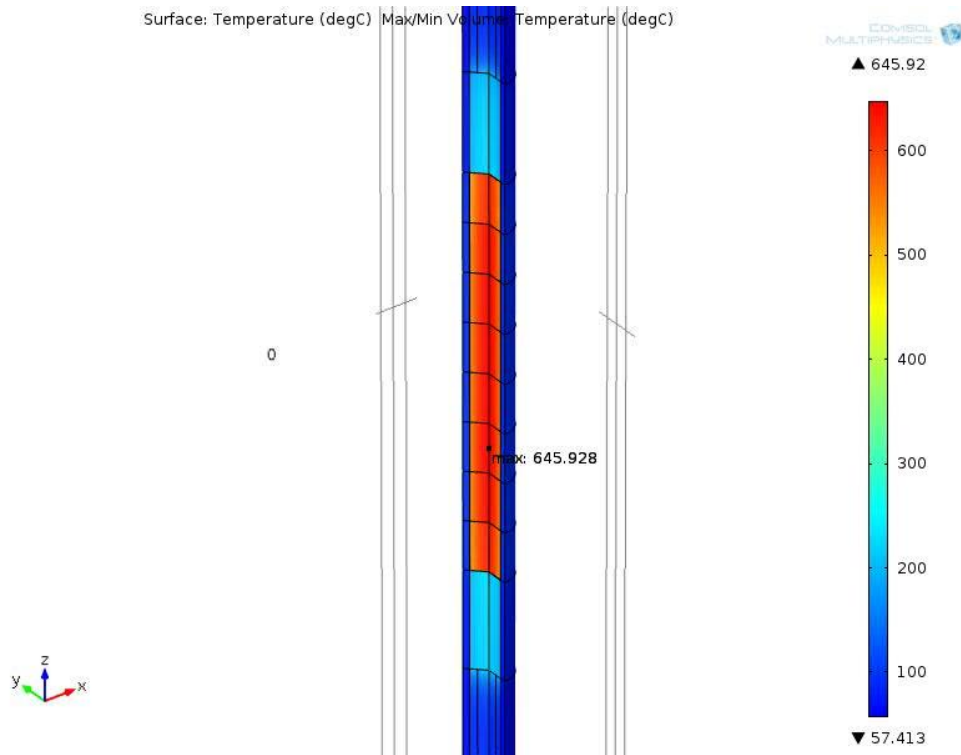


Figure 5.11: 3-D rotated temperature contour of the 2-D axisymmetric modeled volume of the partially loaded target assembly for the 900°C Pellet EOC-1 DB conditions at 50% flow and 100% power.

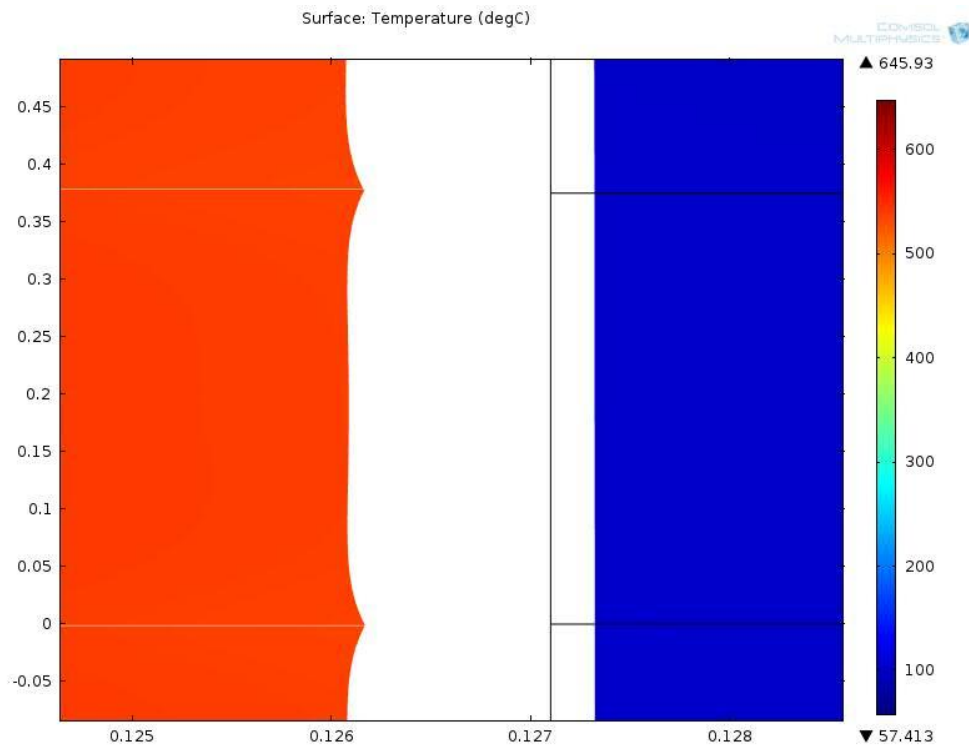


Figure 5.12: Temperature contour with deformation of the 2-D axisymmetric modeled volume of the zoomed-in pellet stack/housing gas gap for the 900°C Pellet EOC-1 SB conditions at 130% power.

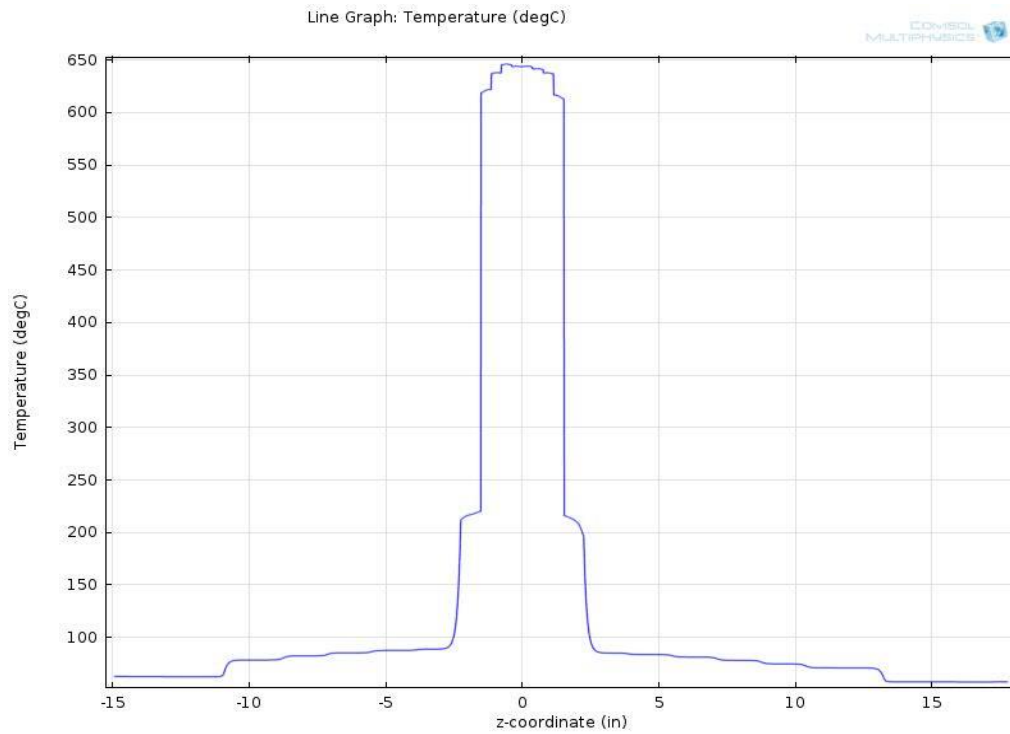


Figure 5.13: Temperature vs. axial position along the axial centerline for the 900°C Pellet EOC-1 SB conditions at 130% power.

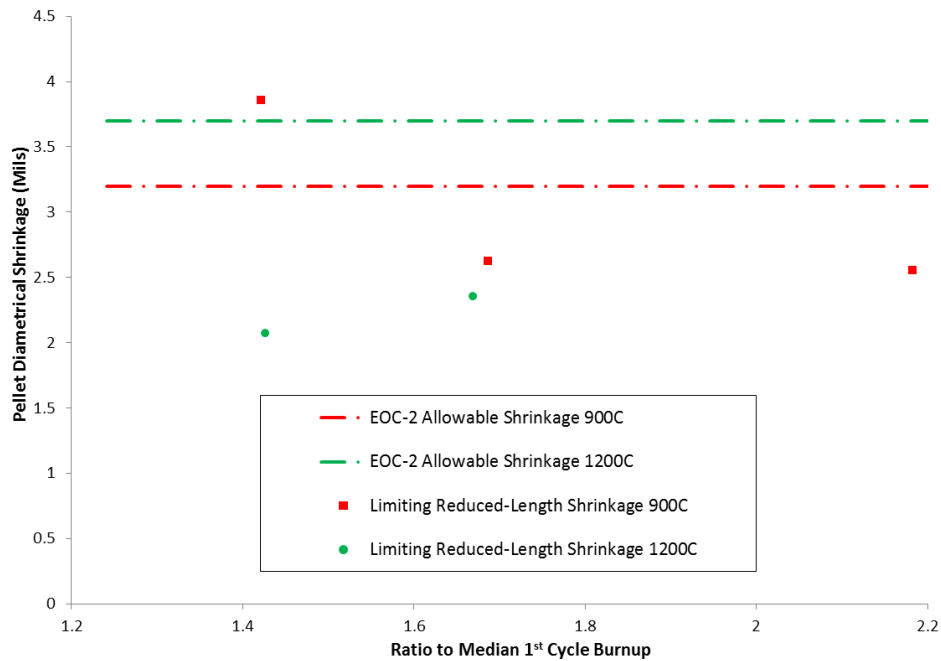


Figure 5.14: The limiting pellet diametrical shrinkage for 0.1-0.3 mil fabrication gap against the measured PIE shrinkages for each pellet heat-treatment.

5.4 Fully Loaded Target Model

This target has a substantially increased loading from previous models, rising from 8 to 50-52 NpO_2/Al pellets, and, as a result, several changes in the scope of the model were required in order to accommodate substantially augmented fission gas releases to the helium plenum, net irradiation-induced swelling/expansion of the pellet stack in the axial direction, and large axial variations in the pellet stack for heat generation rates, burnup, and the resulting effects of these changes. One simplification was that two pellet heat treatments no longer needed to be considered, as the 1200 °C pellets were the only qualified for irradiation for the previous phase partially loaded target. Several official revisions to the model occurred, for purposes of evolving target qualifications and inputs: R0) qualification of the targets for 1 cycle of irradiation, R1) qualification for 2 cycles, R2) repeat R1 to incorporate updated PIE fission gas release fractions, R3) incorporate updated PIE dimensional behavior for axial-dependent effects at a lower flux position VXF-3, and R4) update the R3 for position VXF-15.

5.4.1 Revision 0 calculation

At the time of the revision 0 analysis, the 1200 °C heat-fired pellet had been decided as the only fabrication type used for the fully loaded target. Due primarily to a significant decrease in the helium plenum size and thus a much larger impact on the gas gap thermal conductivity, the allowable diametrical shrinkage decreased from the partially loaded target to fully loaded target. The model was simulated for two irradiation positions, the lower flux position VXF-3 and the highest flux position VXF-15, at EOC-1 in the same parametric solution search method previously described and the results of which are shown in Figure 5.15.

The 3-D rotated temperature contour plots in Figure 5.16, for a spatially undistorted and distorted view, show that the pellet just below the reactor horizontal midplane is the location of maximum temperature for cycle 1 and that the temperatures (as with the input heat generation rates) follows the HFIR core flux cosine curve with respect to axial position. Focusing on the aforementioned “hot pellet”,

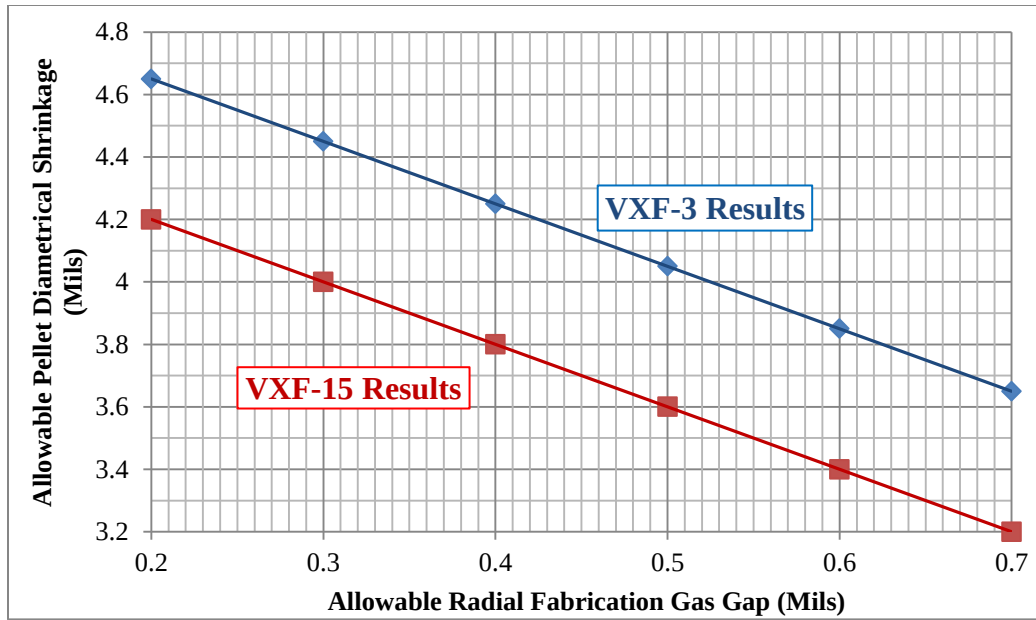


Figure 5.15: Allowable pellet shrinkage vs. fabrication gas gap for safety-basis of a 1 cycle irradiation.

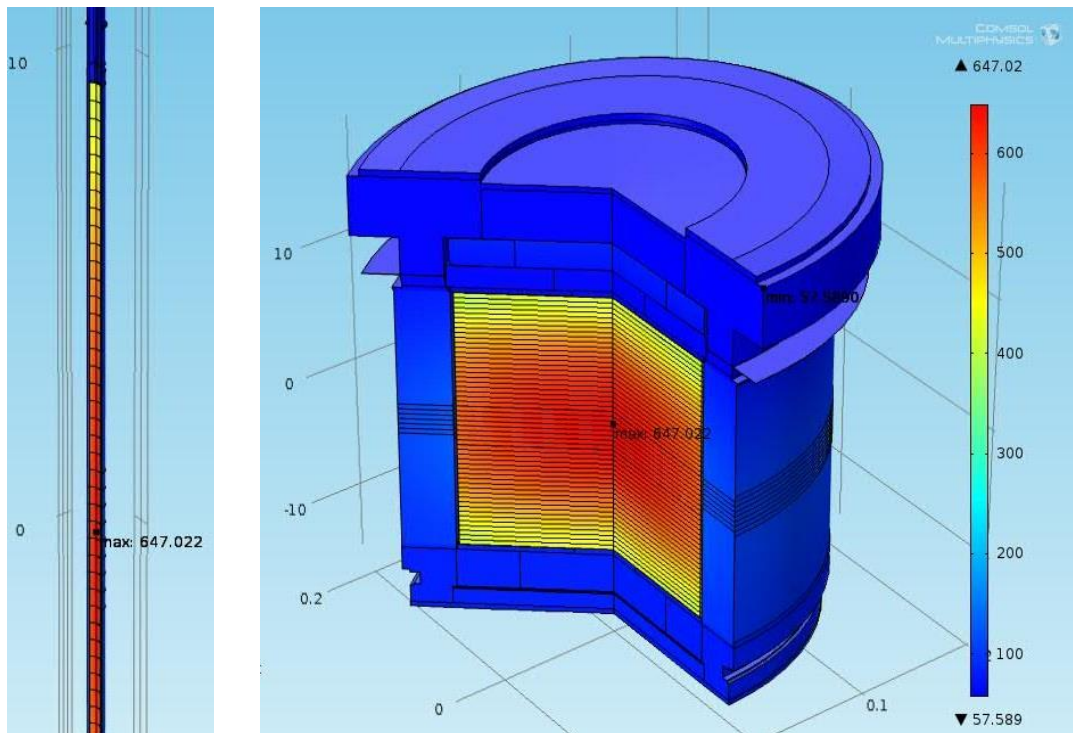


Figure 5.16: 3-D rotated temperature contour for an undistorted and distorted view at VXF-15 EOC-1 SB conditions at 130% power.

its 3-D rotated stress profile with 10000x deformation, plotted in Figure 5.17, shows even more clearly the characteristic hourglass shape expected. The axial centerline temperature profile in Figure 5.18 again shows the cosine curve temperature distribution with only small peaking at the ends (compared to the partially loaded target) due to a greater number of targets and self-shielding.

5.4.2 Revision 1 and 2 calculations

The revision 1 calculation was updated for the second irradiation cycle of the fully loaded target in positions VXF-3 and VXF-15. Unlike previous irradiations, there was a concern for the irradiation burnup-dependent dimensional changes within the cycle's irradiation time and their effect on the peak pellet temperatures. In addition, schedule limitations couldn't allow the calculation to await a wider burnup range of PIE data to define the calculation scope in terms of expected limiting densification values. For this reason, a parametric solution search method was needed in order to calculate the maximum allowable pellet diametrical shrinkage (assuming a ~0.1-0.3 mil fabrication gap) as a function of the heat generation rates in the pellets. This was accomplished via the Java API for COMSOL programming, where an initial guess shrinkage gap value was given at 100 W/g. From there, a default step was taken in the direction of 650 °C for the input shrinkage, and thereafter linear interpolation was used until the maximum temperature was within some tolerance of the melting temperature (649+/- 0.5°C). After that, the current shrinkage input was then used for the next pellet heating rate until 400 W/g (the maximum calculated heating rate in the 2nd cycle) was reached.

Revision 2 analyses consisted of a simple update to this analysis via increased fission gas release fractions. The resulting maximum allowable pellet diametrical shrinkage values are shown in Figure 5.19 below, for both positions VXF-3 and VXF-15. An example of this resulting curve for position VXF-15, along with PIE results from the partially loaded targets is shown in Figure 5.20, which verifies that the fully loaded target is satisfactory with regard to pellet temperatures. This comparison can be created using the calculated maximum pellet HGRs as a function of burnup (a curve not shown here) to transform the pellet dimensional behavior from a function of burnup to HGR. Figure 5.20 shows that an analysis

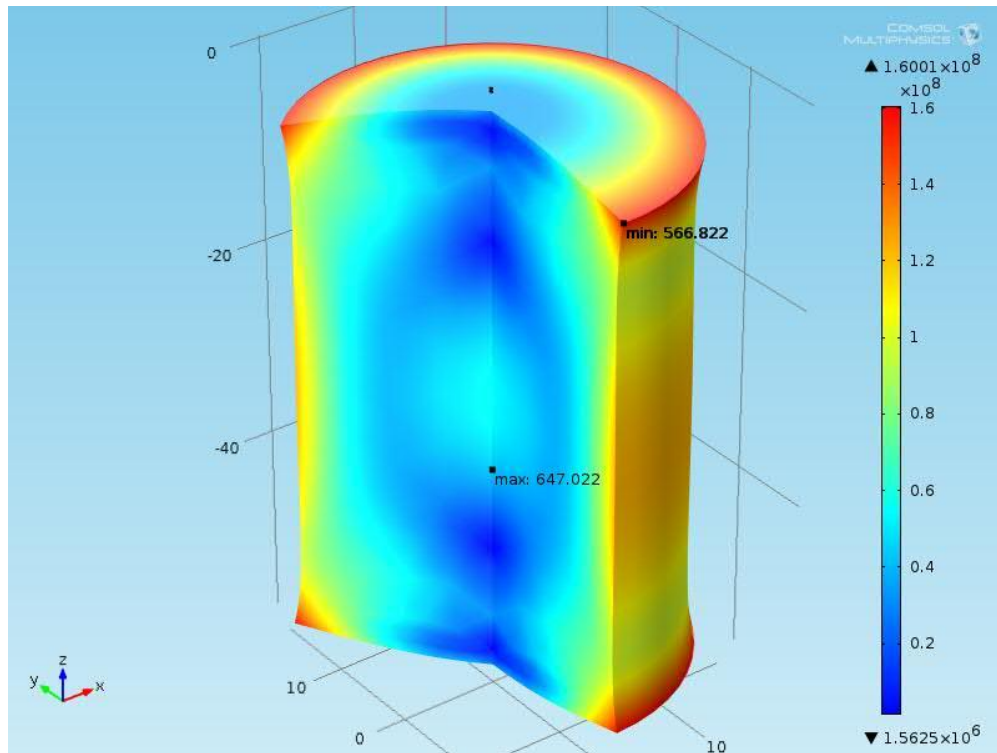


Figure 5.17: 3-D rotated stress contour with 10000x deformation of the 2-D axisymmetric modeled volume of the hot pellet for the VXF-15 EOC-1 SB conditions at 130% power.

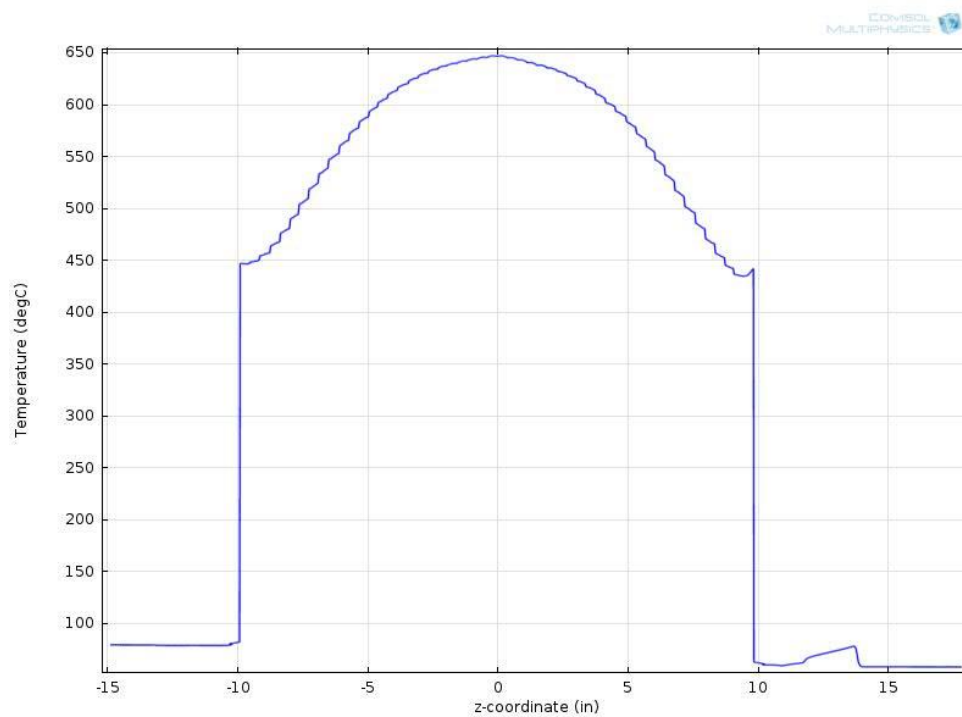


Figure 5.18: Temperature vs. position along the axial centerline for the VXF-15 EOC-1 SB conditions at 130% power.

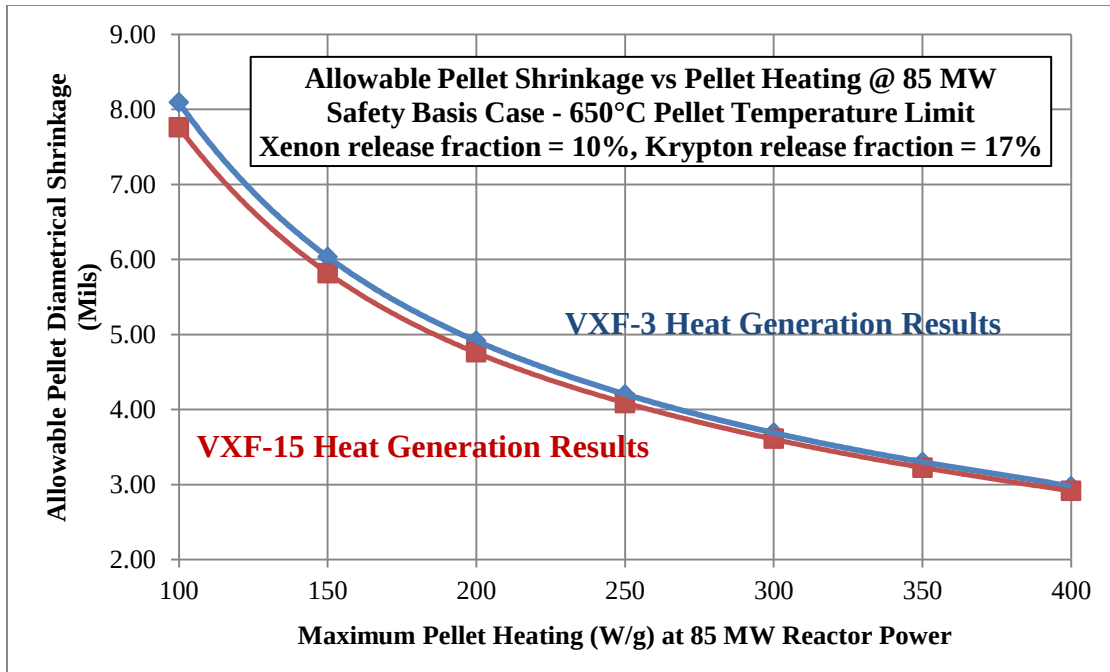


Figure 5.19: Allowable pellet shrinkage vs. maximum pellet heating for safety-basis of a 2 cycle irradiation.

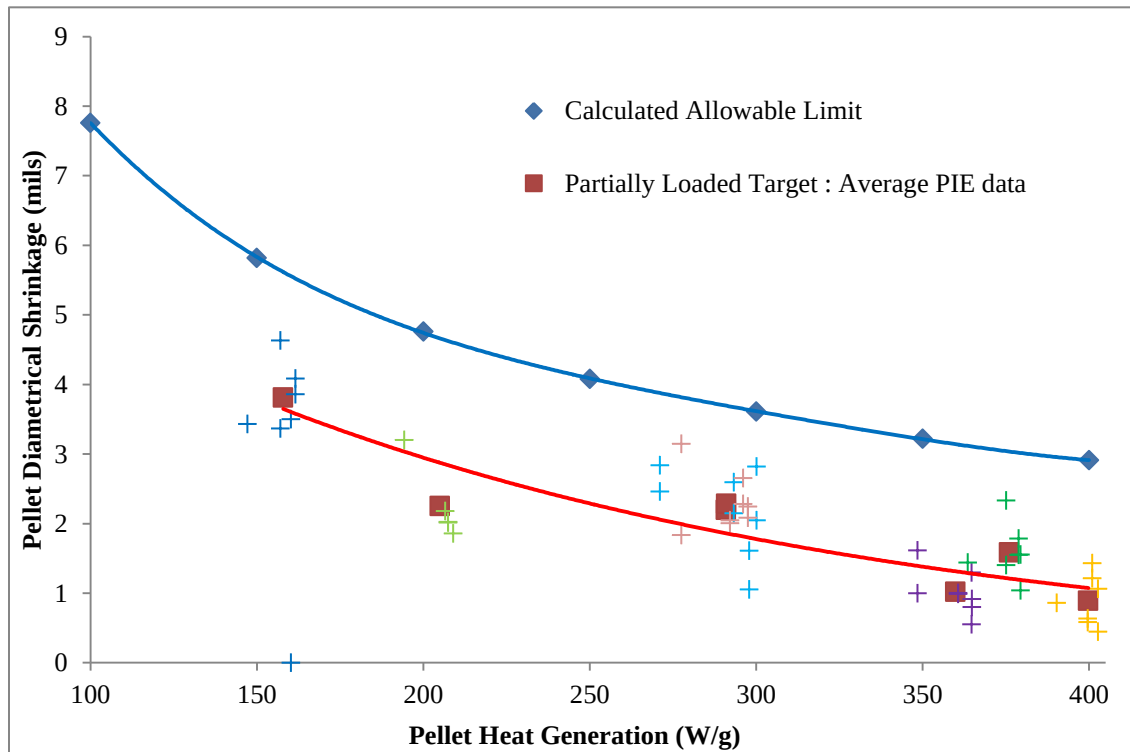


Figure 5.20: Calculated allowable pellet shrinkage with respect to fully loaded target temperatures along with partially loaded PIE data as a function of pellet heat generation.

that did not take credit for burnup-dependent behavior would not have passed qualification, as the maximum observed shrinkage (~4 mils) exceeds the minimum allowable shrinkage (~3 mils).

5.4.3 Revision 3 calculation

At the time of the revision 3 analysis, recent PIE data from the partially loaded target prototype had indicated a potential safety concern for the axial stresses and clearance in the fully loaded target design under second cycle irradiation swelling and thermal expansion conditions. The purpose of this analysis was then to perform best estimate computations of the axially-segmented temperatures and axial thermal expansion in the pellet stack region based on current PIE data. In addition, a special “cold case” is analyzed at the end of the second cycle (EOC-2), where the pellet stack is in contact with (while not applying pressure to) the inside surface of the target housing. These thermal data outputs were then input into a separate hand calculation that calculated a conservative estimate of the axial clearance and stresses.

The PIE dimensional data in Figure 5.21 was available at the time of this revision, using averaged partially loaded target measurements of the diametrical shrinkage of the pellets to yield both a “best-estimate” and bounding curve fit for use as inputs.

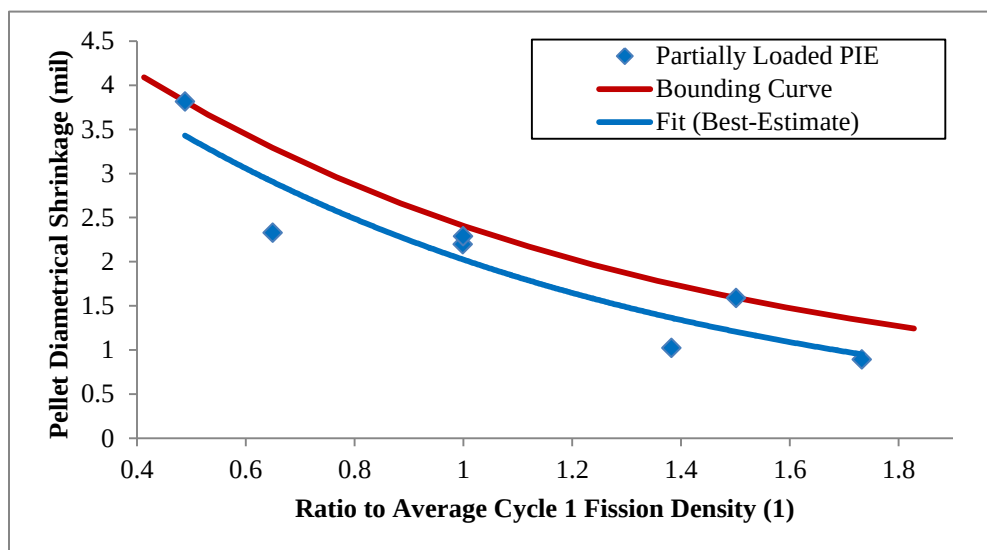


Figure 5.21: PIE data and fitted curves for pellet shrinkage vs. fission density.

The cold case model concerns the case where the NpO_2 pellets, in response to axial compression from the surrounding target components, deform to fill the radial gap between the pellet stack and adjacent target housing. Pressure applied by the pellets to the target housing is not credited in this model. The physical radial gap will thus be the RMS sum of the pellet and housing surface roughness values. For the cold case model, no structural mechanics equations are solved, instead only the temperature field is solved with a modified geometry to put the pellets in contact with the target housing inside surface.

Since previous assessments (revisions 0 through 2) provide a bounding estimate of the maximum pellet temperature with respect to this target design, the SB results from this case do not provide any new insights to the behavior of the target. However, renewed interest in the time- or burnup-dependence of the target temperatures and other behavior gave rise to confirm that end-of-cycle conditions were thermally limiting. Constant pellet temperatures over discrete material regions, as were reported in tables in the analyses for input to a separate calculation, are plotted in Figure 5.22 below for discrete time steps in the 2nd cycle, confirming that EOC-2 is still the bounding estimate with regard to maximum and average pellet temperatures. However, taking into account the burnup-dependence of pellet dimensional behavior yields a more complex axial temperature profile than previously observed in fully loaded target models. As pellets diameters recover from maximum densification and swell outward, closing the radial gas gap, the maximum temperature location moves from the center of the pellet stack to the outer ends, where densification/shrinkage is still dominant. This creates a sinuous axial temperature curve at EOC-2 and an almost constant maximum temperature with respect to cycle time after day 5. Figure 5.23 plots the raw COMSOL pellet temperature values, averaged temperatures by material region and a moving average of the temperatures as a function of axial position.

5.4.4 Revision 4 calculation

The purpose of the revision 4 analyses was to extend the second cycle analyses in the VXF- 3 position, documented in Revision 3, to second cycle irradiation times in the VXF-15 position and the end of the first cycle in both positions. As in Revision 3, the purpose of Revision 4 was not to ensure that

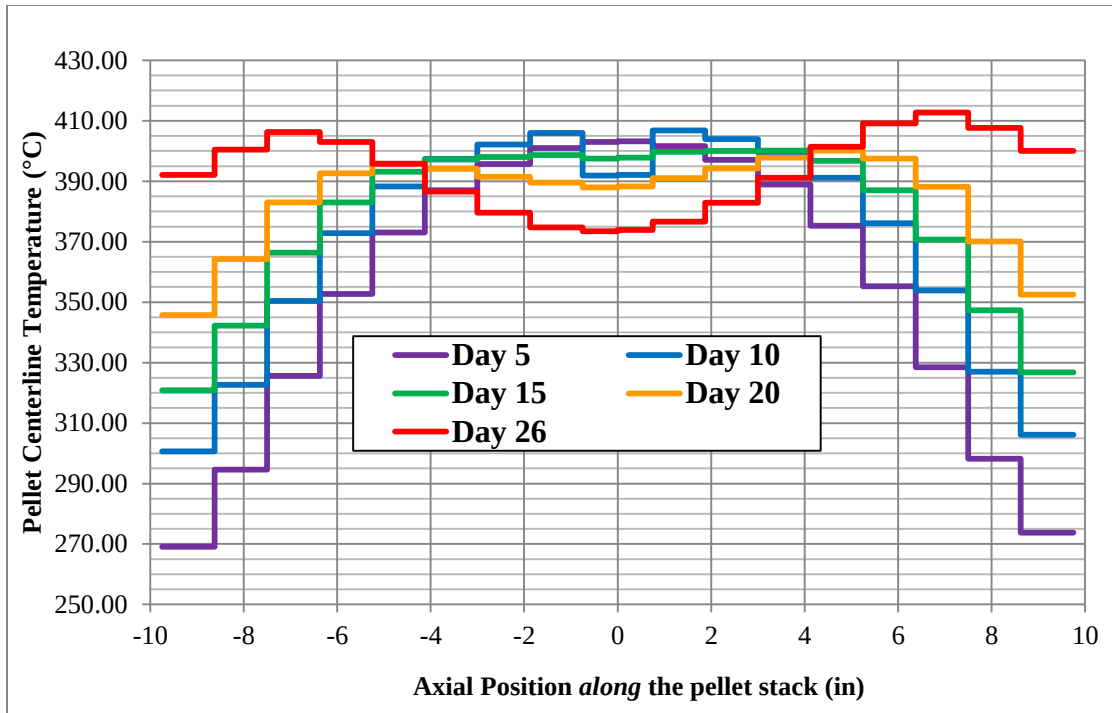


Figure 5.22: Temperature profile along the pellet centerline at 100% power for 5, 10, 15, 20, and 26 days into the 2nd cycle for VXF-3 position.

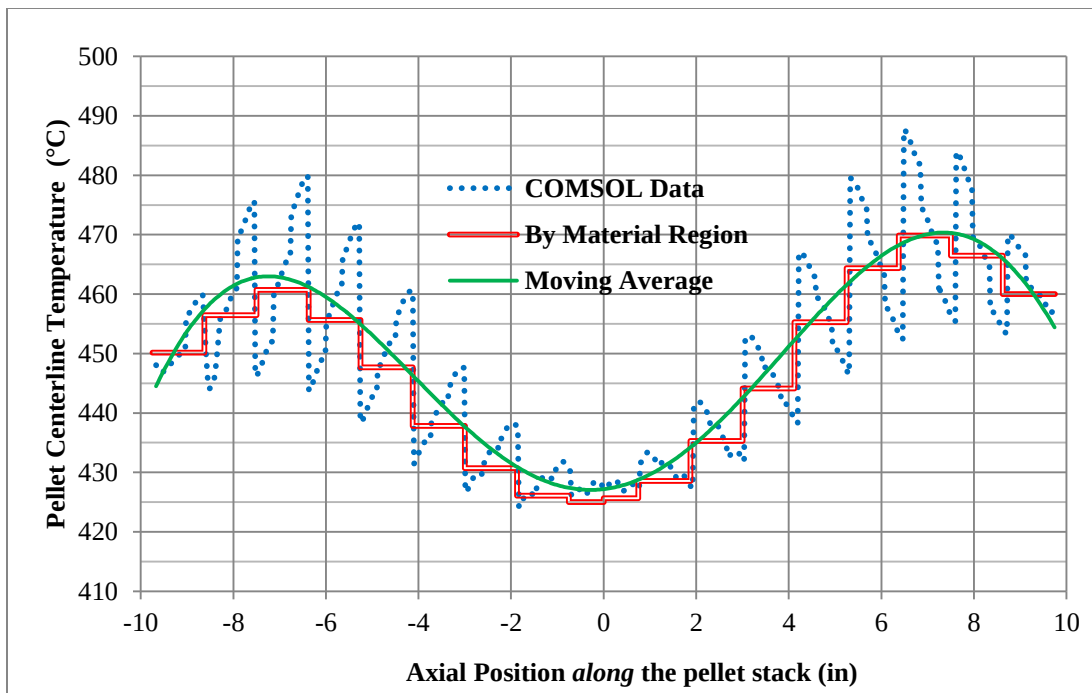


Figure 5.23: Day 26 of 2nd cycle at VXF-3 temperature profile along the pellet axial centerline at 130% power.

internal temperatures in the target do not exceed their melting temperature under safety-basis conditions, which was conservatively addressed in Revisions 0, 1, and 2. The purpose of Revisions 3 and 4 is to provide data to address a potential structural failure in target cladding, a safety analysis which was completed in a subsequent calculation.

The concluding remarks on the burnup or time-dependent temperature behavior during the 2nd irradiation cycle were expanded for these analyses. Plots of the running average of the pellet temperature along the axial centerline for five discrete times in the 2nd cycle are shown in Figure 5.24, and plotted along with the EOC-1 axial centerline pellet temperatures for VXF-3 and VXF-15 in Figure 5.25. The same relationship is shown, with the maximum temperature moving to the outer ends of the pellet stack towards the EOC-2, in addition the EOC-1 maximum temperature is shown to be higher than those seen in the 2nd cycle, including EOC-2. As expected, temperatures are higher in the VXF-15 position. Figure 5.26 and Figure 5.27 show the spatial temperature profile in the pellet stack for a distorted spatial scale for days 0, 5, 10, 15, 20 and 26 into the 2nd cycle, giving a much clearer image of pellet stack temperatures throughout the 2nd cycle.

5.4.4.1 Revision 4 Mesh Refinement

A mesh refinement study was performed for the revision 4 analysis of the fully loaded target model that is now briefly discussed. The study was performed at 130% power, EOC-2 for both the best estimate and “cold case” (which denotes that structural mechanic equations are not solved and zero radial gap distance is assumed) models to demonstrate the increased convergence for the latter model method (where structural mechanics equations are not included and the nonlinear coupling at the pellet/housing gap does not negatively impact convergence).

The number of mesh elements in the pellet/housing region was roughly doubled at each convergence step, using a quadratic basis function, and an error estimate was made from one to two post-processing results: the pellet centerline average temperature, the maximum pellet centerline temperature, and/or the

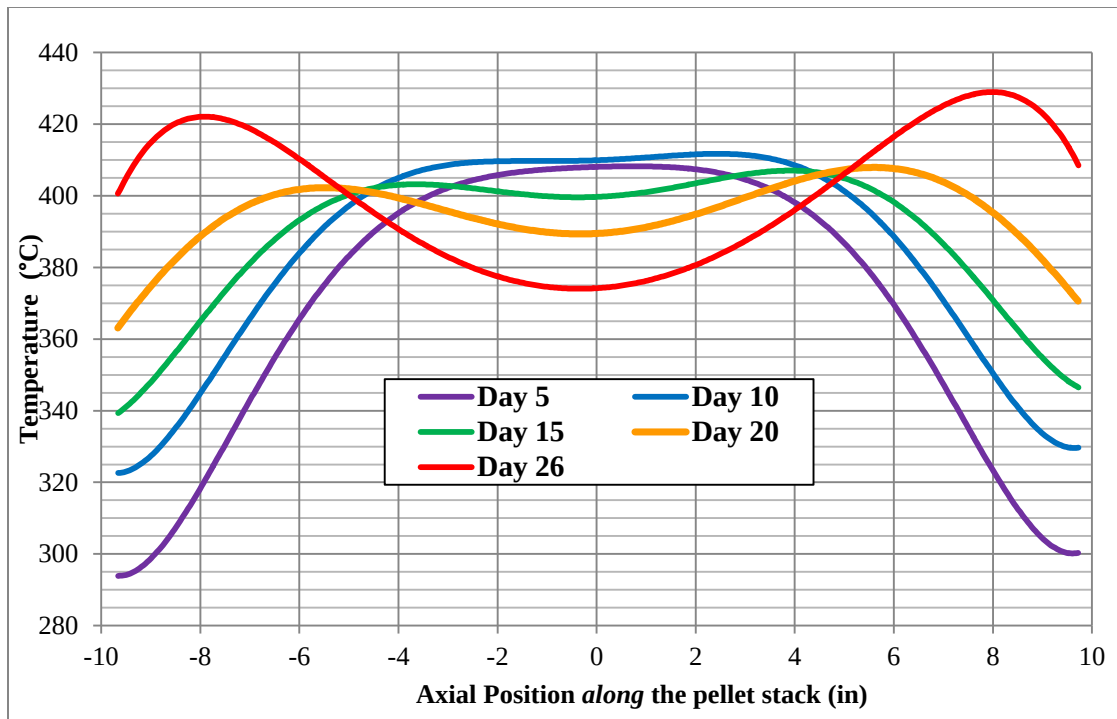


Figure 5.24: COMSOL data-fitted temperature profiles along the pellet centerline at 100% power for 5, 10, 15, 20, and 26 days into the second cycle at position VXF-15.

