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ISOTOPIC AND REACTOR PHYSICS CHARACTERIZATION OF A GAS-COOLED, PEBBLE-BED
MICROREACTOR

BY

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THESIS

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Abstract

Pebble-bed High Temperature Gas-Cooled Reactor (HTGR) designs present a unique modeling challenge. Pebble-beds can have a variety of pebble compositions due to varying levels of burnup and the pebbles are mobile in the core — entering from the top and exiting through the bottom — and may fall in a haphazard arrangement. This work introduces a 20 MWth pebble-bed HTGR reactor design (which will be referred to as Sangamon20) and investigates not only the neutronics of the base model, but the changes to core neutronics after making modifications to the simulation: heterogenizing versus homogenizing the pebble center, imposing a universal symmetry assumption, and changing the arrangement of pebble fuel compositions, all using Serpent and Python. This model of Sangamon20 uses a random dispersal of seven different pebble compositions, each corresponding to a different level of burnup. The heterogenization tests compare k_{eff} , thermal and fast flux profiles, and the neutron lethargy-adjusted energy spectra in the core, reflector, coolant, a random fresh, and a random discharge-burnup pebble. Shuffling and symmetry tests monitor changes to k_{eff} and the outward neutron current at the outer reflector boundary; the latter because it can be used to find the anticipated neutron flux the Reactor Pressure Vessel (RPV) would experience. This informs the level of radiation damage one could expect the RPV to experience each year - which is useful from a design and safety perspective. All of this is in support of the ultimate goal of this project — to establish a baseline source term and to determine what simplifications, if any, can be made in the model without sacrificing accuracy in the results. This is crucial for any future licensing effort, safety analysis, or accident analysis involving this sort of pebble-bed microreactor. Neither the symmetry test nor the shuffling test caused a major difference in either the k_{eff} or the outer-bounds outward neutron current. However, for the heterogenization tests, k_{eff} differed by over 4.0%, and the pebble spectra at certain higher energies disagreed by a factor of 2-4. A complete fuel isotopic composition is accessible at [1], and this thesis discusses select isotopic inventories.

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List of Abbreviations

HTGR	High Temperature Gas-Cooled Reactor
LWR	Light Water Reactor
TRISO	Tri-Structural Isotropic
BISO	Bi-Structural Isotropic
SMR	Small Modular Reactor
HTG-SMR	High Temperature Gas-Cooled Small Modular Reactor
RPV	Reactor Pressure Vessel
SBO	Station Black-Out
ORNL	Oak Ridge national Laboratory
AVR	Arbeitsgemeinschaft Versuchsreaktor
LEU	Low-Enriched Uranium
CSG	Constructive Solid Geometry
ENDF	Evaluated Nuclear Data Format
ACE	A Compact ENDF
MCNP	Monte Carlo N-Particle transport
BEAU	Burnup Equilibrium Analysis Utility
BCT	Body Centered Tetragonal
HCP	Hexagonal Close Packed
INL	Idaho National Laboratory
VSOP	Very Superior Old Programs
PB-FHR	Pebble-Bed Fluoride High Temperature Reactor
FCC	Face Centered Cubic
BCC	Body Centered Cubic
MOL	Middle Of Life
PBMR	Pebble Bed Molten salt Reactor

HTR	High Temperature Reactor
SC	Simple Cubic
EFPD	Effective Full Power Days
NGNP	Next Generation Nuclear Plant
RMC	Reactor Monte Carlo
RSA	Random Sequential Addition
DEM	Discrete Element Method
RUG	Random Universe Geometry
UCO	Uranium Oxycarbide
OTTO	Once Through Then Out
RGB	Red-Green-Blue
VHTRC	Very High Temperature Reactor Critical Assembly
IAEA	International Atomic Energy Agency
CRP	Coordinated Research Project
UAM	Uncertainty Analysis in Modeling
GIF	GEN IV International Forum

Chapter 1

Introduction

1.1 Motivation

The effects of climate change increase in severity every year. From 1980 to present, the global temperature anomaly — defined as the difference between the current average global temperature and the average temperature from 1951 to 1980 — has steadily increased to 1.02°C . One factor contributing to this global climate change is the use of fossil fuels. In relatively recent years, there has been a growing push for energy technologies that do not rely on fossil fuels, such as nuclear power. While nuclear technology is currently in use across the world, many of these reactors are older, and facing closure as their licenses run out. As licenses run out and nuclear power plants are forced to close when there is no replacement reactor, energy companies may be forced to return to fossil fuels to supply the baseline power that nuclear once did. In addition, most of the current global fleet consists of Gen III reactors, which do not feature the passive safety features and advanced designs of Gen IV reactors. There is an international effort to support the development of these reactors, led by the GEN IV International Forum (GIF). GIF identified eight goals the design of Gen IV reactors should fulfill, encompassing improvements to sustainability, economics, safety, and non-proliferation [?].

One such class of Gen IV reactor, the high temperature gas-cooled reactor (HTGR), can have a variety of fuel forms. This work concerns itself with pebble-bed HTGR. Pebble-type fuels consist of a sphere of graphite, approximately the size of a billiard ball, embedded with tri-structural isotropic (TRISO) particles. TRISO-based fuels are popular in Gen IV reactor design because they are a robust fuel form — not prone to cracking and stable to higher temperatures than standard Light Water Reactor (LWR) fuel. This is advantageous to long-term spent fuel safety (though it does make reprocessing much more difficult). Pebble-type fuels in particular can be refueled online, which reduces the need for planned shutdowns. However, HTGRs are typically very large designs, which can be prohibitively costly, or simply unneeded in some use cases.

To avoid this size restriction, another class of reactor was designed - the Small Modular Reactor (SMR). These reactors are smaller than the conventional LWR seen in the USA today. SMRs are often small enough to be shipped in a standard shipping truck or train. Owing to their small size, they are also easier and cheaper to manufacture.

One can deploy an SMR in a variety of new settings, such as isolated towns or work sites, or station many together in one location to fill the role of a single larger reactor. But there exists a class of reactor even smaller than the SMR — the microreactor. Microreactors generally have a capacity of 70 MWth or less and are often deployed in areas only needing a small amount of power, used for research and testing, or used to supply heat for other industrial processes, such as producing hydrogen. Down-sized reactors, such as SMRs or microreactors, have a few inherent safety benefits over their larger cousins, prompting their development. The smaller scale of the reactor pressure vessel (RPV) makes the large active cooling loops of contemporary commercial nuclear reactors unnecessary. For smaller reactors, passive systems relying on natural convection and surface heat transfer remove decay heat after something such as a station black-out (SBO). Under normal operation with station power, supplementary fans and surface coolers can aid heat removal [2].

This work modeled a 200MWth pebble-bed high-temperature gas-cooled SMR based on existing designs. We call this 200MWth reactor the Sangamon200. Sangamon200 is meant to reflect a "classic" Gen IV reactor design. A smaller 20MWth design was created by scaling down the Sangamon200 model. The 20MWth model, hereafter referred to as Sangamon20, is a generic design for use in testing and analysis. This model is simplified to provide a foundation for investigating core neutronics and fuel isotopes without additional features beyond the randomness and heterogeneity of the pebbles inside, which is the focus of this study.

1.2 Objectives

This work briefly describes a 200 MWth pebble-bed HTGR SMR, inspired by concepts from the PBMR [3], [4] and X-Energy [5] reactors, henceforth named Sangamon200. This work established the larger reactor as a baseline for the scaled-down 20 MWth model, Sangamon20 that is the focus of this work.

However, any full-core pebble-bed reactor model will have significant computational load. In order to make running such models less demanding, it is sometimes necessary to make simplifications that are not reflected in a real-world core. A pebble-bed reactor already has multiple layers of heterogeneity - the locations of the TRISO particles in the pebbles are randomly generated as well as the location of the fuel pebbles in the core. Pebble location aside, there are seven fuel compositions also distributed uniformly and randomly throughout the core. Previous work, in contrast, often used a lattice arrangement to set pebble locations. As said before, Sangamon20 uses random pebble dispersal. This means that there are a theoretically infinite number of Sangamon20 designs that *could* exist, with only pebble location changing. This randomness presents a design and licensing challenge — even if one can demonstrate a particular permutation of a given pebble bed reactor is safe, is that model sufficient to prove all variations are? To help answer this question, the shuffling test was performed (see: Methods) to provide

a few variations to compare with the "control" model. Another source of variation in the model is using a symmetry assumption. When a symmetry condition is used, Serpent takes a user-defined fraction of the core (for this thesis, $\frac{1}{6}$) and uses it to represent the entire core. Assuming a symmetry condition may make the core easier to model, but it also introduces error. One can imagine that if this user-defined region happens to have a higher fraction of a particular burnup of pebbles than the rest of the reactor, the results wouldn't accurately reflect the whole-core. To investigate the a series of simulations running the Sangamon20 model while utilizing a radial symmetry condition were analyzed (henceforth called the symmetry test, see section section 3.8, Table ??). This not only shows the impact on this specific design, but also provides insight on the effects such a simplification may have on a more intricate model (where simplification may become a necessity).

1.3 Background

While HTGRs and pebble bed reactors have had a recent resurgence in interest and research, they are, in fact, an older concept. The following subsections describe early HTGR concepts, reactors, and how they contributed to our present knowledge of HTGRs. Even though experimental data collection and analysis is not the goal nor focus of this thesis, the previous empirical data and experience informs modern-day HTGR design and modeling. Additionally, as there have not been many modern-day HTGR designs that have come to fruition — many have been terminated in one form or another before they were built — these early experimental and commercial reactors provide us with valuable insight that may otherwise be inaccessible.

1.3.1 The High Temperature Gas Cooled Reactor: Beginnings and Concepts

HTGRs are a prominent Generation IV reactor design which often uses helium as a coolant, and graphite as a moderator. Their fuel form uses TRISO particles, which consist of a small kernel of fuel, less than half a millimeter across, surrounded by layers of carbon and silicon carbide to protect the fuel kernel and prevent the leakage of radioisotopes. Fuel elements are made by embedding these TRISO particles in graphite. In prismatic HTGRs, the graphite is in the shape of hexagonal columns. In pebble-bed reactors, the graphite is in the shape of six cm diameter spheres. Many of these pebbles enter the core through the top, and slowly move down in a manner similar to grain in silos.

Preliminary concepts for a gas-cooled reactor existed as early as 1942. Farrington Daniels is attributed with establishing the first theoretical designs. Professor Daniel's work with Oak Ridge National Laboratory (ORNL) nailed-down the most basic characteristics of the HTGR. The choice of helium for coolant, graphite for moderator, the direct gas turbine cycle, and the use of uranium or thorium carbides for fuel all came from his work [6].