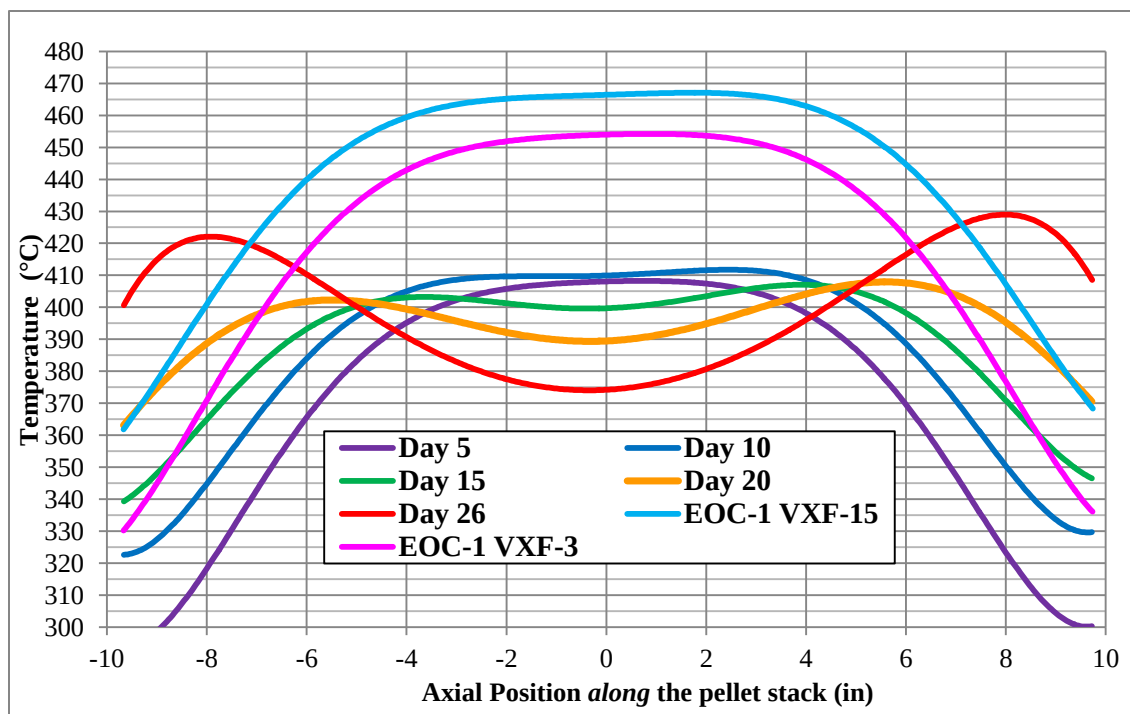


Figure 5.25: COMSOL data-fitted pellet centerline temperature profiles at 100% power for second cycle times at VXF15 as well as EOC-1 for positions VXF-3 and VXF-15.

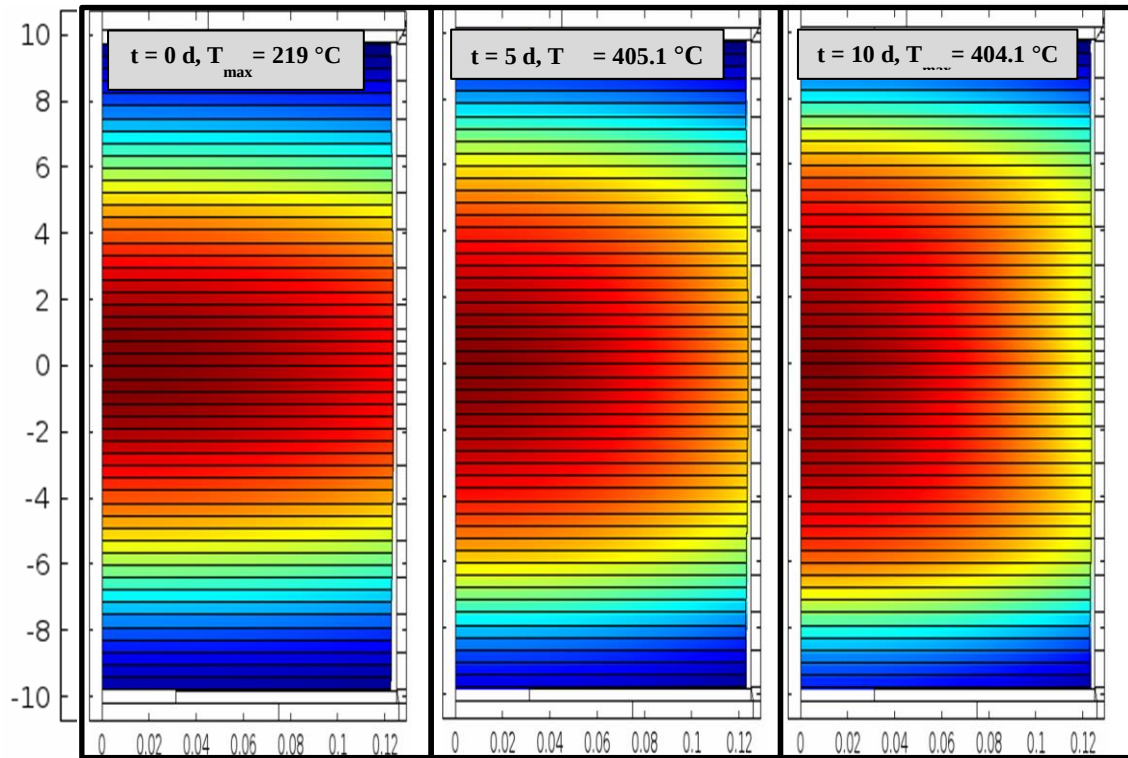


Figure 5.26: Pellet stack temperature profiles for day 0, 5, and 10 into the 2nd cycle, not to same scale.

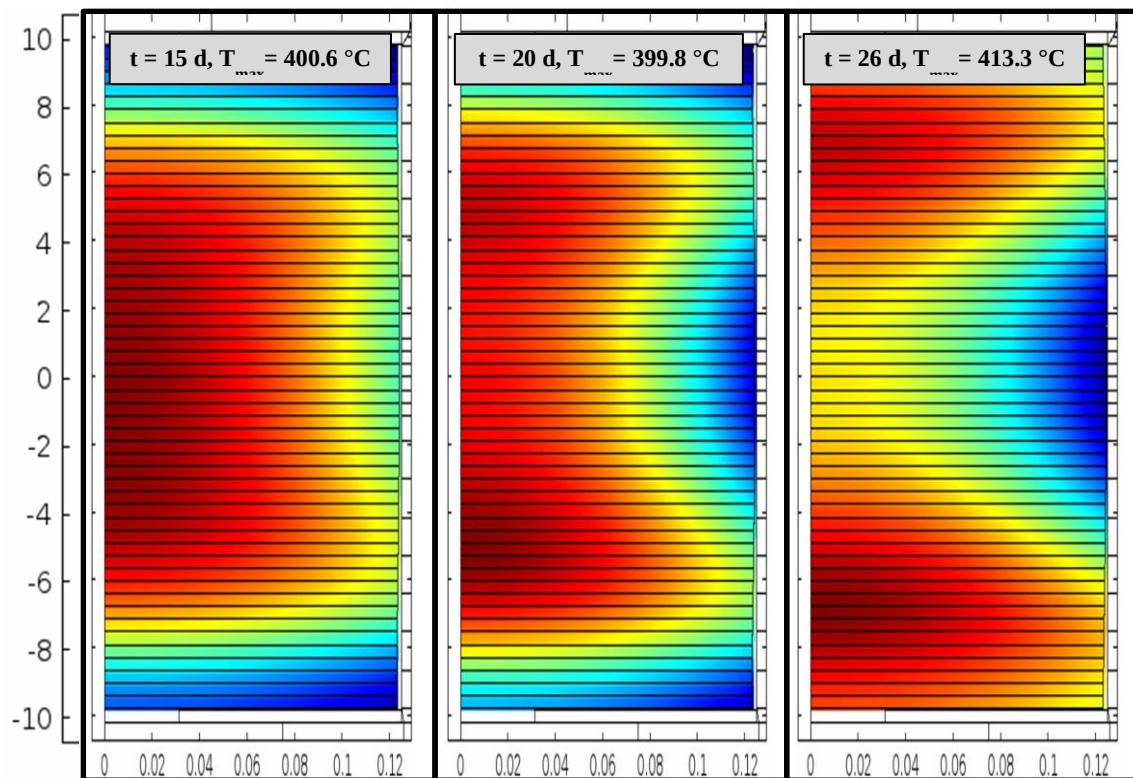


Figure 5.27: Pellet stack temperature profiles for day 15, 20 and 26 into the 2nd cycle, not to same scale.

maximum axial displacement of the pellet stack. The individual error estimates, e^P are defined in Equation 5.1:

$$e^P = \frac{\Delta P}{3}$$

Equation 5.1

Where P is the safety parameter of interest. Finally, the root of the product of the errors was used as a final error “norm”.

The error norm is plotted against the reciprocal of the mesh number in the log-log plot in Figure 5.28. The increased rate of convergence and reduced error in the cold case model can be clearly seen. More specifically, the finite element order of convergence approximately doubles and is a better comparison to the theoretical slope value of 4 for smooth convergence with a 2nd order basis function (quadratic).

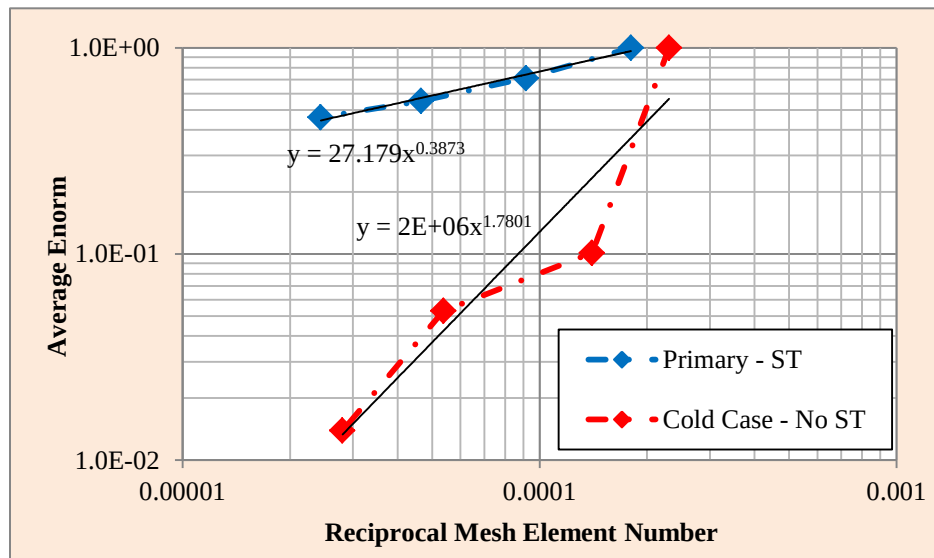


Figure 5.28: Mesh refinement for best estimate (primary) and cold case (no structural mechanics) models for the fully loaded target

6 Plutonium-238 Production Studies: Production Target Model

The production model in COMSOL extends the analysis to three irradiation cycles and makes use of the most up-to-date PIE data, material property inputs, and modeling methodology. The fully coupled thermo-mechanical equations are solved over the entire domain, significantly increasing the degrees of freedom required for a solution, in addition to several other improvements in the computational methodology of the model. In addition, a significantly expanded solution space is covered using this model, given the updated inputs, including each of the seven target holder pins in position VXF-15 and pin 1 in VXF-3, as well as 10 discrete time steps for each of all 3 cycles of irradiation. This detailed solution space allows the verification of “pin 1” at the irradiation end of cycles to be the limiting safety cases for the production target.

There are three primary cases solved for this model, each designed for its own purpose. The “best-estimate” case uses the inputs and methodology designed to solve for conditions in the range of the expected nominal behavior, with a subcase for 50% coolant flow conditions. The thermally limiting safety basis (TLB) is designed to maximize temperatures in the target, specifically the pellet stack, in order to conservatively satisfy the 130% overpower case with regard to melting temperatures. The structurally limiting safety basis (SLB) is designed to maximize stresses in the target, with subcases for optimizing radial stresses on the cladding from the pellets and to optimize axial stresses on the target from aggregate swelling of the pellet stack.

6.1 *Inputs and Methodology*

6.1.1 Pellet properties

PIE dimensional data in the form of pre- and post-irradiation measurements of the pellets’ diameter and length for six fully loaded targets was available and documented for this model. These targets were irradiated for either 1 (2 targets) or 2 (4 targets) cycles, in either the hottest (4 targets) or coldest (2 targets) positions in the holder, and in either the ISVXF-15 (2 targets) or ISVXF-3 (4 targets) positions in

the permanent beryllium reflector. This data was processed in MATLAB in order to assess a statistical trend.

A curve was fitted to the volumetric swelling data as a function of burnup or fission density in Equation 6.1, following previous guidance on UO₂ oxide/cermet pellets for the functional form.

$$Vol. Swell. (BU) = \frac{\Delta V}{V_0} = a * 1e - 20 * BU + c(e^{-b*1e-20*BU} - 1)$$

Equation 6.1

where a,b,c = fit parameters,

BU = burnup or accumulated fission density (fissions/cm³), and

$\frac{\Delta V}{V_0}$ = change in pellet volume (%).

From this fit, predictive confidence intervals of 95% were created based on simultaneous observation, and these were fitted with fifth degree polynomials to create upper and lower bounds to the dimensional behavior of the pellets under irradiation. The original curve fit was determined the “best-estimate” fit. Figure 6.1 shows the spread of the data vs the upper and lower bounds as a function of fission density:

In order to input the volumetric swelling effect into COMSOL, it was determined that incorporating it under the thermal expansion coefficient was most effective. It is useful to recall the original definition of the linear thermal expansion coefficient, $\alpha_L(-)$, in terms of the volumetric expansion coefficient, $\alpha_V(-)$, in Equation 6.2.

$$\frac{V(T)}{V_0} = (1 + \alpha_V \Delta T) = (1 + \alpha_L \Delta T)^3 = 1 + 3\alpha_L \Delta T + \dots \gg \alpha_L \cong \frac{\alpha_V}{3}$$

Equation 6.2

Now define the modified linear “thermal” expansion as a variable in Equation 6.3, $\alpha_{modified}(-)$, that is no longer only expansion due to thermal effects but also swelling/densification due to fission density (FD)-dependent irradiation effects, as previously defined in 4.3.2.1.

$$\alpha_{modified} = \alpha_L(T) + \frac{1}{3} \frac{dV}{V} (FD(z)) \frac{1}{(T - T_{ref})}$$

Equation 6.3

Updated thermal expansion measurement results for NpO_2/Al pellets heat-treated at 1200 °C were also available, which were fit to a 4th degree polynomial to determine a temperature-dependent thermal expansion coefficient in the secant form. This polynomial was then input into COMSOL to recreate the measurement results and compare to the experiment, thus verifying the correct implementation, as shown in Figure 6.2 below where the raw data, averaged data and COMSOL probe results are plotted against each other as a function of temperature.

Other updated properties included the fission gas release fractions, which were set at a constant value during cycles 1 and 2, and increased to another constant during cycle 3. Measurements of the hydrostatically collapsed fabrication gas gap between the pellet stack and housing tube were also made available in order to estimate bounding and best-estimate values.

6.1.2 Structurally Limiting Basis Methods

The methodology to create a conservative assurance of adequate target cooling was well-explored prior to this model however the methodology to assess structural integrity in the target was not as well developed. In addition to using 130% overpower conditions, a bounding Poisson's ratio, best-estimate fabrication gap, and the bounding volumetric swelling curve in the direction of maximum swelling, several other changes were made in order to make this assessment sufficiently conservative.

The first case run is an intermediary step, using the above inputs except for the best-estimate swelling curve (which is conservative for this use), to calculate a temperature profile for the target that is saved for a later subcase. The subcase to assess radial stresses on the cladding from the pellet is denoted SLB-1 and uses the documented tensile yield strength of the cladding material as a safety limit, with observations that the yield strength of the material increases under irradiation [109]. In addition, the inside cylindrical surface of the housing tube was made rigid, not allowed to deform under pressure or axially expand, in order to maximize stress onto the cladding. Finally, documented failure tests of the target specified a minimum elongation of the target itself which was set as a prescribed limit on the target and bounding internal components like the weld support tube.

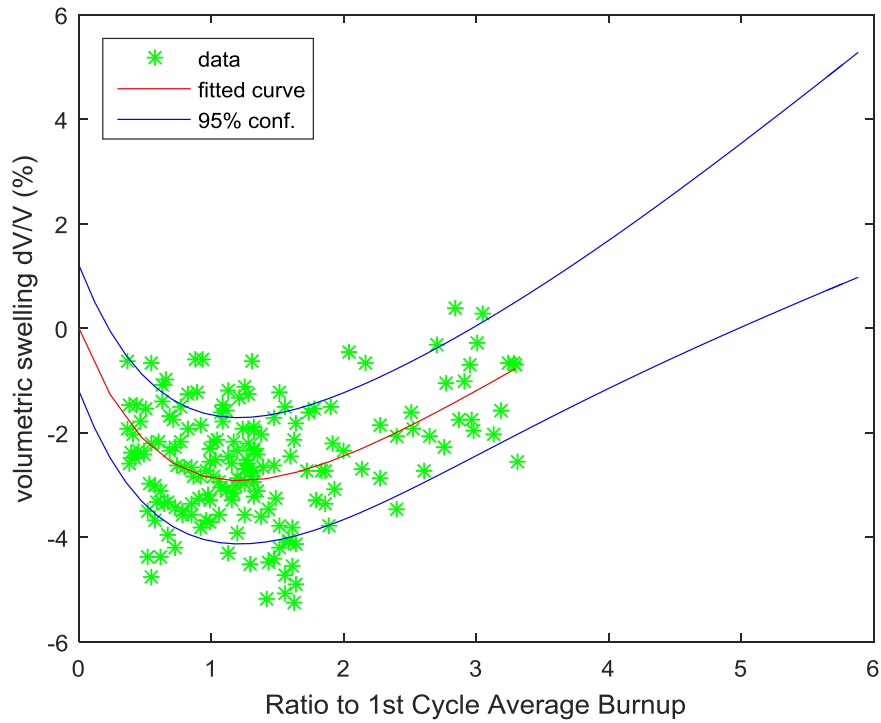


Figure 6.1: Simultaneous observation confidence intervals and their curve fits along with the raw PIE data.

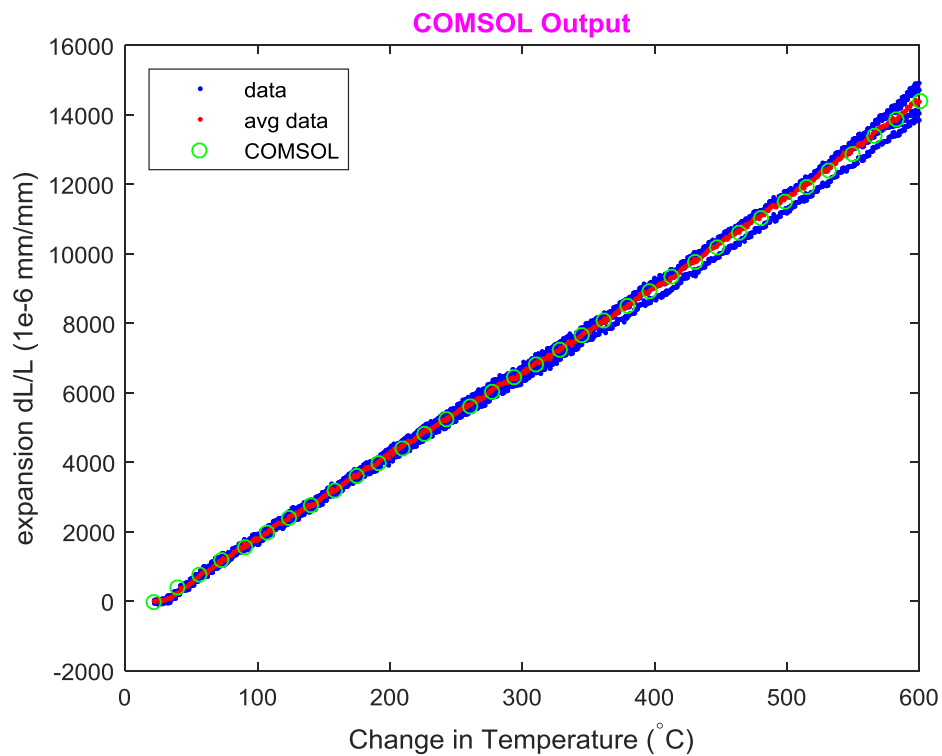


Figure 6.2: Thermal expansion measurement data, averaged data, and the COMSOL probe results.

The subcase utilized to conservatively assess axial stresses in the target is denoted SLB-2 and uses as its safety limit a minimal tensile failure force from the aforementioned destructive target tests. A major conservative assumption desired is to limit the radial expansion of the pellets due to thermal expansion and irradiation swelling to only meet the target cladding inside surface, thereafter letting expansion due to these effects be exhibited only in the axial direction. Therefore, a limiting expansion variable is defined in Equation 6.4 that is the linear expansion variable that would cause the diameter of the pellet to increase to the collapsed diameter of the housing.

$$\alpha_{lim} = \frac{\left[\frac{D_{housing}}{D_{pellet}} - 1 \right]}{\Delta T}$$

Equation 6.4

The diametrical expansion variable is then set as the minimum of the nominal expansion and this limiting expansion value, thus not allowing the pellet to expand into the housing due to only thermal or irradiation effects.

It is now useful to examine the expanded volume in a pellet between a nominal state and the limited state where the pellet is just in radial contact with the housing, as shown in Equation 6.5. The first form is in terms of the linear “thermal” expansion coefficient, then in terms of the utilized modified coefficients including a new coefficient to be applied to linear expansion in the axial direction.

$$V(T, FD) = V_0(1 + \alpha_L \Delta T)^3 = V_0(1 + \alpha_{lim} \Delta T)^2(1 + \alpha_{zmod} \Delta T)$$

Equation 6.5

In order to conserve volume expansion due to thermal and irradiation effects, these two forms must be equal. Now solve the above equation for the new coefficient where it is the only unknown in Equation 6.6.

$$\alpha_{zmod} = \frac{\left[\frac{(1 + \alpha_L \Delta T)^3}{(1 + \alpha_{lim} \Delta T)^2} - 1 \right]}{\Delta T}$$

Equation 6.6

And the axial linear expansion coefficient is defined as either the modified coefficient or the nominal, in Equation 6.7, depending on how much expansion has occurred.

$$\alpha_{axial} = \begin{cases} \alpha_L > \alpha_{lim} & \alpha_{zmod} \\ \alpha_L < \alpha_{lim} & \alpha_L \end{cases}$$

Equation 6.7

Using these terms yields anisotropic expansion that will only allow the diameter of the pellets to expand to a certain diameter, followed then by only axial expansion. Due to this assumption, any solution to the temperature field values would be unrealistic and artificial, thus only the solid mechanics equations are solved for subcase SLB-2 and the temperature field is input from the previous intermediary solution using SLB inputs with otherwise default methodology.

6.2 Production Model Geometry

The geometry of the production model target is an extension of the target designed for the prototypical targets, where a pellet stack is contained within an aluminum housing tube, as shown in Figure 6.3. Similar features to the prototypical targets include: dummy pellets at either end of the pellet stack, a top end cap (TEC) with a large helium plenum and threaded top for HFIR operations removal, a bottom end cap (BEC) with a swage joint, spacer tubes at either end of the target (UST and LST), a support tube (WBT) for the E-beam weld, and welds at either end to attach the end caps. Expansion spacer assemblies of SST316 were added on either end of the pin each consisting of a roll pin that slides

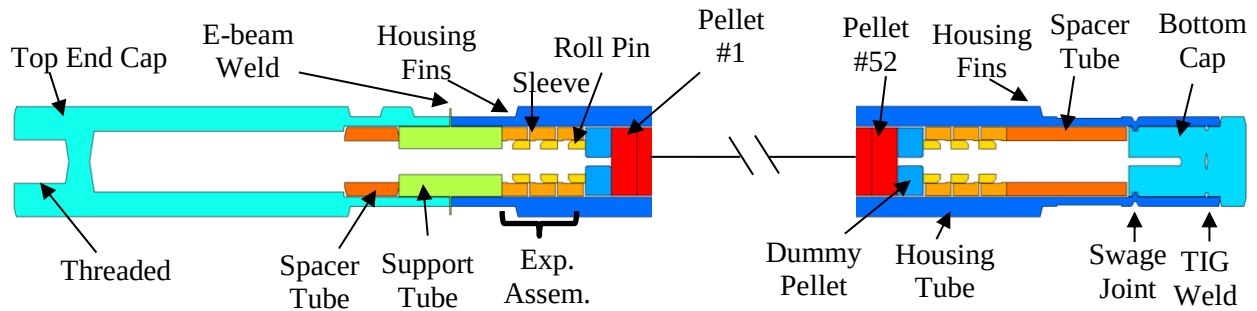


Figure 6.3: Representation of production model target pin components.

into a sleeve under axial compression, designed to create greater axial clearance in the event of axial stresses in the target due to pellet stack swelling, as a result spacer tube lengths decreased. In addition, the nominal pellet length increased by a few mils.

6.3 *Production Mesh*

A total of five mesh cases were designed to analyze this problem. These 5 cases are designated, in order of increasing detail: (1) extra coarse, (2) normal, (3) finer, (4) extra fine, and (5) extremely fine. All 5 mesh cases are similarly formed and differ primarily by the selection of their free mesh size types as defined by COMSOL predefined settings which are sometimes custom adjusted (in terms of minimum and maximum element sizes, or ratio for element growth) in order to optimize the mesh ratios in the side gap (best at a pellet/housing ratio of 2 or greater). These free mesh size settings include four boundary size settings on the pellet sides, housing inside surface, and pellet tops (applying to each pellet top surface) as well as the universal domain size setting.

The boundary settings are calibrated for fluid dynamics (a finer mesh category to allow for more exact solutions in these domains of high interest) at Coarser on the housing tube sides and Normal on the pellet sides for the normal (2nd) case mesh level, as an example for the mesh 2 or normal case. Where commonly the housing boundary default mesh size settings are one or two levels lower than the pellet boundary's size (see the 9 COMSOL default settings listed in section 5.2) in order to achieve a ratio of 1:2 which is optimal for the stable convergence of non-linear contact pairs. The universal domain free mesh size is calibrated for general physics at a Normal setting for the normal case.

The mesh is designed so that the pellet mesh is the dominate control feature of the mesh design. This was done after preliminary analysis revealed that the predominate temperature change in the problem occurs in and around the pellet, with all other temperature features extending out beyond the pellet requiring less detail than within the pellet.

An extensive mesh-density evaluation of this problem was performed early in the study and revealed that the extra coarse mesh with linear finite-element basis function was sufficient to analyze this problem's time-dependent values provided that a quadratic finite-element basis function was also exercised with the extremely fine-mesh to confirm extra coarse mesh values at the times yielding safety basis values, EOC-1 and EOC-3. Therefore, the time-dependent results corresponding to mesh cases 2, 3, and 4 are not documented herein. Only the first and last mesh case (extra coarse and extremely fine) results are directly documented in the analysis, and as a result will be more closely examined in this section. Should it become necessary to examine time-dependent results for finer meshes, all mesh cases were retained in the model for that potential purpose.

The pellet and adjacent housing domain mesh have the highest impact on the solution and are shown below for all 5 mesh cases in Figure 6.4 through Figure 6.6. Note that the mesh density is refined near the cylinder radius edge as recommended by the COMSOL documentation for contact-pair problems, with a desired ratio of 2 to 1 for the adjacent cladding surface mesh density, as well as on the top surfaces of each pellet which is evident for the finer meshes. This is a noted improvement from previous models that did not control the mesh as closely in this manner. The housing is chosen as the source boundary as it is both the stiffer and concave-shaped surface under contact, the destination boundary (pellet radial surface) is then more finely meshed as a result.

Each individual domain is meshed separately. Extra care is exercised between domains that are combined as a union and those domains that are left separately to be combined as an assembly during the geometry creation process. If an assembly is used to form the geometry, adjacent mesh surfaces are not imprinted automatically. The domains outside the pellet stack/housing regions experience less change with increasing mesh fineness as they are governed by a general physics mesh calibration, instead of a fluid dynamics calibration for the surface settings. Figure 6.7 shows the mesh in the WBT, housing and upper expansion spacer regions (where mesh refinement is seen at the expansion spacer/WBT contact boundaries) and Figure 6.8 shows the mesh for the BEC, LST, and lower expansion spacer regions.

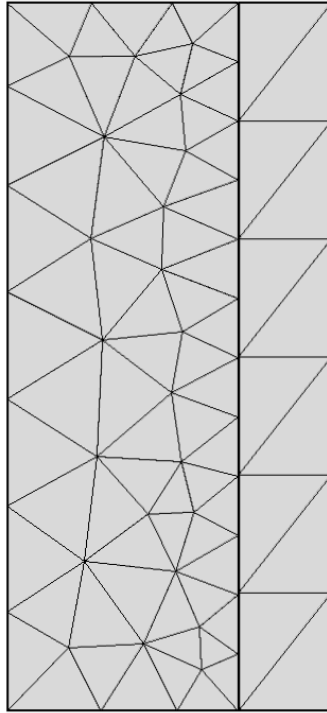


Figure 6.4: Extra coarse mesh in the pellet/cladding region.

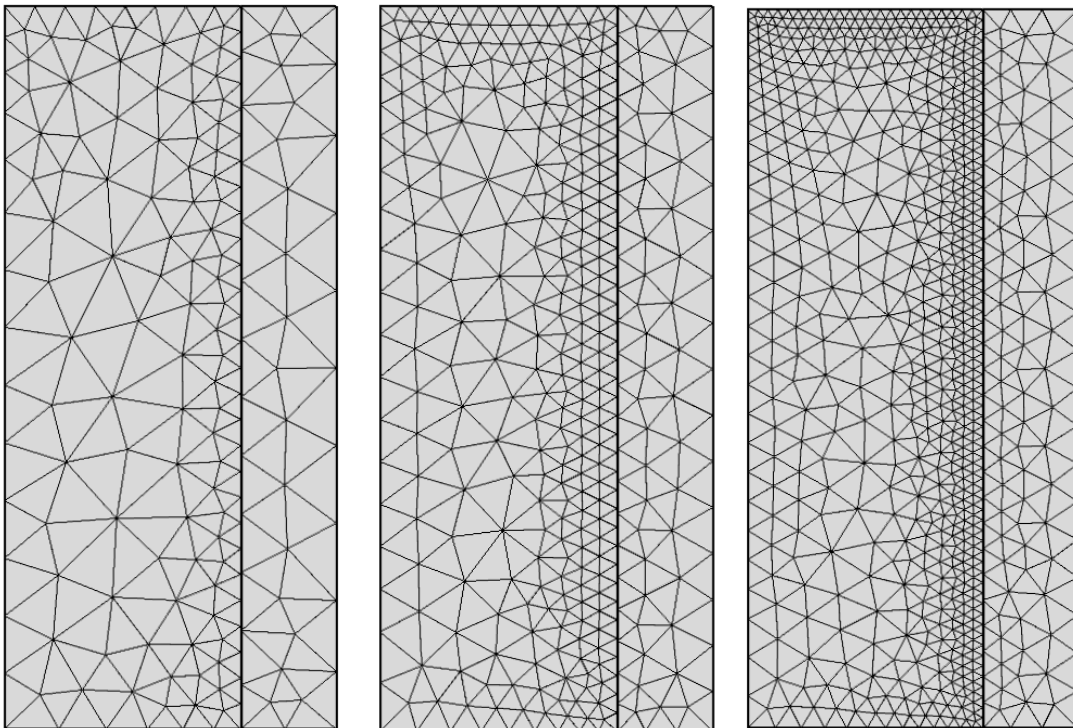


Figure 6.5: Normal, finer and extra fine meshes in the pellet/cladding region.

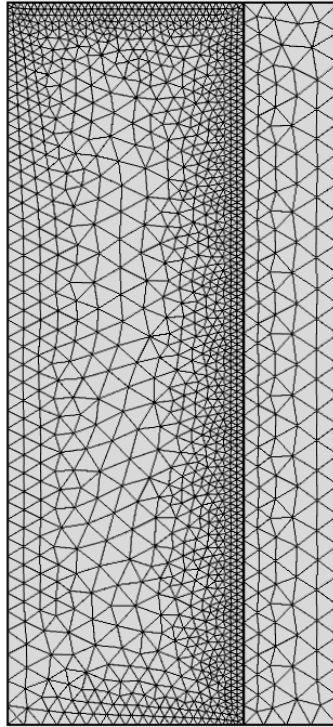


Figure 6.6: Extremely fine mesh in the pellet/cladding region.

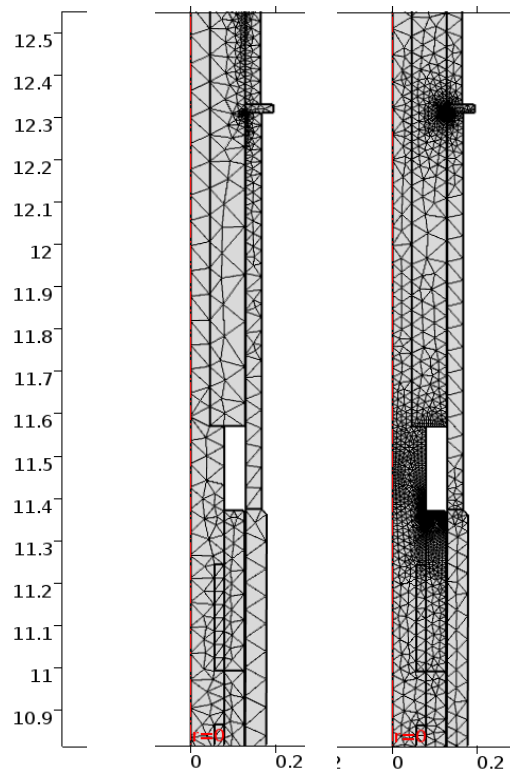


Figure 6.7: Extra coarse and extremely fine meshes in the upper region near the WBT.

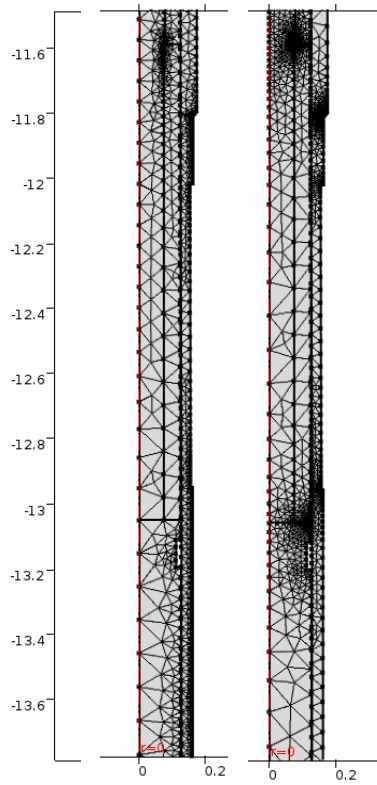


Figure 6.8: Extra coarse and extremely fine meshes in the lower region near the BEC, LST, lower expansion spacers and housing.

6.4 Analyses and Discussion

In the previous fully loaded target analyses, three of the five revisions addressed the maximum target temperatures with respect to the melting temperature and the final two revisions supported the assessment of target axial stresses with axially-dependent thermal data. The analyses for the production model address the bounding temperatures and provide supported axially-dependent thermal data in one assessment, while also providing an assessment of the structural integrity of the target (in terms of the axial stresses among other features).

There are four different model cases analyzed: 1) design-basis (DB) case at steady-state 100% flow, or “best-estimate” 2) DB case at steady-state 50% flow, and 3) thermally limiting basis (TLB) case at 130% overpower conditions, and 4) structurally limiting basis (SLB) case at 130% overpower conditions. Case 2 and 3 are run for the hot pin (or Pin 1) in position VXF-15, and for the DB case at 100% flow (also referred to as the “best-estimate” model) the model is run for all 7 pins in position VXF-15 and pin 1 in position VXF-3. The SLB case is run only for EOC-3, where maximum irradiation swelling leads the limiting conditions for structural integrity.

6.4.1 Best-estimate Analyses

The best-estimate case is analyzed for all irradiation pins, all seven positions in the holder in position VXF-15 and the hot pin (pin 1) in position VXF-3 which is referred to as a “Pin 8”. All eight pins are analyzed over the course of 3 cycles, at 10 discrete time periods (0, 1, 3, 5, 10, 15, 20, 22, 24, and 26 days into each irradiation cycles). Figure 6.9 below provides a summary of the analyses for the eight pins with their maximum target temperatures plotted against irradiation days into the cycle, where Pin 1 of VXF-15 has the highest temperatures over the 3 cycles, Pin 8 (or pin 1 of VXF-3) has the second highest, and the highest temperature pins (1, 2, 3, and 8) have their maximum temperatures at EOC-1.

Figure 6.10 shows the target side pressure for pin 1 over 3 cycles as a function of irradiation days,

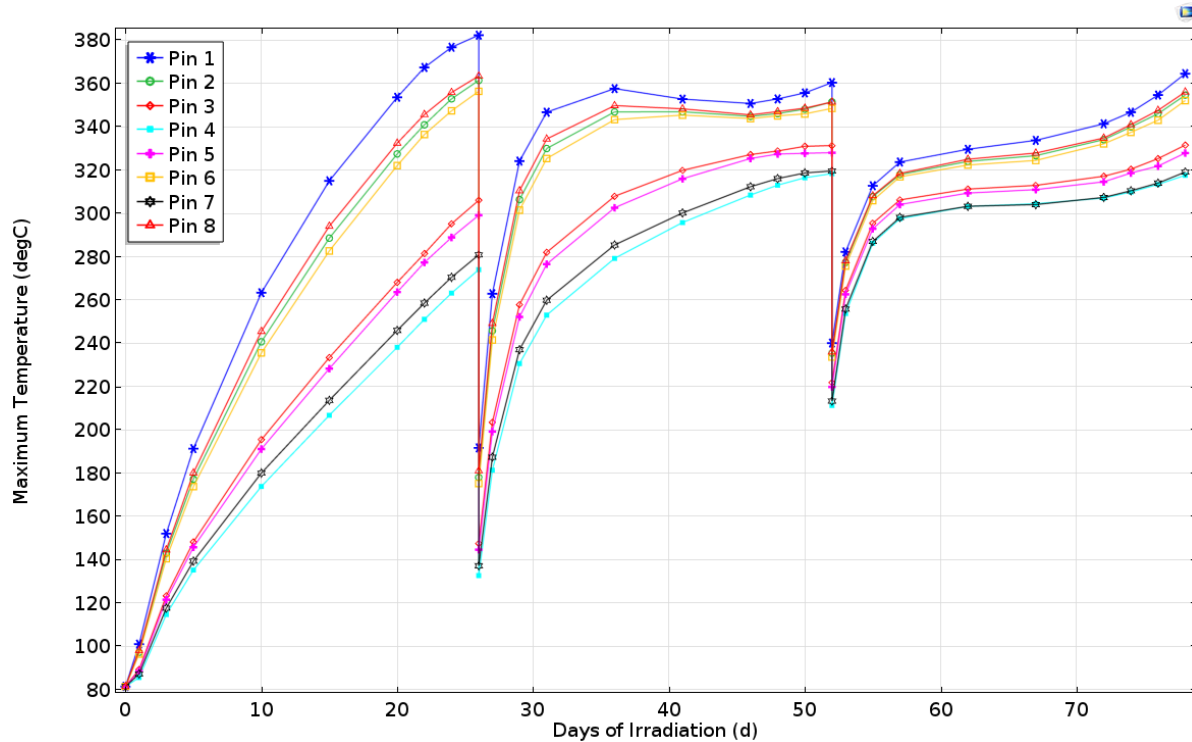


Figure 6.9: Maximum target temperatures over 3 irradiation cycles (78 days) for all 7 pins in VXF-15 and pin 1 in VXF-3 (“Pin 8”).

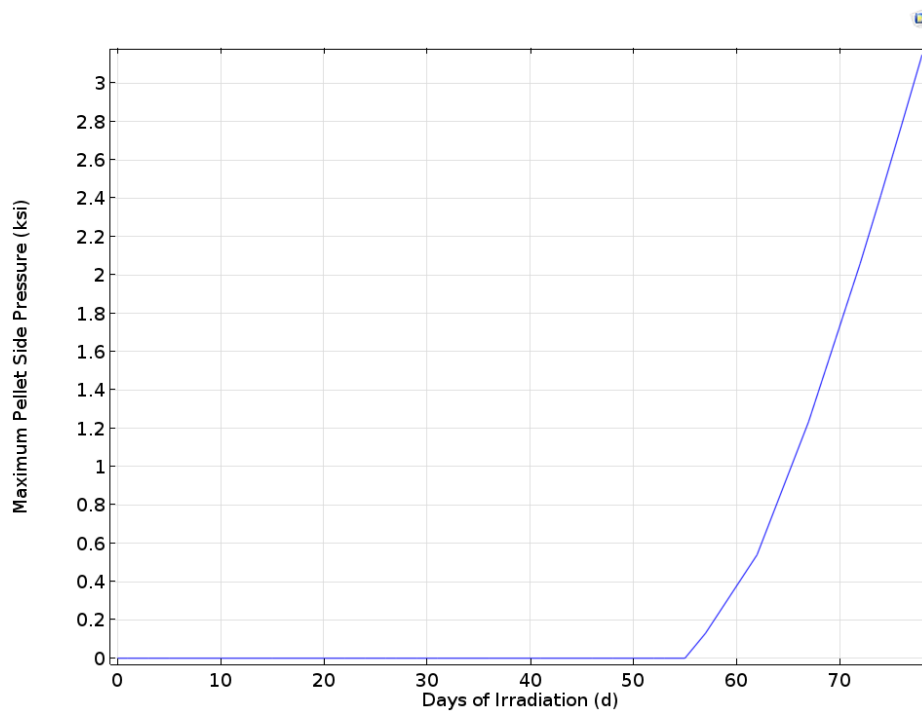


Figure 6.10: Maximum side pressure over 3 irradiation cycles (78 days) for pin 1 in VXF-15.

where the peak pressure occurs at EOC-3. Figure 6.11 shows the temperature profiles in the VXF-15 pin 1 NpO_2/Al pellet stack on a 2-D R-Z section (spatially not-to-scale) for the EOC-1, 2, and 3, while Figure 6.12 shows the effect of irradiation-induced swelling/densification in the pellet/housing gap at the end of each cycle. Figure 6.13 through Figure 6.15 show the pellet centerline temperature profiles for cycles 1, 2, and 3, respectively at ten discrete time steps in each cycle. Figure 6.16 and Figure 6.17 show pellet side temperature and pressures, respectively, for cycle 3 at ten discrete time steps in the cycle. Altogether, the figures show the similar dynamic previously observed where due to higher burnups in the center of the pellet stack linear swelling begins to close the gap and the maximum temperature regions move to the “outer ends” where the gap is larger. During cycle 3, contact is made with the pellet housing at around day 5 and pellet temperatures are reduced as a result.