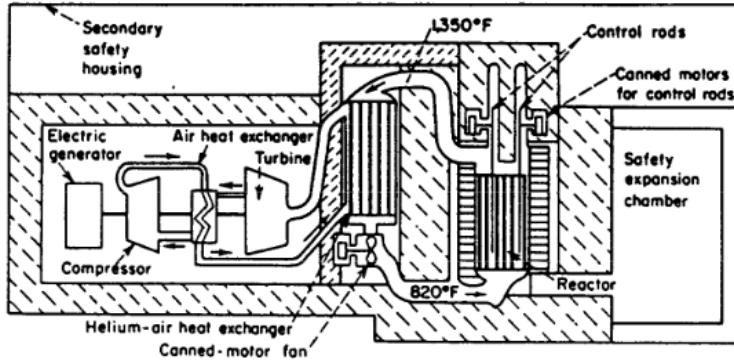


Figure 1.1: Side-View of Daniels et al. (1955) Reactor Concept, from [6]

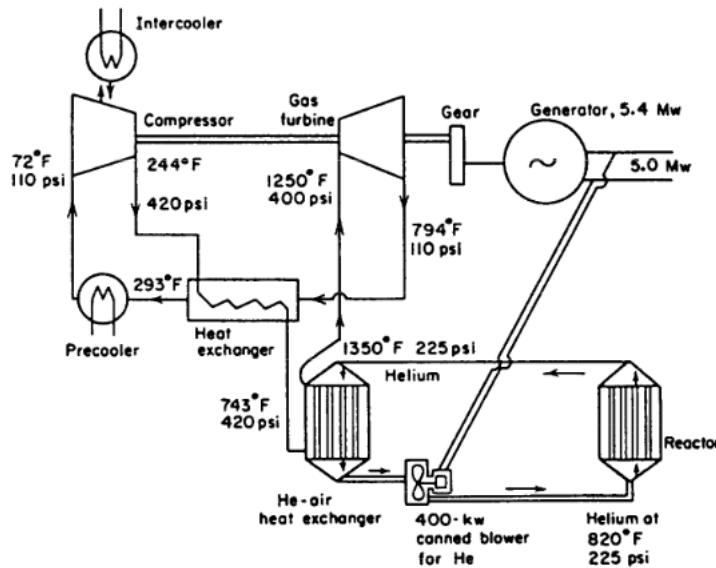


Figure 1.2: Diagram of Coolant Flow in Daniels et al. (1955) Concept, from [6]

Figures 1.1 and 1.2 show the 1955 concept in the design by Daniels et al. A key difference between the Farrington Daniels et al designs and modern HTGRs is the fuel form. While modern designs use TRISO particles embedded in graphite, the Daniels et al design used solid graphite blocks, with channels for both coolant and fuel. Within the fuel channels, fuel loaded in either a pellet or cartridge form, both a mixture of 10% uranium dicarbide and graphite powder. In addition to these fuel channels, the design included an outer ring of graphite reflector in which used thorium to breed ^{233}U . Control rods were of a boron-containing molybdenum. Steel wires that would melt in the case of an accident held more of the same above the core, and would drop the safety rods in case of an accident [6].

1.3.2 Earliest Operational HTGRs

The earliest operational HTGRs came online in the 1960s. These early reactors are discussed in the sections below: Dragon, operating in the UK; Peach Bottom 1, in the US; and the AVR, from Germany. Of these three, only Peach Bottom 1 was a commercial-scale demonstration - the others, Dragon and the AVR, were experimental reactors. Of particular interest is the AVR which is the only pebble-bed reactor of the three. Experiments in the AVR not only provided empirical data on the inner-core temperatures inside the AVR core, but also tested accident response, and observed a "pebble dust" that accumulated in the AVR over its operation — including its activity.

Dragon

The Dragon prismatic HTGR was a test reactor operated in Winfrith, UK, by the Organization for Economic Co-operation and Development from 1964 to 1975, making it the oldest of the reactors discussed in this chapter. It operated with inlet and outlet temperatures of 350 °C and 750 °C, respectively, and at 20MWt [7]. Dragon's main purpose was to test reactor materials, with an emphasis on fuels. It originally used uranium and thorium as fuel but switched to a purely uranium-based fuel with a lower enrichment later in life. The fuel elements themselves were similar in shape to the Daniels et al design: hexagonal prisms with fuel rod channels.

Contrary to the fuel philosophy seen today, Dragon originally allowed fission products released from fuel elements into the circulating helium coolant. The fission products are then purged from the helium. However, Dragon later switched to a coated-particle fuel when it became clear that having such fission product releases were difficult to manage [6].

Peach Bottom 1

Peach Bottom 1 operated from 1966 to 1974, by the Philadelphia Electric Company and was located in Delta, Pennsylvania [7],[8]. It was the first operational HTGR in the US, and the first to produce electric power. It was slightly larger than Dragon, at a nameplate capacity of 115 MWt/40MWe and a slightly lower operating temperature range at 327°C to 700°C inlet to outlet [7]. Like Dragon, Peach Bottom 1 was a prismatic reactor; however, Peach Bottom used coated uranium and thorium carbide particles coated by a single layer of pyrolytic carbon. However, after multiple fuel failures, Peach Bottom upgraded to bistructural isotropic, or BISO, fuels by adding an additional layer of pyrolytic carbon. Peach Bottom would later upgrade the fuel once again by adding a silicon carbide layer, forming TRISO particles [7]. One operational benefit of upgrading to TRISO particles from BISO particles was that the superior fission product retention meant that Peach Bottom 1 could remove the helium purging systems. In addition to the inner fuel region, Peach Bottom, like the Daniels et al design, bred ^{233}U in an outer region using

thorium.

Beyond changing the number and materials for fuel coatings, the experiences in Peach Bottom 1 helped to develop HTGR fuel elements. Operators saw that they could dilute the fuel with graphite moderating material more so than other diluents. This has the advantage of saving fuel material, improving heat transfer, and reducing radiation damage. Additionally, operational experience showed that, in order to prevent the creation and buildup of ^{236}U and ^{237}Np , which are neutron poisons, the ^{235}U and ^{233}U should be kept separate [6]. In the end, however; Peach Bottom 1 closed after the Philadelphia Electric Company determined its size made it no longer economically viable.

AVR

The Arbeitsgemeinschaft Versuchsreaktor (AVR) was an experimental pebble-bed reactor operated in and by the Jülich Research Center (in Jülich, Germany) from 1967 to 1988. It had a capacity of 46 MWt/15MWe, with inlet and outlet temperatures of 275°C and 950°C [7]. The AVR used a combination of uranium and thorium fuels, though it began with bi-structural isotropic (BISO) particles. The core held around 100,000 graphite pebbles, only a third of which had fuel in them.

Despite not being built for experimental purposes, the AVR still housed many experiments that improved our body of knowledge on HTGR technology. During the first few years of its life, the goal of the AVR was to demonstrate that it was a reliable technology — that the reactor could operate safely, that they could control the core power and temperatures, safely shutdown, and remain sub-critical for long periods of time. After this initial period, the AVR shifted focus to allow various experiments including: observing core temperature distributions, accident analysis, and fuel testing. The AVR also shifted from highly enriched to low enriched fuel over time, which caused a variation in fuel pebble compositions, on top of the range of compositions inherent to a multi-pass pebble cycle due to varying burnup.

The AVR also provided data to validate simulations of pebble-bed reactors, and conducted an experiment to better characterize the radial distribution of temperatures in the core [9]. Operators loaded a number of marked pebbles into the core, each housing a series of wires that would melt at a certain temperature, the lowest being 655°C, the highest 1280°C. Those conducting the test tracked pebble location using flow data, and examined them after they were ejected to determine what temperatures the pebbles experienced. Despite the outlet temperature being 950°C, multiple pebbles experienced a temperature greater than or equal to the 1280°C maximum temperature in the melt wires. The results noted that these pebbles went through a zone with a spike in local power density, which could account for the temperature spike [9].

The AVR also demonstrated the inherent safety of HTGR reactors in accident scenarios by purposefully causing

failures of the active cooling system. In the first, the coolant blowers were shutoff, and no shutdown rods inserted, while operating at full power. The operators additionally shut the main circuit valves to prevent natural circulation to regions outside the active core. Overall, the changes to core temperatures were unremarkable. The hottest regions cooled, while the coldest regions warmed up. Additionally, due to negative temperature feedback coefficients, the reactor power immediately declined in response to the transient event. The temperature slowly rose to 2 MW again over 24 hours, leveling out around 300 kW. A further test provided data on loss of coolant and depressurization accidents. As before, the core temperature changes were unremarkable. The upper core region cooled, while the lower, originally cooler core region slowly rose in temperature. The experiment's thermal data helped validate HTGR computer models by providing a real-world benchmark. This meant that the results to aid in the analysis of other HTGRs [9].

Beyond accident safety, the AVR allowed for testing and demonstration of the safety qualities of TRISO and BISO fuel elements; especially relating to high temperature tolerance, and fission product retention. Initial tests used BISO based pebbles, then later transitioned to TRISO, then to low-enriched-uranium (LEU) TRISO pebbles. The TRISO-LEU pebbles had good fission product retention compared with their BISO-based predecessors, based on the activity of samples taken from the circulating helium. Beyond radioisotopes being directly released into the coolant gas, the AVR also showed that in order to accurately characterize the source term of an HTGR pebble bed reactor, one must take the dust from the pebbles into account. Dust from the pebbles bumping and scraping against each other deposited on reactor surfaces in the primary loop. Sixty kg of dust had accumulated by the end of the reactor's life, which averages to 3 kg of dust each year. Measurements of specific activity in the dust showed that the activities of ^{137}Cs , ^{134}Cs , ^{131}I , ^{90}Sr , and ^{60}Co were on the order of $\frac{Bq}{g}$ (see Table 1.1 and Table 1.2). Even though relatively little dust accumulates, the activity of this dust is fairly high, especially compared to the activity of the coolant gas [9]. This dust can become mobile in an accident scenario, potentially being released into the environment, or inhaled.

Isotope	Specific Activity in Primary Coolant Gas [$\frac{Bq}{m^3}$]
Σ Fission noble gas	4.6×10^{08}
3H	3.7×10^{07}
^{14}C	1.9×10^{07}
^{137}Cs	3.0×10^{02}
^{131}I	5.2×10^{02}
^{110m}Ag	4.9×10^{01}
^{90}Sr	2.0×10^{02}
^{60}Co	1.0×10^{01}

Table 1.1: Helium Coolant Specific Activities in the AVR, reproduced from Table 2 in [9] — Results of experiments at the AVR Reactor by H.Gottaut and K.Krüger

Isotope	Specific Activity in Dust [$\frac{Bq}{g}$]
^{137}Cs	2 - 96
^{134}Cs	0.7 - 27
^{131}I	0 - 3
^{110m}Ag	0.1 - 43
^{89}Sr	0.6 - 42
^{90}Sr	19 - 363
^{60}Co	0.2 - 8

Table 1.2: Pebble Dust Specific Activities, reproduced from Table 3 in [9] — Results of experiments at the AVR Reactor by H.Gottaut and K.Krüger

1.3.3 Earliest HTGRs: Conclusion

The three earliest operational HTGRs have been discussed in Sections section 1.3.2, section 1.3.2, and section 1.3.2. Even though Dragon and Peach Bottom 1 are not pebble-bed reactors, they still used TRISO particle fuels, and still provided experience in HTGR operation and management. The AVR, meanwhile, was a pebble-bed reactor, and not only provided general HTGR experience, but also provided pebble-fuel specific data, such as on pebble dust accumulation and activity. The experience from these reactors helped to inform the design of modern HTGRs, especially in regards to providing experimental data to validate computational models against.

Chapter 2

Literature Review

2.1 Computational Modeling and Software

The subsections of section 2.1 below focus on more recent modeling efforts in the pebble bed, HTGR, and SMR/microreactor areas. The first sections provide highlights of some relevant work in specific software, including MCNP and BEAU [10] (see subsection 2.1.2). The later sections discuss an analysis of the effects that the pebble-distribution lattice has on the reactor core as a whole. These will set up the available tools to analyze the reactors summarized in Section section 2.2, which includes a description of the Pebble Bed Molten salt Reactor (PBMR), Next Generation Nuclear Plant (NGNP), Xe-100, and HTR-10 reactors. These descriptions will be supplemented with a discussion of modeling experience or progress achieved by the respective reactor design teams.

2.1.1 Serpent

Serpent uses Constructive Solid Geometry (CSG) to allow user-defined, complex geometries. This includes particles, lattices, and nested components [11]. TRISO particles have locations defined by the three-dimensional coordinates for their centers and their outermost radius. To generate thousands or even millions of particles — Serpent has been tested with up to 60 million of them [11] — Serpent has a built-in particle dispersal routine. The mechanics of the dispersal routine are discussed in greater detail in the Methods Chapter (see chapter 3).

A 2016 study by Friederike Bostelmann et al compared the Very High Temperature Reactor Critical Assembly (VHTRC) [?] benchmark (originally made by the International Atomic Energy Agency (IAEA) Coordinated Research Project (CRP) on Uncertainty Analysis in Modeling (UAM)) to computational models of the VHTRC made in Serpent and SCALE [12]. The VHTRC is a single hexagonal fuel assembly made of graphite, with holes for fuel pins. Normally, a fuel-pin based assembly would not be of interest, however; the VHTRC fuel rods are composed of a graphite in which BISO particles have been uniformly distributed, and so it still has the complexities of particle-based fuels. Friederike et al makes use of two Serpent models — one with a random dispersal and one with a lattice arrangement of BISO particles in the fuel pins. The SCALE model does the same. In general, Serpent had fairly good agreement with the experimental data in criticality calculations (less than 50 pcm), while SCALE 6.1.2 models differed from the

Serpent model by as much as 150 pcm. SCALE 6.2b4, which was in beta at the time, had a disagreement of less than 60 pcm to the Serpent model [12].

2.1.2 MCNP

There has been significant work in the aforementioned Monte Carlo code MCNP to aid HTGR modeling. A 1996 effort developed a new sampling method for particle placement in Monte Carlo to be used in MCNP, which would answer the difficulties of modeling "double heterogeneity" — having two or more types of pebble in a single reactor. Its creators dubbed the version of MCNP that used the sampling algorithm as MCNP-BALL [13]. After testing by performing isotopic inventory and criticality calculations the MCNP-BALL code results were accurate to 0.2% [13].

An additional look into MCNP HTGR simulations examined the ability to create what would normally be a stochastic geometry with a uniform design. Specifically, it used a body-centered-tetragonal (BCT) and hexagonal close pack (HCP) lattice for the TRISO particles. Defining pebble and particle locations in this way is often easier to define in the model, and requires no secondary utility to generate the particle locations randomly. However, this regular arrangement doesn't reflect reality, and can cause pebbles to be cut-off, rather than having their locations conform to the boundaries of the container. For low packing fractions the particles are far enough apart that the differences between two crystal lattice structures are insignificant. In smaller cores, with strong reflectors, the differences between the pebble packing lattices were more significant. Additionally, completely homogenizing the coating of the TRISO particles — blending them with the graphite matrix — lowered k_{eff} by as much as 0.20%. For methods using less dramatic homogenization methods, such as blending the four TRISO coatings into one uniform layer, the computational load decreased (due to the simpler geometry definitions), and the results were marginally (less than 0.05%) different from the 4-coating TRISO particle [14].

2.1.3 BEAU

Beyond steady-state codes such as Serpent, burnup calculation and fuel composition is also of importance. Burnup calculations are required for determining the isotopic composition of fuel, which is a necessity in source-term analysis and determination. Burnup Equilibrium Analysis Utility (BEAU) is a Python-based coupling software that combines either MCNP5 or Serpent with ORIGEN2, using new interface inspired by the MOCUP software named `mocup.py` [10],[?]. `Mocup.py` takes the output files from an MCNP5 or Serpent simulation, and turns them into an object for aiding in depletion simulations. BEAU is for fuel cycle analysis and finding the maximum burnup equilibrium. It was bench-marked against results for a pebble-bed HTGR in INL's PEBBED and VSOP [10]. A lattice of mixed-burnup pebbles (corresponding to passes through the core) was defined according to the benchmark definitions for the core, pebbles, and TRISO particles [10].

BEAU models depletion and multiple burnup states for a continuously refueled pebble bed reactor [10]. It uses the novel multiple burnup state method (MBSM) to do so, which improves on most full-core pebble bed computational methods by including all burnup states for a pebble rather than homogenizing them into a representative average pebble.

Though the benchmark also included a test of a Once Through Then Out (OTTO) fuel cycle. BEAU was found to agree fairly well with PEBBED and VSOP in calculating the equilibrium k_{eff} , burnup, and the isotopic concentrations of uranium and plutonium. However, BEAU consistently under-predicted the isotopic concentrations of ^{244}Am and ^{155}Gd by an order of magnitude [10].

BEAU aided in the design of the Mark-1 pebble bed fluoride high temperature reactor (PB-FHR [10]). The model of the Mark-1 PB-FHR handles pebble locations using a face-centered cubic (FCC) lattice in which all burnup states corresponding to a pass through the core are present in the lattice.

2.1.4 Fuel Modeling

A more general study than the parametric PB-FHR study using BEAU examined the effects of pebble packing on the core neutronics in an HTGR [15]. Rather than model a full core, the study created a unit cell as a reference. The study considers body centered cubic (BCC) and hexagonal close-packed (HCP) lattice unit cells. Instead of using a variety of compositions to represent an equilibrium, middle-of-life (MOL) core, the study used an enrichment of 9.6% — lower than the standard 15% for fresh HTGR pebble-fuel — for all pebbles. For each lattice configuration, tests varied the fuel/moderator (F/M) ratio, and examined the effects on core neutronics and isotopic compositions. The analysis showed no significant difference between BCC and HCP cells. The study determined it would be difficult to select a truly 'optimal' energy spectrum for minimizing the accumulation of particularly harmful fission products. The authors concluded that F/M ratios less than 1/1 favor reducing actinide inventories, while ratios greater than 1/1 can reduce the generation of fission products that would corrode the layers of the TRISO fuel.

Earlier work on HTGRs by General Atomics determined the composition of discharged thorium/uranium prismatic fuel elements. The study assumed fuel recycling to complement the proposed breed/burn fuel cycle. Additionally, the fuel cycle assumes the reactor can start with an initial feed material of 93% ^{235}U , which is currently infeasible (at least in commercial reactors in the United States) [16]. While the Sangamon20 is not a prismatic reactor it helps inform the isotopic compositions of fuel that has reached its end burnup, and provides a comparison.

2.2 Modern HTGRs

The following discusses more recent HTGR designs, which are the inspiration for Sangamon200 and Sangamon20. These modern designs were chosen so that the two Sangamon models more accurately reflect designs that may be deployed in the future.

2.2.1 PBMR

The PBMR is a South African pebble bed HTGR design. While it did not ultimately make it to construction, its design has offered invaluable insight to later HTGR pebble bed designs. The PBMR is heavily based on the German High Temperature Reactor (HTR) design, and has a nameplate thermal power of 400 MW, with inlet-outlet temperatures of 500 °C to 900 °C. It is a modular design, with each unit containing a graphite moderated, helium-cooled-core housed in a steel pressure vessel. In accident scenarios, the PBMR would rely on passive safety features using conduction and convection to provide cooling.

Each core unit would hold around half a million pebbles, which used LEU fueled TRISO particles as the fuel form. These TRISO particles are pressed into a 2.5 [cm] radius graphite sphere, which then has an additional 0.5 [cm] thick layer of graphite pressed around it, to form a 3.0 [cm] radius pebble. The pebbles would undergo a six-pass cycle to reach a target end burnup of 92,000 $\left[\frac{MWd}{tU} \right]$ [3].

As part of the design process, multiple 400 MWth PBMR computational models underwent development and testing. An early version using MCNP5 simplified the fuel by assuming an equilibrium pebble enrichment of 9.6 wt%. It also used a BCC lattice for pebble positions. Its calculated k_{eff} differed from previous MCNP4b results by as much as 1,315 pcm when the model explicitly modeled the bottom cone-shaped regions of the reactor as opposed to a flat surface approximation [17].

An improved design modeled the original VSOP model more closely. A full-core model used a cubic array to map TRISO particles inside the pebbles, while an HCP lattice defined pebble locations [18]. As an improvement on previous iterations, it adds back in the fuel regions from the VSOP model, which tracks pebbles in channels and axial layers to simulate their movement through the core. These layers are modeled in the simplified scheme shown in Fig 2.1.

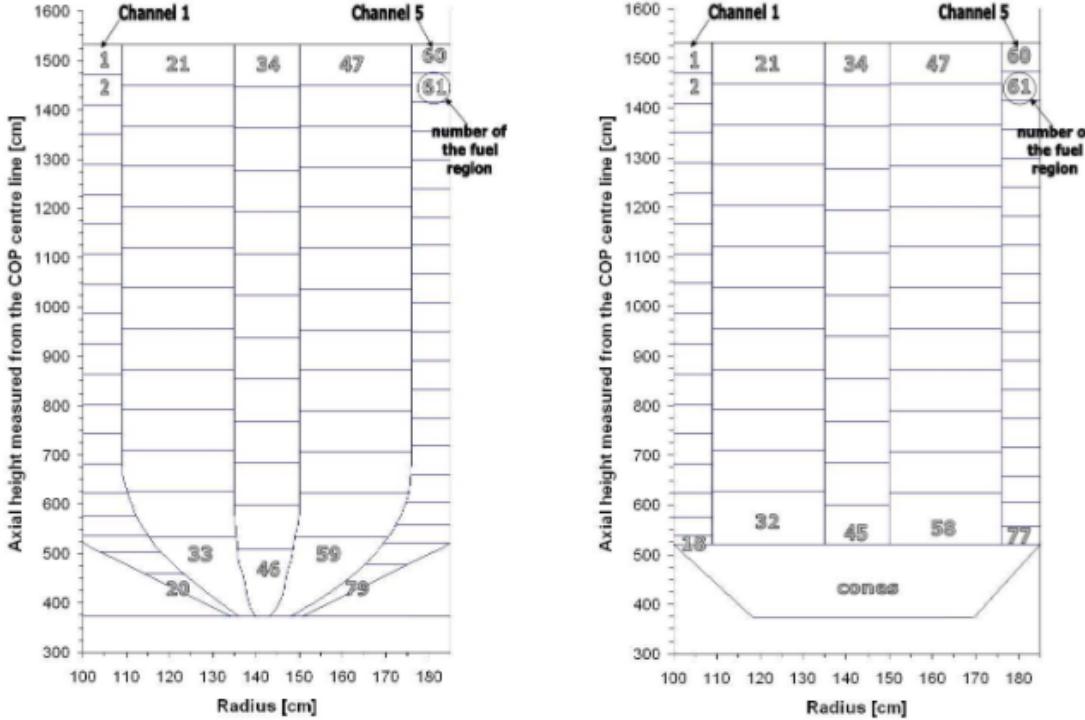


Figure 2.1: Diagram of fuel regions in an equilibrium core model, reproduced from [18]. Axial fuel zones defined for use in MCNP model validation (right) against a previous VSOP model (left).

To simplify, the different pebble burnups in each region are averaged. This study also investigated the effects of different pebble packing arrangements, but rather than use a full-core, a representative one-meter cube of pebbles defines a reference model. The study tested random, HCP, BCC, and FCC at packing fractions of 0.542 and 0.61. It found that across identical packing fractions, differences in reactivity were less than 350 pcm, though k_{eff} values differed by several standard deviations [18].

A separate study by Adem Acr et al performed criticality and burnup calculations using MCNP5 and MONTEBURNS 2.0. It used an averaged 9.6% enriched fuel to simulate an equilibrium core [19]. It tested three pebble arrangements: a BCC lattice with a packing fraction of 0.68, a random arrangement with a packing fraction of 0.61, and a simple cubic (SC) lattice with a packing fraction of 0.52. The initial k_{eff} were similar: 1.2395, 1.2357, and 1.2223, respectively. However, the effective full power days (EFPDs) and end of life burnup required to reach an end k_{eff} of 1.02 differed considerably. BCC required 1200 EFPDs and ended on 99,000 [$\frac{MWD}{T}$], the random arrangement ended on 1000 EFPDs and a burnup of 92,000 [$\frac{MWD}{T}$], and the SC lattice required 800 EFPDs and achieved a final burnup of 86,000 [$\frac{MWD}{T}$] [19]. However, for the random pebble arrangement, which was used to validate the model, the disagreement in excess reactivity was approximately 14%.

Finally, a study using VSOP focused on possible power peaking and the potential consequences of hot spots [20] from fresh pebbles "lumping together". To test this, a mass of fresh pebbles were purposefully introduced in the

fuel region corresponding to the peak power. Even for a very large cluster of fresh pebbles, maximum fuel power only increased by 16%. However, the volumetric power density increased to $18.66 \left[\frac{MW}{m^3} \right]$ from $11.32 \left[\frac{MW}{m^3} \right]$ [20]. The authors noted that this scenario is highly unlikely — the region of highest power is three meters into the core, by which point fresh pebbles would've undergone fission and would have some fission products. This is in addition to the already accidental loading of over one thousand fresh pebbles at once.