6.4.2 Thermally Limiting Safety-Basis

As previously noted, the TLB yields the highest pellet temperature and the minimum safety factor for the calculation. The TLB case is analyzed for the VXF-15 hot pin only over 3 cycles, as the best-estimate case analyses of all pins establishes that Pin 1 is the “hottest” pin and most important for thermal safety analyses. Figure 6.18 shows the maximum pellet temperatures in material regions 5611-5619 where lower numbers denote pellets closer to the horizontal midplane. Figure 6.19 shows the von Mises stress profile in the center pellet at EOC-2 and 3 for a rotated 3-D view, with 100x deformation included. At EOC-2, the pellet expected hourglass shape is clearly shown. By EOC-3 internal strains have clearly risen as the pellet makes side contact with the cladding and, as a result, expansion is expressed as axial elongation, making it more difficult to observe the characteristic hourglass shape. In addition, peak stresses in the pellet have moved from the pellet “corners” to the pellet radial side.

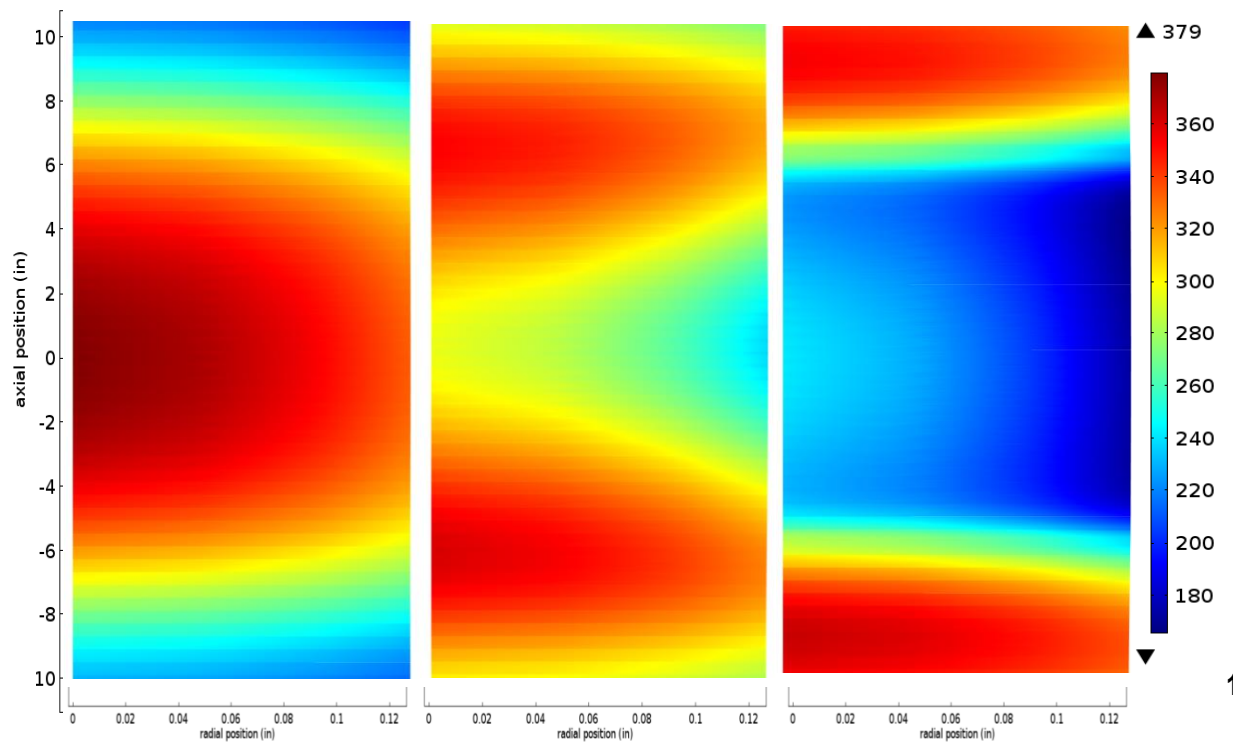


Figure 6.11: 2-D R-Z (distorted) VXF-15 pin 1 pellet temperature profiles (°C) for EOC-1, 2, and 3.

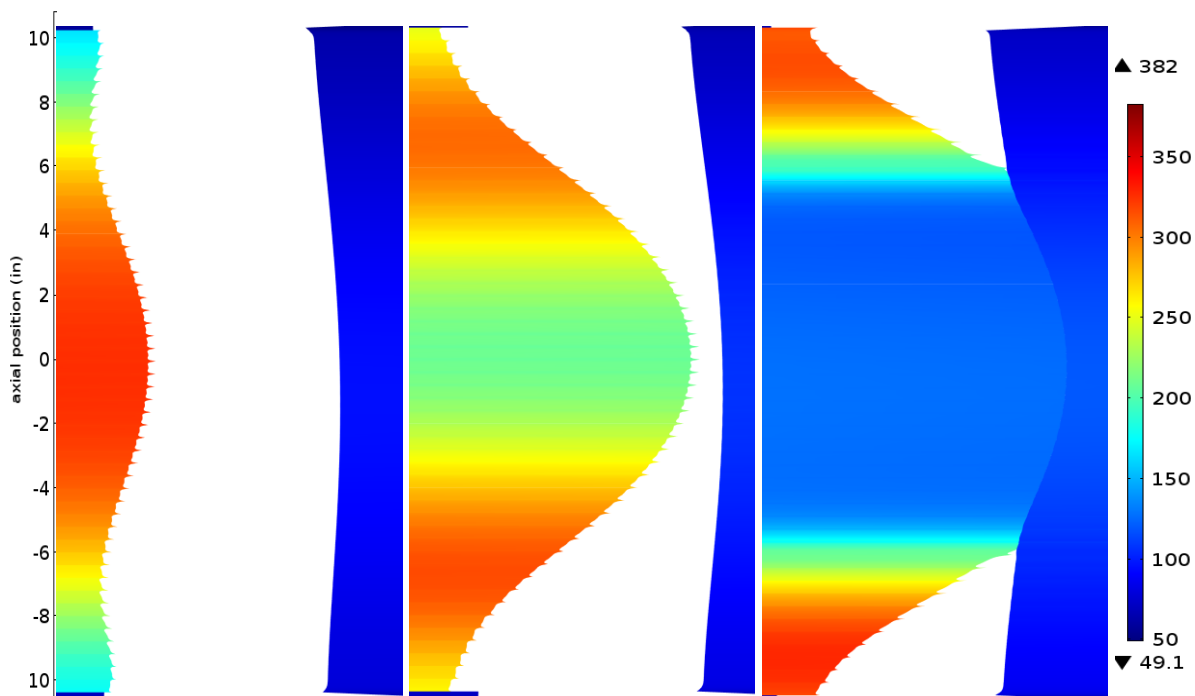


Figure 6.12: 2-D R-Z (distorted) VXF-15 pin 1 pellet temperature profiles (°C) showing radial gap for EOC-1, 2, and 3 where gap width shown is approximately 1 mil.

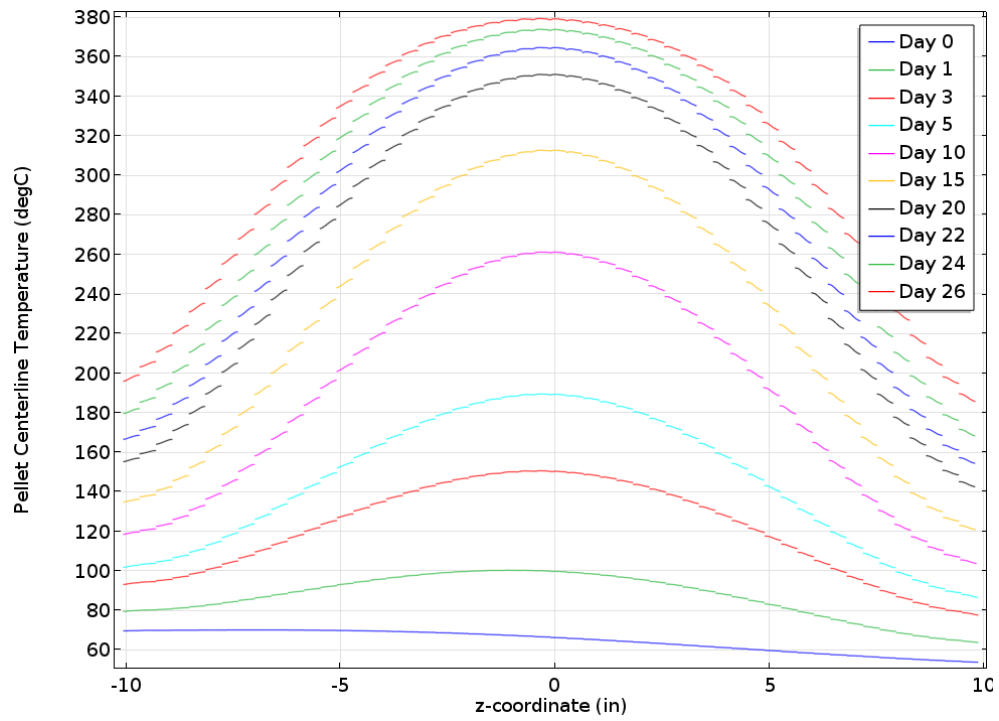


Figure 6.13: Pin 1, cycle 1 pellet centerline temperatures as a function of axial position.

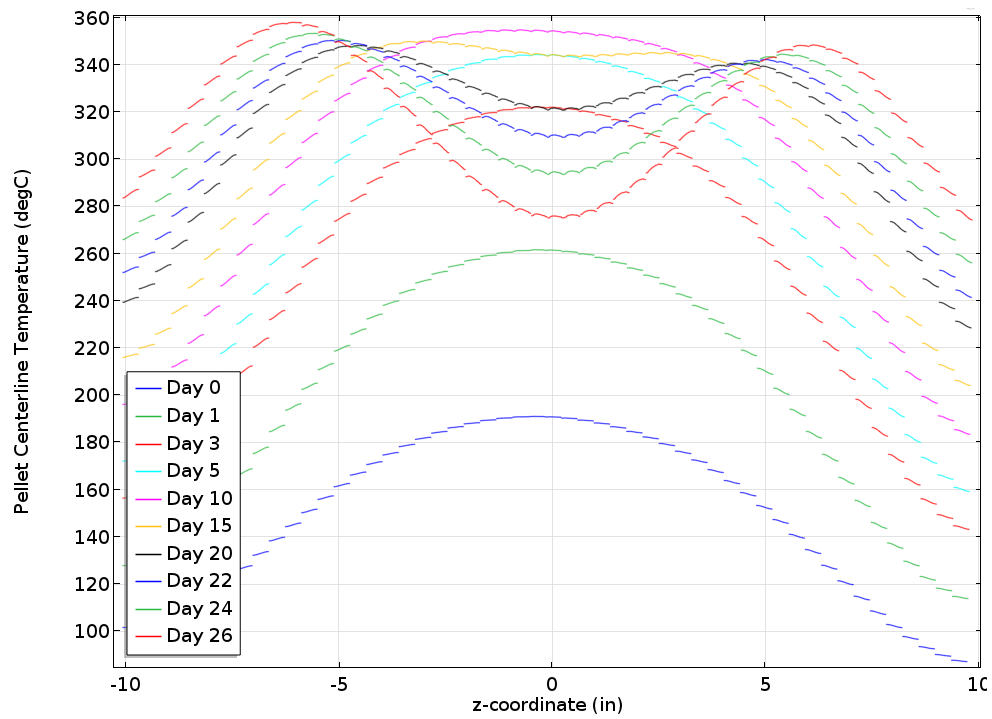


Figure 6.14: Pin 1, cycle 2 pellet centerline temperatures as a function of axial position.

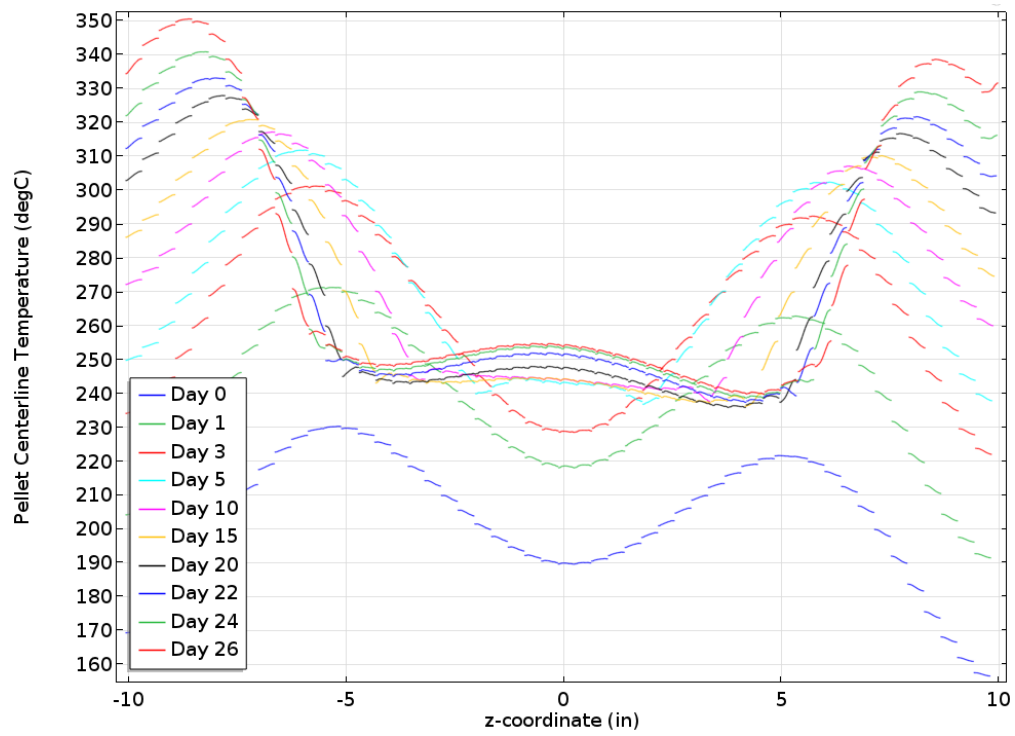


Figure 6.15: Pin 1, cycle 3 pellet centerline temperatures as a function of axial position.

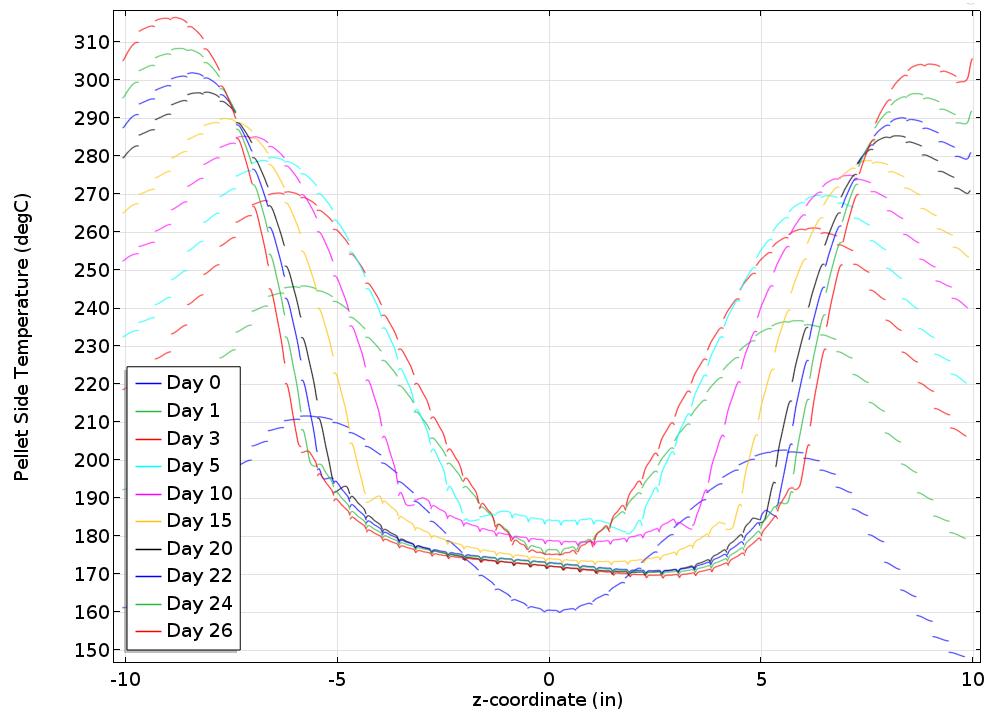


Figure 6.16: Pin 1, cycle 3 pellet side temperatures as a function of axial position.

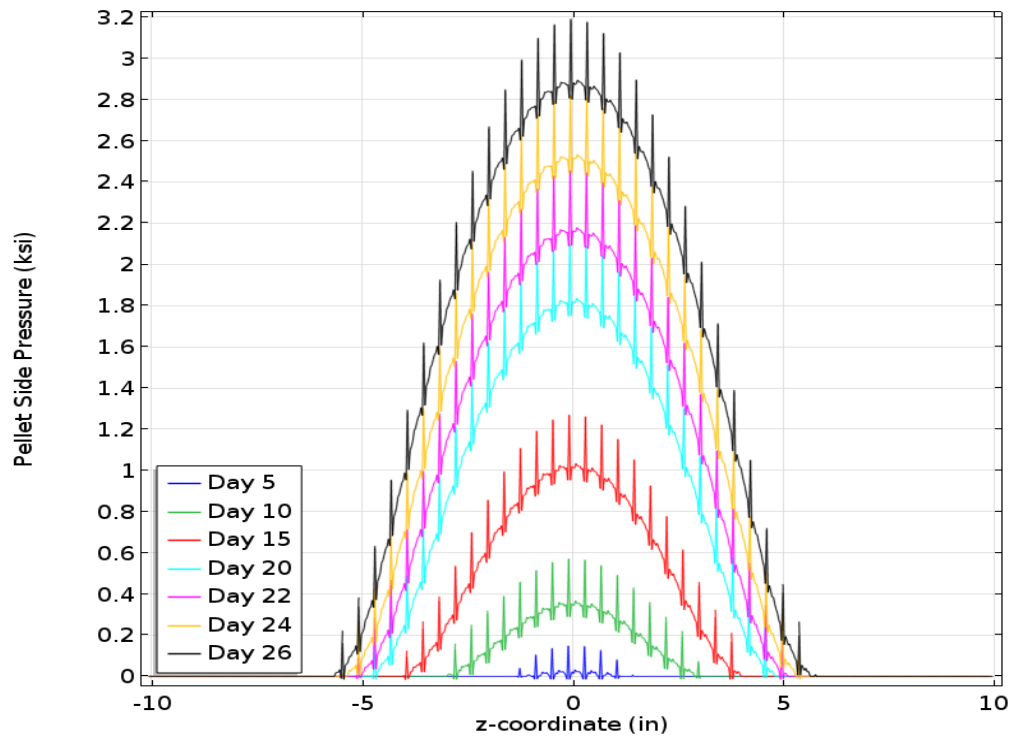


Figure 6.17: Pin 1, cycle 3 pellet side pressures as a function of axial position.

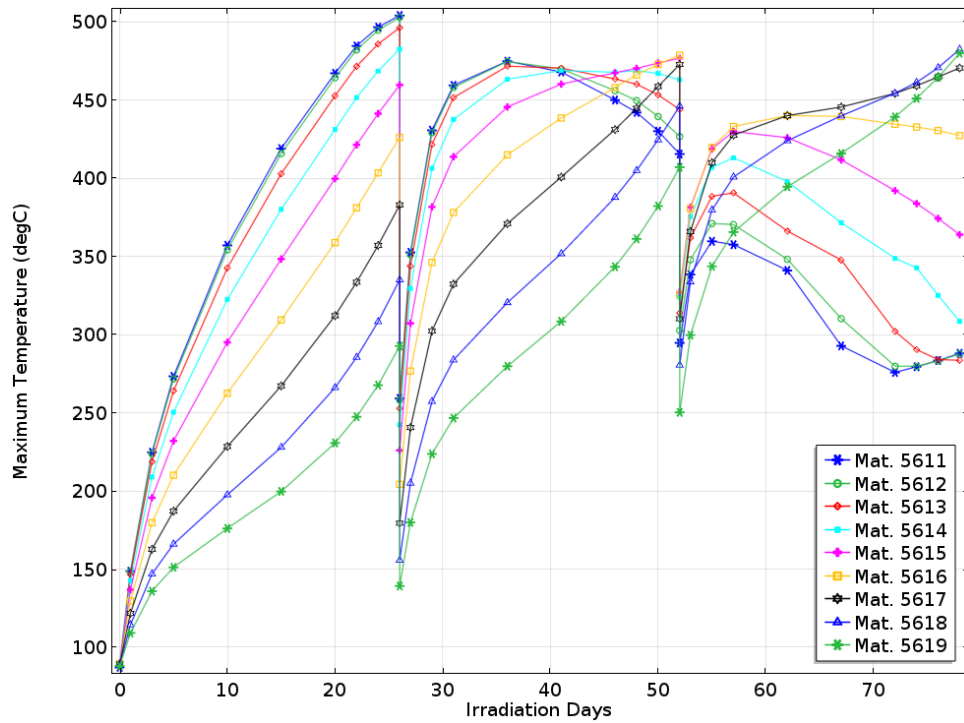


Figure 6.18: Pin 1 maximum material region temperatures as a function of irradiation days over 3 cycles.

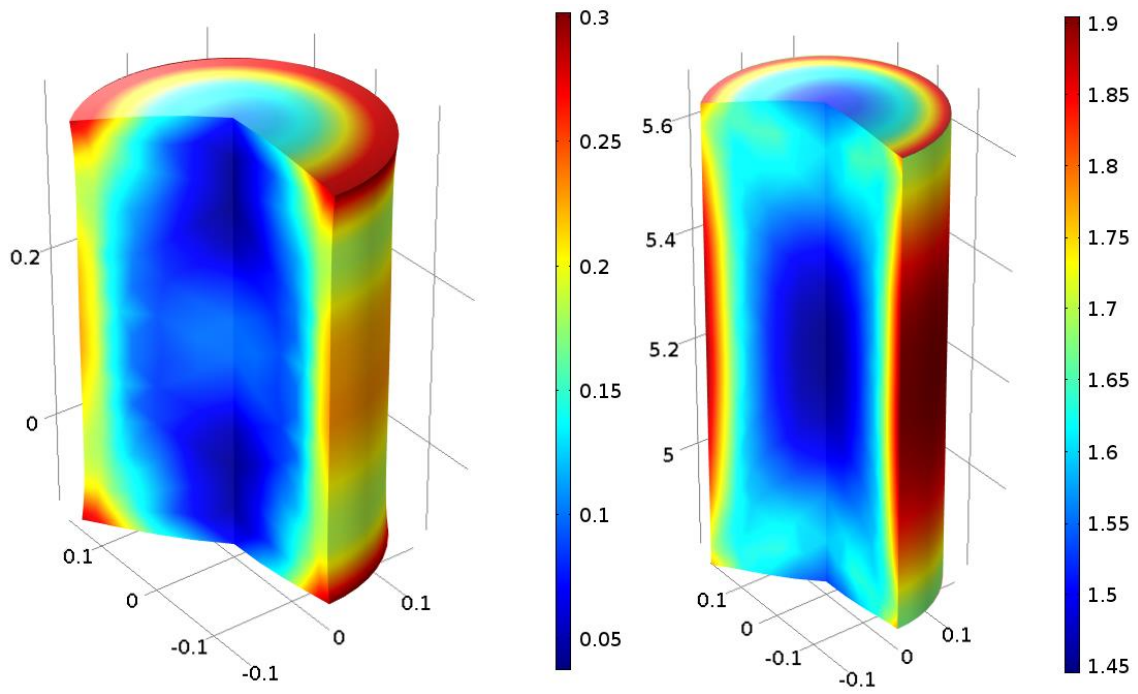


Figure 6.19: 3-D center pellet von Mises stress profile at TLB EOC-2 and 3 with 100x deformation.

6.4.3 Design-Basis 50% Flow

The worst-case steady-state flow reduction of 50% is analyzed at DB or normal reactor operating conditions per EG-6 [110]. As the best-estimate case analyses of all pins establishes that Pin 1 is the “hottest” pin and most important for thermal safety analyses, the DB 50% flow case only analyzes the VXF-15 pin 1 conditions for 3 cycles.

The bulk temperature and target surface temperature profiles as a function of distance into the coolant flow (starting from the top of the target) are shown in Figure 6.20 and Figure 6.21 at EOC-3 for both the DB 50% flow case as well as the DB 100% flow (or best-estimate) case and TLB case. The end of the third cycle is the time period of highest steady-state coolant and target surface temperatures as the highest heat generation rates occur in this cycle. Although the highest target surface and bulk temperatures occur in the DB at 50% flow case, the TLB results remain the bounding safety factor for coolant burnout as they are at 130% overpower conditions which includes a reduced inlet coolant pressure of 343 psig (from nominal at 468 psig) that, with pressure drop, yields a lower water saturation temperature of 391.7 °F (from nominal at 431.7 °F) [111].

6.4.4 Structurally Limiting Safety-Basis

The SLB conditions previously described are only analyzed at EOC-3, for the two primary cases that serve to maximize either radial or axial stresses/forces in the target and are denoted SLB-1 and SLB-2, respectively. The reason for this limited solution space is that the structurally limiting conditions, as confirmed by analysis of the previous case results, are driven by the pellet volume swelling under irradiation, which is at its maximum at the highest burnup at EOC-3.

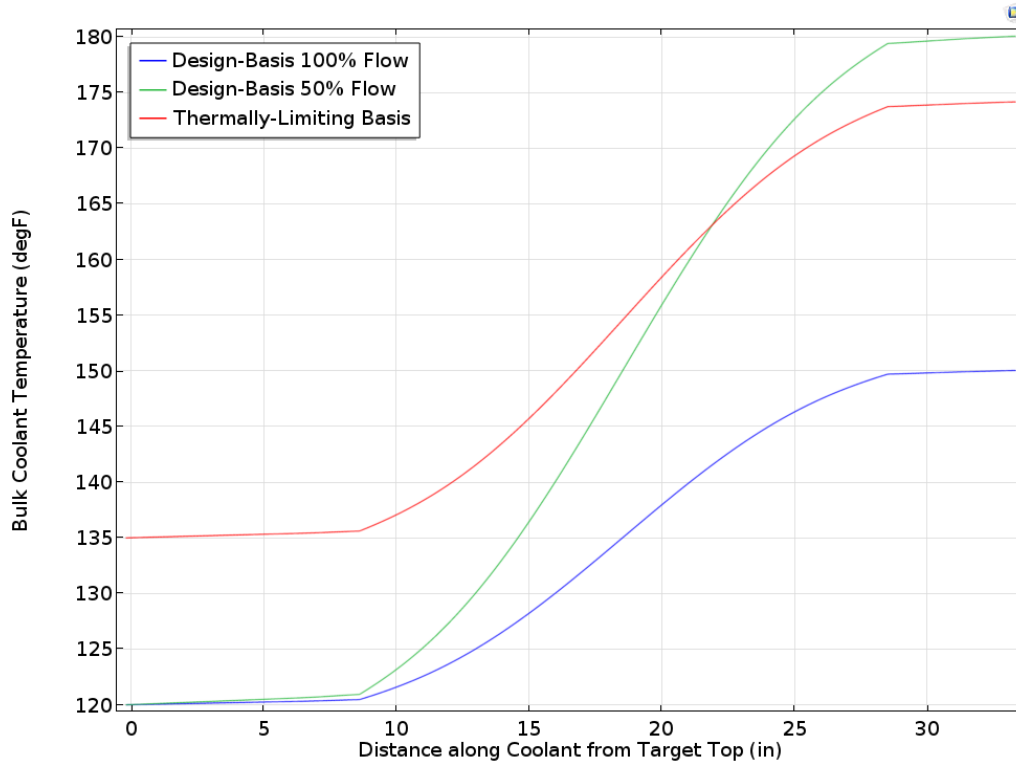


Figure 6.20: EOC-3 bulk coolant temperature as a function of axial position for all cases.

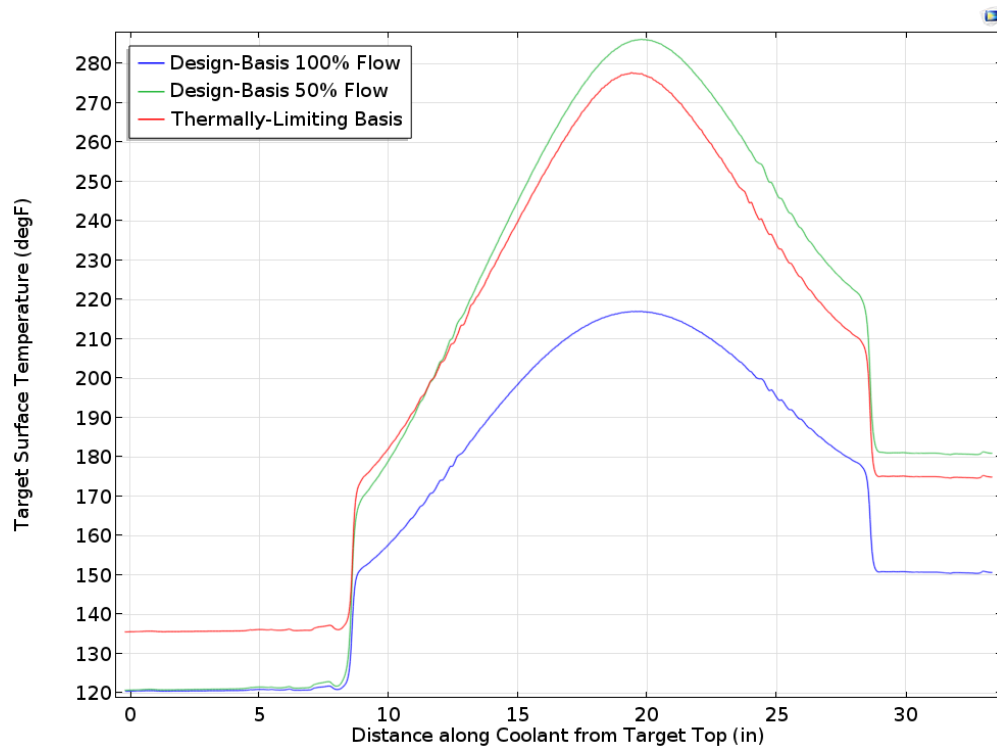


Figure 6.21: EOC-3 target surface temperature as a function of axial position for all cases.

For both cases, the resulting stresses/forces were within their safety limits, as later described in the following section. The “hot pellet” or center pellet stress profile at EOC-3 is shown for a 3-D rotation of 225° for the TLB case (previously shown in Figure 6.19), SLB-1 and SLB-2 cases in Figure 6.22. The axial elongation due to pellet side contact previously noted in Figure 6.19 is extended even further for the SLB cases, where pellet volumetric swelling is significantly increased. For the SLB-1 case, side stresses approximately triple and the pellet deforms upward. For the SLB-2 case stresses maxima are in the center of the target, since for this case axial compression occurs on the pellet stack and expansion into the cladding side wall is minimized. The stress maxima in the pellet stack are higher for the SLB-1 case, however average stress profiles are closer between SLB-1 and SLB-2 where the stress of axial compression is spread throughout the entire pellet stack, as shown in the distorted 3-D stress plots in Figure 6.23 where stress minima for SLB-2 are higher than for SLB-1.

It is important to note the changing scales (on the right of each plot) in Figure 6.22 and Figure 6.23, which if unnoticed could lead to misleading interpretations of the results. These plots are therefore best used for comparing differing behavioral trends in the different cases, and only cautiously for comparisons of magnitude.

6.4.5 Mesh Refinement Study

Mesh refinement studies were performed for both the best-estimate and TLB cases that will now be discussed. The TLB study was performed at EOC-1 and the best-estimate study was performed at 100% flow EOC-3 in order to assess a sufficient variety of the solution space.

The number of mesh elements in the pellet/housing region was roughly doubled at each convergence step and an error estimate was made from three post-processing results: 1) the net energy balance loss in the pellets (energy generated minus energy removal), 2) the maximum pellet centerline temperature, and 3) the maximum pellet side pressure (for EOC-3 study) or minimum axial clearance (for EOC-1).

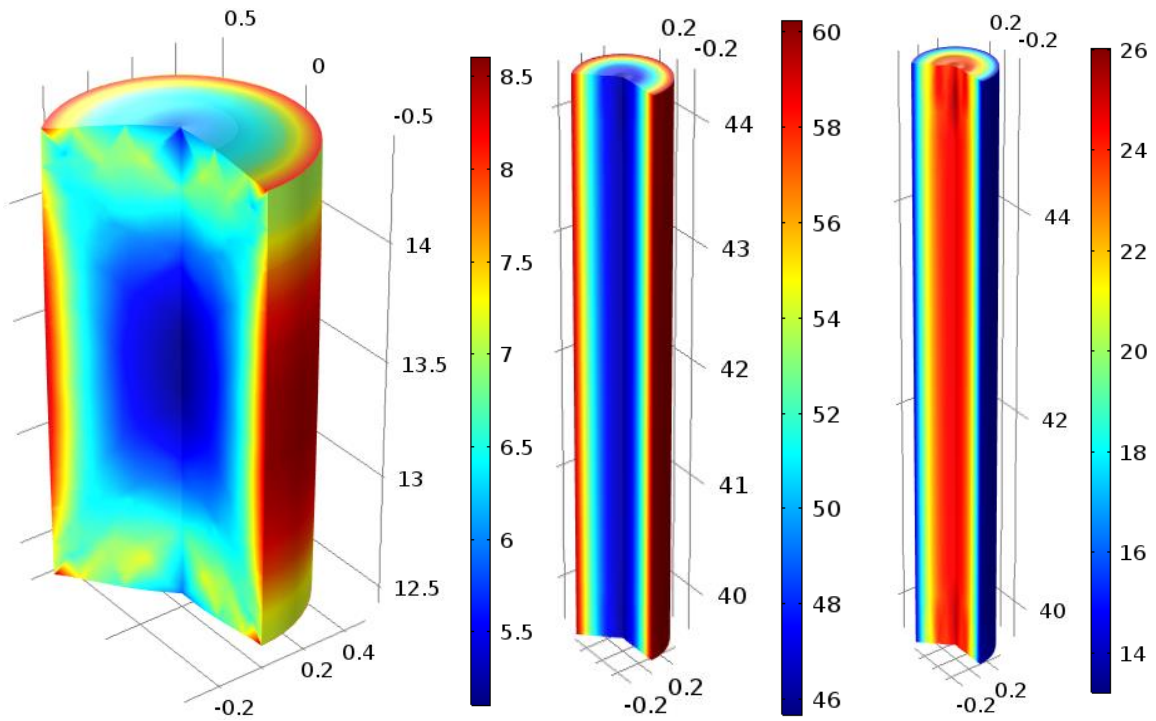


Figure 6.22: 3-D center pellet von Mises stress profile (in MPa) at EOC-3 for TLB, SLB-1 and SLB-2 cases with 100x deformation (dimensions in cm).

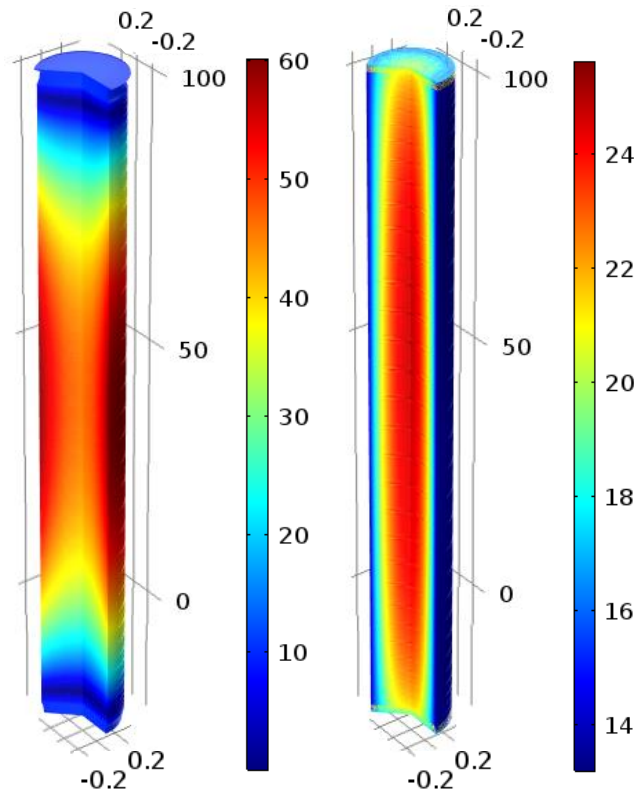


Figure 6.23: 3-D pellet stack von Mises stress profile (in MPa) at EOC-3 for SLB-1 and SLB-2 cases with 100x deformation and 20x distortion in R direction (dimensions in cm).

The individual error estimates were defined in Equation 6.8, where e is the error norm, T is the parameter of interest, k is the element order or basis, and $h/2$ denotes the doubling of the mesh number:

$$e^{h/2} = \frac{\Delta T^{h/2}}{2^{2k} - 1}$$

Equation 6.8

The final error “norm” is defined as the p-norm of the three individual estimates in Equation 6.9:

$$\|e^{h/2}\| = \left(\prod_{i=1}^3 e_i^{h/2} \right)^{1/3}$$

Equation 6.9

There are some limitations to this error norm estimation method, in that its derivation assumes equal size mesh elements, which is not true for this refinement study, and that it assumes doubling of the mesh number for each refinement step, which is approximately true for this refinement study. The error norm is plotted against the reciprocal of the mesh number in log-log scaling in Figure 6.24 and Figure 6.25 using the error norm based on an average of all three parameters and the maximum temperature, respectively. Each plot contains refinement curves using linear ($k=1$) and quadratic ($k=2$) basis elements as well as EOC-1 and EOC-3 inputs. The refinement study for the higher basis quadratic elements have both lower error norms and an increased convergence “slope”. The EOC-1 and EOC-3 refinement studies exhibit very similar convergence slopes and error values.

The error norm estimate using only the maximum temperature shows a clear increased convergence slope compared to the 3-parameter averaged error norm, possibly due to the increased role of non-linear physics in the other two parameters. The convergence slopes for all refinement studies fall short of the theoretical values of 2 (for linear basis) and 4 (for quadratic basis), where a value of ~ 0.85 - 1.54 is observed for the linear basis studies and ~ 1.28 - 2.92 is observed for the quadratic basis studies. This is likely due to the non-linear thermo-mechanical feedbacks and complexity of the model, as well as the limitations in this refinement study previously mentioned. Comparing the convergence slopes to those in

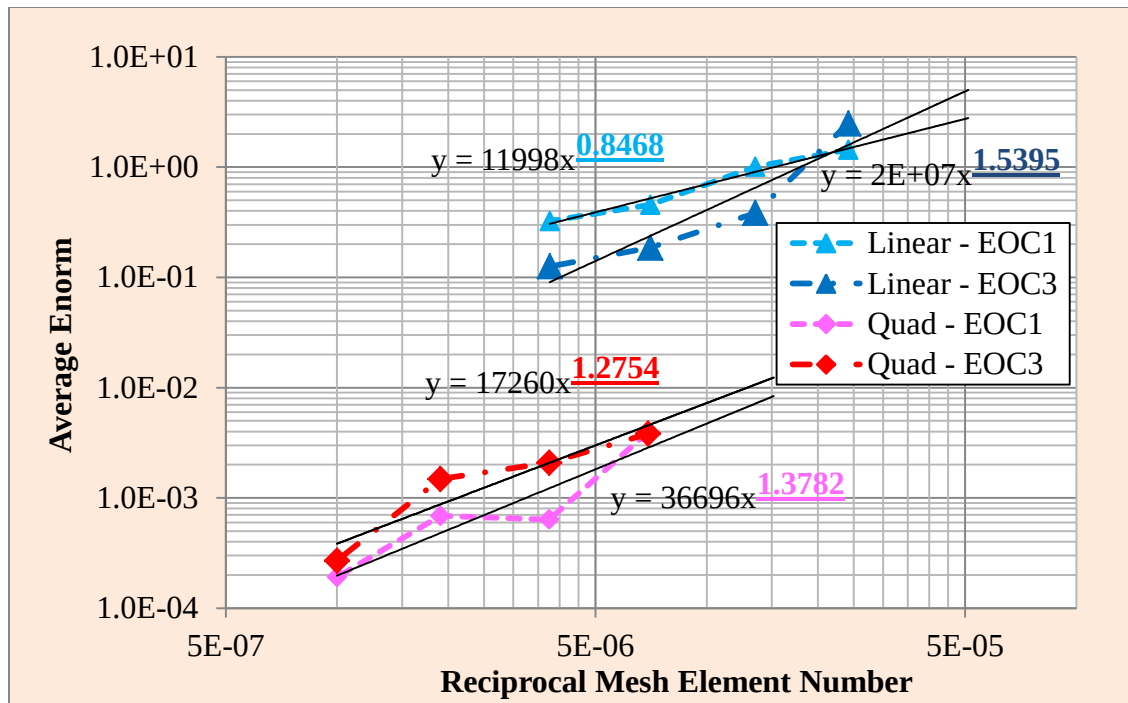


Figure 6.24: Mesh refinement results for EOC1/EOC3 and linear/quadratic bases using an averaged error norm.

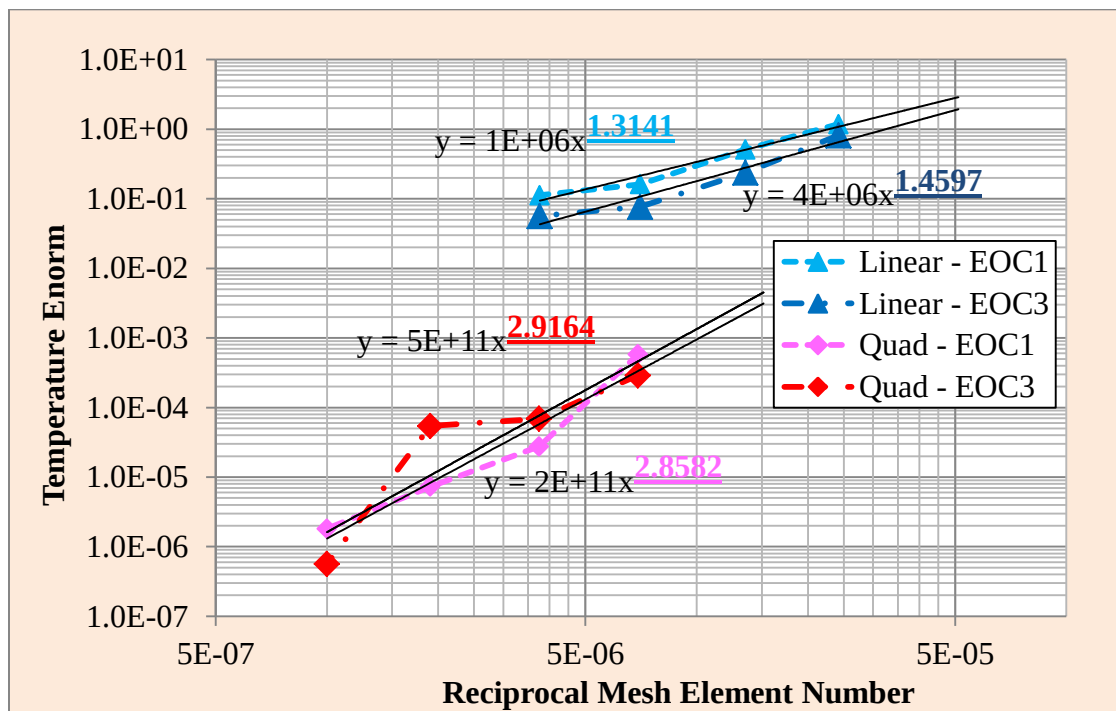


Figure 6.25: Mesh refinement results for EOC1/EOC3 and linear/quadratic bases using the maximum temperature error norm.

the revision 4 analysis of the fully loaded target model, there is a considerable increase in the convergence slope likely due to improved methodology in the production model (including augmented Lagrangian contact instead of penalty factor, more detailed meshing control, etc.). For reference, the local convergence slope would be determined as shown in Equation 6.10, where M is the number of mesh elements:

$$slope = \frac{\log(e^{h/M} / e^{h/2M})}{\log(2)}$$

Equation 6.10

6.4.6 Summary of Production Target Analyses

A summary of the limiting parameter results for each case and identification of the case which yields the lowest safety factor ratio are given in Table 6.1. The primary safety limits of interest over the entire 3 cycle irradiation period are: 1) the maximum target temperature, 2) the maximum side/radial pressure on

Table 6.1: Summary of safety limit results for the production target analyses.

<i>Model Case</i>	$T_{\max}$ (°C)	$P_{\max\text{-side}}$ (ksi)	$\delta_{\min\text{-axial}}$ (mils)	$F_{\max\text{-axial}}$ (lbf)	$T_{\max\text{-surf}}$ (°F)	$\epsilon_{\max\text{-local}}$
<i>DB at 100% flow</i>	382.40	3.30	115.45	0	213.45 ^a	3.79%
<i>DB at 50% flow</i>	403.91	3.10	116.83	0	281.79 ^a	4.05%
<i>TLB</i>	494.95	1.86	158.34	0	270.49 ^b	2.74%
<i>SLB-1</i>	308.93	8.50	41.28	49.31	268.00 ^b	5.62%
<i>SLB-2</i>	404.87	3.50	0	253.65	268.00 ^b	5.72%
<i>Safety Limit</i>	650	21	N/A	659.675	392 ^a -432 ^b	10.27%
<i>Safety Factor</i>	1.31	2.47	N/A	2.60	1.59	1.79

Note a: Model cases with note “a” use a DB inlet pressure and thus surface saturation temperature of ~432 °F.

Note b: Model cases with note “b” use a DB inlet pressure and thus surface saturation temperature of ~392 °F.

the cladding wall by the NpO_2/Al pellets, 3) the maximum estimate of the force on the target axially, 4) the maximum target surface temperature, and 5) the maximum local linear cladding strain due to single pellet expansion. The axial clearance was also included, since many cases did not put any load on the target axially. The maximum target temperature typically occurs at end-of-cycle 1 (EOC-1), with other temperature local maxima occurring at EOC-2, EOC-3 and around day 10 into cycle 2. The maximum target stress/strains and target surface temperatures occur at the EOC-3.

The lower two rows of the table show the safety limits and minimum safety factors (ratio of safety limit to analyzed value), where the value that yields the minimum safety factor for each parameter is highlighted in **bold** in the upper portion of the table. In order to satisfy structural integrity of the target, the side pressure safety limit will be set to the tensile yield strength of the cladding material Al-6061-t4 at 21 ksi [85] and the axial force safety limit of the target will be set to 659.675 lb-f as taken from the minimum of failure tests documented in Attachments 3 through 6 of [86]. Tests have shown that the yield strength of 6061 grade aluminum increases under irradiation [109].

A special case where the hydrostatic collapse of the target causes the cladding to surround each pellet individually – a concern raised from PIE gamma scans of the irradiated targets – is considered here. To address this, the local strain maxima for each pellet, conservatively allowing no diametrical strain to occur against the adjacent housing, are considered for this case. The unirradiated failure strain for clad material 6061-t4 is 22%. Under irradiation, the failure elongation decreases and tests [109] for 6061-t6 showed a decrease from 15% to 9-5% (from 50 to 150 °C). Considering that the T4 temper has a greater unirradiated elongation than the T6 temper, that temperatures in the housing are below 150 °C, and that neutron fluence in the reference case were on the order of 10^{27} n/m²-s which is two orders of magnitude greater than those expected over 3 cycles ($\sim 10^{24}$ - 10^{25}) the 5% elongation failure is likely an overly conservative estimate. Taking the middle ground between 50 and 150 °C loss of elongations and the ratio of the greater elongation for T4 to T6, a better still conservative estimate is given as $\sim 10.27\%$. In addition, this conservatively assumes that no elastic compression of the pellets will occur, that is the

pellets are expanding and incompressible. The saturation temperature of water at reactor pressures is used for the surface temperature limit, as previously described in section 6.4.3.

The minimum safety factor comes from the pellet melting temperature shown in **bold**, where the calculated maximum temperature for the TLB case at EOC-3 is approximately 150 °C below the melting temperature. Figure 6.26 and Figure 6.27 show a parametric sweep case of the power factor at EOC-3 for the three primary cases (no rigid surface is set for SLB), where the TLB is shown to be constricting for maximum target temperatures, the SLB for target side pressure and the BE between the two cases.

It is worthwhile to note that although for case SLB-2 no radial expansion due to thermal or irradiation effects is allowed to occur past the cladding side wall, some significant side pressure still occurs. This is due to elastic axial compression of the pellet stack that causes a transverse strain into the side wall, a result of the calculated stress/strain equations in COMSOL that are not easily adjusted.

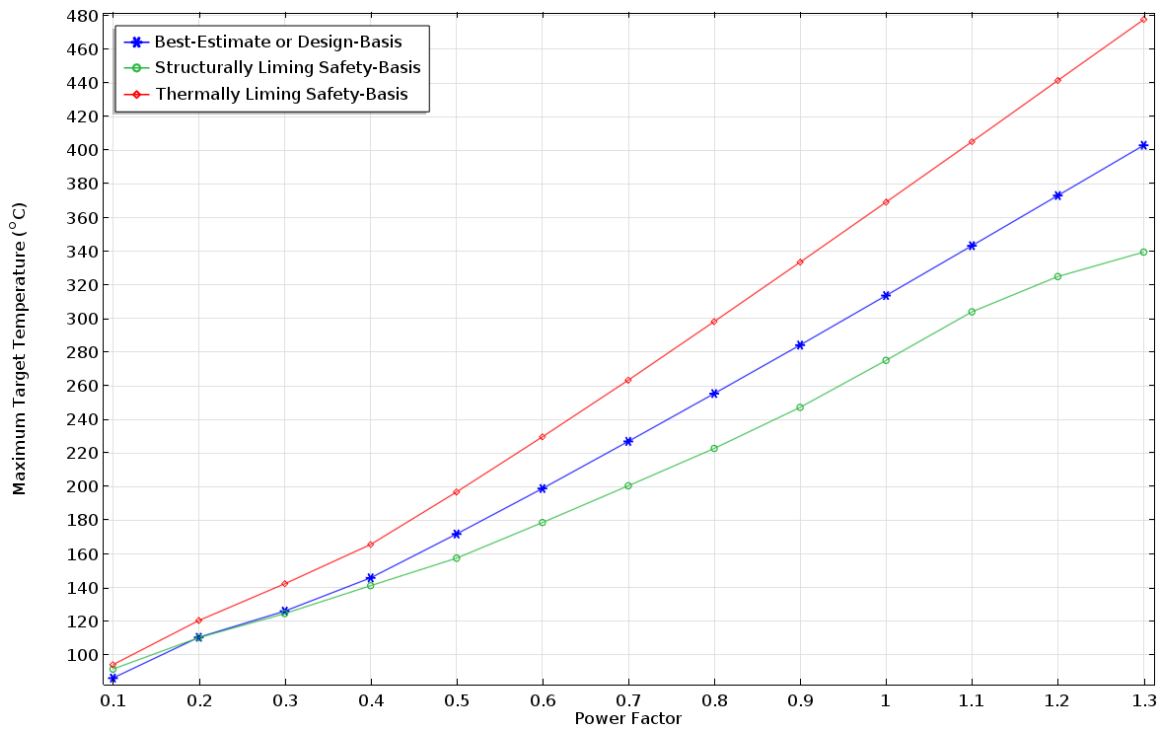


Figure 6.26: EOC-3 maximum target temperature as a function of the power/volume factor for the BE, SLB, and TLB cases.

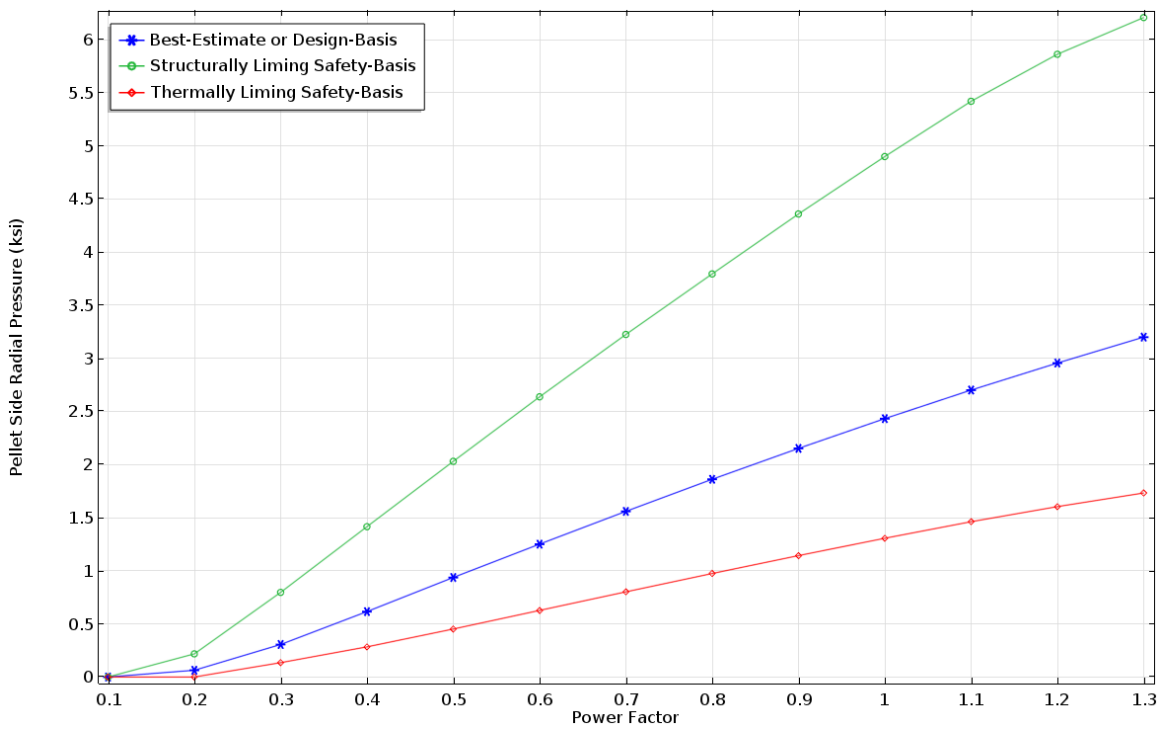


Figure 6.27: EOC-3 pellet radial side pressure as a function of the power/volume factor for the BE, SLB, and TLB cases.

7 Developing Discrete Ordinates in COMSOL Multiphysics

In this chapter, the development of COMSOL multi-dimensional and angularly-dependent neutron transport physics using the discrete ordinates method [114] is discussed. The development of this solution method was intended to serve a variety of potential purposes at the HFIR, in studying more detailed and accurate spatially-dependent flux/power distributions in the HFIR core for different conditions (both stationary and transient) as well as suited to studying other fixed source problems related to reactor operations, including deep-penetration problems in the HFIR beam tubes.

7.1 Discrete Ordinates Derivation and Methodology

The solution of neutral particle (neutron or photon) transport generally requires seven independent variables: 3 spatial coordinate variables specifying the particle position, 2 angular variables specifying the particle direction of travel, 1 variable for particle energy, and 1 variable for time. In this case, the spatial variables are solved using the finite element method, the angular variables using discrete ordinates, the energy variable using the multi-group method and the time variable with implicit time steps.

The static or time-independent neutron transport equation, as shown in Equation 7.1 [115], [116], may be solved in terms of the neutron angular flux, ψ , and includes source terms on the right hand side (RHS) of the equation (the fission source, scattering source and external fixed source, respectively) and the streaming/leakage and annihilation terms on the left hand side (LHS), respectively. The static 3-D neutron angular flux is dependent on six variables: three variables that characterize the particle position (e.g. x,y,z or r,θ,z), two variables to characterize the angular direction of particle movement (the direction cosines), and one variable for the particle energy (whose impact is seen on neutron probability cross sections), where an addition time variable makes seven total variables for a transient solution. The transient or time-dependent form of the transport equation (shown in Chapter 8) includes time-dependence terms, kinetics parameters and precursor concentration equations, as well as an additional time derivative operator in the streaming term not included in the static form.

$$\begin{aligned}
& [\hat{\Omega} \cdot \vec{\nabla} + \Sigma_t(\vec{r}, E)] \psi(\vec{r}, E, \hat{\Omega}) \\
&= \frac{\chi(E)}{k_{eff}} \int_0^\infty dE' \nu(E') \Sigma_f(\vec{r}, E') \int_{4\pi} d\Omega' \psi(\vec{r}, E', \hat{\Omega}') \\
&+ \int_{4\pi} d\Omega' \int_0^\infty dE' \Sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \psi(\vec{r}, E', \hat{\Omega}') + q_{ext}(\vec{r}, E, \hat{\Omega})
\end{aligned}$$

Equation 7.1

where: $\hat{\Omega}$ is the particle direction vector,

$\vec{\nabla}$ is the gradient operator = $\left(\frac{\partial}{\partial x} \hat{e}_x + \frac{\partial}{\partial y} \hat{e}_y + \frac{\partial}{\partial z} \hat{e}_z \right)$ in rectangular coordinates and

= $\left(\frac{\partial}{\partial r} \hat{e}_r + \frac{1}{r} \frac{\partial}{\partial \theta} \hat{e}_\theta + \frac{\partial}{\partial z} \hat{e}_z \right)$ in cylindrical coordinates,

$\Sigma_t, \Sigma_f, \Sigma_s$ are the total, fission and scattering macroscopic cross sections,

$\vec{r}$ is the particle position vector = $\vec{r}(x, y, z)$ in rectangular coordinates and

= $\vec{r}(\rho, \theta, z)$ in cylindrical coordinates,

E is the particle energy,

ψ is the angular particle flux,

χ is the fission distribution,

k_{eff} is the k-eigenvalue or effective multiplication factor,

ν is the average number of neutrons produced per fission, and

q_{ext} is the external fixed source term.

To begin the application of the discrete ordinates to the directions, a first simplification can be made to Equation 7.2 by including the definition of the scalar flux, ϕ , as the integration of the angular flux over all directions, where w_n is a quadrature weighting factor.

$$\phi(\vec{r}, E) = \int_{4\pi} \psi(\vec{r}, E, \hat{\Omega}') d\Omega' = \sum_{n=1}^N w_n \psi(\vec{r}, E, \hat{\Omega}_n)$$

Equation 7.2

In Equation 7.2 the transport equation is solved for N distinct angles and a quadrature approximation [117] is utilized to numerically integrate over the angular domain using weighting factors at each discrete direction. An example of the sampling of the unit sphere in discrete directions is shown in Figure 7.1, where an eighth sphere is shown for three discrete directions which are characterized according to their direction cosines:

where: μ is the direction cosine along the x unit vector $= \hat{\Omega} \cdot \hat{e}_x$ in rectangular coordinates, and

along the ρ unit vector $= \hat{\Omega} \cdot \hat{e}_\rho$ in cylindrical coordinates,

η is the direction cosine along the y unit vector $= \hat{\Omega} \cdot \hat{e}_y$ in rectangular coordinates, and

along the θ unit vector $= \hat{\Omega} \cdot \hat{e}_\theta$ in cylindrical coordinates, and

ξ is the direction cosine along the z unit vector $= \hat{\Omega} \cdot \hat{e}_z$.

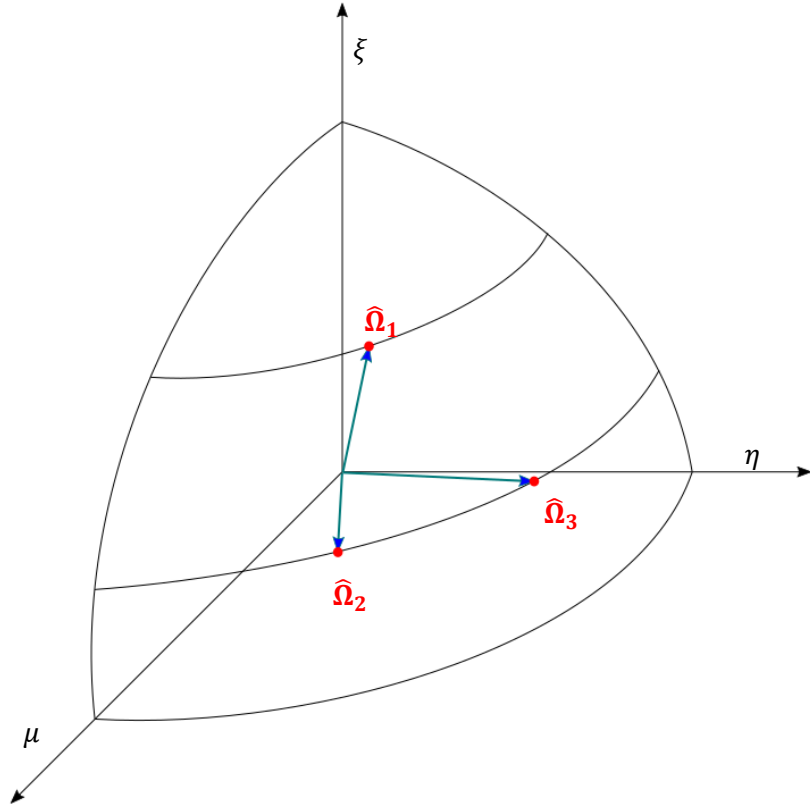


Figure 7.1: Eighth unit sphere with discrete ordinate directions sampled.

Furthermore, as later explained in section 7.1.2, it's found to be advantageous to define scalar flux moments in terms of spherical harmonics as shown in Equation 7.3. See Equation 7.22 in section 7.1.2 which simplifies the scattering source term using the definitions of spherical harmonic moments of the angular flux, which uses the discrete ordinate form of the transport equation.

$$\phi_l^m(\vec{r}, E) = \int_{4\pi} Y_{lm}(\hat{\Omega}') \psi(\vec{r}, E, \hat{\Omega}') d\Omega' = \sum_{n=1}^N w_n Y_{lm}(\hat{\Omega}_n) \psi(\vec{r}, E, \hat{\Omega}_n)$$

Equation 7.3

Having dealt with angular discretization through discrete ordinates, and understanding that COMSOL Multiphysics handles the spatial and time discretization through the FEM and implicit steps, respectively, the remaining independent variable to be discretized is particle energy. Begin by defining a group flux for energy group g , where the particle energy is subdivided into G intervals called groups and the G^{th} group is the lowest energy group:

$$\psi^g(\vec{r}, \hat{\Omega}_n) = \int_{E_g}^{E_{g-1}} \psi(\vec{r}, E', \hat{\Omega}_n) dE'$$

Equation 7.4

If one takes the transport equation in Equation 7.1 and integrates over the group domain from E_g to E_{g-1} , the group definitions for other parameters must be defined in order to conserve reaction rates:

$$\Sigma_t^g(\vec{r}) = \frac{\int_{E_g}^{E_{g-1}} \Sigma_t(\vec{r}, E') \psi(\vec{r}, E', \hat{\Omega}_n) dE'}{\phi^g(\vec{r})}$$

Equation 7.5

$$\chi^g = \int_{E_g}^{E_{g-1}} \chi(E') dE'$$

Equation 7.6

$$\nu \Sigma_f^g(\vec{r}) = \frac{\int_{E_g}^{E_{g-1}} \Sigma_t(\vec{r}, E') \phi(\vec{r}, E') dE'}{\phi^g(\vec{r})}$$

Equation 7.7

$$\mathbf{q}_{\text{ext}}^g(\vec{r}, \hat{\Omega}_n) = \int_{E_g}^{E_{g-1}} \mathbf{q}_{\text{ext}}(\vec{r}, E', \hat{\Omega}_n) dE'$$

Equation 7.8

$$\Sigma_{sl}^{g' \rightarrow g}(\vec{r}) = \frac{\int_{E_g}^{E_{g-1}} \int_{E_{g'}}^{E_{g'-1}} \Sigma_{sl}(\vec{r}, E' \rightarrow E) \Phi_l^m(\vec{r}, E') dE' dE}{\Phi_{lm}^{g'}(\vec{r})}$$

Equation 7.9

The immediate difficulty here is that in order to derive these group constants, the energy dependent fluxes and nuclear data must be known in advance. Fortunately, nuclear data with detailed time dependence is calculated in various data libraries and there are other codes that may be utilized to pre-process these cross sections given expected localized flux curves – an accurate method for fine energy group selections. The ideal approach is to start with simple problems for fine energy groups and use the scalar flux solutions to collapse to a lower number of energy groups, if broader group intervals are desired.

Applying the above discretizations in energy and angle to Equation 7.1 yields the multigroup neutron transport equation for discrete ordinates in Equation 7.10: ISCT represents the truncated number of scattering orders, or the P_N order, where isotropic scattering requires only the leading term (P_0). The number of discrete ordinates is represented by the S_N order, where for 3-D, there are $N(N+2)$ distinct directions. So for a given problem, there are $G*N(N+2)$ governing weak equations of starting form Equation 7.10.

$$\begin{aligned} & [\hat{\Omega}_n \cdot \vec{\nabla} + \Sigma_t^g(\vec{r})] \Psi_n^g(\vec{r}, \hat{\Omega}_n) \\ &= \frac{\chi^g}{k_{\text{eff}}} \sum_{g'=1}^G \nu \Sigma_f^{g'}(\vec{r}) \Phi^{g'}(\vec{r}) + \sum_{l=0}^{\text{ISCT}} \sum_{m=-1}^1 Y_{lm}^*(\hat{\Omega}_n) \sum_{g'=1}^G \Sigma_{sl}^{g' \rightarrow g}(\vec{r}) \Phi_{lm}^{g'}(\vec{r}) + \mathbf{q}_{\text{ext}}^g(\vec{r}) \end{aligned}$$

Equation 7.10

In Equation 7.10, most of the terms have the same expansion for all coordinate systems and thus their formulation varies little and need no additional derivations. However, two terms, the “streaming” or

“leakage” term and the scattering source vary significantly between each coordinate system and thus warrant further discussion in sections 7.1.1 and 7.1.2.

7.1.1 Streaming operator

The “streaming” term in the neutron transport equation is the projection or dot product of the neutron direction vector and the spatial gradient of the angular neutron flux. This term represents the movement or streaming of neutrons within the problem geometry and to the outside of its borders (thus it is also known as the “leakage” term) and its proper formulation is therefore very important to neutron transport. Table 7.1 below gives a summary of the different formulations for the coordinate systems utilized: 1-, 2-, 3-D Cartesian as well as 2-D cylindrical geometries, where ω is the angle between the unit vector $\hat{e}_\rho$ and the line made by the projection of the direction onto the plane of the unit vectors $\hat{e}_\rho$ and $\hat{e}_\theta$.

As shown in the 3-D Cartesian example in Equation 7.11, the formulation for Cartesian coordinates can be done by expanding the derivative of the neutron flux with respect to the streaming direction, s , in terms of the partial derivatives of the seven independent variables. The angular and energy derivatives are eliminated as they do not change along the streaming direction in Cartesian coordinates. For lower coordinate systems, the spatial flux gradients $\frac{\partial \psi}{\partial z}$ and $\frac{\partial \psi}{\partial y}$ are eliminated progressively for 2- and 1-D

Table 7.1: Neutron streaming operators for 1-, 2-, 3-D Cartesian and 2-D cylindrical coordinate systems.

Dimension	Spatial Variables	Angular Variables	$\hat{\Omega} \cdot \vec{\nabla}$
1D Cartesian	x	μ	$\mu \frac{\partial}{\partial x}$
2D Cartesian	x,y	μ, η	$\mu \frac{\partial}{\partial x} + \eta \frac{\partial}{\partial y}$
3D Cartesian	x,y,z	μ, η, ξ	$\mu \frac{\partial}{\partial x} + \eta \frac{\partial}{\partial y} + \xi \frac{\partial}{\partial z}$
2D Cylindrical	ρ, z	ω, ξ	$\frac{\mu}{\rho} \frac{\partial}{\partial \rho} \rho + \xi \frac{\partial}{\partial z} - \frac{1}{\rho} \frac{\partial}{\partial \omega} \eta$

Cartesian coordinates due to the infinite expansion of the problem along those axes. The time derivative is nonzero for time-dependent or transient studies, which are not considered in this work.

$$\begin{aligned}\frac{d\psi}{ds} &= \frac{\partial x}{\partial s} \frac{\partial \psi}{\partial x} + \frac{\partial y}{\partial s} \frac{\partial \psi}{\partial y} + \frac{\partial z}{\partial s} \frac{\partial \psi}{\partial z} + \frac{\partial \mu}{\partial s} \frac{\partial \psi}{\partial \mu} + \frac{\partial \eta}{\partial s} \frac{\partial \psi}{\partial \eta} + \frac{\partial \xi}{\partial s} \frac{\partial \psi}{\partial \xi} + \frac{\partial E}{\partial s} \frac{\partial \psi}{\partial E} + \frac{\partial t}{\partial s} \frac{\partial \psi}{\partial t} \\ &= \mu \frac{\partial \psi}{\partial x} + \eta \frac{\partial \psi}{\partial y} + \xi \frac{\partial \psi}{\partial z} + \frac{1}{v} \frac{\partial \psi}{\partial t}\end{aligned}$$

Equation 7.11

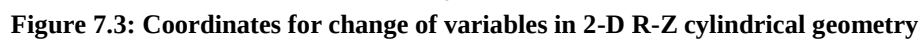
In 2-D cylindrical coordinate systems, two of the four angular variables can be used to describe the direction of the angular flux for all dimensions, as shown in Table 7.1. The streaming term for 2D cylindrical coordinate systems can be seen in Equation 7.12, where the partial derivative with respect to angular variable ω is utilized in place of μ . As opposed to the Cartesian geometries, there is an angular derivative term in the cylindrical coordinate system (see Figure 7.2) that cannot be eliminated as the angular flux varies with angular variable ω or μ – as can be seen in Figure 7.2, the angular variable ω will vary as the particle moves along a straight line. The change in angular variables is examined more closely in Figure 7.3. There the relation derived in Equation 7.13 can be seen, where the projected length dh is shown to be equal to product of the differential streaming length, ds , and θ vector direction cosine, η , as well as the product of the radius, ρ , and the negative change in angular variable ω , $-d\omega$ (noting that $\sin(-d\omega) \approx -d\omega$). Using this relation on Equation 7.12 yields the non-conservative form of the 2-D cylindrical static streaming operator in Equation 7.14.

$$\begin{aligned}\frac{d\psi}{ds} &= \frac{\partial \rho}{\partial s} \frac{\partial \psi}{\partial \rho} + \frac{\partial \theta}{\partial s} \frac{\partial \psi}{\partial \theta} + \frac{\partial z}{\partial s} \frac{\partial \psi}{\partial z} + \frac{\partial \omega}{\partial s} \frac{\partial \psi}{\partial \omega} + \frac{\partial \eta}{\partial s} \frac{\partial \psi}{\partial \eta} + \frac{\partial \xi}{\partial s} \frac{\partial \psi}{\partial \xi} + \frac{\partial E}{\partial s} \frac{\partial \psi}{\partial E} + \frac{\partial t}{\partial s} \frac{\partial \psi}{\partial t} \\ &= \mu \frac{\partial \psi}{\partial \rho} + \xi \frac{\partial \psi}{\partial z} + \left[\frac{\partial \omega}{\partial s} \right] \frac{\partial \psi}{\partial \omega} + \frac{1}{v} \frac{\partial \psi}{\partial t}\end{aligned}$$

Equation 7.12

$$dh = \eta ds = -\rho d\omega \rightarrow \frac{d\omega}{ds} = -\frac{\eta}{\rho}$$

Equation 7.13



$$\mu \frac{\partial \psi}{\partial \rho} + \xi \frac{\partial \psi}{\partial z} - \frac{\eta}{\rho} \frac{\partial \psi}{\partial \omega} + \frac{1}{v} \frac{\partial \psi}{\partial t}$$

Equation 7.14

The conservative form of the static cylindrical streaming operator is shown in Equation 7.15, and is thus named as it conserves neutrons in the finite difference scheme. Equation 7.16 uses the product differentiation rule to show the equivalence between the conservative and non-conservative forms – excluding the z-derivative term, which is identical in both.

$$\frac{\mu}{\rho} \frac{\partial}{\partial \rho} \rho \psi + \xi \frac{\partial \psi}{\partial z} - \frac{1}{\rho} \frac{\partial}{\partial \omega} \eta \psi$$

Equation 7.15

$$\frac{\mu}{\rho} \frac{\partial}{\partial \rho} \rho \psi - \frac{1}{\rho} \frac{\partial}{\partial \omega} \eta \psi = \mu \frac{\partial \psi}{\partial \rho} + \frac{\mu}{\rho} \psi - \frac{\psi}{\rho} \frac{\partial \eta}{\partial \mu} - \frac{\eta}{\rho} \frac{\partial \psi}{\partial \omega} = \mu \frac{\partial \psi}{\partial \rho} - \frac{\eta}{\rho} \frac{\partial \psi}{\partial \omega}$$

Equation 7.16

Integrating the conservative form of the streaming operator in Equation 7.15 and using integration by parts it can be shown that the angular terms cancel out, leaving only the gradient of the particle current as expected. A similar operation using the non-conservative form in Equation 7.14 yields leftover terms.

7.1.2 Scattering Source

Start with the scattering source from the neutron transport equation (Equation 7.1) as depicted in Equation 7.17, which is the integral over all energies and angles of the product of the differential scattering cross section and angular flux. The differential scattering cross section, as in Equation 7.18, is commonly expanded in terms of Legendre polynomials in order to separate the angular dependence of the scattering source. The scattering moments are subsequently defined using the orthogonality of the Legendre polynomials in Equation 7.19.

$$q_s(\vec{r}, E, \hat{\Omega}) = \int_{4\pi} d\Omega' \int_0^\infty dE' \Sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \psi(\vec{r}, E', \hat{\Omega}')$$

Equation 7.17

$$\Sigma_s(\vec{r}, E' \rightarrow E, \Omega \cdot \Omega') = \sum_{l=0}^{\infty} (2l+1) \Sigma_{sl}(\vec{r}, E' \rightarrow E) P_l(\Omega \cdot \Omega')$$

Equation 7.18

$$\Sigma_{sl}(\vec{r}, E' \rightarrow E) = \int_{-1}^1 d\mu_0 \Sigma_s(\vec{r}, E' \rightarrow E, \Omega \cdot \Omega') P_l(\Omega \cdot \Omega')$$

Equation 7.19

Substituting the Legendre Addition Theorem (Equation 7.21) and Equation 7.18 into Equation 7.17, the scattering source can be simplified as shown in Equation 7.22 and then further simplified using the definition of the scalar flux moments in Equation 7.3. Application of the discrete ordinates and multigroup methods, in addition to truncating the scattering source to some finite scattering order (P_n order) of value ISCT will yield the scattering source in Equation 7.22 in the form depicted in Equation 7.10. Table 7.2 shows the differing required flux moments for increasing characterization of the scattering order, as well as increasing dimensions, where for dimension D and order i the total flux moments required is increasing by $1+(D-1)*i$ for each order i where the total is for a scattering order ISCT is then:

$$\#of \text{ flux moments} = \sum_{i=0}^{ISCT} 1 + i(D-1)$$

Equation 7.20

Table 7.2: Required flux moments for 1-, 2-, and 3-D coordinate systems currently analyzed.

P_N	1-D	2-D	3-D
0	ϕ_0	ϕ_{00}	ϕ_{00}
1	ϕ_1	ϕ_{10}, ϕ_{11}	$\phi_{10}, \phi_{11}, \phi_{11}^i$
2	ϕ_2	$\phi_{20}, \phi_{21}, \phi_{22}$	$\phi_{20}, \phi_{21}, \phi_{21}^i, \phi_{22}, \phi_{22}^i$
3	ϕ_3	$\phi_{30}, \phi_{31}, \phi_{32}, \phi_{33}$	$\phi_{30}, \phi_{31}, \phi_{31}^i, \phi_{32}, \phi_{32}^i, \phi_{33}, \phi_{33}^i$

$$P_l(\Omega \cdot \Omega') = \frac{1}{2l+1} \sum_{m=-l}^l Y_{lm}^*(\Omega) Y_{lm}(\Omega')$$

Equation 7.21

$$\begin{aligned} \mathbf{q}_s(\vec{r}, \mathbf{E}, \hat{\Omega}) &= \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}^*(\hat{\Omega}) \int_0^{\infty} \Sigma_{sl}(\vec{r}, \mathbf{E}' \rightarrow \mathbf{E}) \int_{4\pi} Y_{lm}(\Omega') \Psi(\vec{r}, \mathbf{E}', \hat{\Omega}') d\Omega' d\mathbf{E}' \\ &= \sum_{l=0}^{\infty} \sum_{m=-l}^l Y_{lm}^*(\hat{\Omega}) \int_0^{\infty} \Sigma_{sl}(\vec{r}, \mathbf{E}' \rightarrow \mathbf{E}) \Phi_{lm}(\vec{r}, \mathbf{E}') d\mathbf{E}' \end{aligned}$$

Equation 7.22

The Legendre Addition Theorem can be expanded using the definition of the spherical harmonics function (Equation 7.23) and this can be simplified, depending on which dimension the problem is solved in, as summarized in Table 7.2 through P_3 scattering. The P_N order denotes the truncation of the infinite Legendre expansion in Equation 7.22, where isotropic scattering problems require only the leading term.

$$P_l(\Omega \cdot \Omega') = P_l(\mu) P_l(\mu') + 2 \sum_{m=1}^l \frac{(l-m)!}{(l+m)!} P_l^m(\mu) P_l^m(\mu') \cos[m(\omega - \omega')]$$

Equation 7.23

7.1.3 Cylindrical Coordinates Angular Derivative

Recall that the conservative streaming operator for 2-D cylindrical coordinates in Equation 7.15 contains an angular derivative term with respect to the angular variable, ω , which is the rotation about the radial axis as shown in Figure 7.2. Since the developed COMSOL Multiphysics model tool does not numerically solve the angular dimensions of the problem, only the spatial dimensions are meshed, this angular derivative term must be approximated. The implemented approximation of the angular derivative term is a finite difference of two “half-angle” angular flux terms along the same discrete ξ_p levels, where the level is denoted by the subscript p . This requires that the angular discretization scheme be set up upon same ξ_p - and μ_{pq} - levels (denoted by subscripts p and q respectively), in a level symmetric quadrature set as that shown in Figure 7.4, where the ξ_3 level is shown as well as some (μ, ξ) discrete ordinate locations.

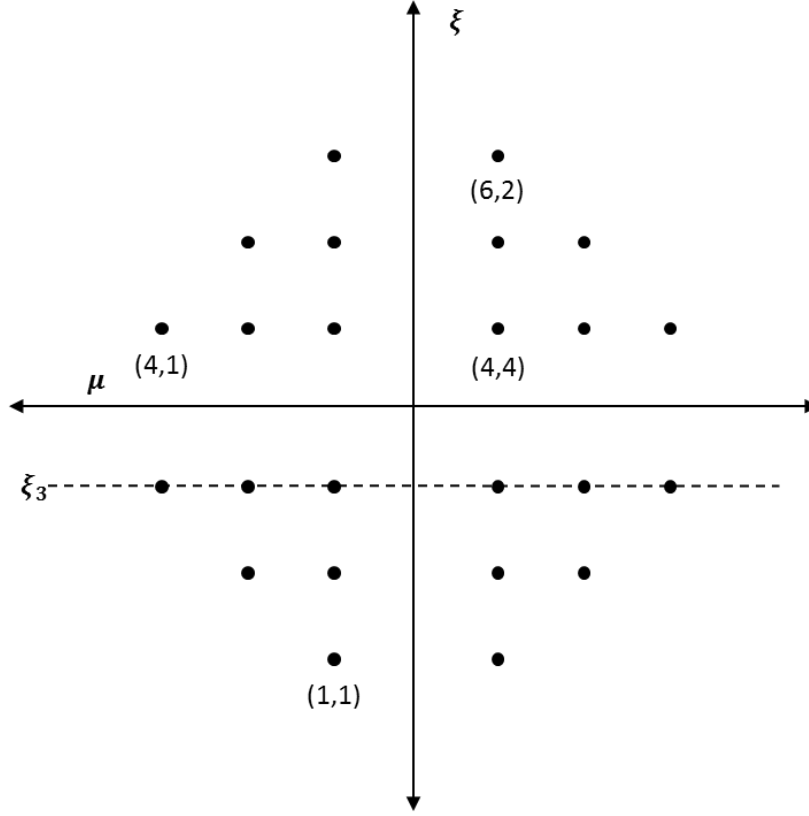


Figure 7.4: Example of the μ, ξ numeration scheme for an S_6 angular quadrature.

Using half-angle angular differencing coefficients, $\alpha_{pq+1/2}$, and angular fluxes, $\psi(\xi_p, \mu_{q+1/2}) = \psi_{pq+1/2}$, the finite difference approximation is accomplished as shown in Equation 7.24, as adapted from Equation 7.15. The angular differencing coefficients are constructed such that neutron conservation is conserved. Looking at for the case of a uniform and isotropic flux, the streaming term will not vanish unless the definition in Equation 7.25 is met. Summing the terms in Equation 7.24 according to quadrature integration, to maintain neutron balance the condition shown in Equation 7.26 must be satisfied, which further simplified shows that $\alpha_{p1/2} = 0$ for all p in conjunction with Equation 7.25 is satisfactory, where the level symmetric quadrature is such that $\alpha_{pN+1/2} = 0$ as well.

$$\frac{\mu_{pq}}{\rho} \frac{\partial}{\partial \rho} \rho \psi_{pq} + \xi_p \frac{\partial \psi_{pq}}{\partial z} - \frac{\alpha_{pq+1/2} \psi_{pq+1/2} - \alpha_{pq-1/2} \psi_{pq-1/2}}{\rho w_{pq}}$$

Equation 7.24

$$\alpha_{pq+1/2} = \alpha_{pq-1/2} - \mu_{pq} w_{pq}$$

Equation 7.25

$$\sum_{p=1}^N \sum_{q=1}^{N_p} (\alpha_{pq+1/2} \psi_{pq+1/2} - \alpha_{pq-1/2} \psi_{pq-1/2}) = \sum_{p=1}^N (\alpha_{p1/2} \psi_{p1/2} - \alpha_{pN+1/2} \psi_{pN+1/2}) = 0$$

Equation 7.26

The relation between the half-angle angular flux variables to the nominal variables is quantified in Equation 7.27, where the relation is transformed into a function of the next half-angle angular flux. The initial half-angle angular flux, $\psi_{p1/2}$, must then be known to solve Equation 7.24 and Equation 7.27. Starting at $\omega=\pi$ the initial half-angle streaming term is defined from Equation 7.15 at $\mu_{p1/2}$ in Equation 7.28, where the solved differential equation is given. Therefore for two-dimensional cylindrical coordinates, the angular flux must be solved at an additional N quadrature locations where the total angular quadrature locations (and therefore flux variables) is then $N(N+2)/2+N$.

$$\psi_{pq} = \frac{1}{2} (\psi_{pq+1/2} + \psi_{pq-1/2}) \rightarrow \psi_{pq+1/2} = 2\psi_{pq} - \psi_{pq-1/2}$$

Equation 7.27

$$(1 - \xi_p^2)^{1/2} \frac{\partial \psi_{p1/2}}{\partial \rho} + \xi_p \frac{\partial \psi_{p1/2}}{\partial z}$$

Equation 7.28

7.1.4 Weak Form Interface Methodology

All finite element analysis in COMSOL Multiphysics uses the weak form to derive solutions to a system of partial differential equations (PDEs), therefore the weak form interface, where the discrete ordinates variables are placed, is in a sense COMSOL's unformatted equation interface. What follows is a brief and simplified explanation of the weak form approach as implemented in COMSOL.