2.2.2 Next Generation Nuclear Plant (NGNP)

Like the PBMR, the NGNP did not make it to construction though it provides many insights to our design of HTGRs. The NGNP project downselected its design choices to two reactors — a prismatic HTGR and a pebble-bed HTGR. While the NGNP project eventually opted for the Areva prismatic HTGR design [21] due to reasons related to pebble costs, studies noted that, technologically speaking, there was no inherent advantage or disadvantage between the two technologies [22]. Another project supporting the NGNP was a whole-core depletion model that used a once through fuel cycle, and assumed an average burnup of $100\text{-}150 \left[\frac{GWd}{t} \right]$ after an 18 to 24 month residence time in the core [23]. Much of the work from this study is applicable only to prismatic designs, such as the effects of the number of batches cycling, and fuel shuffling on core neutronics [23].

2.2.3 X-100

Based on experience from the PBMR project, the X-energy Xe-100 is a 200 MWt HTGR pebble-bed SMR. It is similar in design to all of its predecessors, featuring LEU TRISO particle fuel in $3.0 \left[cm \right]$ radius pebbles. While the Xe-100, or a similar design from X-energy, is not in operation as of this publication, the project is still ongoing. It is this reactor that the micro-reactor described in this thesis is most heavily influenced by as it is an active reactor concept that builds on the experience gained from the PBMR project.

The Xe-100 uses approximately 220,000 pebbles in a six-pass cycle, and TRISO particles using Uranium Oxycarbide (UCO) — identical to the ones intended for the PBMR [5]. However, while the number of passes is unchanged, the target end burnup for the pebbles is higher, at $160,000 \left[\frac{MWd}{tU} \right]$ [24]. While the Xe-100 hasn't been built yet, there have been studies conducted by ORNL providing data on the production and material properties of the UCO-based fuel particles [25] and pebbles utilizing them, which the Sangamon20 and Sangamon200 models reference for fuel material data such as density.

2.2.4 HTR-10

The HTR-10 is a 10 MW, HTGR design. Multiple studies exist examining the effects of pebble and TRISO arrangement on the HTR model. These studies primarily work with the Reactor Monte Carlo (RMC) or MCNP5 programs. A base

benchmark study created the HTR-10 in MCNP. Pebbles contained 8335 TRISO particles on average, dispersed in a cubic lattice. Pebbles, meanwhile, are in a BCC arrangement, such that F/M ratios and void fractions stay constant [26].

A later study used RMC to study the explicit modeling of the random nature of both the pebbles and particles in the core, a 'double heterogeneity' [27]. The Random Sequential Addition (RSA) method was used to distribute the TRISO particles within the pebbles (the packing fraction was less than 30%, the maximum RSA can achieve). The Discrete Element Method (DEM) dispersed pebbles. To simplify the model, it assumed that all pebbles have identical TRISO dispersal patterns. Testing showed this caused little (σ less than 0.00014) error between this simplification and a model using different TRISO arrangements in each pebble. The RMC model had good agreement with VSOP HTR-10 simulations [27].

Other work with the HTR-10 introduces a new method of explicit random particle dispersion for use in RMC, called the Random Universe Geometry method (RUG). RUG improves on RSA by allowing a higher particle packing fraction, and on the DEM by being faster and simpler to implement [28]. Whenever a particle enters a cell that is stochastic, the algorithm randomly samples from a list of possible materials, and determines the contents of the cell mid-transport. The RUG method has good agreement with preliminary testing using HTR-10 benchmarks [28].

2.2.5 Modern HTGRs: Conclusion

While the PBMR and Xe-100 are the most closely related to the Sangamon20 and Sangamon200 models, the HTR-10 is a helpful point of reference, as it's closest in size to Sangamon20. Beyond the reactor parameters, the work investigating the effects of pebble and particle arrangement helped to direct the shuffling and sensitivity tests.

Chapter 3

Methodology

This chapter introduces the Sangamon reactors: the Sangamon200, and a scaled-down version, the Sangamon20; inspired by the PBMR [3], [4] and Xe-100 [29], [5]. Both Sangamon200 and Sangamon20 are UCO-pebble fueled, helium cooled reactors. All simulations used Serpent version 2 [30] with postprocessing and analysis performed using Python [31] and the Python libraries numpy [32] and PyNE [33].

3.1 Modeling Particle Dispersal

Often in HTGR modeling, a uniform lattice is used to approximate the locations of TRISO particles and fuel pebbles. However, this doesn't reflect real life — pebbles are not perfectly stacked in the core. On top of this, models utilizing lattices often cut-off portions of pebbles at the boundaries that don't perfectly fit. Instead, the Sangamon200 and Sangamon20 use a random placement of pebbles. This random dispersal is not only truer to a real pebble-bed, but conforms pebble locations to the boundaries of the core.

In order to determine the locations of random TRISO particles and pebbles, the Serpent particle dispersal routine was leveraged. It takes the number of particles, defined by the user, or η_{pf} , the packing fraction (the total volume of particles divided by the volume of that space). The dispersal routine has the user define the particle radius, and the size and shape of the volume housing the particles. The routine first randomly determines a single point for each particle contained in the volume. Then, the routine uses the 'growth factor' and 'shake factor' - both described as fractions of the particle radius, and iterates. During each iteration, the size of the point's radius increases by the growth factor. Additionally, the center will move in a random direction a distance equal to the shake factor. If the particle growth causes the particle to overlap with another particle or leave the volume, it doesn't grow that cycle. Similarly, if the center's movement causes overlap or the particle to leave the containing volume, it doesn't move. The dispersal routine iterates until all particles are to their full size, contained in the volume, and not overlapping with any other particles. The routine generates an output file, in which each line gives the location of a particle center (in x,y,z coordinates), a particle radius, and the name of the particle type, to associate it with the "pbcd" (short for pebble bed) card (see the input syntax manual from [30]) later.

3.2 Run Parameters and Conditions

All Serpent 2 simulations and post-processing were run on an Ubuntu 18.04 machine using Python version 3.8.5, numpy version 1.19.2, and PyNe version 0.7.1. Cross-section data uses the JEFF 3.1.2 data libraries. Below, Table 3.1 gives the Monte Carlo run parameters for each Serpent model.

Table 3.1: Relevant Monte Carlo Parameters for Single Pebble and Sangamon Reactor Simulations

Parameter	Single Pebble	Sangamon200	Sangamon20
Active Cycles	500	150	100
Inactive Cycles	250	50	50
Neutron Population	20000	70000	50000

All input files are available on github at [34].

3.3 Burnup and Depletion Methodology

In order to determine isotopic compositions in the pebbles, a Serpent burnup simulation of a single pebble ran in burnup steps of 180, 360, 540, 720, 900, and 1080 days — to represent a number of six-month passes. The single pebbles are the only simulations that utilize individually defined TRISO particles by default. Each pebble has an inner region containing the TRISO particles embedded in graphite, and an outer region consisting only of graphite as illustrated by Figure 3.1. Each region homogenized by volume fraction using the "mix" card (see [30]) in Serpent. The material properties of fresh UCO are pulled from [25] and [35]. Material properties for TRISO particle layers are from [36], [37], [38], and [39]. The graphite reflector properties are assumed to be the same as the buffer layer in TRISO particles.

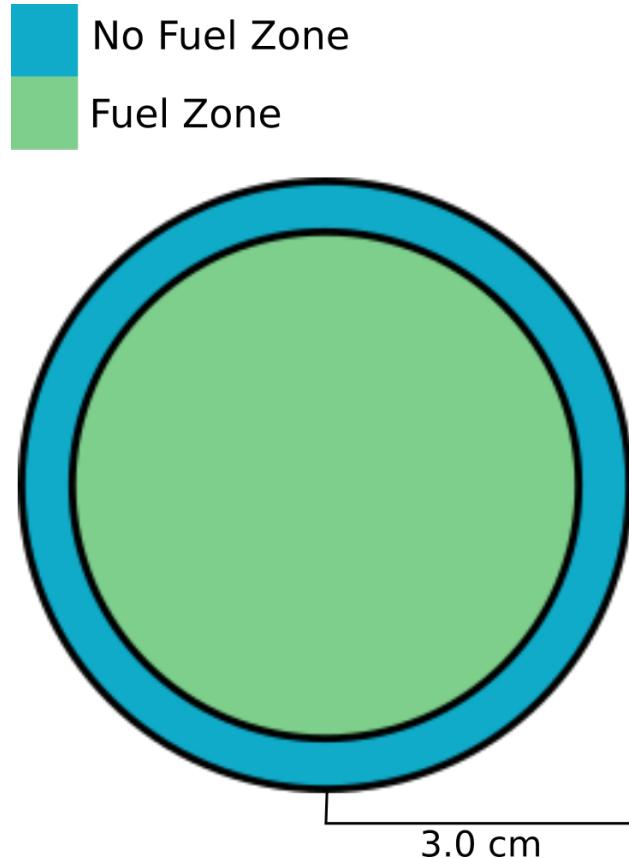


Figure 3.1: Pebble Zones

Table 3.2: Pebble Parameters

Parameter	Value
Fueled-Center Radius [cm]	2.5
Graphite Outer Shell Thickness [cm]	0.5
Total Radius [cm]	3.0
TRISO Particles per Pebble	18,000

Above, Figure 3.1 shows the fueled vs non-fueled regions of the pebbles, while Table 3.2 gives the full measurements of the pebbles. For homogenized pebbles, the fuel region is the homogenized center consisting of dispersed TRISO particle material blended with graphite, while the non-fueled region is pure graphite. In heterogenized models, the fueled region marks the part of the pebble where TRISO particles are located inside a graphite matrix, and the non-fuel region is the area of pure graphite that surrounds it. Below, Figure 3.2 and Table 3.3 give detailed measurements on the size of a TRISO particle and its layers, and gives a visual reference. Figures 3.2 and 3.1 are both to scale.

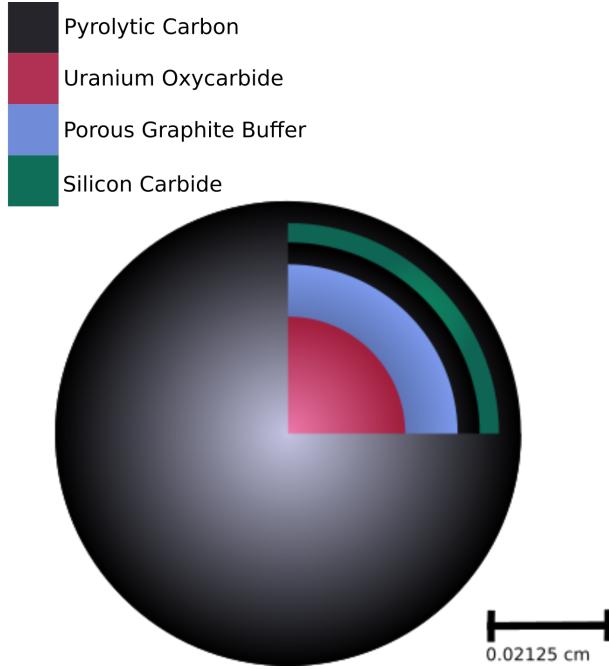


Figure 3.2: TRISO Particle Layers

Table 3.3: Particle Parameters

Parameter	Value [cm]
Uranium Oxycarbide Kernel Radius	0.02125
Graphite Layer Thickness	0.03075
Inner Pyrolytic Carbon Layer Thickness	0.03475
Silicon Carbide Layer Thickness	0.03825
Outer Pyrolytic Carbon Layer Thickness	0.04225

3.4 Fuel Composition

The residence time of a pebble in the active core determines its isotopic composition. We chose to model seven possible pebble compositions exist, one for each of the six 6-month passes, plus an additional composition for fresh pebbles. The seven pebble compositions are equally and randomly distributed in the core.

The design approximates the exact isotopic composition by running a burnup calculation using Serpent for a single pebble in a cube with a reflective boundary condition to create an infinite lattice. The void is filled with helium of the same material properties as in the full core models. Just as with the location of the pebbles in the full core, the Serpent particle dispersal routine generated the TRISO particle locations.

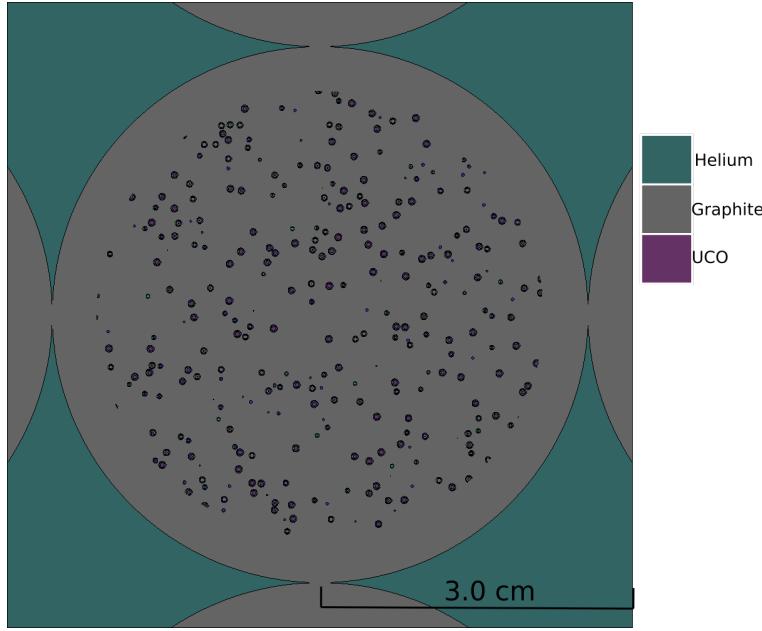


Figure 3.3: Geometry of the Single-Pebble Burnup Calculation for Sangamon20

Figure 3.3 shows the cross-section of the pebble the depletion model is based upon. Once the depletion simulation determines the isotopic compositions for all six burnup states, the model homogenizes the pebbles by volume, to improve performance. The volume of a TRISO particle, and more specifically, a UCO kernel, is constant. The effects of homogenization were explored in the heterogenization tests, which we described in section 3.7.

3.5 Sangamon200

Sangamon200 is a 200 MWth helium cooled reactor, with parameters as defined in Table 3.4. Though the model does use some parameters from pre-established designs, it is a simplification to not only reduce computational load, but to create a generic HTGR pebble-bed whose analysis can more broadly apply to pebble-based HTGRs of similar size. The top and bottom of the reactor core are a flat surface, to create a cylindrical shape. The graphite reflector surrounds it with no barriers between the reflector and active core region. These are the only simulated parts of the reactor - there are no control rods included. In addition, the graphite reflector is a solid cylindrical shell, a container for the pebbles.

While Sangamon200 is not the focus of this assessment, some parameters determined aided in Sangamon20's design. A surface detector placed in the reflector, just inside the outer bound of the reflector, shown in Figure 3.4, tracks the outward neutron current. When determining the appropriate reflector thickness in Sangamon20, this current is used as an upper boundary and reference point — that is, the graphite reflector must not only be sufficient to keep the reactor critical, but must also keep the outward surface current less than or equal to Sangamon20's to

Table 3.4: Geometric and Internal Core Parameters in the Sangamon Reactors

Parameter	Sangamon200 [5], [29]	Sangamon20
Thermal Power [MW]	200	20
Average Core Temperature [K]	800	800
Enrichment [wt%]	15.5%	19.75%
Average Core Pressure [MPa]	5.9	5.9
Outer Core Radius [cm]	216	165
Outer Core Height [cm]	1150	330
Reflector Thickness [cm]	92	75
Number of Pebbles	220,000	23,000

protect the RPV.

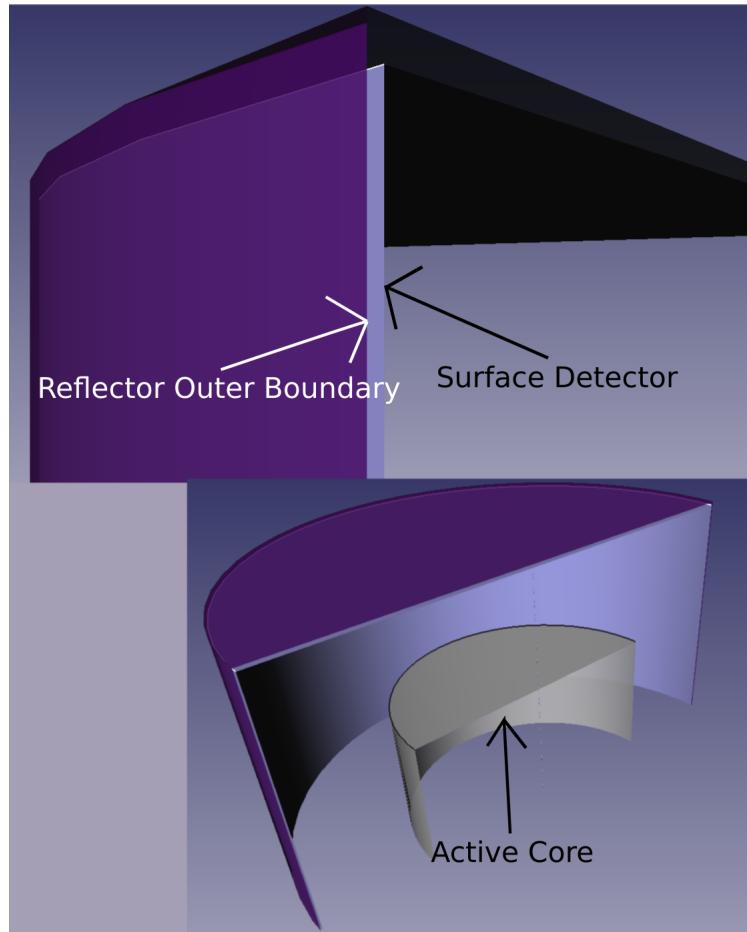


Figure 3.4: Detector Placement Inside Reflector in Sangamon200 and Sangamon20

In Figure 3.4, the graphite reflector outer boundary (dark purple) is shown, with the surface detector shell shown inside of it (light purple). The active core region, which contains the fuel pebbles, is in grey. The detector is centered on the same point as the reactor as a whole. Its height is 2 [cm] less than that of the reflector (e.g., the top of the detector is one [cm] below the top of the reflector) and the radius is one [cm] less than that of the reflector. This

detector measures the outward neutron current in $\left[\frac{\text{neutrons}}{\text{s}} \right]$. To arrive at the unit of $\left[\frac{\#}{\text{cm}^2 \text{s}} \right]$ most are familiar with, we divide by the detector's surface area thusly:

$$J^+ = \frac{J_s^+}{S_d} \quad (3.1)$$

where

$$\begin{aligned} J^+ &= \text{outward neutron current } \left[\frac{\#}{\text{cm}^2 \text{s}} \right] \\ J_s^+ &= \text{surface unadjusted outward neutron current } \left[\frac{\#}{\text{s}} \right] \\ S_d &= \text{detector surface area } [\text{cm}^2] \end{aligned}$$

After accounting for the surface area, the outward current at the detector is $7.351 \times 10^{11} \left[\frac{n}{\text{cm}^2 \text{s}} \right]$.

3.6 Sangamon20

Sangamon20 is a 20 MWth helium-cooled pebble bed reactor, fueled with 19.75% enriched uranium oxycarbide. While the thermal power of Sangamon20 is 10% that of Sangamon200, it isn't sufficient to simply scale Sangamon200's dimensions down to 10% of their original values, as that wouldn't have the correct volume for the required pebbles, and the neutronics — such as leakage — would be inconsistent. An inner core volume that is 10% Sangamon200's should be a good approximation, but in order to be certain that this volume would hold the mass of fuel needed, a simple calculation was carried out, which is detailed in subsection 3.6.1.

3.6.1 Inner Core Volume Determination

The first assumption made in the scale-down is that Sangamon200 and Sangamon20 have the same specific power, or $\left[\frac{\text{kW}}{\text{g UCO}} \right]$.

To calculate the mass of fuel in Sangamon200:

$$M_{f,200} = \frac{4}{3} \pi r_u^3 \rho_u n_T n_{p,200} \quad (3.2)$$

where

$$M_{f,200} = \text{mass of fuel in Sangamon200 [g]}$$

r_u = the radius of the UCO kernel inside a TRISO particle [cm]

ρ_u = the density of UCO in [$\frac{g}{cc}$]

n_T = number of TRISO particles in one pebble

n_p = number of pebbles in Sangamon200

Using the parameters from Table 3.4, the power density of Sangamon200 and Sangamon20 is 0.11 [$\frac{kW}{g}$]. With a power capacity of 20 MWth, one can calculate the total mass of UCO in Sangamon20 as

$$M_{f,20} = \frac{P}{\rho_p} = 181818.18 \text{ [g]} \quad (3.3)$$

where

$$M_{f,20} = \text{total mass of UCO in Sangamon20 [g]}$$

P = Thermal power of Sangamon20 [kW]

ρ_p = Sangamon20's power density [$\frac{kW}{g}$]

Equation 3.2 calculates the total mass of fuel in the Sangamon200 reactor by first calculating the mass of UCO in a single pebble using the density of UCO and the total volume of UCO kernels in a single pebble. This value is then multiplied by the number of pebbles in Sangamon 200 (see Table 3.4). The total mass of fuel in the reactor divided by the mass of fuel in a single pebble gives the number of pebbles in the reactor, as follows:

$$n_{p,20} = \frac{M_{f,20}}{\frac{4}{3}r_u^3 n_T \rho_u} \quad (3.4)$$

where

$n_{p,20}$ = number of pebbles in Sangamon20 [-]

$M_{f,20}$ = total mass of UCO in Sangamon20 [g]

r_u = radius of a UCO kernel [cm]

n_T = number of TRISO particles in a single pebble [-]

ρ_u = density of UCO [$\frac{g}{cm^3}$]

Rounding up - there can only be complete pebbles - we arrive at the number of pebbles for the Sangamon20 as shown in Table 3.4.

Knowing the number of pebbles is insufficient - the exact dimensions of the active core region are still undefined. To determine the volume of this space, the formula uses concept of the packing fraction. The packing of even uniform objects in a 3-dimensional space is a complicated problem [40]. Assuming the pebble behavior is random loose packing [40] - the pebbles have unsystematically fallen into the core and the core is unshaken - the packing fraction in the range of 0.56 to 0.60 [40]. Using the definitions above, the active core volume is

$$V_{c,20} = \frac{n_{p,20} \frac{4}{3} \pi r_p^3}{\eta_{pf}} \quad (3.5)$$

where

$V_{c,20}$ = volume of the active core in Sangamon20 [cm^3]

$n_{p,20}$ = number of pebbles in Sangamon20 [-]

r_p = radius of a pebble [cm]

η_{pf} = packing fraction [-]

Using the formula for the volume of a cylinder, one can plot possible sets of $r_{c,20}$ and $h_{c,20}$ that satisfy the volume requirement.

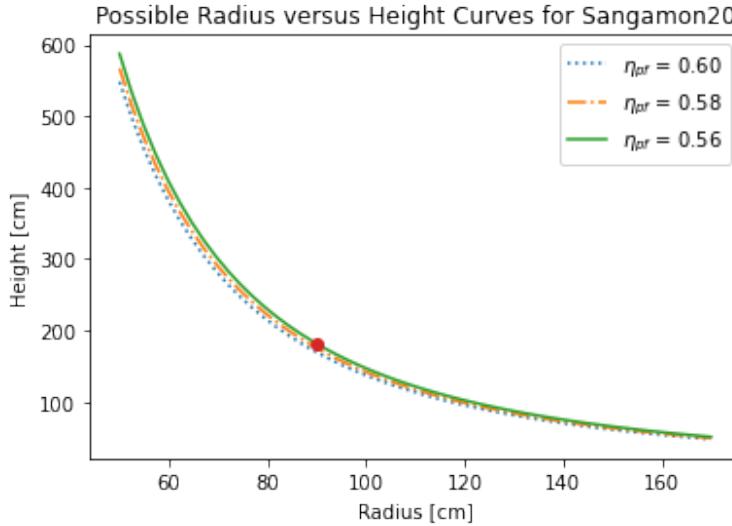


Figure 3.5: Curve of possible height and radii that satisfy the volume requirements imposed by packing fraction(s) η_{pf}

The most critical configurations for a cylinder are either a *square* shape, in which the height is equal to the diameter, or a *flat* shape in which diameter is significantly greater than height. As most designs use a height that is greater than or equal to the diameter, Sangamon20 is a square cylinder. The point indicated in 3.5 shows the radius and height selected for Sangamon20 - a radius of 90 [cm], and a height of 180 [cm].