Consider a PDE, $L(f)$, that is desired to be solved, that is itself a function of a functional f over a given domain. The desired function to be calculated is defined as $q(\vec{r})$ such that Equation 7.29 is satisfied over the real domain R^n where the superscript n denotes the domain dimension order. The boundary conditions or constraints, $l(q)$, are also solved for $q(\vec{r})$ over the real domain R^{n-1} as shown in Equation 7.30.

$$L(q) = 0 \text{ on } \Omega \in R^n$$

Equation 7.29

$$l(q) = 0 \text{ on } \partial\Omega \in R^{n-1}$$

Equation 7.30

The desired function is then approximated as a weak solution, q^N , that is presented as a summation of basis functions, ϕ_{ai} , and their coefficients, α_i , that have a value of zero outside their respective nodes, see Equation 7.31, where there is some error, e^N , between the desired exact solution and weak solution as shown in Equation 7.32.

$$q \approx q^N = \sum \alpha_i \phi_{ai}$$

Equation 7.31

$$q(\vec{r}) = q^N(\vec{r}) + e^N(\vec{r})$$

Equation 7.32

Test functions, ϕ_β , are applied to the PDE and boundary conditions and are integrated over their domains to yield the weak form statement as shown in Equation 7.33. The Ritz-Galerkin approach treats these equations as a variational problem to find a weak solution, q^N , that solves the weak statement for some set of well-chosen test functions. Application of the divergence theorem by integration by parts to the PDE integrand will yield the natural boundary conditions for the FEA domain. Test and basis functions are applied across each finite mesh element in order to represent a complex solution as a

combination of simple functions. These functions are typically represented with Lagrangian shape functions (where linear, quadratic, and cubic are used in this work).

$$\int_{\Omega} \phi_{\beta} \mathbf{L}(\mathbf{q}^N) + \int_{\partial\Omega} \phi_{\beta} \mathbf{l}(\mathbf{q}^N) = \mathbf{0}$$

Equation 7.33

7.1.5 Discrete Ordinates Boundary Conditions

Having defined PDEs that make up the G by N(N+2) weak statements that are solved over the problem domains in Equation 7.10, it remains to define boundary conditions that yield a unique (and therefore solvable) problem. Since there are G by N(N+2) discrete weak statements and flux variables, there will be the same number of boundary constraints at each problem boundary corresponding to each flux. The two boundary conditions set up to be defined by default for the discrete ordinates tool are the (1) Vacuum, and (2) Reflective conditions.

The constraint shown in Equation 7.34 is applied to boundaries that are set to the Vacuum condition, where the flux is set to zero for those variables whose sum of the direction cosines and surface normal cosines products sum to less than zero (that is to say, those angular fluxes that are incoming into the vacuum surface). The constraint shown in Equation 7.35 is applied to boundaries that are set to the Reflective condition, where the flux is set to the surface normal dot product sum of those flux variables who share a reflective angle at the boundary.

$$\psi_n^g(\vec{r}, t) = 0, \sum_{i=1}^{N_D} \hat{n}_i \hat{\Omega}_i^n < 0, \vec{r} \in \Gamma_{vac}$$

Equation 7.34

$$\psi_n^g(\vec{r}, t) = \sum_{i=1}^{N_D} \sum_{m=1}^{N(N+2)} \hat{n}_i \psi_m^g(\vec{r}, t), \hat{\Omega}_i^n = \hat{\Omega}_i^m, \vec{r} \in \Gamma_{refl}$$

Equation 7.35

7.1.6 K-Eigenvalue Global ODE

For eigenvalue problems, the PDEs are solved for an eigenvalue that exemplifies the “criticality” of the system. Under this definition, a supercritical system is that where *more* neutrons are born in each generation than were born in the previous generation, and therefore (assuming no reactivity feedbacks) the number of neutrons will approach infinity as time approaches infinity. A subcritical system is that where *less* neutrons are born in each generation than were born in the previous generation, and therefore (assuming no reactivity feedbacks) the number of neutrons will approach zero as time approaches infinity. A perfectly critical system then has the same number of neutrons between generations and its neutron count will be static. The eigenvalue flux solution to a system therefore represents the calculated shape of the flux distribution, which would depend on the system power (in a critical system) or the time (in a transient subcritical or supercritical system).

The k-eigenvalue, k_{eff} , is shown in Equation 7.10 and is also known as the neutron multiplication factor. For eigenvalue problems (where this option is added), a global ODE is added in the form of Equation 7.36. The triple integral which represents the integration over the entire fissionable domain, V_F , is defined as a local integration operator definition, $intop1$. The eigenvalue k_{eff} is then the sum of all neutrons born to fission, and since it is applied as a divisor to the fission source term on the right hand side of Equation 7.10, it imposes that a balance of 1 neutron is born per generation. Therefore the relationship as shown in Equation 7.37 shows how k_{eff} characterizes the criticality of the problem.

$$\iiint_{V_F} \sum_{g'=1}^G \nu \Sigma_f^{g'}(r) \phi^{g'}(r) dr - k_{eff} = 0$$

Equation 7.36

$$\begin{aligned} k_{eff} &> 1 && \textit{supercritical} \\ k_{eff} &= 1 && \textit{critical} \\ k_{eff} &< 1 && \textit{subcritical} \end{aligned}$$

Equation 7.37

7.1.7 Process Flow Methodology

Physics are built using the Java API programming of COMSOL, which provides the user java utilities to edit and create COMSOL features. This physics-builder program is built into the COMSOL Application Builder for its convenient graphical user interface features (however any Java compiler would be sufficient, or alternatively using the COMSOL LiveLink to MATLAB). Figure 7.5 shows the process for building a single discrete ordinates model, which is further discussed below:

1. In the course of defining the problem, the user must choose the appropriate cross sections – whether they come from a utility or can be manually entered. In the case of this research, cross sections were processed in the SCALE 6.1 code package: the CSAS-MG or T-XSEC control sequences run BONAMI and CENTRM/PMC or NITAWL (for 1-D) and the AWL utility is used to save an AMPX working directory.
2. Alternatively, a KENO problem may be run, using CSAS5 or CSAS6 (for KENO V.a or -VI, respectively) for an intended cross section collapse.
3. In the application builder window (see Figure 7.6), the user simply has to select the choices available: dimension, S_N order, P_N order, energy groups, type of sources (eigenvalue and/or fixed source).
 - a. Upon clicking cross section mixing or collapse one of two utilities will run that post-process an AMPX working directory or KENO output file, respectively, into a text file.
 - b. Upon clicking run, the model will be built with its given local model variables (flux moments, scattering sources, etc.), weak form interface with weak statements and BCs, global ODE for k-eff, and default solvers, mesh, and geometry.
 - c. The user must then save the model file.
4. From the model file, the user must set up the problem details and import cross sections. If there are any errors, one can edit them manually or using an editing utility.
5. Finally, the user may run the model and post-process the results.

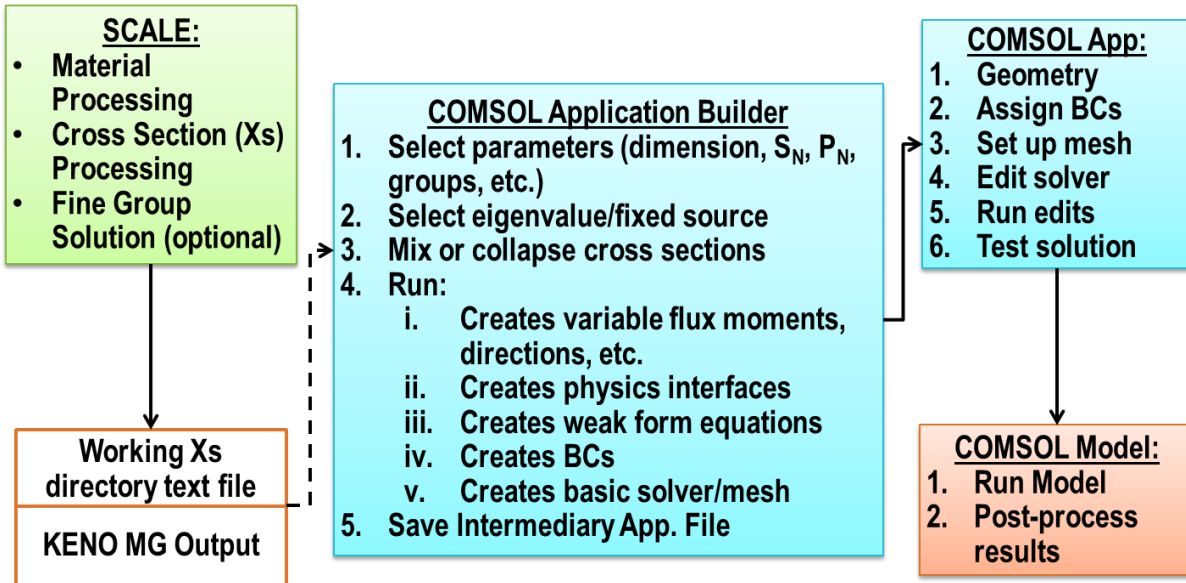


Figure 7.5: Simple flow diagram showing the process of building a discrete ordinates model

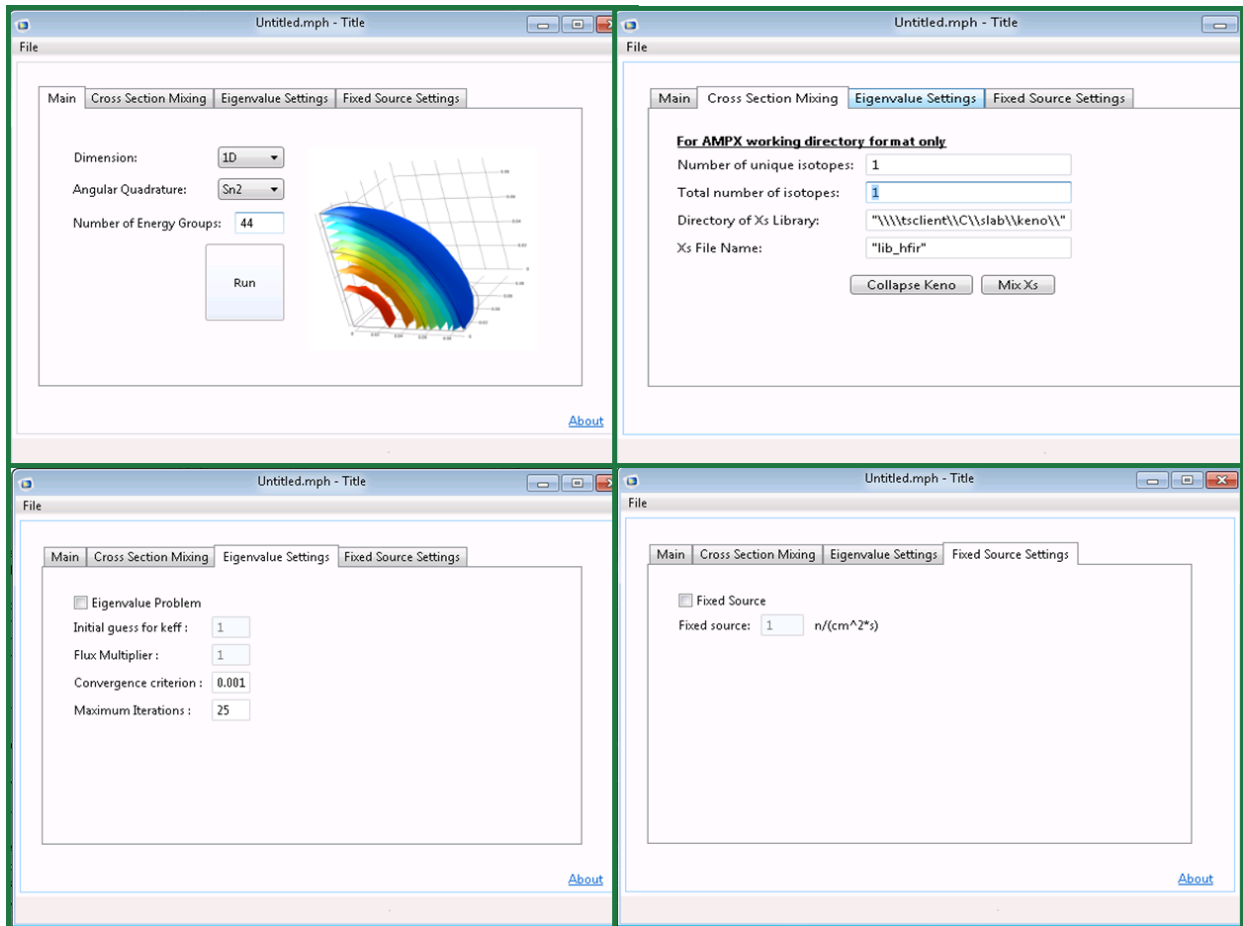


Figure 7.6: Windows of the COMSOL discrete ordinates physics-builder application.

7.2 *Benchmark Problems and Results*

There are currently three sets of benchmark problems that have been run: 1) Kobayashi benchmarks designed for difficult flux profiles that exhibit ray effects and compared to PARTISN, 2) Water-reflected sphere problem compared to Attila, 3) Example problems created for various dimensions and compared to SCALE code package transport solvers. In addition, the verification of a static clean core model of the HFIR is compared against available flux distributions and results presented.

7.2.1 **Kobayashi Benchmarks**

The Kobayashi benchmarks [118] are difficult problems that are designed to assess the accuracy of the flux distributions in highly absorbing medium systems with void regions. This is the ideal common condition for exhibiting ray effects [119][120], that of an isolated isotropic source in a purely absorbing medium. There are three set problem geometries and for each, there is a case without scattering and one with a 50% scattering cross section. Provided in the benchmark are analytical solutions – numerically integrated for no scattering and Monte Carlo for 50% scattering – of the flux distribution along straight lines that can be used for comparison. A short problem setup summary for the three cases is given in Figure 7.7 and Table 7.3, and an example of the Cartesian mesh is given in Figure 7.8.

For each problem, analytical solutions are provided to point fluxes along three straight lines in the geometry in 5 cm intervals. To be concise, only results for the 3rd problem will be summarized for both cases here, the duct geometry with three 90° turns as shown on the right in Figure 7.7 which would be expected to be the most difficult solution for the discrete ordinates method.

No ray effect remedies, including first collision source methods [121], are used for two reasons: 1) In order to allow the ray effects to manifest and see how the code handles the resulting discrepancies from this expected limitation to discrete ordinates, and 2) ray effect remedies like the first collision source method are not practical for distributed sources including common eigenvalue calculations.

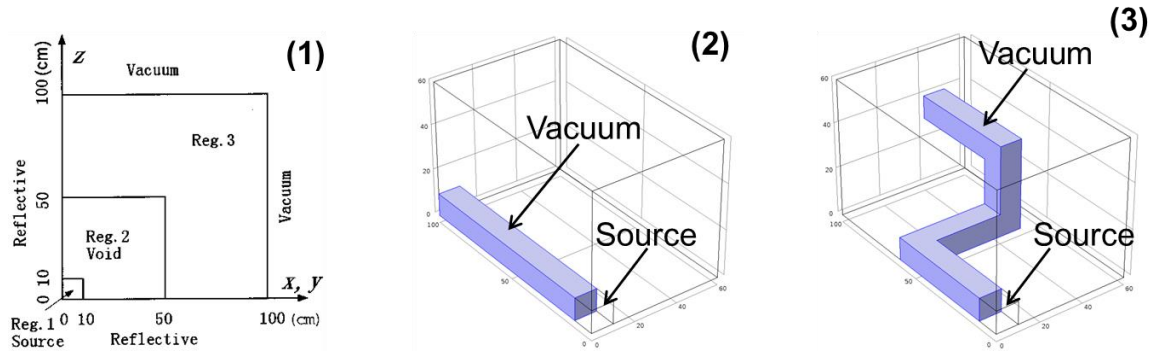


Figure 7.7: Kobayashi benchmark geometry setups for all 3 problems.

Table 7.3: Problem parameters for the Kobayashi benchmarks.

Region	S (n/cm ³ -s)	Σ_t (1/cm)	Case i	Case ii
			Σ_s (1/cm)	
1	1	0.1	0	0.05
2	0	10^{-4}	0	5e-5
3	0	0.1	0	0.05

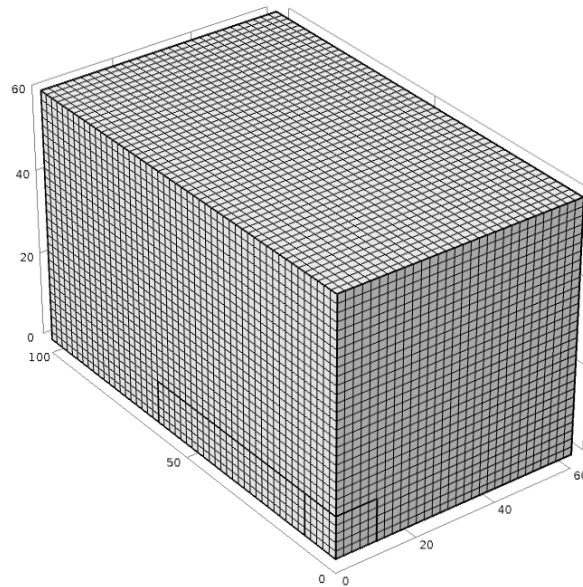


Figure 7.8: Mesh with 2 cm intervals for Kobayashi problem 3 in COMSOL using a mapped swept mesh.

For this research, the PARTISN discrete ordinates code is used for comparison purposes by the author. S16 angular quadrature is utilized, P0 scattering, and a mesh width intervals of 2 cm using a mapped/swept mesh for 45 – 125,000 mesh elements (see Figure 7.8). In the COMSOL solver settings, the PARDISO linear solver was used with the segregated solver that utilizes a “lower limit” feature that simulates the negative flux fixup which is also in PARTISN. The flux comparison results for problem 3 along four individual lines are presented in Figure 7.9 – Figure 7.14. The solution time was 1-2 hours using 14-28 million DOF, with memory usage distributed across two 128 GB computational clusters on the RRD computational cluster.

The scalar flux plots along the four chosen lines in Figure 7.9 and Figure 7.11 show good comparison across the three solutions. The ratio to analytical flux plots for these paths shown in Figure 7.10 and Figure 7.12 more clearly indicate the variation shown as these lines move away from the source location, which is expected, as previously indicated due to the ray effects of the discrete ordinates formulation, yet where COMSOL compares well within these limitations in comparison to the PARTISN code. The paired plots in Figure 7.13 and Figure 7.14 further demonstrate this comparison, where the strong ray effects from the no-scattering case i resulted in a negative flux fixup in Figure 7.13. Furthermore, a 3-D plot of the log-flux in Figure 7.15 further shows the ray effect variation of the COMSOL solution.

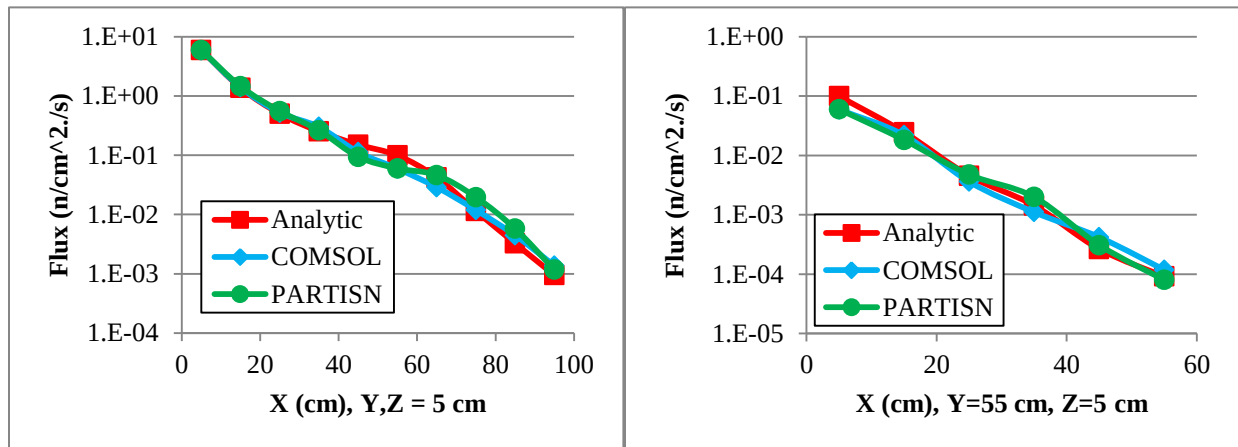


Figure 7.9: Kobayashi problem 3, case i, fluxes along indicated lines for analytical, COMSOL, and PARTISN solutions.

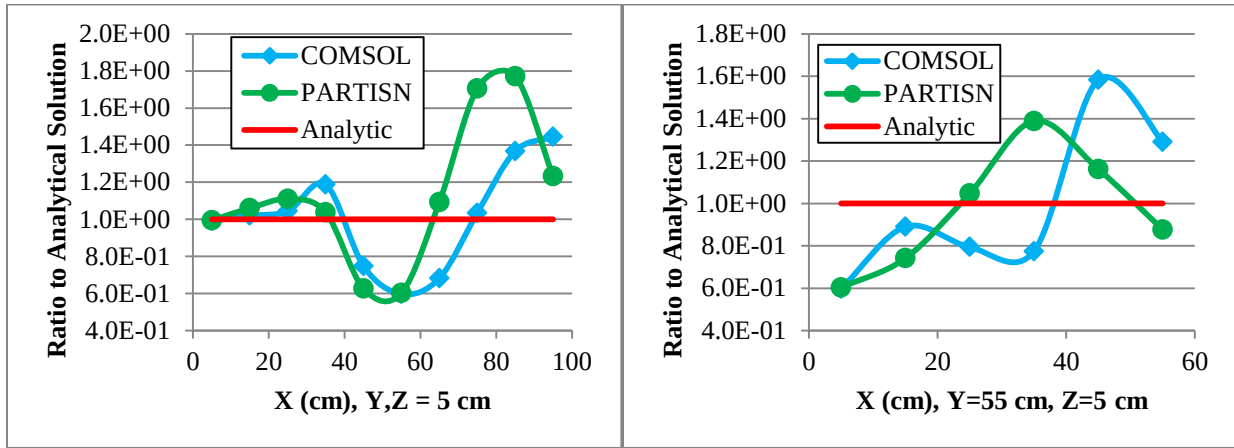


Figure 7.10: Kobayashi problem 3, case i, flux ratio to analytical solution along indicated lines for COMSOL and PARTISN solutions.

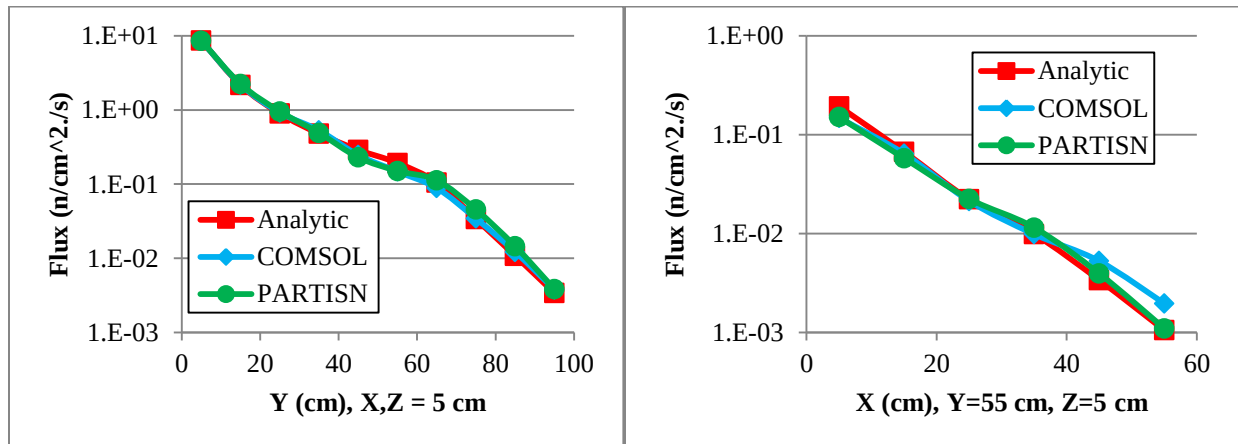


Figure 7.11: Kobayashi problem 3, case ii, flux along indicated lines for analytic, COMSOL and PARTISN solutions.

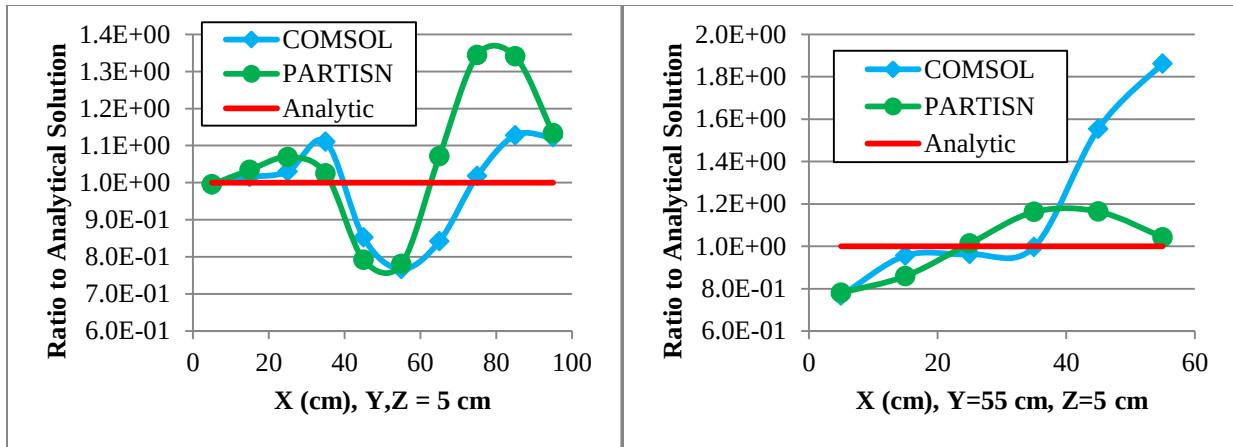


Figure 7.12: Kobayashi problem 3, case ii, flux ratio to analytical solution along indicated lines for COMSOL and PARTISN solutions.

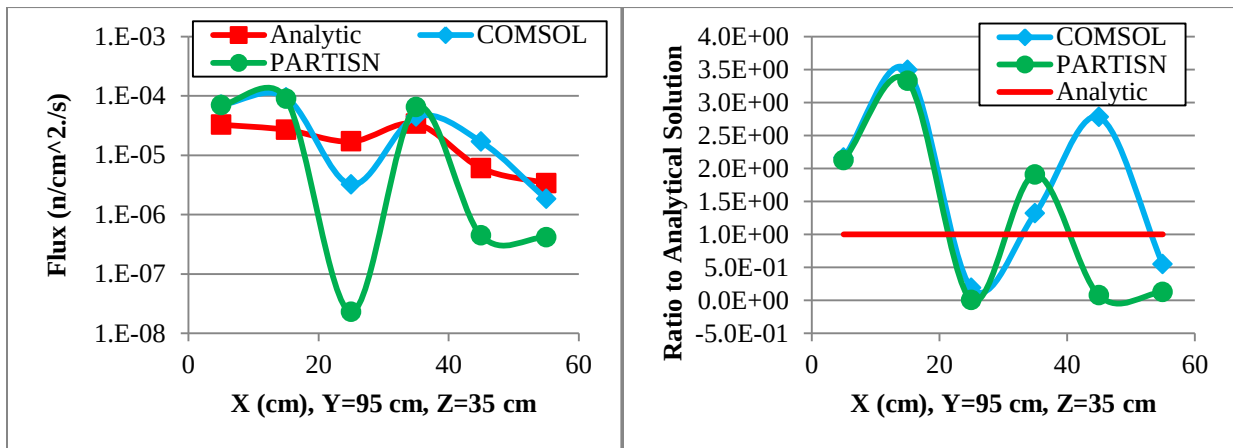


Figure 7.13: Kobayashi problem 3, case i, flux and flux ratio to analytical solution along indicated line for analytical, COMSOL and PARTISN solutions.

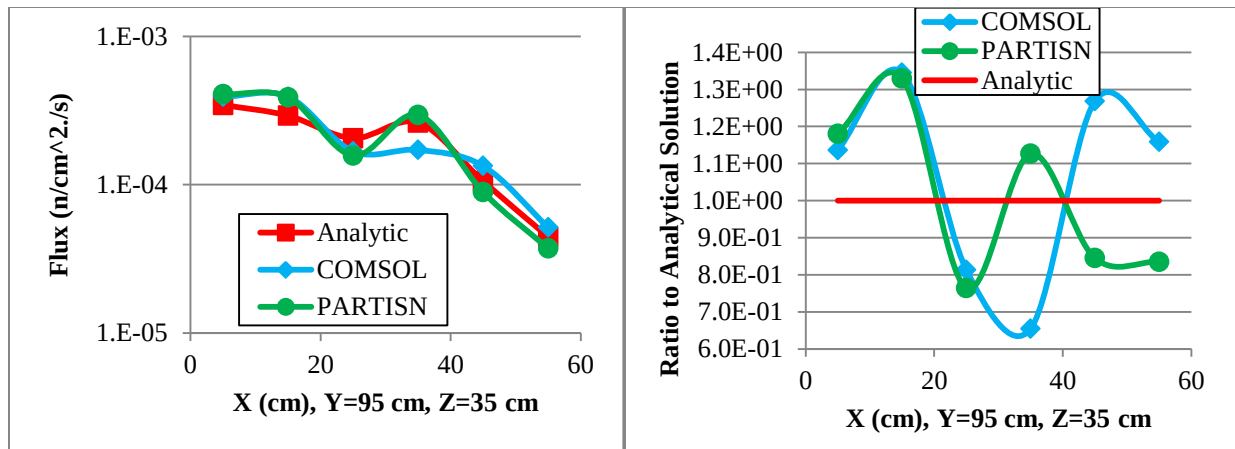


Figure 7.14: Kobayashi problem 3, case ii, flux and flux ratio to analytical solution along indicated line for analytical, COMSOL and PARTISN solutions.

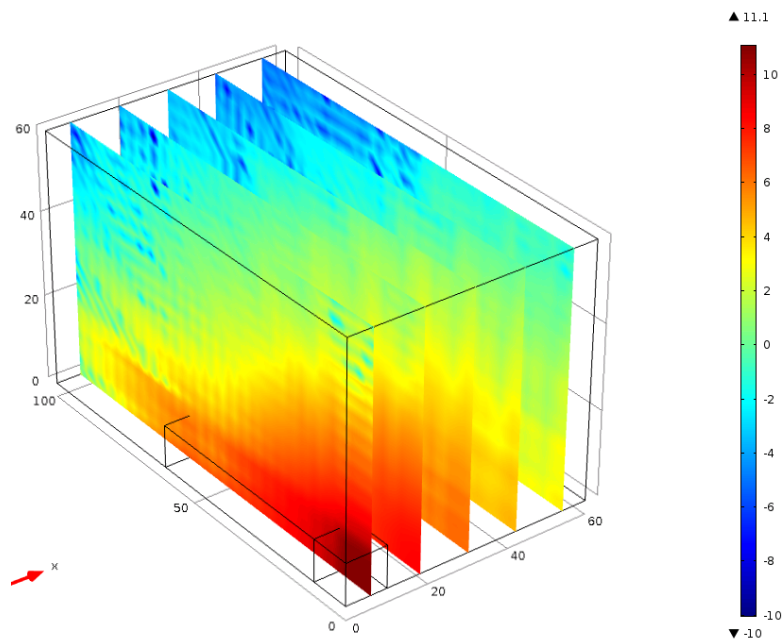


Figure 7.15: 3-D slice plot of the log-flux for case i of Kobayashi problem 3.

7.2.2 Water-reflected sphere

A simple and straightforward water-reflected sphere problem is presented in this section. Table 7.4 that follows gives the short summary of the problem, including 1-group cross sections and the outer radius of the materials. The anticipated result for this benchmark problem is a k_{eff} of unity. Chosen problem parameters are S4 quadrature, with P0 scattering and a convergence criterion of $1e-4$. The problem uses 39 thousand DOF, 1-2 GB of RAM and has a 1-2 minutes solution time for the MUMPS linear solver and fully-coupled Jacobian. The k-eigenvalue comparison is presented in Table 7.5 with good comparison to reference discrete ordinates code Attila and a contour representation of the scalar flux is shown in Figure 7.16.

7.2.3 Miscellaneous problems

In this section, HFIR HEU fuel material is assembled in several configurations that were arbitrarily chosen and the eigenvalues/fluxes compared to the available SCALE codes to ensure that the same nuclear data was being used as input. The SCALE 44 energy group cross section libraries are used and processed with the same functional modules and, where possible, similar solution methods were used. However, for the 3-D comparisons, it should be noted that the Monte Carlo code KENO V.a or KENO-VI cannot give a direct comparison to the COMSOL solutions, due to the angular quadrature approximation of the discrete ordinates method.

First presented are two very simple one-region eigenvalue problems in 1-D and 2-D. Both are computed using S_2 quadrature, however at the time the mesh intervals are different for each study so that control parameter isn't available. The 1-D case uses simple uranyl fluoride solution of 93 wt.% enrichment $^{235}\text{U}/\text{U}$ in a 16 cm slab with reflective BC on the left boundary and vacuum BC on the right. This case is compared to XSDRNPM and is presented in Figure 7.17 and Table 7.6.

Table 7.4: Problem parameters for the water-reflected sphere problem.

Material	$\Sigma_t(1/\text{cm})$	$\Sigma_f(1/\text{cm})$	$\Sigma_s(1/\text{cm})$	$R_o(\text{cm})$
^{235}U	0.326400	0.182595	0.248064	6.12745
Water	0.326400	0.000000	0.293760	9.191176

Table 7.5: K-eigenvalues for simple water-reflected sphere.

Material	keff	%Error
Analytical	1.0000000	--
COMSOL	0.9994911	0.05%
Attila	0.9990156	0.10%

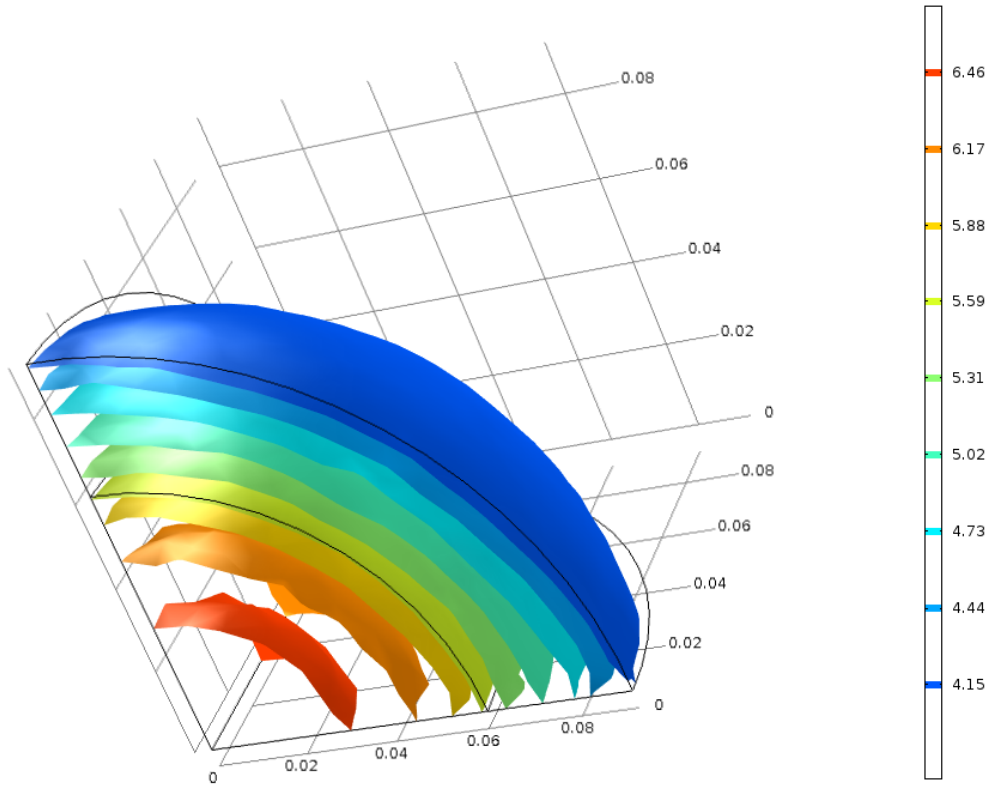


Figure 7.16: Scalar flux ($\text{n/cm}^2\text{-s}$) profile in 8th core 3-D water-reflected sphere.

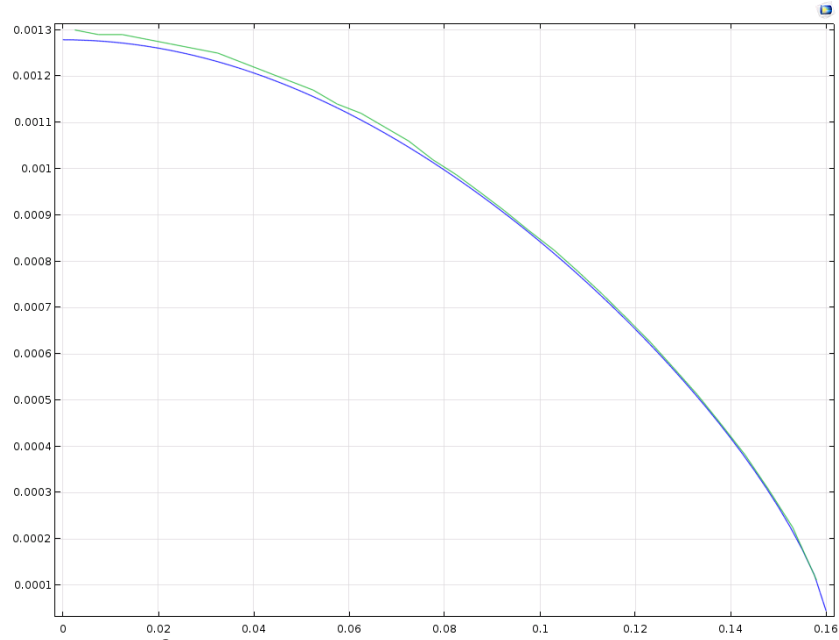


Figure 7.17: Neutron flux (n/cm²-s) comparisons between XSDRNPM and COMSOL for energy groups 44 for uranyl fluoride solution.

Table 7.6: K-eigenvalue comparisons for COMSOL between SCALE codes NEWT and XSDRNPM.

Material	1-D	%Diff	2-D	%Diff
COMSOL	1.527118	0.77%	1.247174	-0.44%
SCALE	1.538999	--	1.252748	--

The 2-D case uses the same uranyl fluoride solution as the 1-D case in a square 16-by-16 cm, with reflective BC on the left and bottom boundaries and vacuum BCs on the right and top boundaries. This case is compared against NEWT and the comparison is presented in Figure 7.18 and Table 7.6. The expected flux distribution over the one-region problem is observed in Figure 7.19. Agreement is found between the results, although a return to these studies with closer control on input parameters should allow closer agreement.

7.2.4 Beginning-of-Cycle HFIR Model

The static beginning-of-cycle (BOC) or clean core model for the HFIR core has been developed for the discrete ordinates formulation in COMSOL. The geometry used is a simplified representation documented in previous calculations, and shown in Figure 7.20, and the BOC material compositions are documented in Appendix C of [34]. The left of Figure 7.20 shows the simplified geometry, with important features highlighted including the inner and outer fuel element (IFE and OFE) regions which are subdivided into eight and nine axially-averaged radial regions, respectively. The flux trap (FT) region is located at the center of the reactor, with the removable beryllium (RB) and PB reflector regions on the radial outer edges of the core, and the control element (CE) region in between the fuel and reflector regions, which includes an inner and outer control element (ICE and OCE) region as well as water regions between the CEs. Reactor pool water surrounds all core components and is extended to 70 cm. Both 3 and 44 energy group neutron cross sections have been input, although due to limitations in computation time, a 3 energy group approach is preferred.

The 3 group cross sections are generated by collapsing finer group calculations in KENO V.a (in the case of results exhibited here, a 44 group ENDF/B-V library) using the neutron flux spectrum and reaction rates calculated therein into the energy spectrum shown in (as used in and comparable to original HFIRCE-4 energy range results). The KENO V.a model is run using the CSAS5 control sequence BONAMI/CENTRM cross section processing modules for resonance shelf-shielding and production of multigroup cross sections.

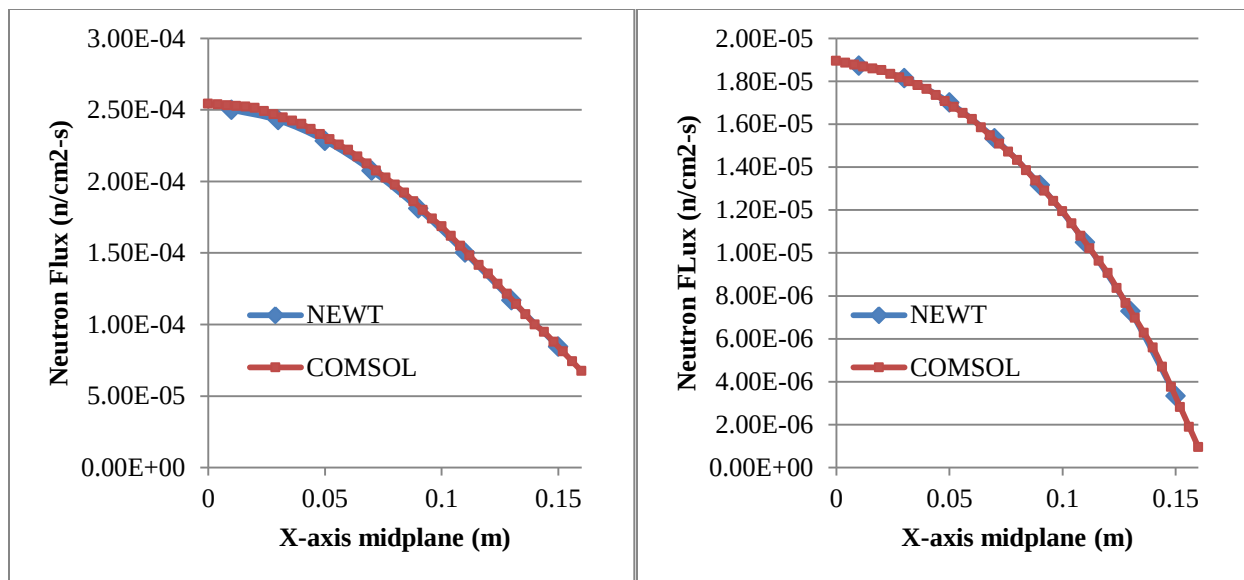


Figure 7.18: Neutron flux comparisons between NEWT and COMSOL for energy groups 1 (left) and 44 (right) for uranyl fluoride solution.

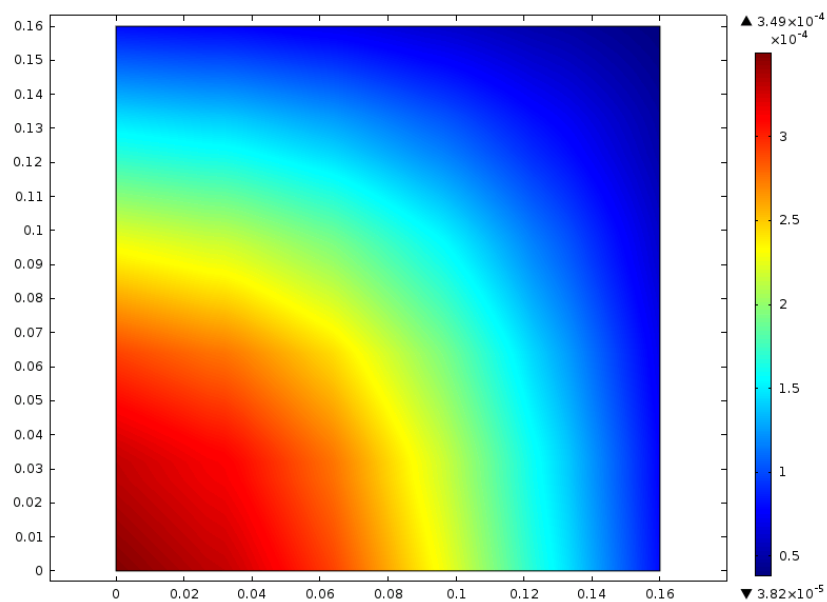


Figure 7.19: Neutron flux (n/cm²s) surface profile for group 1 in COMSOL 2-D discrete ordinates uranyl fluoride.

An unstructured, free triangular coarse mesh of ~67 thousand mesh elements is used, as shown in the right of Figure 7.20, and the problem is solved using 42 GB of RAM and 5 million DOF. The MUMPS direct linear solver is used with the fully-coupled solver (note: no negative flux fixups). S_8 angular quadrature is used, with P_1 scattering order and a raised convergence criterion of $1e-2$.

The BOC HFIR scalar flux contour/surface plots for the three groups are presented in Figure 7.21 and a raised tube-contour plot for the relative fission rate is presented in Figure 7.22. These R-Z flux distributions are in very good agreement with previously calculated HFIR flux distributions for Cycle 400 [122]. Fast fluxes are concentrated in their places of origin, in the IFE and OFE with a largest peak in the center of the IFE at the horizontal midplane. Fast fluxes born in the fuel regions leak into the FT and beryllium reflector regions, where the fast flux quickly decreases due to moderation to lower neutron energies. The epithermal flux experiences its peak in the center of the fuel regions, leaking into the FT and reflector regions with less decrease than the fast flux. The thermal flux increases with increasing penetration into the FT towards the $R=0$ axial centerline, with strong thermal flux peaks in the center of the HFIR core. The thermal flux also increases with penetration into the reflector region for a few centimeters, before falling off into the outer reflector and reactor pool.

The fission density distribution is also in very good agreement with previously calculated distributions [122], with peak powers occurring along the reactor midplane at the inner and outer radial edges of the IFE and the greatest power peak observed at the inner radial edge of the OFE.

The scalar fluxes for the three groups along the reactor midplane ($z=0$) to 60 cm is shown in Figure 7.23 and a comparison along the midplane for each group is made between a user-generated KENO V.a simulation (44 energy groups), the COMSOL discrete ordinates results and a 3-group diffusion theory simulation in COMSOL [15] for the same mesh in Figure 7.24 - Figure 7.26.

A further comparison for the fast flux is made in Figure 7.27 between the previously discussed methods to solve the HFIR simplified core to previous studies of a more detailed 3-D HFIR core (where the primary simplification is homogenizing explicit involute fuel plates into radial and axial fuel regions)

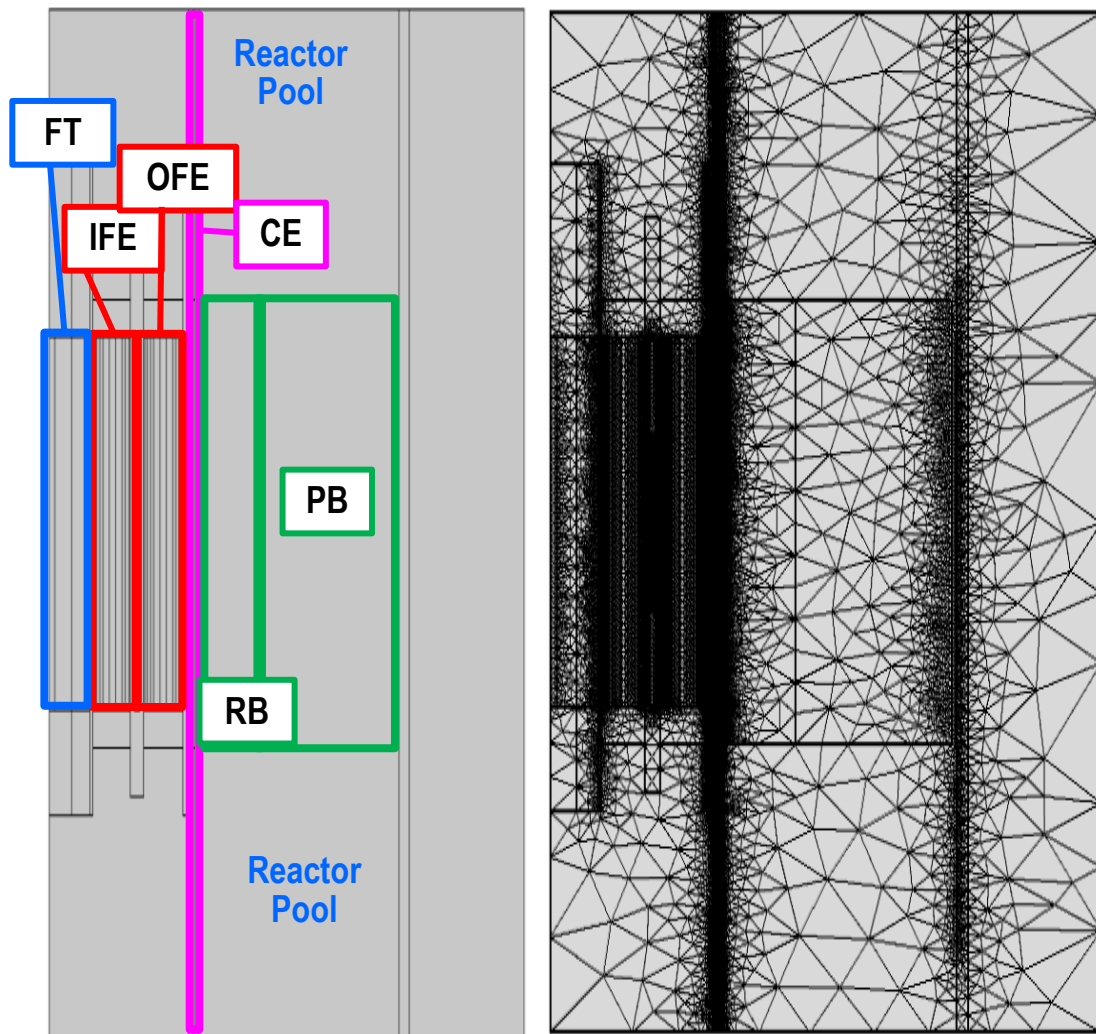


Figure 7.20: Simplified HFIR core geometry (left) and extremely coarse mesh (right).

Table 7.7: Three-group energy structure.

Group #	Group Name	Lower Neutron Energy	Upper Neutron Energy
1	Fast	100 keV	20 MeV
2	Epithermal	0.625 eV	100 keV
3	Thermal	10^{-5} eV	0.625 eV

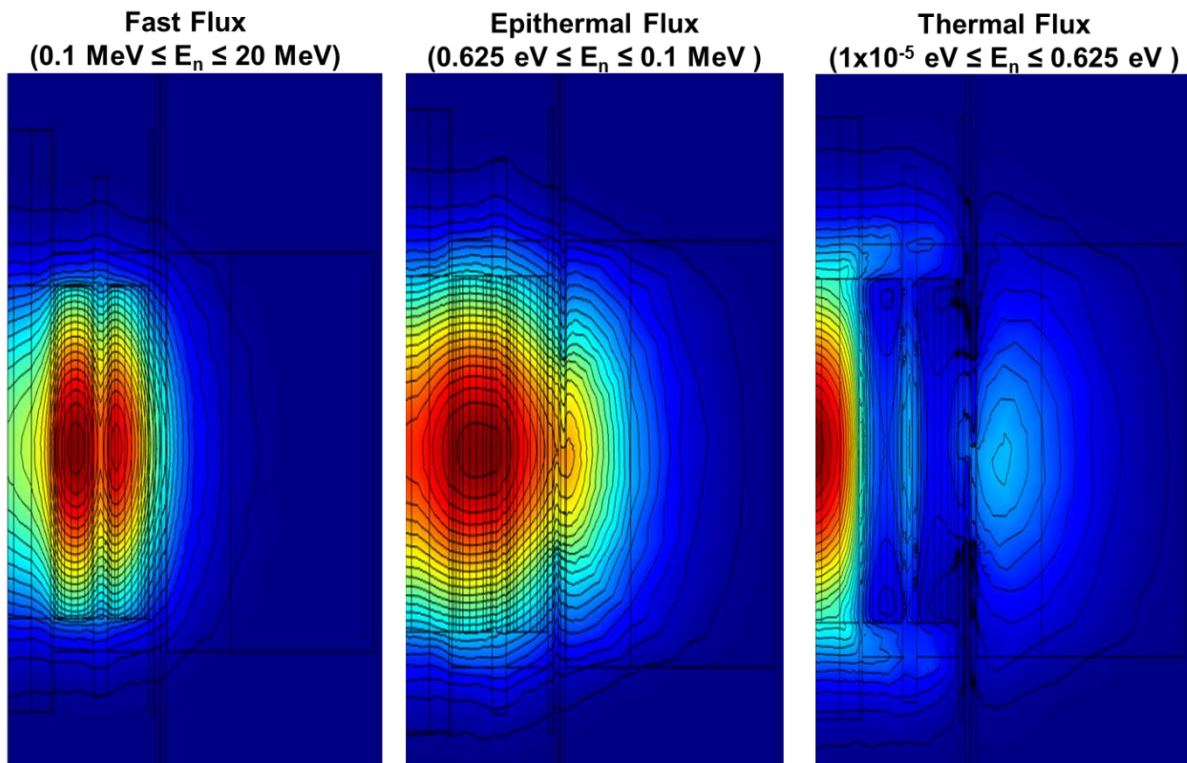


Figure 7.21: Flux surface/contour plots for the fast, epithermal and thermal energy groups from left to right.

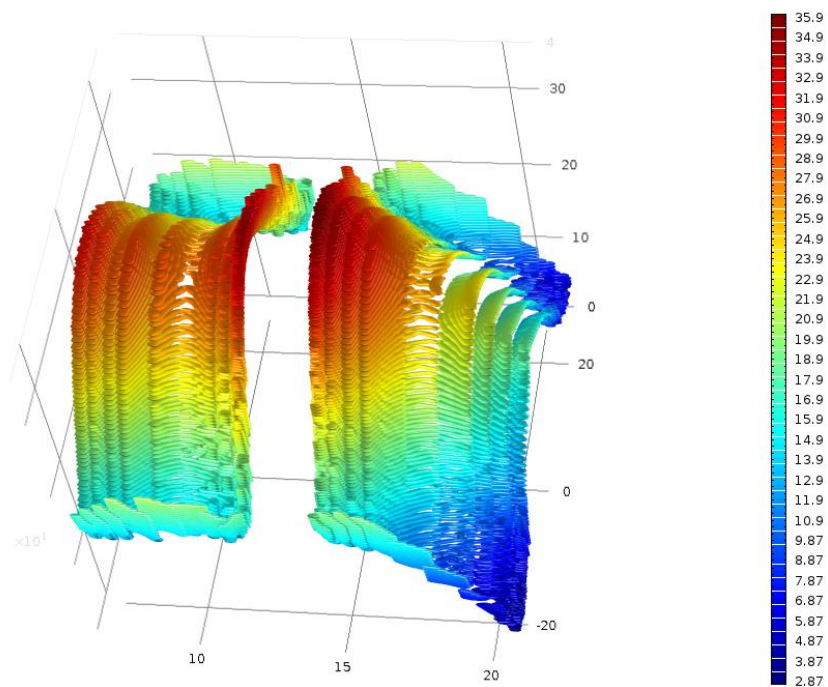


Figure 7.22: Raised tube-contour plot of the fission rate for an eigenvalue calculation.

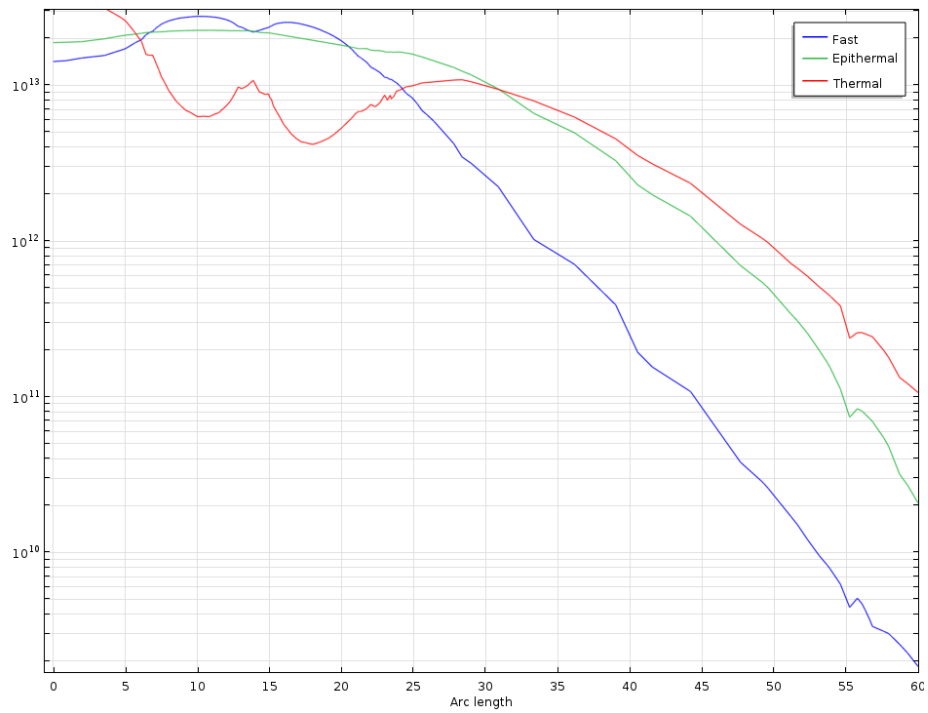


Figure 7.23: Scalar fluxes along reactor midplane for fast, epithermal and thermal fluxes.

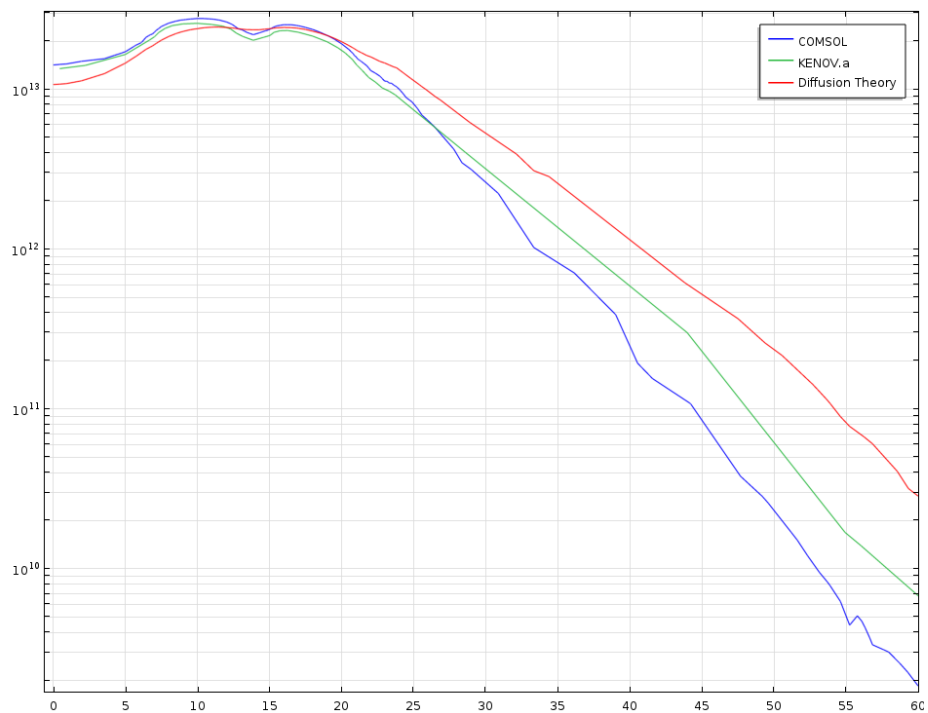


Figure 7.24: Scalar fast fluxes along the reactor midplane for COMSOL discrete ordinates, KENO V.a, and COMSOL diffusion theory models.

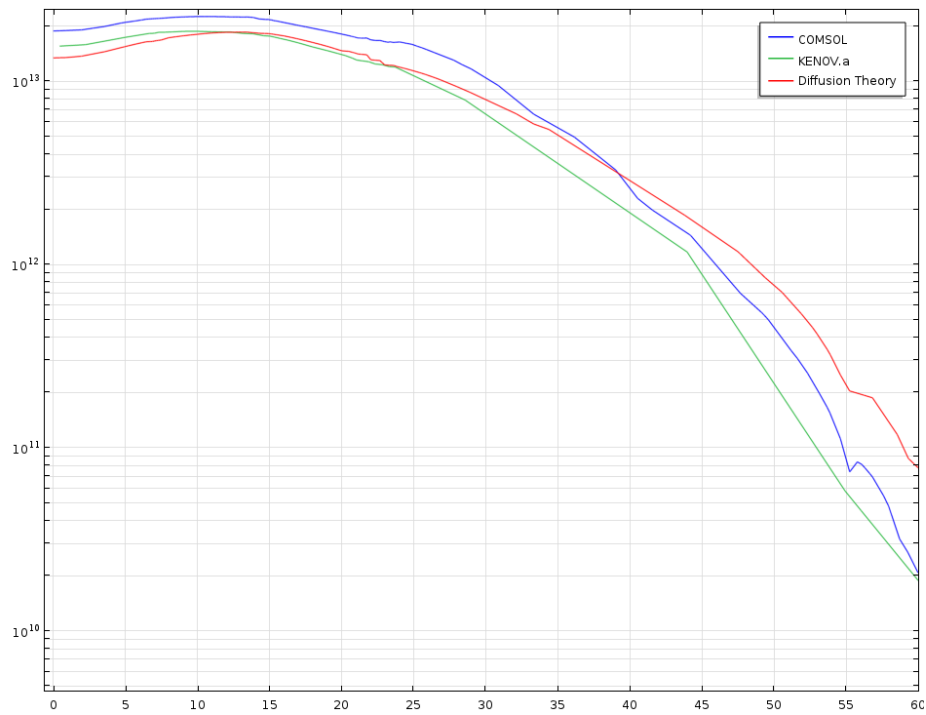


Figure 7.25: Scalar epithermal fluxes along the reactor midplane for COMSOL discrete ordinates, KENO V.a, and COMSOL diffusion theory models.

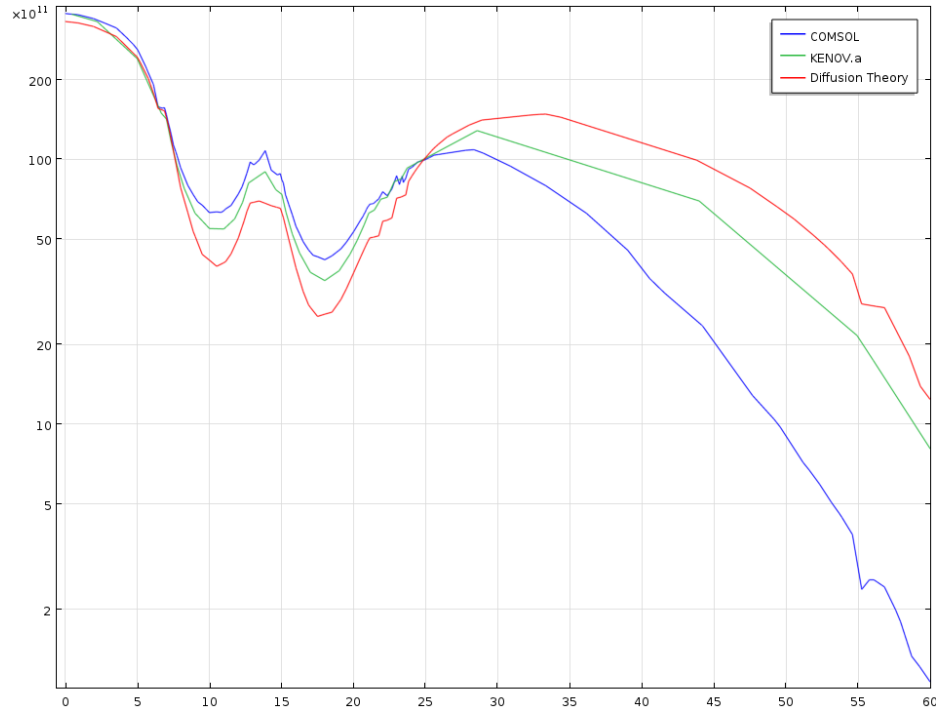


Figure 7.26: Scalar thermal fluxes along the reactor midplane for COMSOL discrete ordinates, KENO V.a, and COMSOL diffusion theory models.

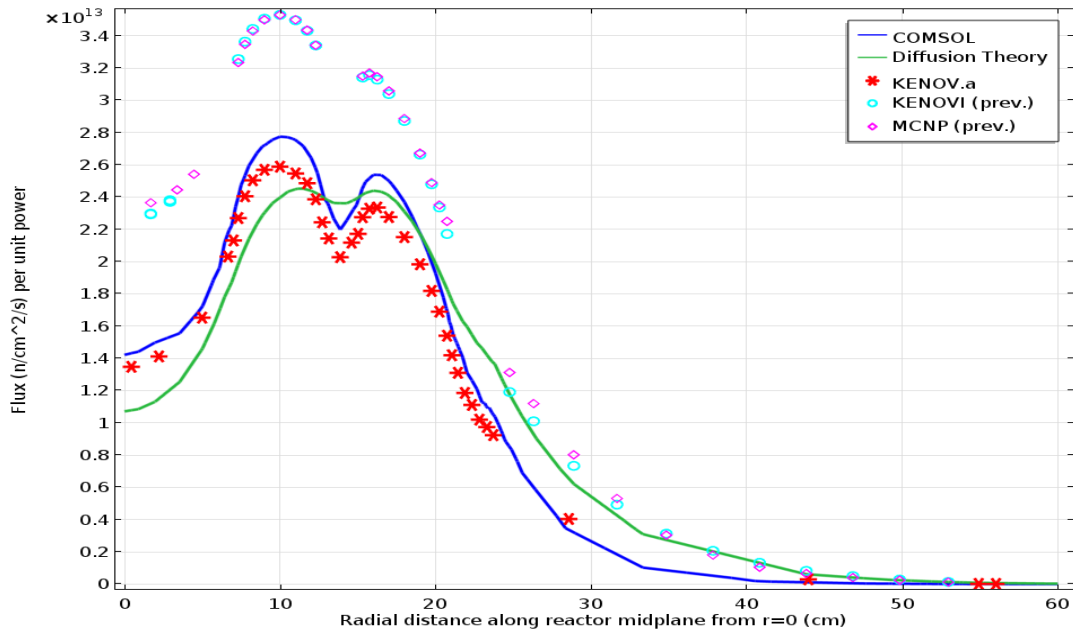


Figure 7.27: Scalar fast fluxes along the reactor midplane for COMSOL discrete ordinates, KENO V.a, and COMSOL diffusion theory simplified HFIR core models and for KENO-VI and MCNP5 more detailed HFIR core models.

in KENO-VI [123] and MCNP5 [124] . As can be seen from the results, the discrete ordinates solution in COMSOL offers good agreement to other methods of modelling the HFIR core, with some improvements in agreement over previous diffusion theory FEA methods in the fuel region.

7.3 Discrete Ordinates Development Summary

A physics-building application for the discrete ordinates method solution to the transport equation is created in COMSOL Multiphysics for all 3 Cartesian geometries and 2-D R-Z, making use of the Java API programming and Application Builder GUI. The method makes full use of finite element analysis and is readily applicable to multiphysics applications involving the over 30 physics modules built into COMSOL. The application is tested against several benchmark problems with modest success and comparison against other discrete ordinates (and Monte Carlo) codes, including XSDRN-PM, NEWT, KENO, MCNP, PARTISN, and ATILLA. In addition, a static BOC HFIR core model is developed and verified to be made available for use and examination in future HFIR core safety analyses.

8 Time-Dependent Discrete Ordinates

In this chapter, the extension of the COMSOL multi-dimensional and angularly-dependent neutron transport physics discussed in the previous chapter to include time-dependent capabilities is included, as well as comparison with a 1-D benchmark problem. The development of this added capability is intended to serve a variety of potential purposes for reactor kinetics at the HFIR, including solutions to reactor kinetics problems in the HFIR SAR, comparison against documented kinetics results, and utilization of time-dependent flux data for multiphysics problems in COMSOL.

8.1 Quasi-Static Development

Recalling the unpacking of the streaming operator term in section 7.1.1, there was derived a time derivative of the neutron angular flux divided by the neutron speed, v . This term was eliminated as the time derivative is zero for the stationary case however it is reintroduced to the transport equation for time-dependent solutions. Furthermore, the time-dependent behavior of delayed neutron precursor groups must be accounted for with kinetic equations for each delayed neutron precursor group, as seen below. This accounts for those precursors generated during fission that decay to release neutrons over a much longer time span (on the order of seconds) than prompt fission neutrons ($\sim 10^{-17}$ seconds to be considered instantaneous).

$$\frac{dC_i(\vec{r}, t)}{dt} + \lambda_i C_i(\vec{r}, t) = \frac{\beta_i}{k_s} \sum_{g'=1}^G v \Sigma_f^{g'}(\vec{r}) \phi^{g'}(\vec{r}, t)$$

Equation 8.1

where: t is the model time variable,

C_i is the concentration for precursor group i ,

λ_i is the decay constant for precursor group i ,

β_i is the delayed neutron fraction for precursor group i , and

k_s is the stationary solution for k_{eff} .

$$\begin{aligned} \frac{1}{v^g} \frac{d\psi_n^g(\vec{r}, \hat{\Omega}_n, t)}{dt} + [\hat{\Omega}_n \cdot \vec{\nabla} + \Sigma_t^g(\vec{r})] \psi_n^g(\vec{r}, \hat{\Omega}_n, t) \\ = \chi_p^g \frac{(1 - \beta_{eff})}{k_s} \sum_{g'=1}^G v \Sigma_f^{g'}(\vec{r}) \phi_{lm}^{g'}(\vec{r}, t) + \sum_{l=0}^{ISCT} \sum_{m=-l}^l Y_{lm}^*(\hat{\Omega}_n) \sum_{g'=1}^G \Sigma_{sl}^{g' \rightarrow g}(\vec{r}) \phi_{lm}^{g'}(\vec{r}, t) \\ + \sum_{i=1}^{np} \chi_{di}^g \lambda_i C_i(\vec{r}, t) + q_{ext}^g(\vec{r}, t) \end{aligned}$$

Equation 8.2

where: v^g is the neutron speed for group g ,

χ_p^g is the prompt fission distribution for group g ,

β_{eff} is the total delayed neutron fraction for all precursors, $\beta_{eff} = \sum_{i=1}^{np} \beta_i$

np is the number of delayed neutron precursor groups, and

χ_{di}^g is the delayed neutron fission distribution for precursor group i into energy group g ,

Thus there is now the added inputs for the kinetics parameters, typically determined for a system or material region, neutron speed by group, and new probability density function for the production of neutrons by delayed neutron precursors. It can be seen that the decay of delayed neutrons will become a driving force for reactivity insertions less than the delayed neutron fraction (delayed-critical).

Preliminary experimentation with this fully-implemented space-time approach has yielded an unstable convergence for all but very small time steps that are too computationally restrictive. Therefore the approach has been adjusted to a quasi-static approach that solves a time-dependent amplitude function, $P(t)$, to the spatial flux shape function, Ψ , that is quasi-statically updated at periodic larger time steps, Δt_ψ , the product of each making up the time-dependent angular flux distribution as shown in Equation 8.3.

$$\psi(\vec{r}, \hat{\Omega}_n, t) = P(t) \Psi_n^g(\vec{r}, \hat{\Omega}_n, \Delta t_\psi)$$

Equation 8.3

8.1.1 Point Kinetics

For the purposes of the current model, a spatially independent neutron amplitude function is desired for the system. The development of the point kinetics equations, which fill this need, may begin with the general angular-independent neutron transport equation as rewritten from Equation 8.2 by integrating over all angles (using the definition of the scalar flux and particle current, J) and removing the fixed source term and multigroup terminology to yield the scalar flux transport equation [116] in Equation 8.4.

$$\begin{aligned} \frac{1}{v} \frac{d\phi(\vec{r}, E)}{dt} + \vec{\nabla} J(\vec{r}, E) + \Sigma_t(\vec{r}, E)\phi(\vec{r}, E) \\ = \chi(E)(1 - \beta_{eff}) \int_0^\infty dE' v \Sigma_f(\vec{r}, E') \phi(\vec{r}, E') + \int_0^\infty dE' \Sigma_s(\vec{r}, E' \rightarrow E) \phi(\vec{r}, E') \end{aligned}$$

Equation 8.4

This equation, along with its static eigenvalue form, is integrated over space, for the volume V , and energy, E , and the precursor equation is integrated over space. Keeping in mind an inner production definition as shown in Equation 8.5 for notation, the resulting equations are given in Equation 8.6 through Equation 8.8. Note that the energy integration is applicable only to the fission distribution fraction, χ , for the fission term (which integrates to a value of 1) and that the integration of the scattering transfer term yields the scattering cross section of E' , $\Sigma_s(r, E')$, therefore simplifying each term into an inner product over energy, E' .

$$\langle a, b \rangle = \int_V d\vec{r} \int_0^\infty dE a(\vec{r}, E) b(\vec{r}, E)$$

Equation 8.5

$$\frac{d}{dt} \langle \frac{1}{v}, \phi \rangle + \langle \vec{\nabla} J \rangle + \langle \Sigma_t, \phi \rangle - \langle \Sigma_s, \phi \rangle = (1 - \beta_{eff}) \langle v \Sigma_f, \phi \rangle + \sum_{i=1}^6 \lambda_i \langle C_i \rangle$$

Equation 8.6

$$\frac{d\langle C_i \rangle}{dt} + \lambda_i \langle C_i \rangle = \beta_i \langle v \Sigma_f, \phi \rangle$$

Equation 8.7

$$\langle \vec{\nabla} J \rangle + \langle \Sigma_t, \phi \rangle - \langle \Sigma_s, \phi \rangle = \frac{\langle \nu \Sigma_f, \phi \rangle}{k}$$

Equation 8.8

Substituting the static equation, Equation 8.8, into the time-dependent form, Equation 8.6, yields Equation 8.9. Reactivity, ρ , is defined in terms of the neutron multiplication factor in Equation 8.10, where $\rho = 0$ denotes a critical system. The neutron density or amplitude function is defined as $P(t) = \langle \frac{1}{v}, \phi \rangle$, the precursors as $C_i(t) = \langle C_i \rangle$, as and the mean generation time, Λ , is defined in terms of the neutron density and fission production rate in Equation 8.11.

$$\frac{d}{dt} \langle \frac{1}{v}, \phi \rangle + \frac{\langle \nu \Sigma_f, \phi \rangle}{k} = (1 - \beta_{eff}) \langle \nu \Sigma_f, \phi \rangle + \sum_{i=1}^6 \lambda_i \langle C_i \rangle$$

Equation 8.9

$$\rho = 1 - \frac{1}{k} = \frac{k - 1}{k}$$

Equation 8.10

$$\Lambda = \frac{\langle n \rangle}{\langle \nu \Sigma_f, \phi \rangle} = \frac{\langle \frac{1}{v}, \phi \rangle}{\langle \nu \Sigma_f, \phi \rangle} = \frac{\langle \frac{1}{v}, \phi \rangle / \langle \phi \rangle}{\langle \nu \Sigma_f, \phi \rangle / \langle \phi \rangle} = \frac{\bar{1}}{\nu \Sigma_f}$$

Equation 8.11

Substituting these definitions into equations Equation 8.9 and Equation 8.7, yield the point kinetics equations as shown in Equation 8.12 and Equation 8.13 corresponding to the amplitude and precursor equations, respectively.

$$\frac{dP(t)}{dt} = \frac{(\rho - \beta_{eff})}{\Lambda} P(t) + \sum_{i=1}^6 \lambda_i C_i$$

Equation 8.12

$$\frac{dC_i}{dt} + \lambda_i C_i = \frac{\beta_i}{\Lambda} P(t), i = 1, \dots, 6$$

Equation 8.13

8.1.2 Quasi-Static Form

At a time point n , t_n , the static spatially dependent neutron flux is solved statically by using a finite difference approximation to the time derivative and utilizing the previously solved neutron flux shape at time t_{n-1} as shown in Equation 8.14. The static angular flux shape is solved at larger time steps Δt_ψ chosen by the user and adjusted in order to yield the most accurate solution, while the time-dependent amplitude function, $P(t)$, is solved at much smaller time steps, Δt_p , which are dictated by the solver settings within COMSOL.

$$\begin{aligned} & \frac{1}{v^g} \frac{\Psi_n^g(\vec{r}, \hat{\Omega}_n, t_n) - \Psi_n^g(\vec{r}, \hat{\Omega}_n, t_{n-1})}{t_n - t_{n-1}} + [\hat{\Omega}_n \cdot \vec{\nabla} + \Sigma_t^g(\vec{r})] \Psi_n^g(\vec{r}, \hat{\Omega}_n, t_n) \\ &= \chi_p^g \frac{(1 - \beta_{\text{eff}})}{k_s} \sum_{g'=1}^G v \Sigma_f^{g'}(\vec{r}) \Phi^{g'}(\vec{r}, t_n) + \sum_{l=0}^{\text{ISCT}} \sum_{m=-1}^1 Y_{lm}^*(\hat{\Omega}_n) \sum_{g'=1}^G \Sigma_{sl}^{g' \rightarrow g}(\vec{r}) \Phi_{lm}^{g'}(\vec{r}, t_n) \\ &+ \sum_{i=1}^{\text{np}} \chi_{di}^g \lambda_i C_i(\vec{r}, t_n) + q_{\text{ext}}^g(\vec{r}, t_n) \end{aligned}$$

Equation 8.14

As previously described, the angular flux is implemented in the weak form interface (w1) and the static eigenvalue within a global equations interface (ge1). A placeholder function for the previous time step angular flux, u_i , is defined with a second weak form interface (w2) per Equation 8.15 and the spatial precursor groups are solved in PDE coefficient mode (c). These steps make up the initial solution study step as shown in Figure 8.1. The point kinetics equations are defined as global equations (ge2) and two other global equations nodes make up global placeholders for the previous time step, t_{prev} (ge3), and current time step, t_{curr} (ge4) as shown in Equation 8.16 and Equation 8.17. The “nojac” operator is applied to exclude these placeholder equations from the solution Jacobian and save computation memory.

$$u_i(\vec{r}) - \text{nojac}[\Psi_n^g(\vec{r}, \hat{\Omega}_n, t_n)] = 0, i = 1, \dots, G * N(N + 2)$$

Equation 8.15

$$t_{\text{prev}} - \text{nojac}[t_{\text{curr}}] = 0$$

Equation 8.16

$$t_{\text{curr}} - \text{nojac}[t] = 0$$

Equation 8.17

The right of Figure 8.1 shows how these physics interface are solved within the quasi-static framework, where intermediate Time-Dependent Study Steps, i , solve the point kinetics and t_{curr} placeholder equations, followed by a Stationary Study Step, $i+1$, update to the angular flux variables, and a Stationary Study Step, $i+2$, update to the placeholder variables u_i and t_{prev} . These study steps are solved in sequence, each study step using the previous solution as its initial values, until after the chosen number of angular flux updates the transient is ended on an intermediate Time-Dependent Study Step $i=M$.

8.2 1-D Benchmark

The 1-D transient benchmark problem 16-A1 [125],[126] is chosen that uses two energy groups and six delayed neutron precursor groups to solve a supercritical fast reactor problem. Seven slab zones are ordered in widths of 40, 47.374, 9, 34, 9, 47.374, and 40 cm in sequential order where zones 1 and 7 are each other's reflection of fuel blanket region, zones 2, 4, and 6 are core regions, and zones 3 and 5 are control rod regions. Vacuum boundary conditions are specified on each outside end. The cross section

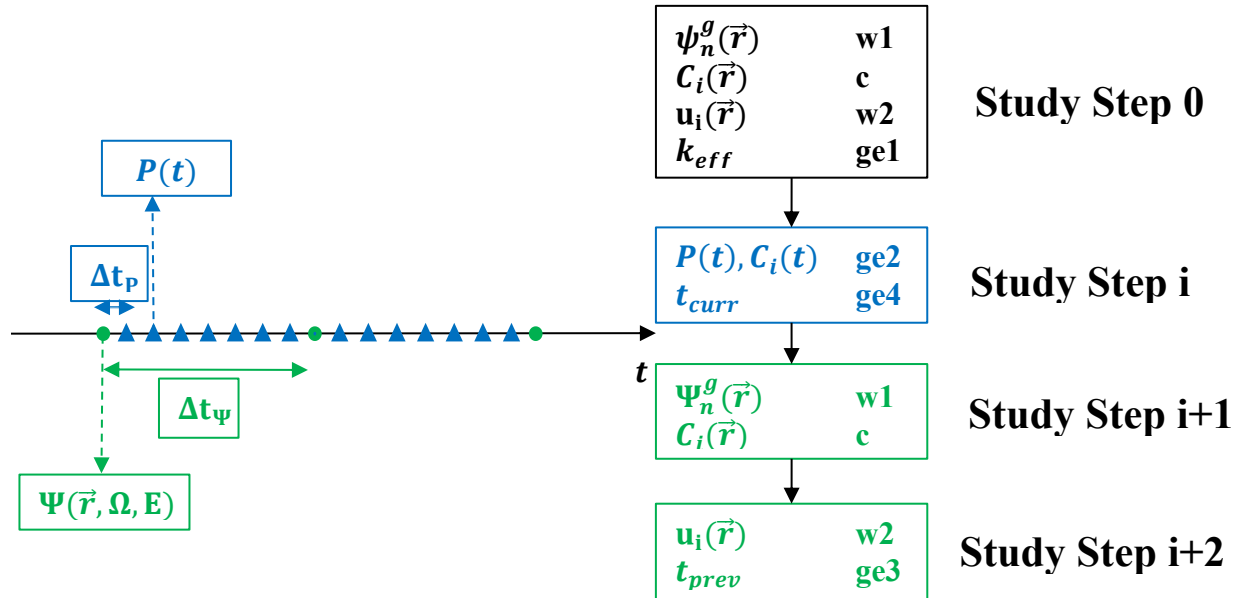


Figure 8.1: Quasi-static solution time-stepping (left) and COMSOL study steps (right).

and time-dependent problem parameters are given in Table 8.1 and the neutron precursor group parameters are shown in Table 8.2. A step perturbation at time zero applies a positive 5% perturbation to the cross section in region 2 and a negative 5% perturbation to the cross section in region 6.

The mesh nodes per zone are shown in the right column of Table 8.1. An S_8 angular flux with P_0 scattering is updated five times at $t=0$, $1e-5$, $1e-4$, $1e-3$, and $1e-2$ seconds. All stationary steps use a fully coupled solver except for the initial solution step which uses a segregated solver with negative flux fixup, with convergence criterion at $1e-5$ and $1e-3$ for angular flux and placeholder updates, respectively. Time-dependent steps use a convergence criterion of $1e-2$ and the generalized alpha method with strict solver time stepping is used and a constant solution predictor. All study step solvers used a direct MUMPS solver with memory usage at ~ 2 GB and solution time at around 20 minutes.

The benchmark [126] is digitized using an online plot digitizer and therefore the results comparison is not completely exact, although it is satisfactory. The resulting relative power profile from $1E-6$ to $1E2$ seconds is shown in Figure 8.2, with close comparison to the benchmark results including an initial “equilibrium” at relative power ~ 1.5 before runaway power increase at ~ 1 seconds. The group 1 and group 2 flux profiles as a function of slab position are shown in Figure 8.3 and Figure 8.4, with good agreement to the digitized benchmark. The symmetric flux profile at time zero and the non-symmetric flux tilt between zone 2 and 6 after time zero are both clearly shown. The calculated reactivity step insertion was ~ 0.00111 .

Table 8.1: Material cross-sections and mesh width for 1-D transient problem 16-A1.