3.6.2 Graphite Reflector Thickness Determination

The reflector must be sufficiently thick to keep the reactor critical, and protect the pressure vessel from radiation damage. To ensure this, we imposed a condition that the outward current in Sangamon20 must be less than or equal to the outward current in Sangamon200 at the outer reflector boundary. The detector layout in Sangamon20 is identical to Figure 3.4.

3.7 Heterogenization Tests

As described above, the pebbles use the approximation of a homogenized 'fueled-center', to reduce computational load. However, a few tests performed undid this change, explicitly defining all TRISO particles in the pebbles, as they are in the single-pebble (infinite lattice) depletion models which generated the equilibrium fuel composition. These so-called heterogenization tests compared the 2-group fast and thermal fluxes in the radial and axial direction. In addition, they compared the lethargy-adjusted neutron energy spectrum using a 315-group energy structure. Beyond showing the full curves for each of these values for comparison, the relative difference is provided graphically

for each. Other than the choice to explicitly model the TRISO particles, the heterogenized model is identical to the Sangamon20 homogenized-pebble model.

3.8 Reactor Sensitivity to Pebble Locations and Symmetry

By the nature of random pebble dispersal, there are a theoretically infinite number of perturbations to the Sangamon reactor models that are no different sans slight variations in pebble locations. It is also entirely possible to have bands in the reactor such that multiple pebbles of same (or similar) burnup form lines or pockets. In the interest of better characterizing the neutronics of this reactor model, a test explored various pebble composition locations. The *shuffling* test maintained the pebble locations, but changed what composition the individual pebbles were (for results, see subsection 4.4.2). The second analyzed the effects of utilizing a symmetry simplification, in order to improve computational speed (see subsection 4.4.1) where $\frac{1}{6}$ of the core is modeled with a periodic boundary condition (neutrons exiting one side of the symmetry slice enter the other at the same height and trajectory). The slice used to simplify changed in each test, shown in Figure 3.6. In each test, all other parameters remain the same.

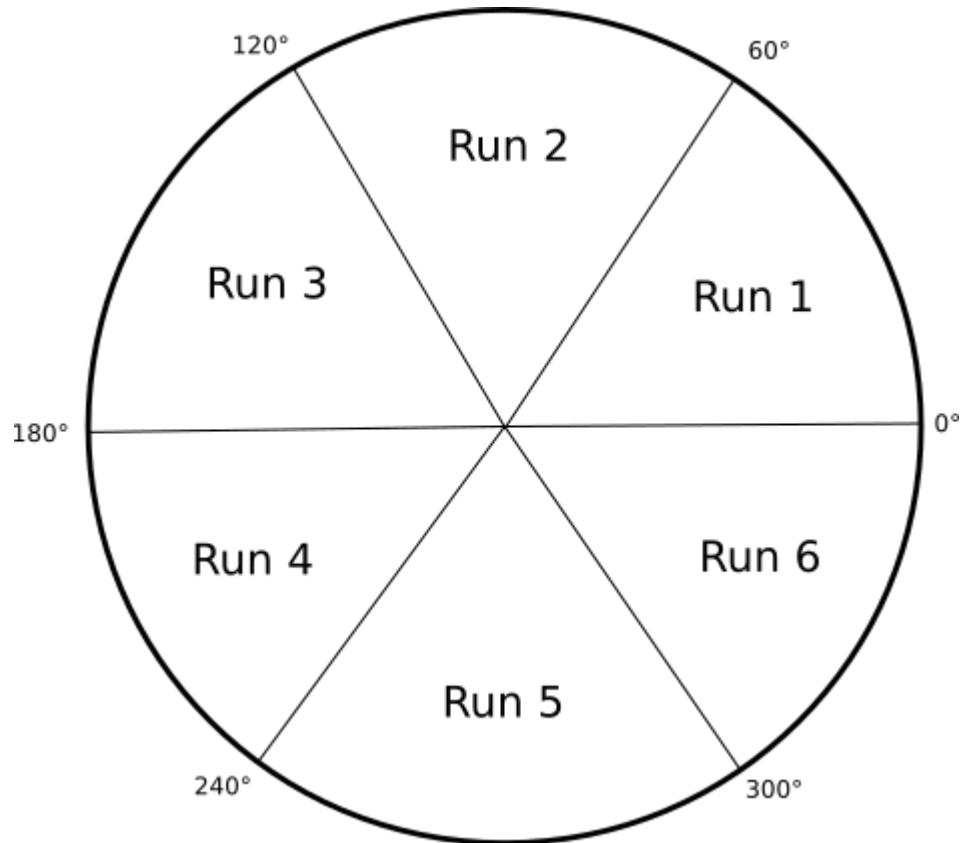


Figure 3.6: Symmetry Test Run Layouts

The shuffle tests change which fuel composition is in which pebble. As an example, Run 1 in the shuffle test

makes all fresh, or "zero-pass" pebbles of the first-pass composition, first-pass pebbles of the second-pass, and so on down the line. Run 2 makes the originally fresh (zero-pass) pebbles the second pass composition, the first-pass pebbles the third-pass composition, and so on. This scheme is described in 3.5.

Table 3.5: Shuffle Test Run Schemes

Original Fuel Position in Control	Position in Test Run					
	Run 1	Run 2	Run 3	Run 4	Run 5	Run 6
0	1	2	3	4	5	6
1	2	3	4	5	6	0
2	3	4	5	6	0	1
3	4	5	6	0	1	2
4	5	6	0	1	2	3
5	6	0	1	2	3	4
6	0	1	2	3	4	5

In both tests, the k_{eff} and outward currents are recorded and compared to the control model's k_{eff} and J^+ (see section 4.2). The appendix contains all geometry and mesh images for each run, and a pixel-by-pixel image difference of the mesh results (see chapter 6).

Chapter 4

Results

This chapter first presents the atomic fractions of select isotopes of interest, and the fission rate/thermal flux mesh corresponding to each depletion time step. Then, section 4.2 covers the results of the basic control model. The final sections — dedicated to homogenization (see section 4.3), symmetry (see subsection 4.4.1), and shuffling (see subsection 4.4.2) — compare the results of these tests to the control model.

4.1 Fuel Isotopic Compositions

Serpent allows the user to set a series of burnup steps in a single simulation if desired. For this work, the burnup steps were defined by the total days that had passed — 6 months, 12 months, 18 months, 24 months, 30 months, and 36 months. Other than this, all conditions are equal at each time step.

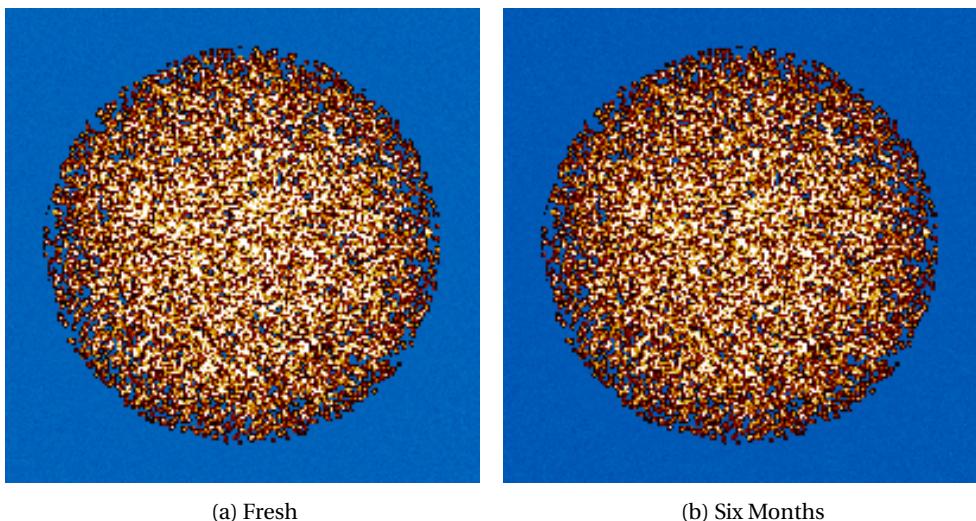


Figure 4.1: Serpent-generated mesh figures of the fission rate (hot color map) and thermal flux (cold color map) for the representative single-pebble at each depletion step. A cold color map is from shades of whitish-blue (high) to blackish-blue (low) while the hot color map is from a whitish-yellow (high) to reddish-brown (low)

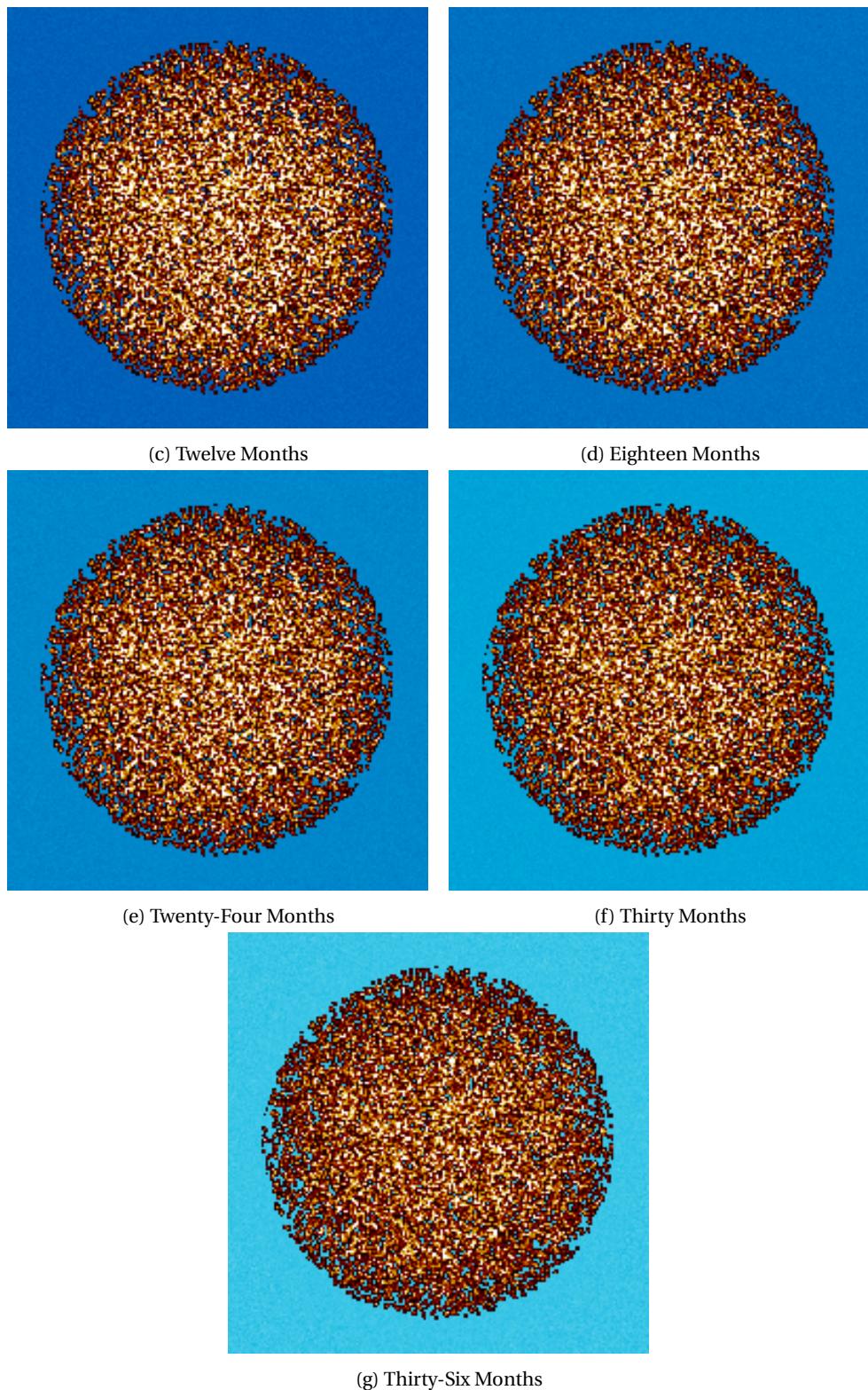
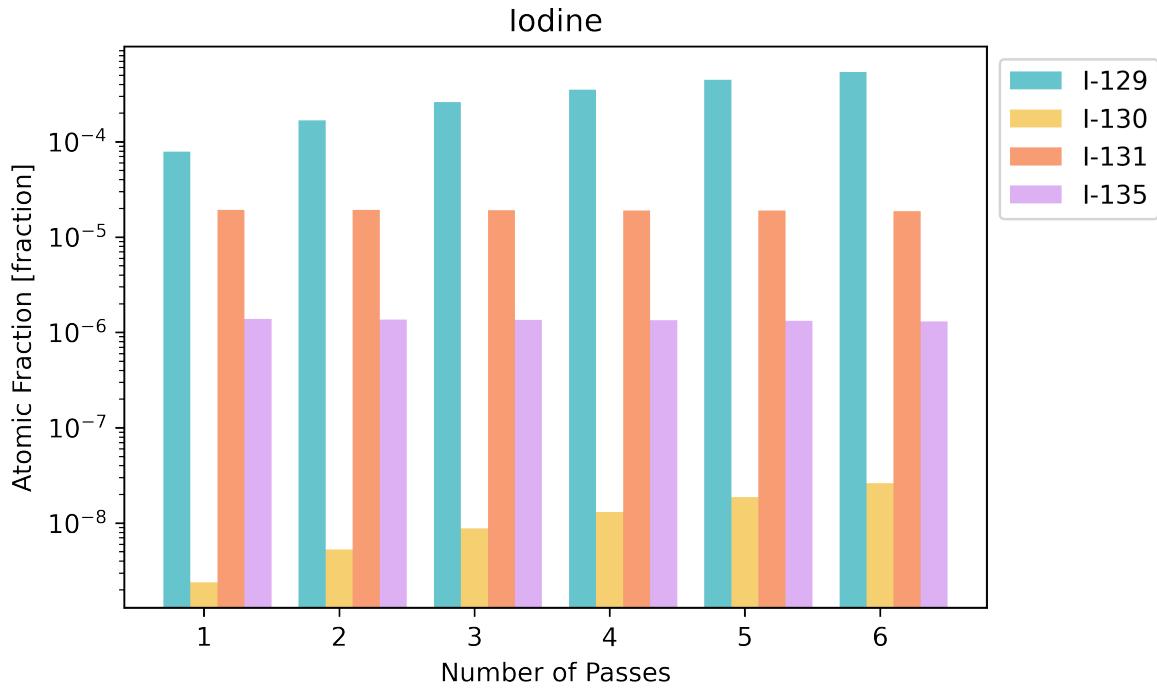