Material	Group	$\Sigma_t(1/\text{cm})$	$\Sigma_f(1/\text{cm})$	$\Sigma_s^{g \rightarrow g}(1/\text{cm})$	$\Sigma_s^{g \rightarrow g'}(1/\text{cm})$	Mesh Nodes
1,7	1	0.2411	8.3441E-4	0.2336	3.598E-3	40
	2	0.4172	3.2776E-4	0.4070	0.0	
2,4,6	1	0.1849	7.4518E-3	0.1777	2.085E-3	48
	2	0.3668	1.1061E-4	0.3537	0.0	
3,5	1	0.09432	0.0	0.08571	1.717E-3	10
	2	0.1876	0.0	0.1713	0.0	

$1/v_1=1.851\text{E-}9 \text{ s/cm}$, $1/v_2=1.088\text{E-}8 \text{ s/cm}$, $\chi_1=0.0$, $\chi_2=0.0$

Table 8.2: Delayed neutron precursor group parameters for 1-D transient problem 16-A1.

Precursor Group i	β_i	$\lambda_i(1/\text{s})$
1	8.1E-5	0.0129
2	6.87E-4	0.0311
3	6.12E-4	0.134
4	1.138E-3	0.331
5	5.12E-4	1.26
6	1.7E-4	3.21

Total effective fraction = 0.0032

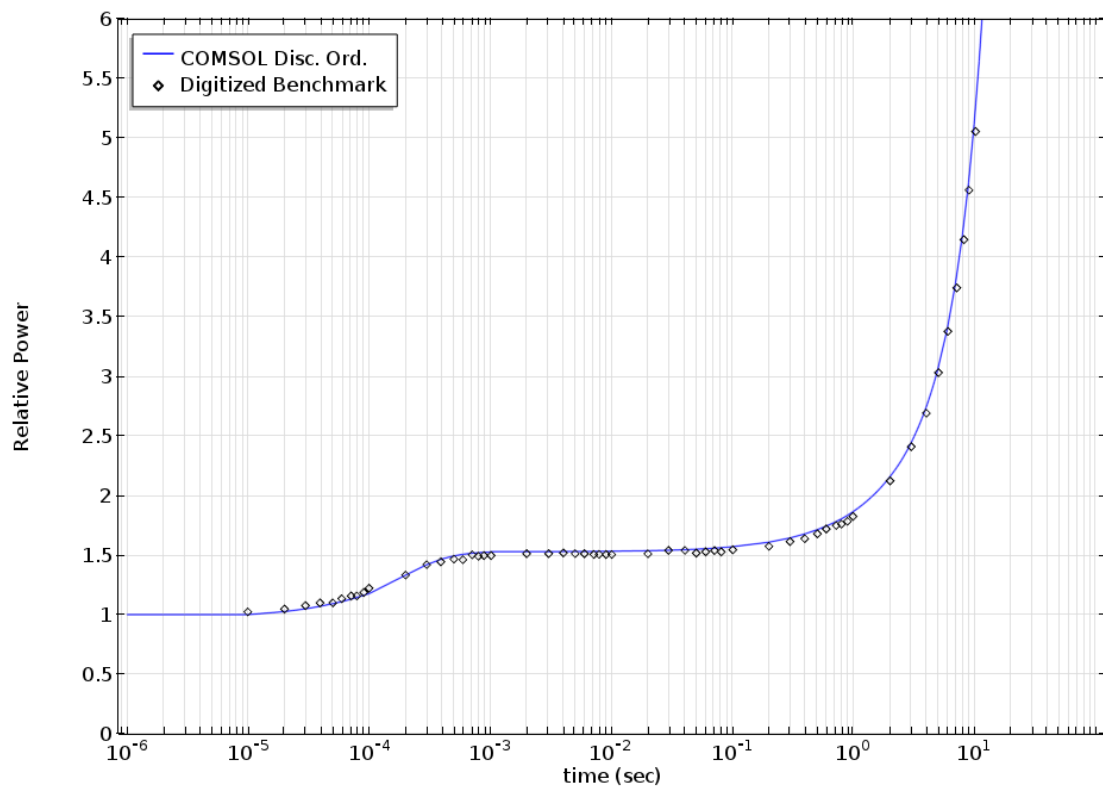


Figure 8.2: Relative power as a function of time for the 16-A1 transient problem.

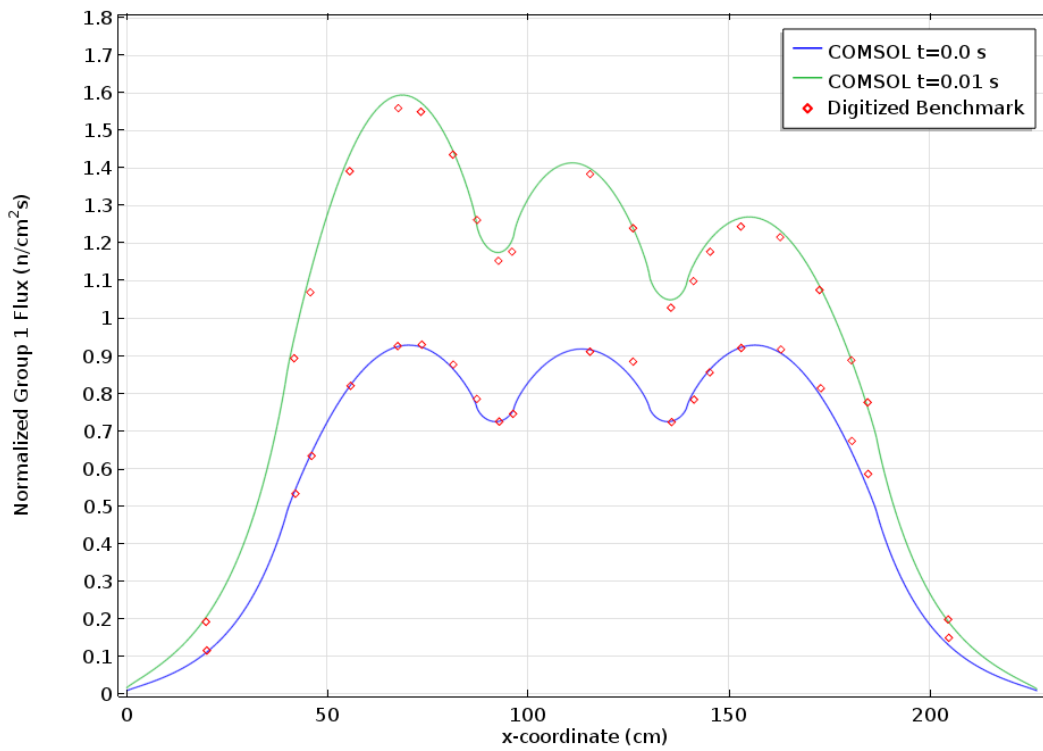


Figure 8.3: Normalized group 1 flux profile at $t=0$ and 0.01 seconds for the 16-A1 transient problem.

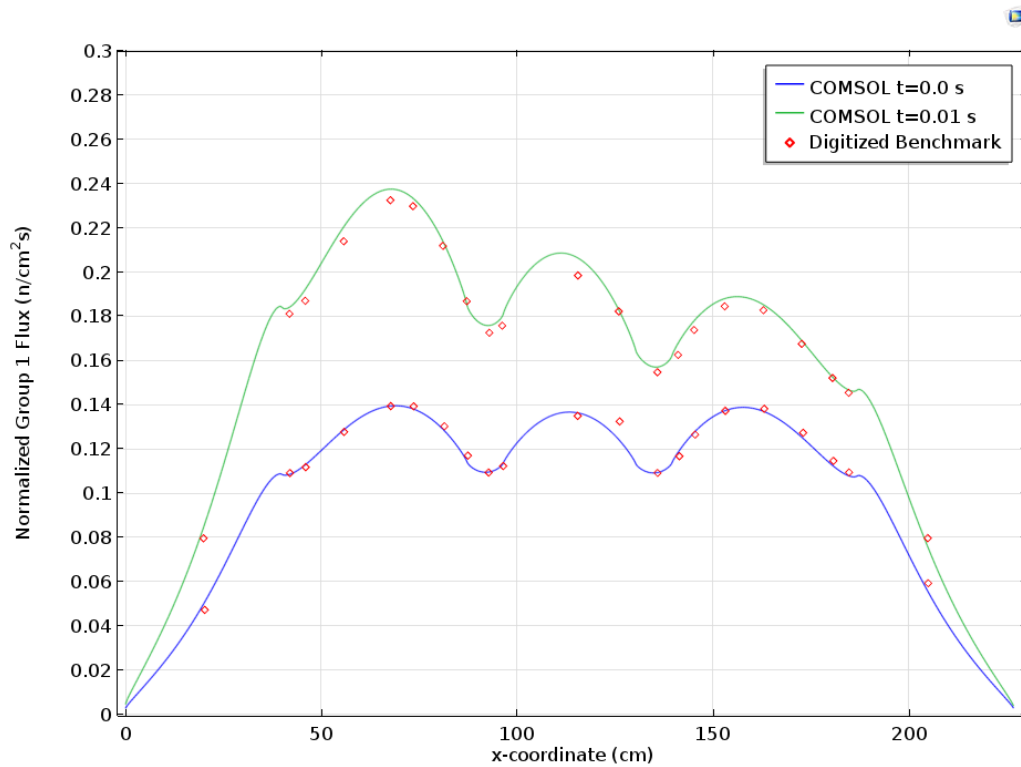


Figure 8.4: Normalized group 2 flux profile at $t=0$ and 0.01 seconds for the 16-A1 transient problem.

9 Concluding Statements

The following two sections summarize the final conclusions for this research and outline future research opportunities generated from this work.

9.1 Conclusions

The primary objective of this research is to develop new methodologies to ensure safe reactor operations and irradiations of experiments at the HFIR. In the course of that goal, strongly coupled thermo-mechanical models are developed for several ^{238}Pu production targets including a comprehensive model for further design optimization efforts, and a discrete ordinates methodology is developed in COMSOL that allows for versatile neutron transport calculations with easy access to multiphysics coupling.

Thermo-mechanical steady-state models were developed for four preliminary target designs to produce ^{238}Pu , for both single pellet capsules (a “bare” pellet and reduced-length pellet) and prototypical targets (a partially loaded or 8 pellet target and a fully loaded or ~50 pellet target). The results demonstrated the safety of the target designs under the given conditions and inputs, the complex tightly coupled thermal-structure behavior that occurs in these targets, and the power of high fidelity multiphysics models to solve unique problems. The purpose of these analyses was to demonstrate the safe irradiation with respect to thermal and structural margins at the HFIR, often intentionally using over-conservative and approximate inputs and methods – however, some in-situ characteristics were observed including deformation behavior due to thermal strain and axially dependent temperature profiles.

A summary of the solution scope for the ^{238}Pu production target models is given in Table 9.1, the details of which are expanded upon below. Throughout the models, thermal margins were the primary items of interest, where the maximum temperature, T_{max} , with respect to melting consistently presented the smallest safety margins, and the maximum target surface temperature, T_{surf} , was conservatively compared to the coolant saturation temperature. In the production model, parameters pertinent to

Table 9.1: Summary of solution scopes for all thermo-mechanical models.

<i>Model</i>	Parametric Sweep	Pellet Heat-Treatments	Solution Search	Pellet Swelling	Time Steps	Positions	Limiting fields
<i>Partially Loaded</i>	No	900 °C, 1200 °C	Yes	Constants	2	1	$T_{\max}, T_{\text{surf}}$
<i>Fully Loaded</i>	Yes	1200 °C	Yes	Constants/2 Functions	2/7	2	$T_{\max}, T_{\text{surf}}$
<i>Production</i>	Yes	1200 °C	No	3 Functions	30	8	$T_{\max}, T_{\text{surf}}, P_{\text{side-max}}, F_{\text{axial}}, \epsilon_{\text{axial-pellet}}$

structural integrity of the model including the maximum pellet side pressure on the cladding/housing, $P_{\text{side-max}}$, the axial force on the placed on the target welds, F_{axial} , and the maximum local axial strain the pellets may place on the cladding/housing given a “locked-in” state from hydrostatic collapse, $\epsilon_{\text{axial-pellet}}$.

The first prototypical model was for the partially loaded target design, including 8 pellets, and the geometry dimensions were 2-D R-Z in order to save on computation resources. Because of the reduced margins and unavailable PIE data from the reduced-length tests, two heat-treatments at 900 °C and 1200 °C were considered, each analyzed using a manual solution search for varying bounding radial shrinkage and fabrication gaps at EOC-1 and EOC-2. As a result of these analyses and the received PIE data, the target with 1200 °C heat-treatment pellets was chosen for irradiation.

The second prototypical target model was for the fully loaded target, containing 52 pellets, and underwent several revisions to its solution scope for evolving results from the incoming PIE data. At first, the same manual solution search method was employed for EOC-1 analysis, analyzed at two different positions VXF-15 and a lower flux location VXF-3. For the EOC-2 analysis, it became necessary to credit the time or burnup-dependent behavior of pellet densification/swelling observed in partially loaded target PIE, using an automated solution search method that found the maximum allowable shrinkage for a range of pellet heat generation rates at EOC-2 conditions. This method, plotted

alongside current PIE data at the time, allowed for the irradiation of 2nd cycle targets. As pellet swelling (or densification recovery) was observed, the potential for aggregated pellet stack expansion to place axial force on the target became a concern. As a result, time-dependent analyses in cycle 2 were completed with two swelling curves and, in addition to further confirming acceptable temperature maxima and revealing target time-dependent behavior, supplied axial temperatures for a separate calculation of axial target stresses.

The production model was then created, as the potential for 3 cycles of irradiation with acceptable isotopic quality was realized and the design updated for greater axial clearance, with thermo-mechanical modeling enabled over the entire target domain as opposed to only the pellets and their surrounding components. A large wealth of PIE data from fully loaded target irradiations allowed three curves (a best-estimate and two bounding fits) for dimensional irradiation behavior to characterize the 7 pins of the VXF-15 holder and pin 1 of VXF-3 for 3 cycles of irradiation for 10 time steps in each cycle. The model cases addressed structural as well as thermal limitations, confirming pin 1 of VXF-15 as the limiting pellet and reaffirming the target maximum temperature as the limiting safety parameter. This model allowed for the safe irradiation over 3 cycles as well as detailed characterization of the target behavior under irradiation.

The COMSOL application builder was used to manage the input, material mixing, and (optionally) collapsing of cross sections from the SCALE code system, create a discrete ordinates physics module in COMSOL suited to the user's needs and setup a segregated solver. The created model may then be setup for the problem-dependent geometry and other settings. The created COMSOL weak form module was then able to be used to solve G by $N(N+2)$ discrete ordinates equations and boundary conditions (either vacuum or reflective), in a form conducive to eigenvalue and/or fixed source neutron transport calculations. The discrete ordinates equations are variable in terms of geometry dimensions (including 1-D, 2-D, and 3-D Cartesian as well as 2-D R-Z), angular quadrature (level symmetric sets from $N=2$ to $N=16$), scattering order ($P_N=0$ to 3), and energy groups (limited by computational memory).

That method is verified for a variety of benchmark studies, including (1) a 3-D fixed source calculations of the Kobayashi benchmark problem with comparison to the PARTISN code, (2) 3-D Godiva-like criticality sphere problem with comparison to the ATILLA code, and (3) various author-created eigenvalue problems (in 1-, 2-, 2- R-Z, and 3- dimensions) that are compared to corresponding SCALE module codes (XSDRN-PM, NEWT, KENO V.a). Finally, a beginning-of-cycle simplified 2-D R-Z HFIR core is analyzed with comparison to simplified HFIR core analysis in KENO V.a and diffusion theory as well as detailed HFIR core analysis in MCNP and KENO-VI. Historically, few versatile discrete ordinates tools have been created for finite element analysis and few non-stochastic analyses of the HFIR core have been conducted, making the application of discrete ordinates in COMSOL a unique tool for future HFIR safety analyses.

The neutron transport methodology in Chapter 7 is extended to time-dependent capabilities in Chapter 8 by using a quasi-static approach that uses the point kinetics equations for fine time-stepping of the flux amplitude and discrete ordinates method as a larger time step quasi-static update to the flux shape function. This is implemented in COMSOL using the weak form, PDE coefficient, and global ODE interfaces in order to implement angular flux, neutron density, precursor group, and spatial flux and time placeholder variables in sequential study steps that are built in the COMSOL Application Builder. This methodology is used to solve a two-group, 1-D Cartesian slab problem with a step cross-section perturbation. The results of this problem compare well with the benchmark, both in terms of the time-dependent flux tilt and relative power.

It has been shown that there is a great potential to utilize discrete ordinates in COMSOL for a variety of applications to accurately model neutron transport. It is also established that there is a motivation and opportunity to analyze the unique discrete ordinates problems with multiphysics and/or reactor kinetics applications at the HFIR using a new and original computational tool.

9.2 *Proposal for Future Work*

Although the documented research has been satisfactorily summarized, there are areas of future potential work, in both thermo-mechanical target analyses and discrete ordinates development in COMSOL, that have been identified. These areas include, but are not limited to, those listed below:

1. Several areas of design optimization may be explored for the production of ^{238}Pu at the HFIR including to the target design (a 2nd generation target to ensure greater axial clearance is being studied which may or may not require further analyses), the pellet fabrication (e.g. increased NpO_2 loading above 20% will allow greater product output, yet require further input data and subsequent analyses), or the target holder (a 2nd generation target holder will require computational flow dynamics analysis to ensure adequate flow distribution to each target pin and may either implement or reference the developed production model).
2. An alternative irradiation program at the HFIR of NpO_2 pellets (with no aluminum powder mixing) in zircaloy cladding is being explored which may use the developed models from Chapters 4 through 6 as reference or starting point for analyses.
3. The discrete ordinates methodology developed in this research utilized neutron transport only, however transport of photons (or gamma rays) is also amenable to the discrete ordinates method and has an important effect in the HFIR and other nuclear applications. By utilizing the previously developed methods, gamma transport could be added to this tool and benchmarked against many existing problems including further analyses on the HFIR core.
4. The discrete ordinates methodology demonstrated in this research was primarily limited to static problems, however by implementation of a quasi-static method with point kinetics in COMSOL (briefly demonstrated in Chapter 8) or implicit discrete ordinate time stepping (a more computationally demanding approach) reactor transient or other time-dependent kinetics problems may be analyzed. Worthwhile implementations at the HFIR may include the scram of

reactor control elements or the ejection of a high neutron absorption rabbit during HFIR operation.

5. A possibility that was briefly explored was applying a deterministic solution to the neutron transport equation in COMSOL using methods for solving the angular domain other than discrete ordinates, including spherical harmonics and direct angular discretization. The latter method was explored using the additional dimension features offered within COMSOL, which unfortunately at the time was not a very versatile or capable tool for this particular purpose. However, ongoing improvements to this tool in future versions of COMSOL may offer further exploration of this approach that would be a unique, challenging, and worthwhile research opportunity.

There are many avenues of research that may arise from the thermo-mechanical and discrete ordinates methodology described in this dissertation in addition to the four areas identified and briefly discussed above.

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APPENDICES

Appendix A – Molybdenum-99 Production Studies

In this chapter, studies are made for the production of molybdenum-99 (^{99}Mo) through irradiation of high density low-enriched uranium (LEU) targets in the HFIR hydraulic tube (HT) facility, located in the HFIR flux trap region. These studies were performed in order to facilitate the design of a HT “rabbit” holder target, which was completed, and followed through to approved HFIR safety calculations to support the irradiation of these targets.

A.1 Background of Molybdenum-99 Experiments

^{99}Mo is a radioactive isotope of molybdenum with a half-life of 2.75 days that beta decays to Technetium-99m ($^{99\text{m}}\text{Tc}$). $^{99\text{m}}\text{Tc}$, a metastable nuclear isomer of ^{99}Tc , is used in 20 million diagnostic medical applications per year as a radioactive tracer and is the most widely used medical isotope constituting 85% usage in nuclear medical imaging. Its short half-life (6 hours) emitting 140.5 keV gamma rays makes it well-suited for medical imaging using scintillation cameras and its biological half-life (1 day) keeps patient exposure low. The radioisotope is used in a wide variety of imaging areas, including the brain, heart, lungs, liver, kidneys, tumors, bones, and blood.

Currently, the primary domestic supply of ^{99}Mo comes from HEU targets irradiated in research reactors. Recently, the usage of LEU targets has been studied and pursued, as the primary ^{99}Mo source at the National Research Universal reactor in Ontario, Canada has been scheduled for shutdown initially in late 2016 and now early 2018. Thus the interest in LEU targets presents both a non-proliferation avenue of approach as well as meeting a very necessary public health requirement.

A.1.1 ^{99}Mo Production at the HFIR

This target is part of a two target campaign to produce ^{99}Mo at the HFIR using neutron irradiation of high-density uranium targets. The two parts involve 1) a lower-enriched, smaller LEU target to be irradiated in the HT facility, and 2) a higher enriched, larger LEU target to be irradiated in the permanent beryllium reflector. Other methods of ^{99}Mo production have been pursued at the HFIR, including

irradiation of aqueous uranyl-based solutions in the Gamma Irradiation Facility (GIF), but this chapter focuses on the high density LEU campaign, specifically part 1, involving the irradiation of an LEU target in the HT facility.

HFIR was originally designed to produce transplutonium isotopes. The FTT region contains 37 experiment sites and is located at the center of the reactor with a the peak thermal neutron flux of approximately 2.2×10^{15} neutrons/cm²-s at full power of 85 MW_{th}. Target removal availability and the high thermal flux in the hydraulic tube makes it well-suited to accommodating a short half-life medical isotope production target that may be irradiated for a shorter time period than the typical 22-26 day HFIR fuel cycle then removed for subsequent separation, recovery, and purification at the Radiochemical Engineering Development Center (REDC). The higher enriched, larger LEU target may be irradiated for a full operating cycle in the permanent beryllium reflector, where lower fluxes and burnup will occur, before removal and chemical filtration.

A.2 Methodology

Version 1.5.1 of the MCNP5 code was utilized to solve neutral particle (neutron and photon) and electron transport for certain neutronics parameters such as reactivity insertion, neutron fluxes and heat generation rates in the targets. Version 6.1 of the SCALE code package is used, specifically the COUPLE and ORIGEN-S modules in order to calculate transmutation and decay of the nuclide inventory in the target. In addition, Mathematica and COMSOL were used for preliminary thermal cooling analysis.

A.3 Preliminary Studies

Preliminary studies use a middle-of-cycle (MOC) neutron flux to calculate the heat generation rates and fluxes for depletion. The methodology is similar to that more fully described in the following subsections in terms of heat generation rates calculated using MCNP5, ORIGEN-S, COUPLE, and OPUS. In addition, a Mathematica script using a coolant control volume is used to conservatively estimate the wall temperature of the capsule for comparison to a flat, conservative estimation of coolant

saturation. The studied input design parameters were primarily the LEU foil enrichment and capsules position in the rabbit stack.

Two example plots from this preliminary phase are shown below for a 10-day irradiation period, a plot of the ^{99}Mo activity as a function of time during and after irradiation in Figure A.1 and the capsule wall temperature as a function of axial position in the rabbit stack compared to the saturation temperature in Figure A.2. Preliminary results in Figure A.1 and Figure A.2 are analyzed for different placements of the capsule in the rabbit stack (from 1 to 8 or 9, where lower numbers indicate the bottom of the rabbit stack and position 5 is at the reactor horizontal midplane), where primarily the center position 5 or the top of the stack (8 or 9) were preferred, and ^{235}U enrichments, where enrichments above 1.0% were determined to be too restrictive for shipping radioactivity and timing requirements. As a result of these preliminary studies and design considerations, a natural enrichment LEU foil capsule was chosen for irradiation at position 8 in the rabbit stack.

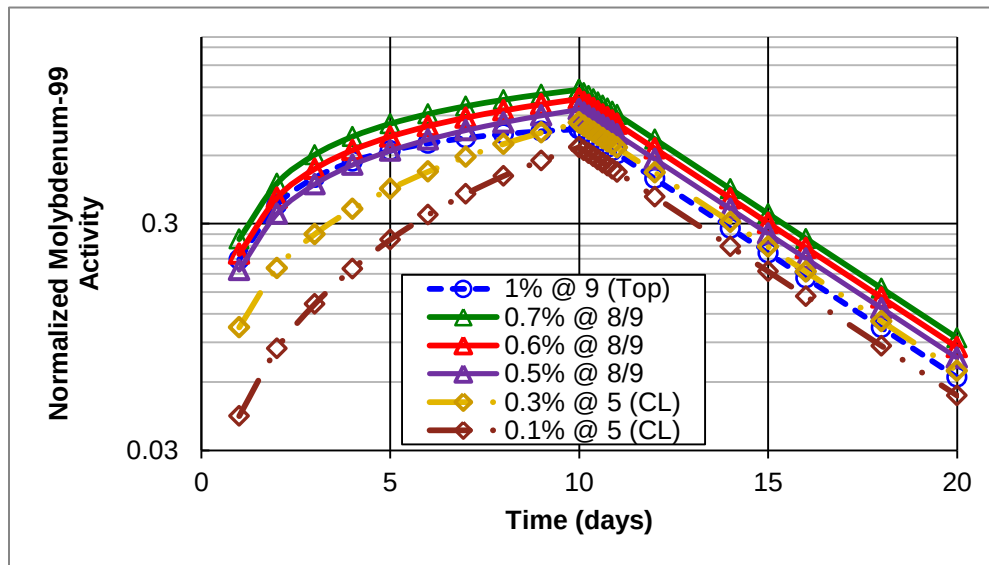


Figure A.1: Normalized ^{99}Mo radioactivity as a function of time in days (for a 10 day irradiation period) for a variety of configurations and foil enrichments.

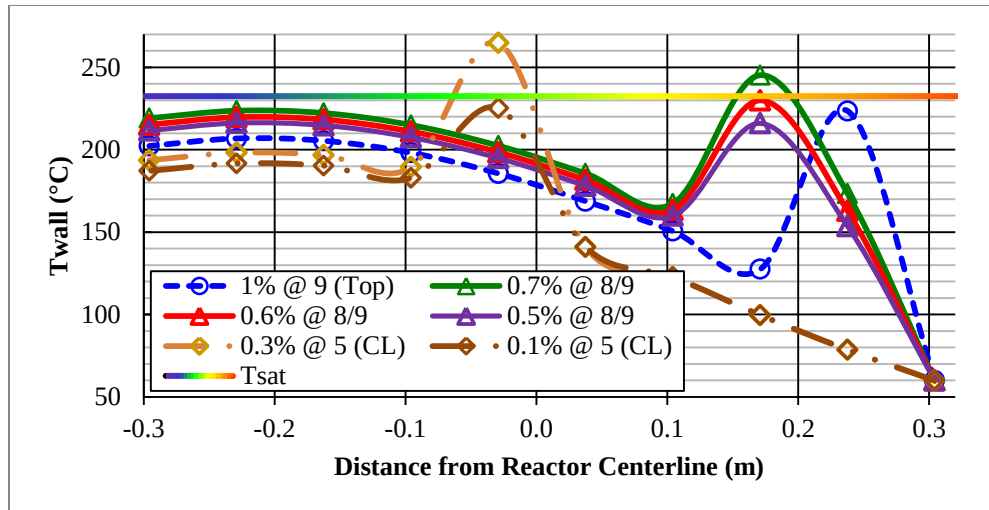


Figure A.2: Maximum capsule wall position as a function of axial position in the rabbit stack for a variety of configurations and foil enrichments.

A.4 Safety and Production Calculations

The final target design and plan consisted of nickel component parts and an LEU coated foil of natural enrichment (~ 0.7 wt.% ^{235}U) to be irradiated in the HT facility at a top position (position 8). In order to assure adequate target cooling, two cases were requested to be modeled: 1) A nominal case of normal target loading at position 8, and 2) A misloading of the target at the reactor centerline position (position 5).

A.4.1 Target Geometry and MCNP Model Input

The two HFIR core MCNP models, modified versions of HFIR fuel cycle 400 [124], occur at beginning-of-cycle (BOC) and end-of-cycle (EOC) for a 26 day fuel cycle and were modified to reflect the current design drawings of the HFIR HT facility and its utilized rabbit components. The rabbit stack was modeled in flux trap position B-3 (HT facility) and the in-vessel drawings of the B-3 tube and surrounding target shrouds were used to update the geometry.

In addition to the LEU target, aluminum rabbits complete the remainder of the rabbit stack in the B-3 tube. HFIR rabbit pushers are placed at the top and bottom (positions 9 and 1, respectively) of rabbit

stacks as large OD capsules that help push/pull the rabbit stack into/out of the hydraulic tube. In this case, since the irradiation capsule is heavy compared to dummy rabbits, only a bottom rabbit pusher is needed. HFIR dummy capsules serve as placeholders, in order to locate the irradiated target in its' desired position.

The target material compositions are hardened 4N5 Nickel and high density LEU foil manufactured at the Y-12 National Security Complex using available natural uranium feedstock (~ 0.711 wt.% ^{235}U), with a back-filled helium gas for the plenum regions of the target. The measured impurities are utilized in the MCNP data cards for these materials.

The target/rabbit assembly geometry is contained in a nickel housing with a maximum length of ~ 2.625 inches, with a welded nickel end cap. A ~ 125 micron thick LEU foil is coated with ~ 7.5 micron thick nickel coating. With the LEU coated foil wrapped outside a nickel inner sleeve, the inner sleeve acts as a spring which pushes the LEU coated foil flush against the inner surface of the housing. The ~ 17 degree gap in the LEU foil is conservatively directed away from the core centerline since the thermal flux is greatest in the center of the core. Figure A.3 and Figure A.4 show the LEU rabbit geometry as modeled within the hydraulic tube in MCNP.

For the nominal case considered, the rabbit pusher is placed at position 1, HFIR dummy capsules at positions 2 thru 7, and the U foil irradiation capsule placed at position 8. For the loading error case, the rabbit pusher is placed at position 1, HFIR dummy capsules at positions 2 thru 4 and 6 thru 8, and the LEU foil irradiation capsule placed at position 5. In the position 5 case, the height of the rabbit pusher is increased to ~ 2.93 (~ 7.45 cm) in order to place the LEU foil at the reactor core horizontal midplane (the location of highest flux and thus highest heat generation). Figure A.5 shows the MCNP as-modeled rabbit stack in the HT facility with the LEU rabbit at position 5.

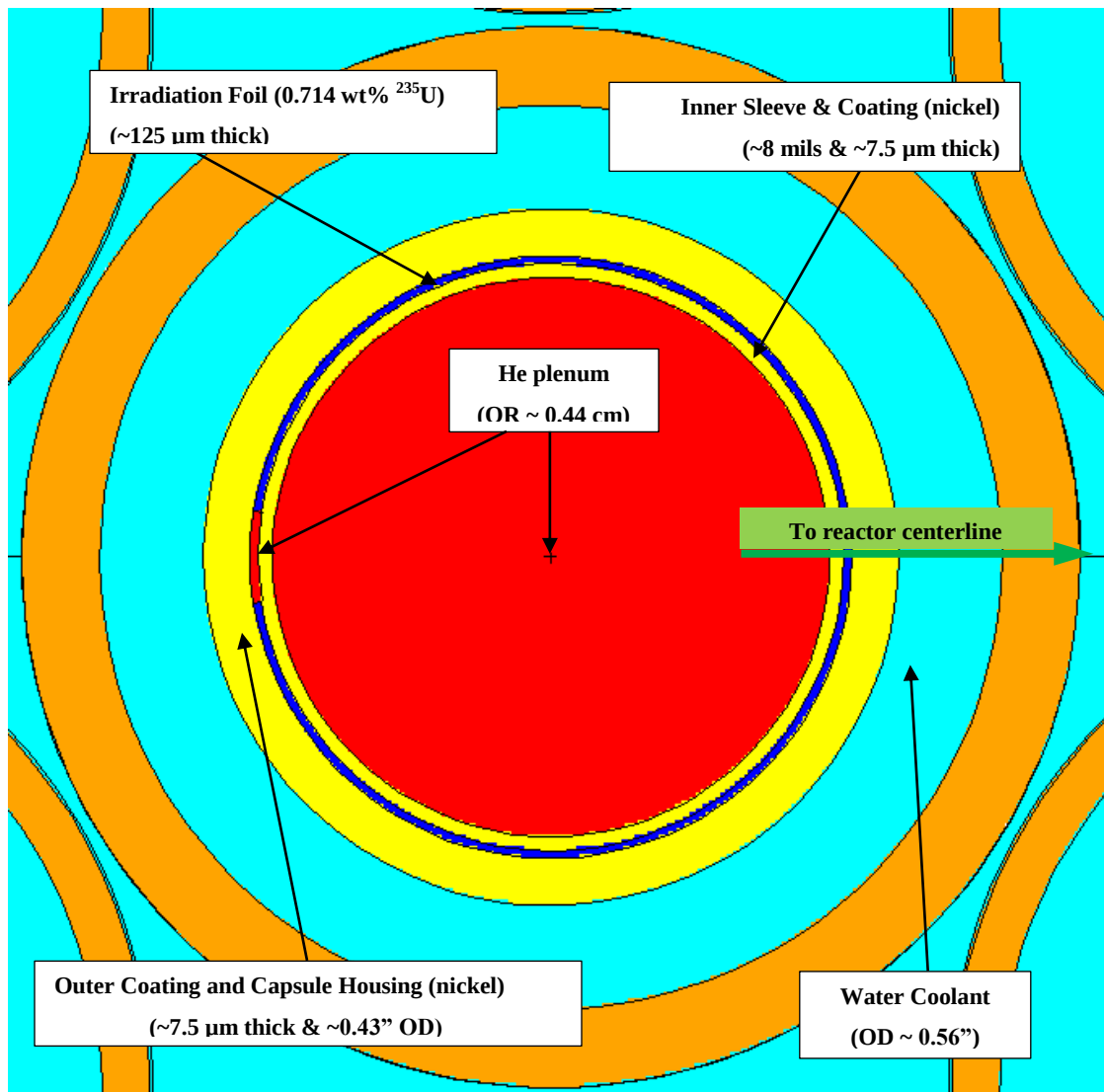


Figure A.3: MCNP as-modeled x-y cross section of HT and LEU capsule at the core horizontal midplane (dimensions are approximate).

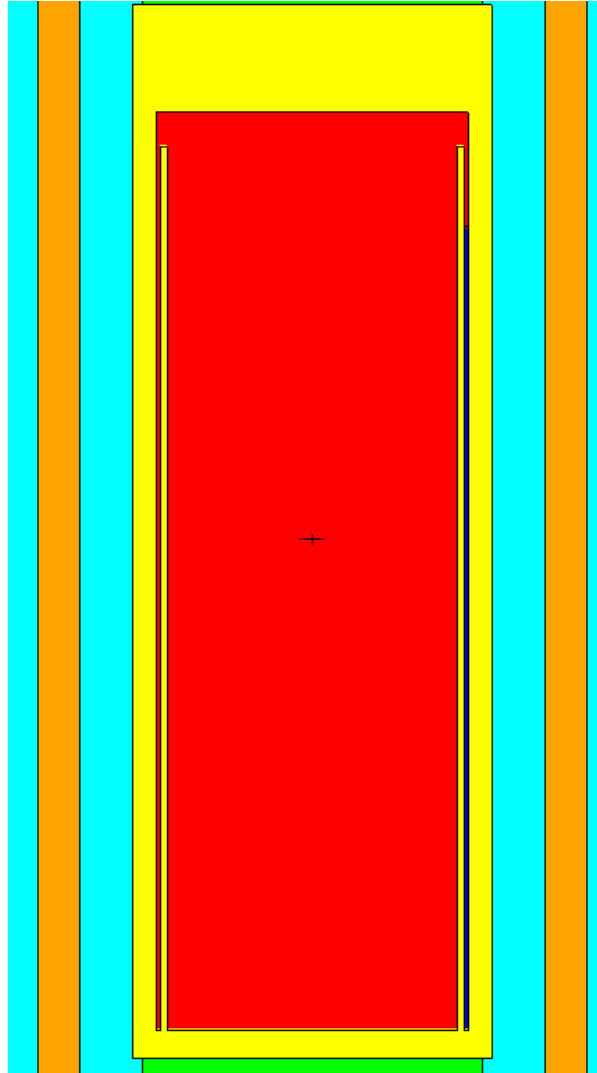


Figure A.4: MCNP as-modeled x-z cross section of LEU irradiation capsule at the core horizontal midplane.

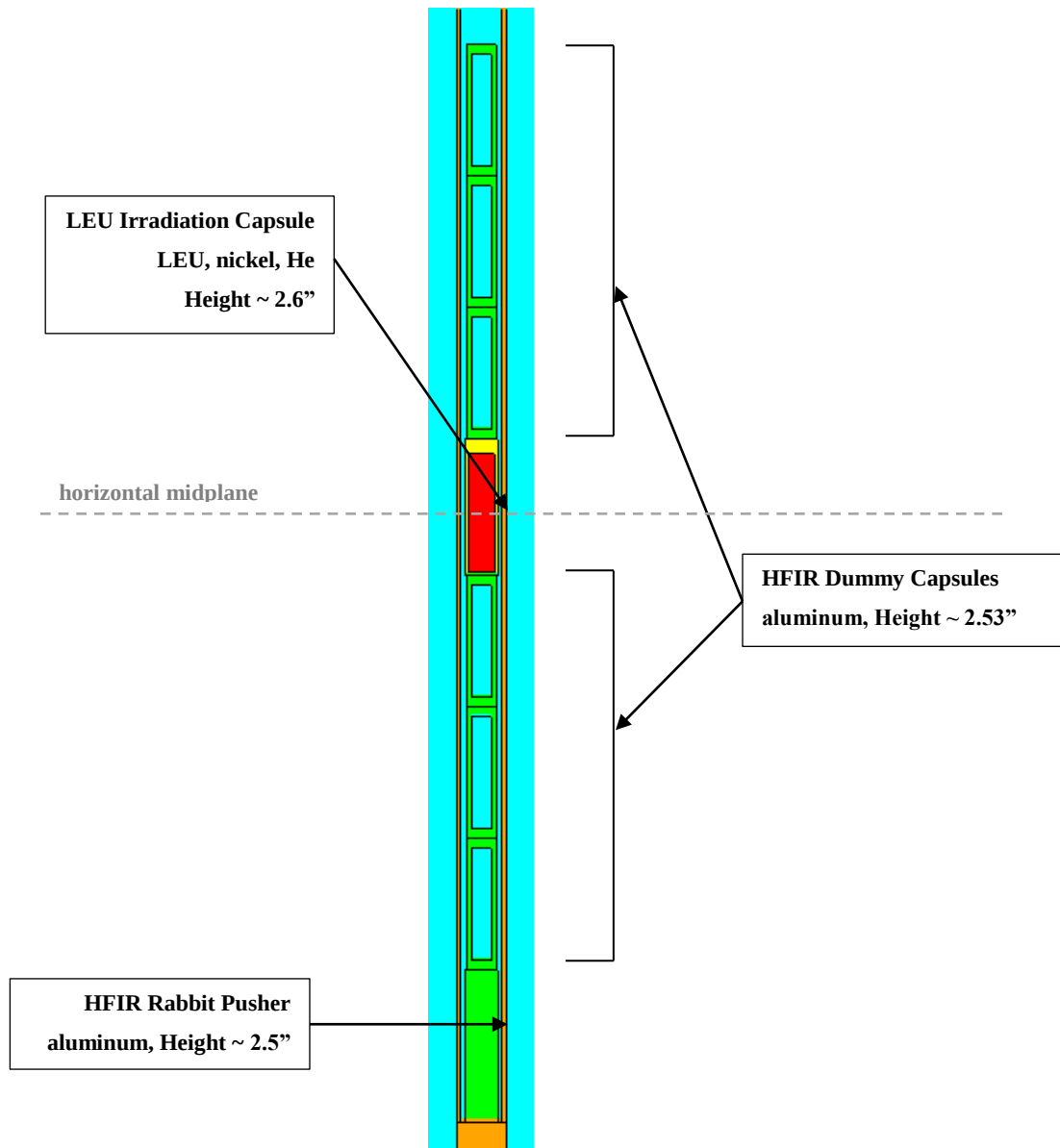


Figure A.5: MCNP as-modeled x-z cross section of HT rabbit stack for LEU irradiation capsule at position 5.

A.4.2 *Heating Mechanisms in a HFIR Target*

It is important to discuss and understand the mechanisms or components that contribute to heating of the target in HFIR. Components of nuclear heating include:

1. Prompt gamma (or photon) radiation arising from the fission process in the reactor fuel components and then imparting energy through absorption or scattering in the target.
2. Capture gamma rays (or photons) from (n, γ) reactions occurring in the surrounding structural materials and then imparting energy through absorption or scattering in the target.
3. Prompt gamma (or photon) radiation arising from the fission process in the target fissionable material and then imparting energy through absorption or scattering in the target.
4. Capture gamma rays (or photons) from (n, γ) reactions occurring in the target materials and then imparting energy through absorption or scattering in the target.
5. Prompt neutrons arising from the fission process in the reactor fuel components and then imparting energy through absorption reactions, scattering or induced fission in the target.
6. Prompt neutrons arising from the fission process in the target fissionable material and then imparting energy through absorption reactions, scattering or induced fission in the target.
7. Fission fragments arising from the fission process in the target fissionable material and then imparting energy locally as ionized daughter nuclei.
8. Decay gamma radiation (or delayed photons) produced from the decay of fission products in the core and imparting energy through absorption or scattering in the target.
9. Decay gamma radiation (or delayed photons) produced from the decay of neutron-activated structural materials surrounding the target and imparting energy through absorption or scattering in the target.
10. Beta and alpha particles produced from the decay of neutron-activated materials and fission products in the target and imparting energy locally as ionizing radiation.

11. Decay gamma radiation (or delayed photons) produced from the decay of neutron-activated materials in the target and imparting energy through absorption or scattering in the target.
12. Decay gamma radiation (or delayed photons) produced from the decay of fission products in the target and imparting energy through absorption or scattering in the target.

Table A.1 below sorts the above components into the calculation methodology by which they are solved, the transient power curve they are dictated by, their physical source location, and particle type.

Components 1 through 7 are “prompt” or “instantaneous” components in that they are directly proportional to the fission rate in the reactor core. During steady state operation this is typically the largest single component of nuclear heating, however during a HFIR transient it falls off very quickly upon the reactor scram along the order of a 3rd of a second (along with the HFIR fuel fission rate).