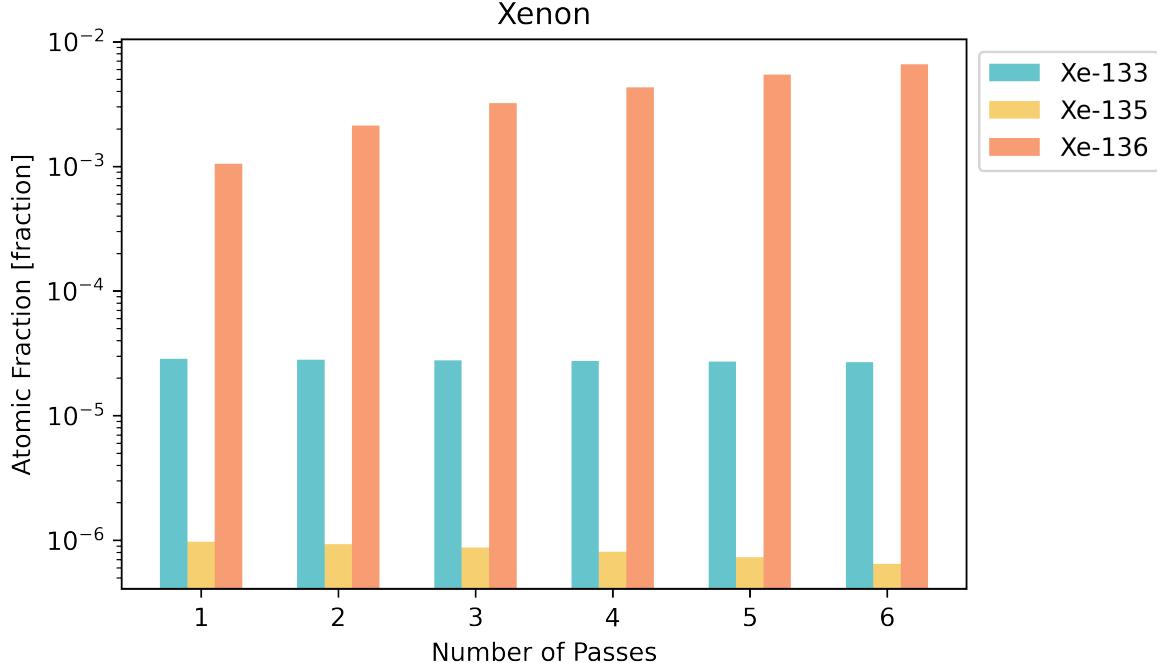
Figure 4.1: Serpent-generated mesh figures of the fission rate (hot color map) and thermal flux (cold color map) for the representative single-pebble at each depletion step. A cold color map is from shades of whitish-blue (high) to blackish-blue (low) while the hot color map is from a whitish-yellow (high) to reddish-brown (low). (cont)

Figure 4.1 depicts the evolution of the fission rate (hot color map) and thermal flux (cold color map) over the seven stages. The maximum cutoff for thermal flux is 0.625 eV in these figures. Over successive depletion steps, the fission rate decreases, and thermal flux increases. This is not unexpected — as the pebble burns, the atomic fraction of fissile ^{235}U decreases, which results in a lower fission rate at each time step. At the same time, the reduction of fissile isotopes and build up of fission products means the neutrons can have a longer lifetime before undergoing capture, resulting in a more thermalized spectrum.

But understanding the effects on simple core neutronics such as the fission rate or thermal flux is not the only reason to find the isotopic composition of the fuel. Fission product buildup in the fuel not only has long term ramifications for spent fuel handling, but matters for our understanding of accident consequence analysis. The potential isotopes — and in what amounts — that a living being or environment might be exposed to after an accident is called a source term. As shown in Tables 1.1 and 1.2, fission products can either leach into the coolant gas, or be found in the fine dust formed when the pebbles bump against each other during operation. In an accident, this dust could be jettisoned from the RPV in the case of a breach, where it could be inhaled or reach the ground or groundwater. In order to fully understand accident consequences, one must understand the source term. Figure 4.2 provides the atomic fractions of isotopes of iodine, xenon, cesium, radium, thorium, uranium, and plutonium within depleted UCO.

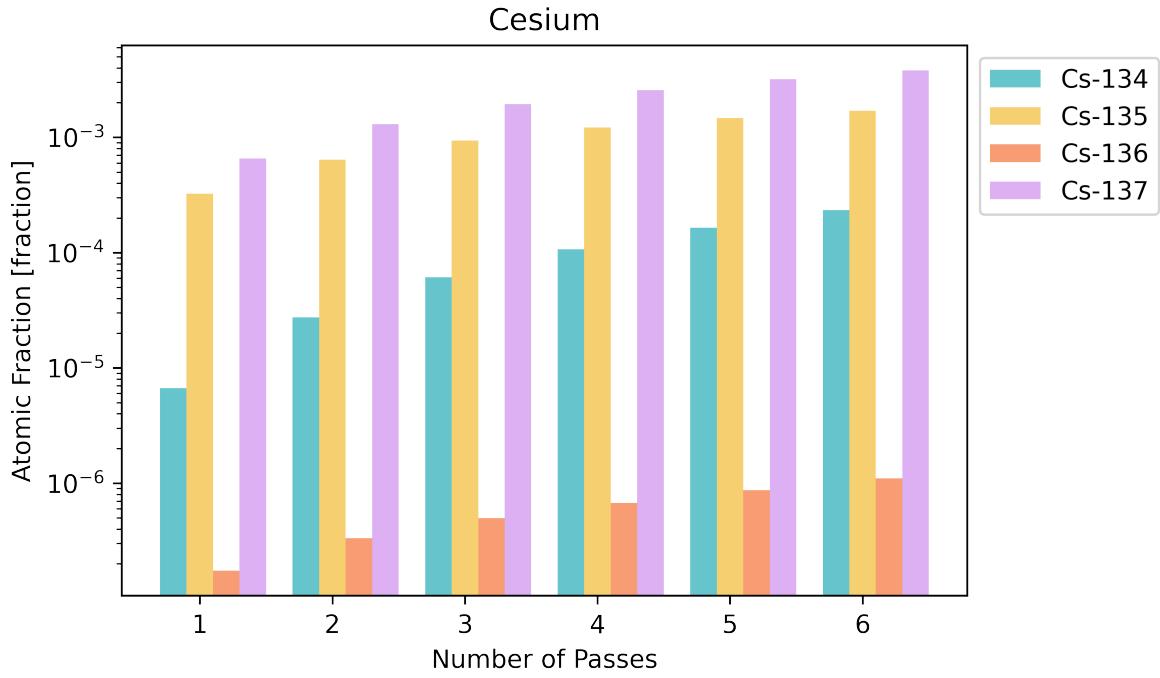


(a) Iodine isotope buildup with each pass

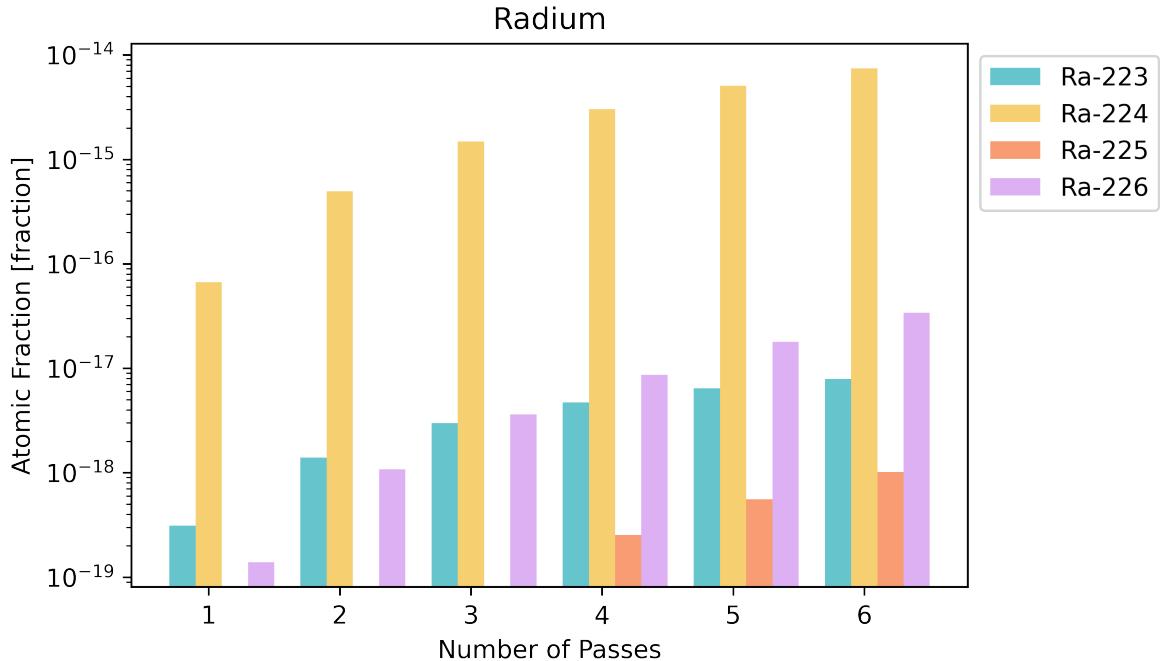


(b) Xenon isotope buildup with each pass

Figure 4.2: Evolution of Safety Relevant Isotopic Concentrations in Pebbles of Sangamon20 over Six Six-Month Passes



(c) Cesium isotope buildup with each pass



(d) Radium isotope buildup with each pass

Figure 4.2: Evolution of Safety Relevant Isotopic Concentrations in Pebbles of Sangamon20 over Six Six-Month Passes (cont.)