Components 8 and 9 are core decay components, in that the radioactive decay of reactor materials outside the target (including fission products from the fuel and neutron-activated structural materials) contribute their delayed photons to the target heating. These follow the radioactive decay of the HFIR core which is a slower decline determined by reactor fission products’ and activated material half-lives.

Components 10 through 12 are target decay components in that the radioactive decay of materials inside the target (including fission products from the LEU foil and neutron-activated materials in the nickel components) contribute to the target heating. Similar to the core decay components, these follow the radioactive decay of the respective materials, where the target decay falls off somewhat faster than the activated materials in the nickel. As opposed to the core materials, it is necessary to include radioactive beta and alpha decay heating in addition to the delayed photon heating from the LEU foil, as these components are locally deposited.

Components of nuclear heating are depicted in Figure A.6.

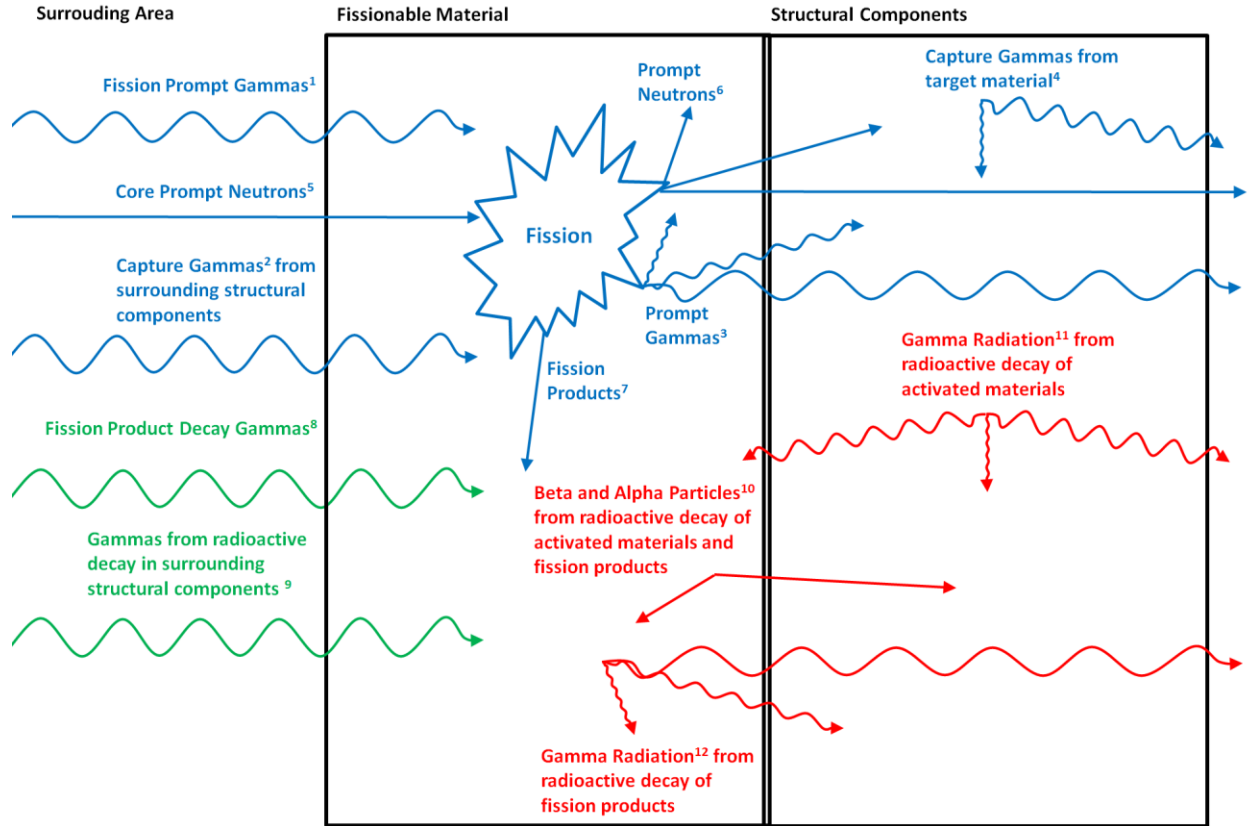


Figure A.6: Target heat generation components.

Table A.1: Sorting of heating components into calculation methodology, transient curve, physical source and particle type.

#	Description	Calculation	Transient	Source	Particle
1	Core Prompt Gammas	F6:p	Prompt	External	Prompt Gammas
2	Structural (n,gamma)			Target Fission	
3	Target Prompt Gammas			Target	Prompt Neutrons
4	Target (n, gamma)			External	
5	Core Prompt Neutrons	F6:n	Prompt	Target Fission	F.P.'s
6	Target Prompt Neutrons			Target Fission	Delayed Photons
7	Fission Fragments	EOC-Core	Core Decay	External	
8	Core Decay Gammas	EOC-LEU	Target Decay	Target Fission	
9	Structural Decay Gammas	EOC-LEU,Ni		Target	Beta+Alpha
10	Target Fission Gammas	ORIGEN-S			
11	Target Activation Gammas				
12	Target Beta+Alpha Decay				

A.4.3 Safety Calculation Methodology

In the following sections the methodology is described behind the safety calculation for the production of ^{99}Mo in an LEU foil rabbit capsule at the HFIR. A concise overview of the methodology for each safety case is shown in Figure A.7, where the codes used (ORIGEN-S, COUPLE, OPUS, & MCNP) as well as controlling scripts written in Python and Fortran are identified. The HFIR BOC model described in section A.4.1 is solved and the resulting fluxes are used to collapse cross sections using COUPLE, which is then used to execute an ORIGEN-S script over 10 to 26 days. The day 26 radionuclide inventory is used in the HFIR EOC model, in addition to beta/alpha/gamma decay from ORIGEN-S, and is run in five separate cases to yield the individual heat generation rate components in the LEU foil and nickel capsule, as well as the EOC eigenvalue for potential reactivity insertion. Using the ORIGEN-S output, OPUS outputs the radionuclide inventories and decay heats for shipping and transient studies.

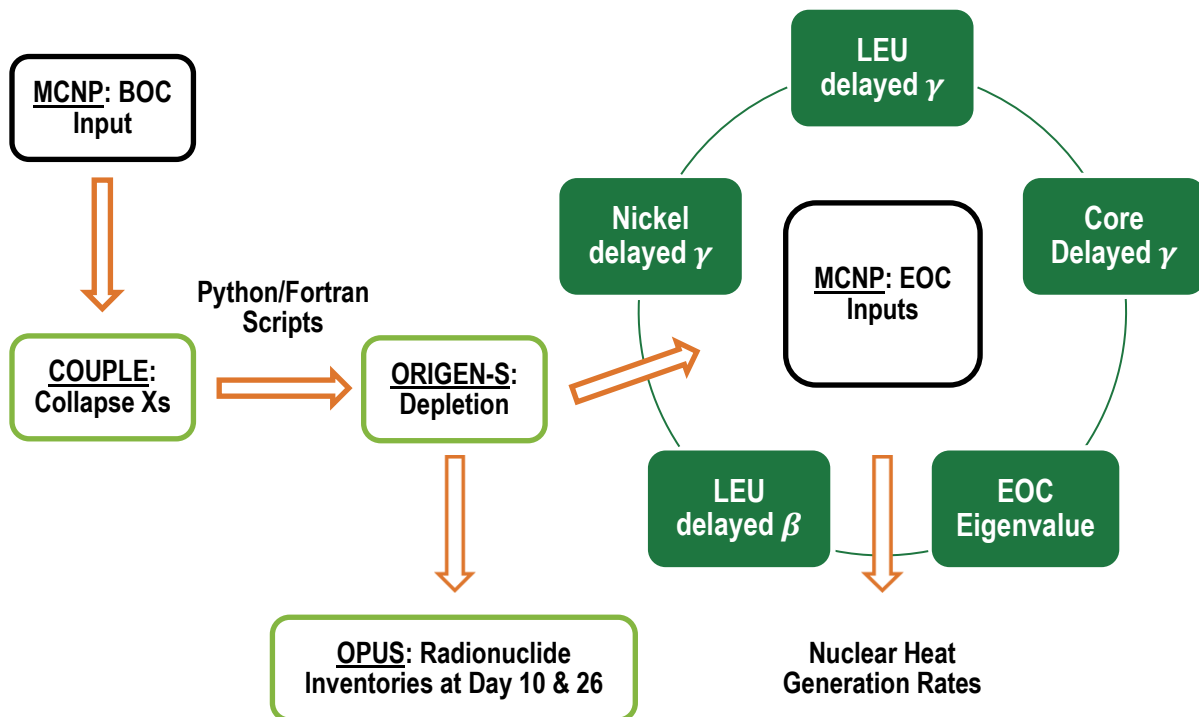


Figure A.7: Overview flow diagram of the ^{99}Mo production safety calculation methodology.

A.4.3.1 Activation, depletion, and decay calculations using SCALE

The SCALE code including the COUPLE, ORIGEN-S, and OPUS modules were used to perform activation, depletion and decay calculations on the LEU foil material and nickel assembly component material including the housing capsule, the inner sleeve, the foil's nickel coating, and the end cap. The COUPLE code, utilizing the BOC 238-group neutron flux spectrum as cross section weighting data, was used to collapse the 238-group AMPX neutron activation cross sections into one-group format as required by ORIGEN-S, unless user-supplied cross sections were made available. A Python script was generated and utilized to execute a Fortran program to extract the fluxes and actinide cross sections from the MCNP output, write an ORIGEN-S calculation, and execute it. COUPLE was provided actinide fission and radiative capture cross sections calculated in the BOC MCNP input, as described later, to account for self-shielding effects in the LEU foil material cross sections. Since self-shielding effects for the nickel components activation calculations are not expected to be significant, the infinite dilute cross sections are utilized. Then, the ORIGEN-S code was used to perform the activation and depletion calculations and OPUS was used to post-process the results into easy to read tables.

For the ORIGEN-S calculations, one 26 day fuel cycle was modeled for limiting safety calculations or a 10 day irradiation for nominal shipping calculations. Both cases utilized a constant total neutron flux to activate the foil and assembly components. Transport calculations were performed on day 0 (BOC) to calculate the materials' spatially dependent neutron fluxes (among other parameters wanting to be studied, but not documented here). The BOC was chosen as it is representative of the neutron flux in the target region over the course of the cycle. The day 26 fluxes were calculated in the EOC transport calculations and it was shown that thermal neutron fluxes were within ± 1 % of the BOC while fast neutron fluxes decreased from their BOC values.

ORIGEN calculations for a 10 day irradiation were performed on the LEU foil and nickel component materials to calculate their post-irradiation radionuclide inventories and decay heats for transportation and PIE requirements. Also, the ORIGEN calculations were utilized to determine the end-of-cycle delayed

photon sources (photons/second) resolved in a 57-energy group structure for each of the LEU foil and nickel component materials. The same energy structure used in HFIR calculation C-HFIR-2012-035 was used in these calculations. Fixed source MCNP photon type calculations were constructed based on these results to determine the photon heating rates due to delayed photons. As described in a later section, the LEU foil's heat generation rates due to the core's and LEU foil's delayed photons can reach up to 47.6 and 2.1 watts/gram, respectively, whereas the nickel components' delayed photons contribute considerably less (less than 0.01 watts/gram).

A.4.3.2 Neutron Flux

The neutron fluxes resolved in a 238-energy group structure were calculated for the irradiation capsule materials with track length estimate of flux tallies (F4:N) in MCNP. The fluxes are resolved into 238-group structures because, in this format, they can be used to define a source weighting spectrum for the SCALE activation calculations, which was described in more detail in A.4.3.1. MCNP tallies are normalized per starting particle (i.e., per source fission neutron), and therefore, the tally results must be multiplied by the fission neutron source strength. The fission neutron source strength is defined by Equation A.1.

$$S_n \left(\text{fission neutrons/second} \right) = \frac{P(W) \times \bar{\nu}(n/\text{fission})}{e(J/\text{MeV}) \times Q(\text{MeV}/\text{fission}) \times k_{eff}}$$

Equation A.1

In Equation A.1, P is the reactor power in watts (85×10^6), $\bar{\nu}$ is the average number of neutrons produced per fission reaction, e is a unit conversion factor (1.60218×10^{-13} J/MeV), Q is the average recoverable energy released per fission reaction, and k_{eff} is the effective multiplication factor. For these calculations, a fixed average recoverable energy of 200.7 MeV per fission was utilized, which is slightly less than the EOC Q -value of 201.3 MeV/fission and slightly greater than the BOC Q -value of 200.2 MeV/fission that were calculated in [128]. The average number of neutrons produced per fission is given

in the MCNP output and typically varies between 2.439 and 2.441 for HFIR calculations. MCNP also outputs the multiplication factor, which should be close to unity for these calculations. Thus, a total fission neutron source of approximately 6.4 to 6.5×10^{18} fission neutrons per second is used for the 85 MW calculations.

A.4.3.3 Neutron and Photon Heating

The most conservative heat generation rates in the LEU foil occur at the end of the cycle, however beginning of cycle heating rates are also calculated and included. Heating due to fission dominates other heating mechanisms in the LEU foil, and the greatest amounts of fissile material (primarily due to ^{239}Pu , ^{235}U , and ^{241}Pu) are present in the foil at the end of the cycle in comparison to any other point in time due to the build-up of ^{239}Pu from the fertile isotope ^{238}U through neutron absorption and subsequent β decays. Thus, the LEU foil's greatest fission rates and heat generation rates occur at EOC. Also, at the end of a cycle, the delayed photon sources from the HFIR fuel and LEU foil are greatest due to the buildup of fission products, resulting in the peak delayed photon source heating at the end of the cycle.

Track length estimate of energy deposition tallies (type 6) were used to calculate heating due to neutrons and fission products (F6:N) and prompt and capture photons (F6:P). The units corresponding to the F6 tally are MeV/g-fission_neutron and the desired units are W/g, so the tally results are multiplied by the total fission neutron source (fission_neutrons/second) and the unit conversion factor (1.60218×10^{-13} W-s/MeV). The source and tally cards used for the EOC MCNP input are provided in Appendix 3.

A.4.3.4 Delayed Photon Heating

Delayed photons are not included in MCNP photon production cross sections, so the delayed photon sources were determined from ORIGEN calculations as previously described. Then, fixed source MCNP calculations in photon mode were run with the BOC and EOC inputs and the photon sources previously described. The delayed photon source heating at the BOC is conservatively determined using the EOC delayed photon source, where the delayed photon source is largest. The photon heating tallies previously

described were used to calculate the photon heating rates due to the delayed photons. Multipliers equal to the product of the total source strength (photons/second) and 1.60218×10^{-13} W-s/MeV were used to convert the photon heating results in terms of MeV/g-source_photon to units of W/g. The EOC core delayed photon source cards generated in C-HFIR-2013-005 [127] were utilized in this set of calculations. The EOC LEU foil delayed photon source cards are shown in Appendix 4 for position 5 and the EOC nickel capsule components delayed photon source cards are shown in Appendix 5 for position 8.

A.4.3.5 *Beta Plus Alpha Heating*

Beta plus alpha heating in the LEU foil material can be calculated with two separate methods. The ORIGEN-S calculations described previously can be used to determine the total heat (watts) due to photons, betas, and alphas and the heat due to photons only. Assuming the betas and alphas are locally deposited, the heat due to betas and alphas only can be calculated by subtracting the heat due to photons only from the total heat. Heating due to beta and alpha radiation is however dominated by the beta radiation.

The second method utilizes the track length estimate of fission energy deposition tally in MCNP (F7:N), which includes the kinetic energy of fission fragments, the kinetic energy of prompt neutrons, and the kinetic energy of prompt photons. Kinetic energy from fission fragments is locally deposited, but the prompt neutrons and photons need to be transported because their energy is deposited throughout the system. The corresponding Q-values for the dominant fissioning nuclides in the LEU foil, namely Pu-239 and Pu-241 at the EOC and U-235 at the BOC, are listed in Table A.2 and were obtained from [129].

The delayed beta Q-values are 6.500 and 5.310 MeV, respectively, for U-235 and Pu-239. If this energy is assumed to be deposited locally in the LEU foil, the heat deposition in the LEU foil due to delayed betas can be approximated by multiplying the result of the F7:N tally (MeV/g-fission_neutron) by the total fission source (fission_neutrons/second), the unit conversion factor of 1.60218×10^{-13} W-s/MeV, and the ratio of Q_{β} to Q_{F7} (Equation A.2, [128]).

Table A.2: Q-values for selected isotopes.

Description	²³⁵ U Q-values (MeV)	²³⁹ Pu Q-values (MeV)	²⁴¹ Pu Q-values (MeV)
Q _f = kinetic energy of the fission fragments	169.130	175.550	175.360
Q _{np} = kinetic energy of the prompt neutrons	4.838	6.128	5.990
Q _{γp} = kinetic energy of the prompt gammas	6.600	6.741	7.640
Q _{F7} = sum of above	180.568	188.419	188.990
Q _β = total energy released by delayed betas	6.500	5.310	6.580
ratio of Q _β to Q _{F7}	3.600%	2.818%	3.482%

$$H_{\beta} = H_{F7} \left(\frac{Q_{\beta}}{Q_{F7}} \right)$$

Equation A.2

The total fission rates for each isotope were taken from the ORIGEN-S depletion calculation and used to find a fission-averaged beta heating ratio at the BOC and EOC. However, the conservatively larger beta heating contribution was generated by the former ORIGEN-based method calculating the difference between the total heat and photon heating in ORIGEN-S. These values, which include the alpha heating, were used for conservatism over those found using the fission deposition method. The ORIGEN-based method was also used to calculate the beta heat generation rates in the nickel capsule assembly components.

A.4.3.6 Actinide Capture and Fission Cross Sections

The radiative capture (MT=102) and fission (FM option -6) reaction rates for 30 important actinides were calculated in the LEU foil, in addition to the total neutron flux, in MCNP for use in the SCALE calculations as previously described. The 30 actinides include those nuclides with recoverable fission energy data in ORIGEN-S (except ²⁴⁵Cm and ²⁴³Pu) and are listed in Table 4.3 below.

The one-group cross sections (barns) were calculated for each actinide as defined by Equation A.3.

$$\overline{\sigma}_x = \frac{\int \sigma_x(E) \phi(E) dE}{\int \phi(E) dE}$$

Equation A.3

In Equation A.3, $\bar{\sigma}$ is the one-group actinide cross section in barns, σ_x is the energy-dependent microscopic cross section for reaction type x in barns, E is energy (in eV), and ϕ is the energy-dependent neutron flux in neutrons/cm²-sec per fission neutron. The total neutron source is applied to both the denominator and numerator and thus cancels itself out. The resulting actinide cross sections are then utilized in the LEU foil's ORIGEN depletion calculations previously described.

A.4.3.7 *Transient Heat Generation*

Three components contribute to the total transient decay heating of the irradiation capsule in this analysis: prompt particle heating, reactor delayed photon heating and target decay heating [130]. The first is due to “prompt” effects; the capsule heating due to reactions from prompt neutrons and photons in the reactor (primarily neutron-induced fission in the LEU foil). This includes all contributions from prompt neutrons and photons produced in the reactor, including those from the irradiation capsule itself. The initial prompt heat generation after reactor scram is determined from MCNP calculations as previously described. This effect is the primary contributor over short time periods (less than 1 second) due to its large value at time zero after reactor shutdown. However, its time-dependent power curve, developed by the HFIR point-kinetics reactivity model [131], falls off rapidly due to the rapid insertion of the safety plates.

The second heating component is “core decay” due to the delayed photons emitted by the reactor fuel and structural materials after shutdown from fission and activation products. The initial heat generation at the start of shutdown is established in the core EOC fixed source MCNP calculation (see Section 4.5.3). The time-dependent power curve of the reactor core's decay is originally described in [132], using both ANSI/ANS 5.1 and ORIGEN2.

The third heating component is the local decay components from the irradiation capsule itself. The radioactive decay of the capsule produces beta (electron or positron), alpha (⁴He), and gamma (photon) particles due to its fission and activation products. All radiation released is conservatively assumed to deposit its energy locally (in the decay material). However, the fixed source calculations transport these

delayed photons and most of the energy is deposited elsewhere in the system. To be conservative, delayed photon heating between the capsule materials (the LEU foil and the nickel assembly components) is counted twice according to the delayed photon EOC fixed source calculations. This additional heating contribution decays according to a conservative decay power fraction which bounds the local decay fraction of the contributing source (the LEU foil or nickel assembly components) as further described in the results.

The total steady-state heat generation rate is used as the initial total heat generation rate at reactor scram. The contributions from the core decay photons and local target decay at time zero are subtracted from this value to determine the initial prompt heat generation rate. Since the local target decay is conservatively overestimated to be locally deposited, this results in a corresponding underestimation of the prompt contribution. However, as the “prompt” power fraction is bounded by the local target decay power fractions this represents a conservative total transient heat generation over all time steps. The time-dependent curves of HFIR prompt and delayed photon heating is that developed for the HFIR RELAP model [58] – documented in Attachment 1 of [133] – and the local target decay is determined by ORIGEN depletion and decay calculations as previously described.

A.4.3.8 Beta particle energy deposition

The beta particle energy spectra resulting from the thermal neutron fission of several fissile isotopes (^{239}Pu , ^{235}U , and ^{241}Pu) is obtained from [135], [136], [137], [138] and confirmed in [139]. The spectra over the energy ranges 1 to 9 MeV are shown in Figure A.8 below.

As can be seen, the spectra are very consistent between the four sets of measurements. However, the energy spectrum of ^{239}Pu was used in this calculation as it is the primary fissioning isotope at the end-of-cycle, where the highest heat generation rates occur. An LEU irradiation capsule surrounded by water was modeled in MCNP for the electron transport mode. The energy deposition in three cells of the irradiation capsule was calculated using the *F8 card (pulse height tally using surface and source weight collections).

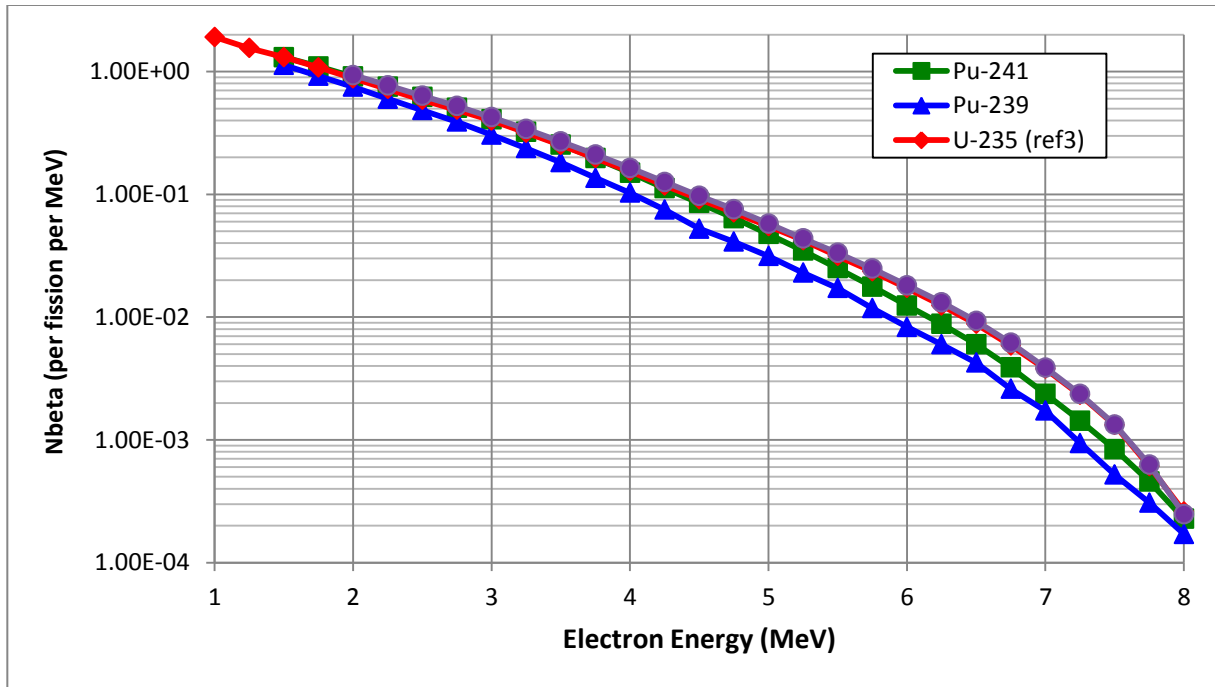


Figure A.8: Fission beta particle energy spectra for fissile isotopes.

A.5 Final Target Design Results

A.5.1 Potential reactivity feedback

To assess the potential impact of the insertion and removal of the two rabbit stack configurations, considered in terms of the rabbit stack reactivity worth, the steady-state effective multiplication factors, k_{eff} , were extracted from the BOC and EOC MCNP outputs, for each rabbit position, and compared to the water-filled hydraulic tube case. For the BOC and EOC cycle inputs, all configurations' (rabbit stack with capsule at position 8, rabbit stack with capsule at position 5, water-filled HT) k_{eff} values compared well to those calculated in ORNL/TM-2010/318, Appendix B. The maximum reactivity worth of the rabbit stack configurations with respect to the water-filled hydraulic tube was calculated to be $+2.38 \pm 0.56$ cents (1 standard deviation provided) at BOC and 1.18 ± 0.56 cents at EOC – both for the irradiation capsule in position 8. A value of 0.0076 was used for β_{eff} .

The water-filled HT introduces a neutron-absorbing material (the hydrogen-rich water) to the HT region, and thus is bounding in terms of a lower reactivity (or a minimal k_{eff} value) compared to the rabbit

stack (which represents a positive reactivity addition by displacing the water with the 6 dummy capsules, 1 HFIR pusher rabbit, and the irradiation capsule). A previous calculation [134] gave a 2.9 cent reactivity worth for 9 dummy rabbits, which is on the order of the calculated results. The placement of the LEU irradiation capsule, which has little fissile material, presents an overall negative reactivity addition in its placement closer to the reactor horizontal midplane (position 5) in the results. The negative reactivity impact of replacing a HFIR dummy rabbit with an LEU irradiation capsule at reactor midplane includes the displacement of relatively neutron-transparent aluminum with better neutron-absorbing materials in the hardened 4N5 nickel (large content of ^{58}Ni) and LEU foil (large content of the naturally abundant isotope ^{238}U). The positive reactivity addition gained by the placement of the capsule, including the fissile content in the LEU foil (primarily ^{235}U) and displacement of the water in the inner annular region of the dummy rabbit, is relatively less significant in the results. Therefore the greatest reactivity worth (and the least neutron-absorbing configuration) is that with the irradiation capsule placed at Position 8. The reactivity worth for the HT rabbit configurations and their associated uncertainties can be seen in Table A.3. Thus the positive reactivity addition associated with the insertion and the subsequent negative reactivity addition associated with the ejection of the hydraulic tube rabbit configurations (containing 1 pusher rabbit, 6 dummy capsules and 1 LEU irradiation capsule) are considerably less than the 9 cent limit.

Table A.3: Multiplication factors and reactivity of rabbit stack configurations.

Case	keff	σ	ρ (¢)*	σ (¢)	$\rho + 2\sigma$ (¢)	$\rho - 2\sigma$ (¢)
BOC water-filled HT	0.99811	0.00003	-	-	-	-
EOC water-filled HT	1.00209	0.00003	-	-	-	-
BOC foil position 8	0.99829	0.00003	2.38	0.56	3.50	1.26
BOC foil position 5	0.99820	0.00003	1.19	0.56	2.31	0.07
EOC foil position 8	1.00218	0.00003	1.18	0.56	2.29	0.07
EOC foil position 5	1.00215	0.00003	0.79	0.56	1.90	-0.33

* with respect to the water filled HT case and calculated as $(k_2 - k_1)/(k_2 * k_1) * (100/\beta_{\text{eff}})$

A.5.2 Thermal Heating & Nuclide Inventory Results

The dominant heating mechanism in the LEU foil is fission-induced heating. The uranium-235 content burns up continuously throughout the cycle while other fissionable isotopes including ^{239}Pu and ^{241}Pu – which have larger fission thermal neutron cross sections and greater energy release per fission than ^{235}U – continuously increase in concentration. Thus, the contribution of fissionable isotopes is greatest at the end of the cycle. The nuclear heat generation rates are broken down into the heating due to fission energy (not included in the total heat generation rates); heating due to neutrons and fission products; heating due to prompt and capture photons; heating due to prompt particle contributions; heating due to delayed betas and alphas; and heating due to the delayed photon sources of the HFIR core, LEU foil and nickel capsule components. The maximum LEU foil heat generation rates were determined to be ~ 500 W/g for position 8 and ~ 800 W/g for position 5. The maximum heat generation rates for the nickel components was determined to be on the order of ~ 25 W/g and ~ 40 W/g for positions 8 and 5.

Per section A.4.3.8, an alternative distribution of the beta energy deposition in the foil may be used in subsequent heat transfer analysis which does not assume all beta particle energy is locally deposited in the foil. The adjusted EOC heat generation rates were approximately 1 to 10 W/g greater in the nickel components and 10 to 40 W/g less in the LEU foil.

The three time-dependent heat generation rate results are expressed as a function of decay time after reactor scram for both irradiation capsule positions (5 and 8). Per section A.4.3.7, the delayed photon heating from the LEU foil to the nickel housing is conservatively added to the initial target decay heating and decays according to the nickel component local decay fraction, which conservatively bounds the decay of the LEU foil. The normalized transient heat generation results for the LEU foil out to 0.6 seconds, 10 minutes, and 10 hours post-shutdown are shown in Figure A.9 through Figure A.11.

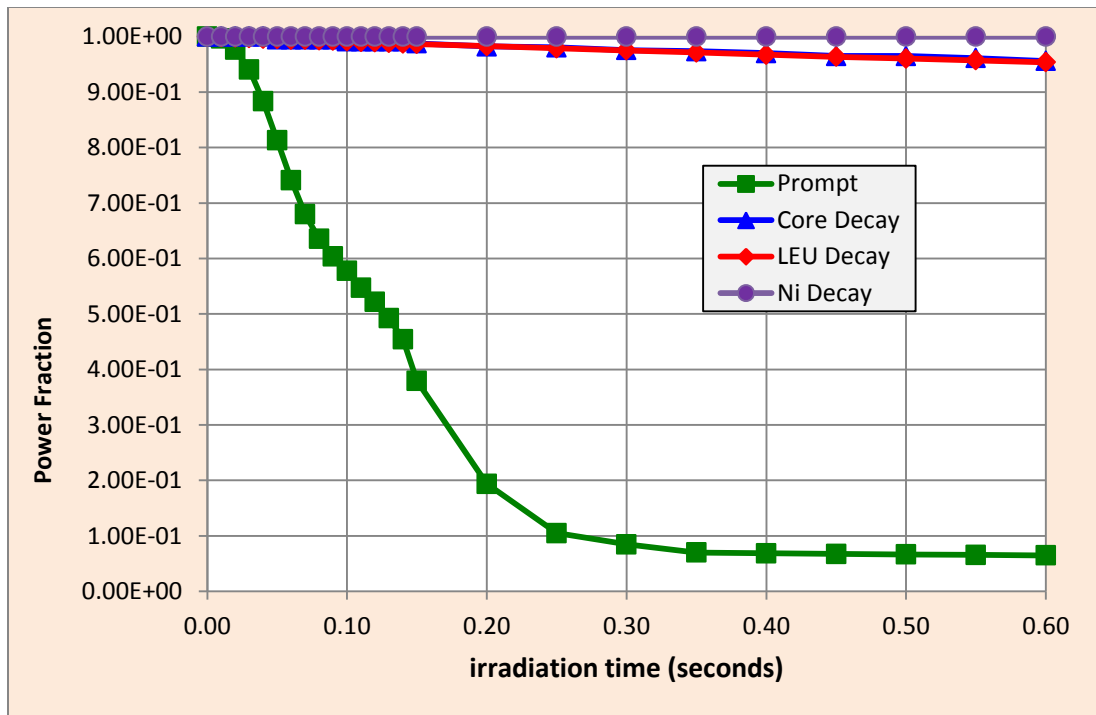


Figure A.9: Transient power fractions for the different heat sources from shutdown to 0.6 seconds decay.

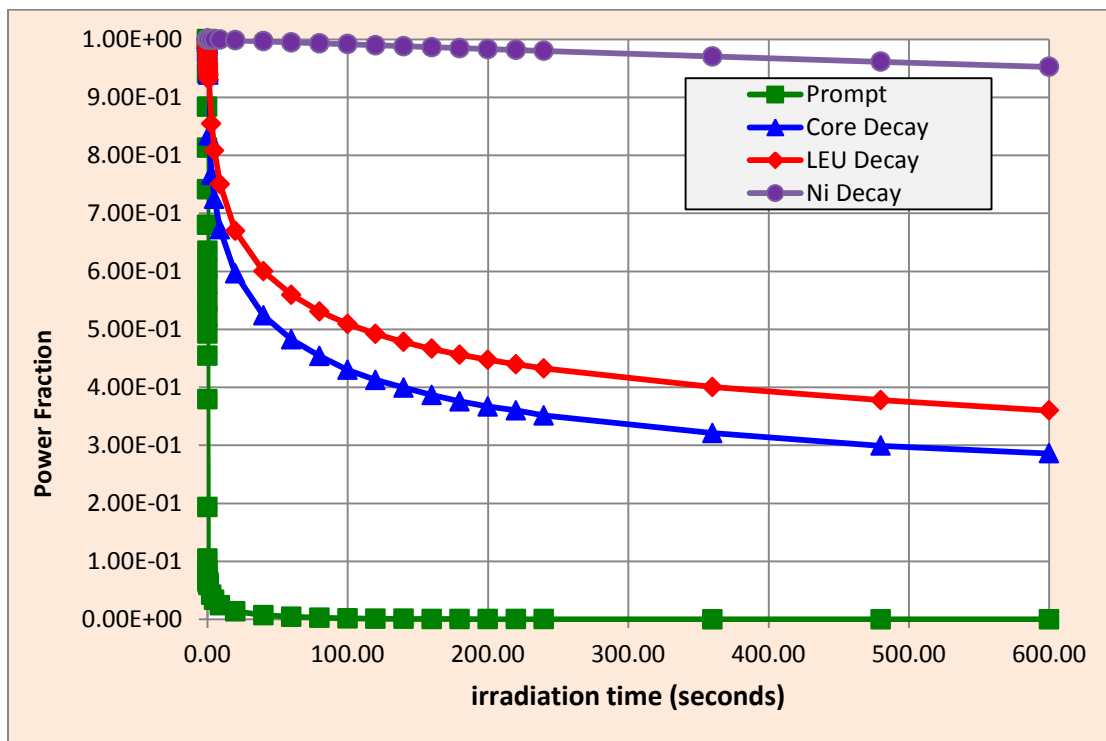


Figure A.10: Transient power fractions for the different heat sources from shutdown to 10 minutes decay.

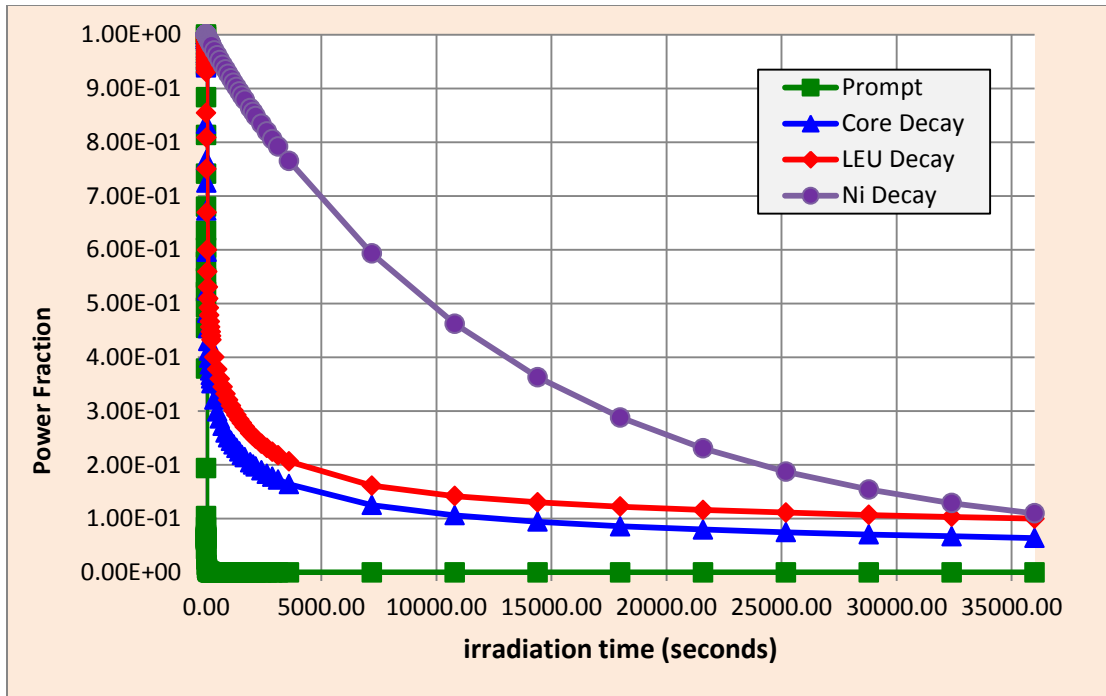


Figure A.11: Transient power fractions for the different heat sources from shutdown to 10 hours decay.

A.5.3 Nuclide Inventory Results

The ongoing and post-irradiation nuclide inventories were calculated and reported for both the LEU foil and nickel components. The fission gas inventory results were used in thermal safety calculations, while radioactivities of isotopes, for example iodine-131, and decay heats were used for assessing post-irradiation shipping safety requirements. As mentioned previously, the initial contribution to heating is dominated by the fission of ^{235}U before the build-in of fissile plutonium isotopes becomes more significant, this is shown for position 5 in terms of the capsule fission rate over a full irradiation cycle in Figure A.12.

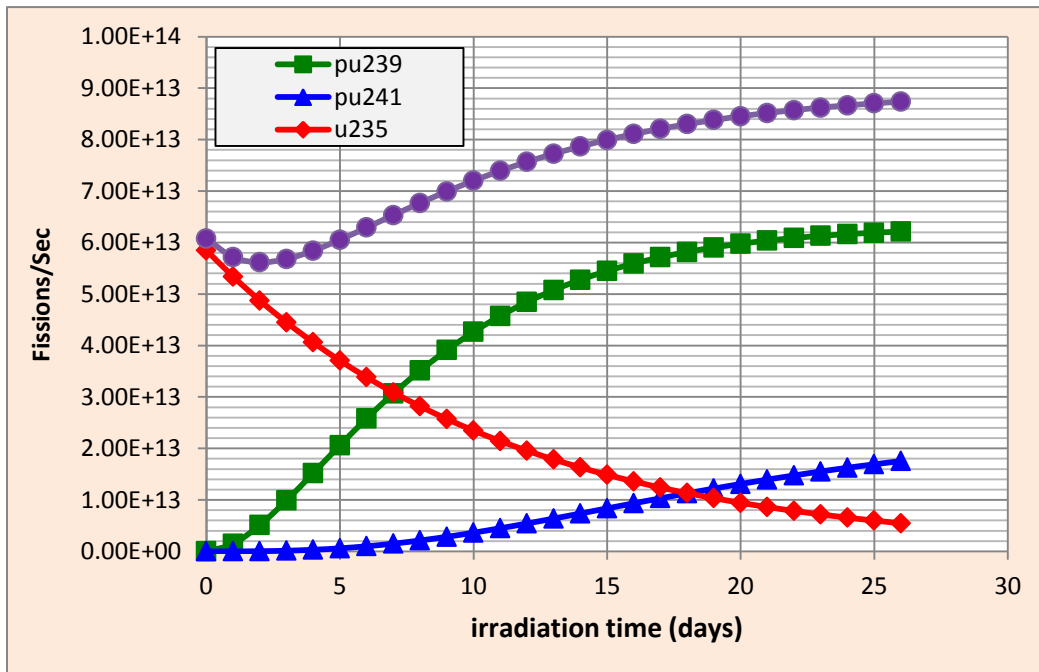


Figure A.12 : Fission contributions over HFIR fuel cycle in LEU foil at position 5 from ORIGEN-S depletion calculation for different fissile isotopes.

A.6 Molybendum-99 Production Summary

A set of neutronics calculations were performed to support the irradiation of a high-density LEU foil and nickel irradiation capsule in the HFIR HT for up to 1 full cycle or 10 days (for shipping requirements). The SCALE code including the COUPLE, ORIGEN-S, and OPUS sequence was used to perform depletion, activation, decay and source term calculations on the LEU foil and nickel capsule assembly components. MCNP, a Monte Carlo-based transport code, was utilized for neutron, photon, and coupled neutron-photon transport calculations to estimate energy-dependent neutron fluxes, actinide cross sections and heat generation rates. Nuclear heat generation rates, nuclide inventories, and decay heating rates for the LEU foil and its associated nickel capsule components. In addition, an alternative heating distribution using electron transport in MCNP was utilized.

VITA

Christopher James (C.J.) Hurt was born on March 29th, 1989 in Richmond, Kentucky, to his parents Mike and Sharnell Hurt from Kentucky and West Virginia, respectively. He is the younger brother of Stanton Hurt, and older brother of Wesley Hurt. C.J. attended Madison Central High School and graduated in May 2007 with honors, 3rd in his class. C.J. subsequently attended the University of Tennessee, where he obtained his Bachelors of Science degree in Nuclear Engineering in May 2011 and began his graduate work at UT in August. During his undergraduate studies, C.J. completed internships at the BlueGrass Chemical Agent-Destruction Pilot Plant in central KY and at the Y-12 National Security Complex in Oak Ridge, Tennessee.

C.J. has continued his Ph.D. graduate work under guidance of his technical mentor, Dr. James D. Freels, and his major professor, Dr. G. Ivan Maldonado. C.J.'s Ph.D. research is in the field of thermo-mechanical analyses and neutron transport in finite element analysis, with additional topics in nuclear reactor physics. While obtaining his Ph. D in Nuclear Engineering at the University of Tennessee, C.J. earned a certificate in nuclear criticality safety. C.J. will graduate with his Ph. D in the fall of 2016. The next step in C.J.'s life will be to pursue a fulltime career in Nuclear Engineering.