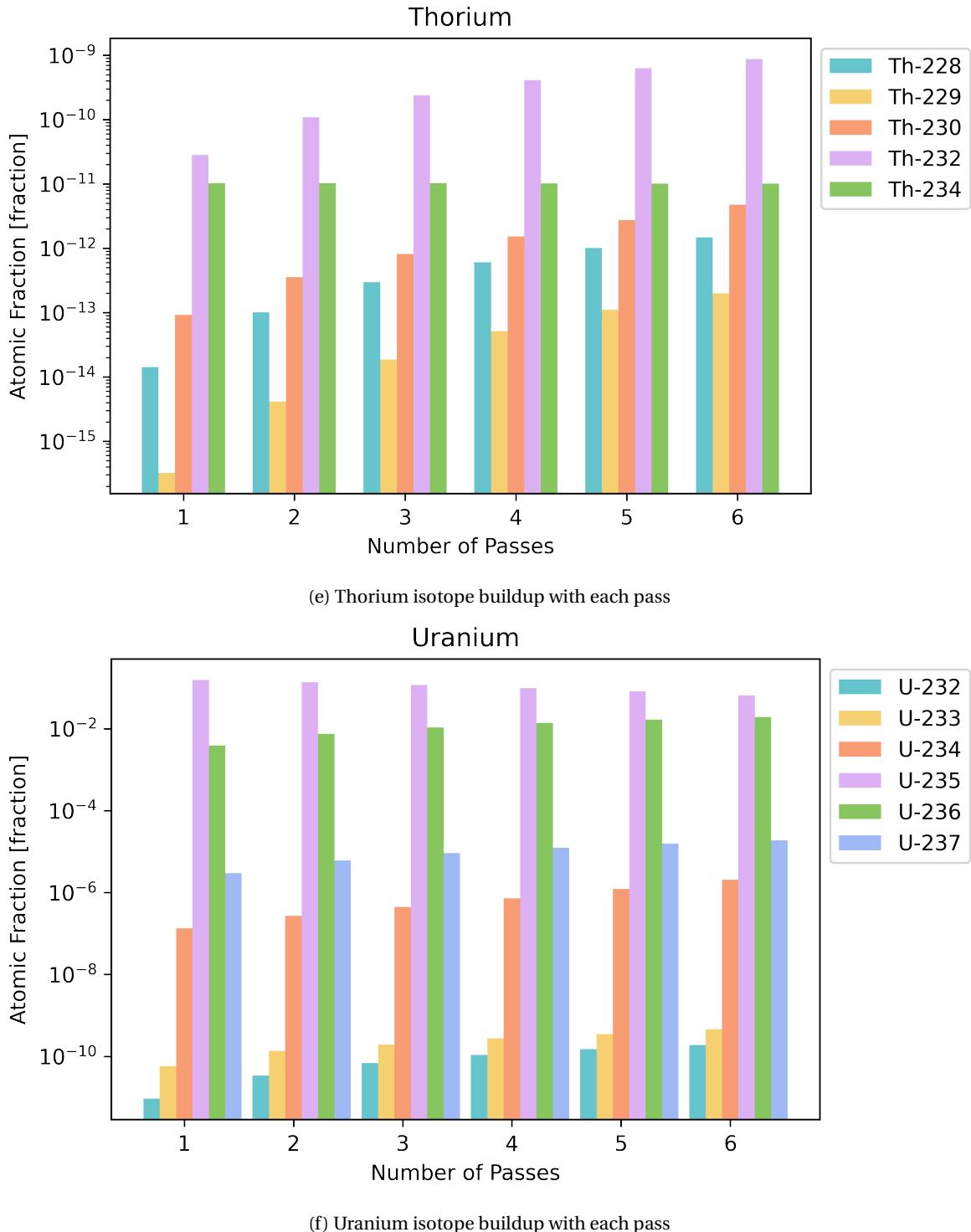
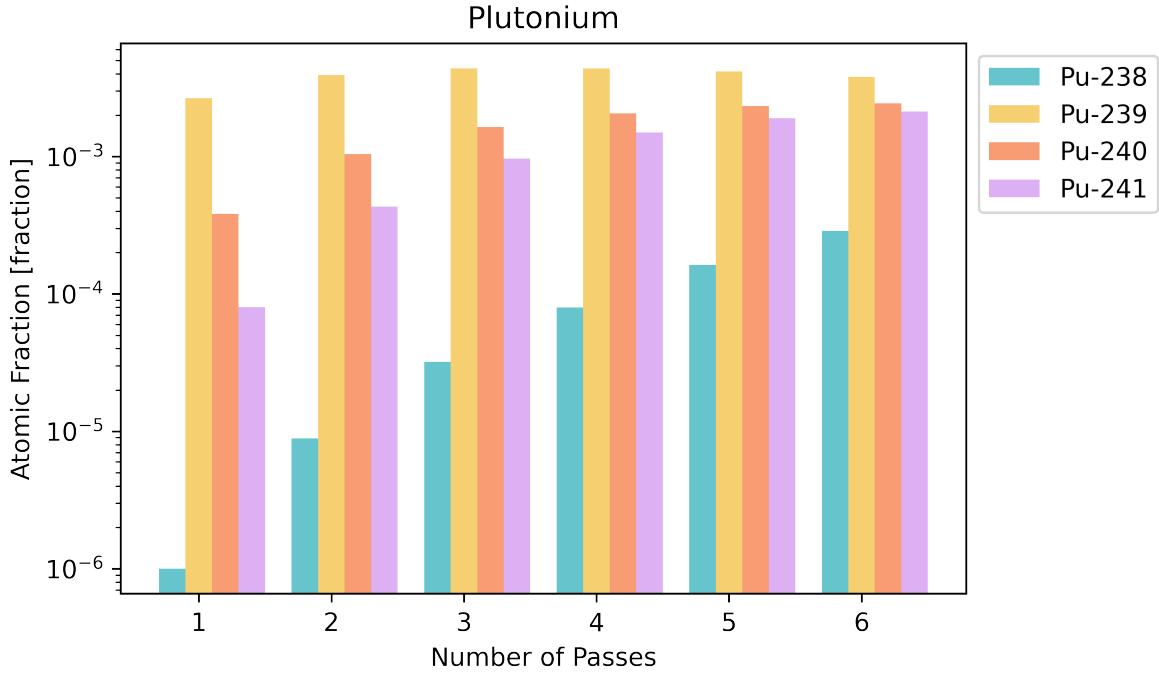


Figure 4.2: Evolution of Safety Relevant Isotopic Concentrations in Pebbles of Sangamon20 over Six Six-Month Passes (cont.)



(g) Plutonium isotope buildup with each pass

Figure 4.2: Evolution of Certain Isotopic Concentrations in Pebbles over Six Six-Month Passes (cont.)

The full isotopic inventory tracked in the Sangamon20 reactor models extends far beyond those supplied in Figure 4.2. For a full list, see [1] for the compositions alone, or [34] for a complete input file and associated output. Figure 4.2 focuses on those of interest in safety analysis, such as those in Table 1.2 and Table 1.1.

Only the xenon content rivals the inventory of uranium. All isotopes of uranium steadily increase over time with the exception of ^{235}U , ending at 0.0647 by atomic fraction in the sixth pass. ^{232}U , initially the smallest fraction of uranium sees the most dramatic increase over time, increasing by two orders of magnitude between the first (9.28×10^{-12}) and sixth (1.9×10^{-10}) cycle. While the atomic fraction doesn't reach an equilibrium, the rate at which it increases each cycle is steady - increasing by 4.02×10^{-11} , 4.2×10^{-11} , and 3.9×10^{-11} from the third to fourth, fourth to fifth, and fifth to sixth pass, respectively. Plutonium content is also fairly high, with ^{239}Pu peaking at 0.00439. However, unlike many other isotopes, which peak in the sixth cycle, ^{239}Pu crests in the third and fourth passes, decreasing from 0.00439 in the fourth pass to 0.00380 in the sixth. ^{238}Pu , meanwhile, is the least abundant, but does experience the most dramatic increase over time (especially between the first and second passes).

^{133}Xe appears to be steady around its initial concentration of 2.86×10^{-5} atomic fraction, decreasing only to 2.68×10^{-5} by the sixth pass. ^{135}Xe decreases a bit more dramatically, going from an initial 9.70×10^{-7} after its first six months, to 6.46×10^{-7} after thirty-six months. ^{136}Xe is both the greatest contributor to xenon content in

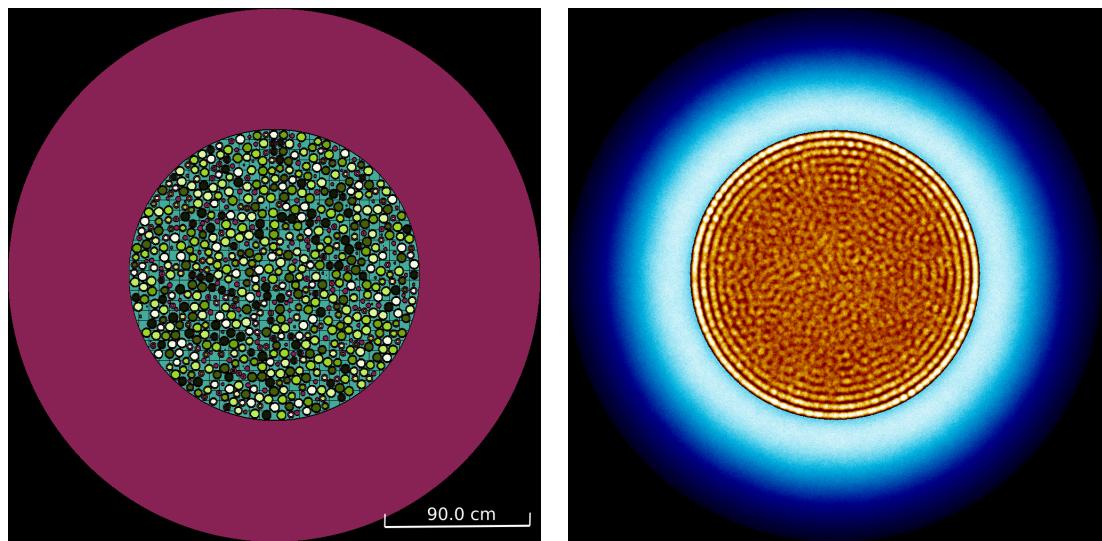
the fuel, and the only isotope reported in Figure 4.2b to increase, owing to its long half life. Each cycle increases ^{136}Xe content by 0.0011, beginning at a concentration of 0.00105 in the first cycle and ending at 0.0066 after the sixth. Isotopes of iodine form a smaller portion of fission products than xenon or caesium (still a relatively high magnitude) which is of concern due to its high mobility in water and uptake in the thyroid. ^{129}I is the most abundant isotope of iodine reported here. It increases for the entirety of the pebble's life, beginning at 7.38×10^{-5} and peaking at 0.000538 at its discharge burnup. ^{130}I and ^{135}I are both relatively stable, most likely due to their short half-lives, combined with transmutation after undergoing neutron capture. While ^{130}I is the least abundant, it increases over time. Caesium has a net concentration similar to xenon's. Unsurprisingly ^{135}Cs and ^{137}Cs , which both have half-lives longer than a pebble's residency time in the reactor, are in greatest abundance, and increase over time. These, too, are of concern, due to their long half-life.

Of the elements reported here, radium and thorium are in lowest abundance. ^{225}Ra only appears in trace amounts (less than or equal to 9.99×10^{-20}) for the first three passes. ^{224}Ra far outweighs the other reported isotopes of radium, with an atomic fraction of 7.46×10^{-15} after thirty-six months - two orders of magnitude higher than all other isotopes of radium combined at this depletion step. Thorium has the second-least abundant atomic fractions, with fertile ^{232}Th being the most abundant, at 8.80×10^{-10} in the sixth pass. However, being present only in low concentrations is not enough to ensure that it is not a risk in an accident scenario. An isotope with a very short half-life, or ones that are toxic in addition to being radioactive can pose a serious threat even in relatively low amounts.

4.2 Full-Core Control Model

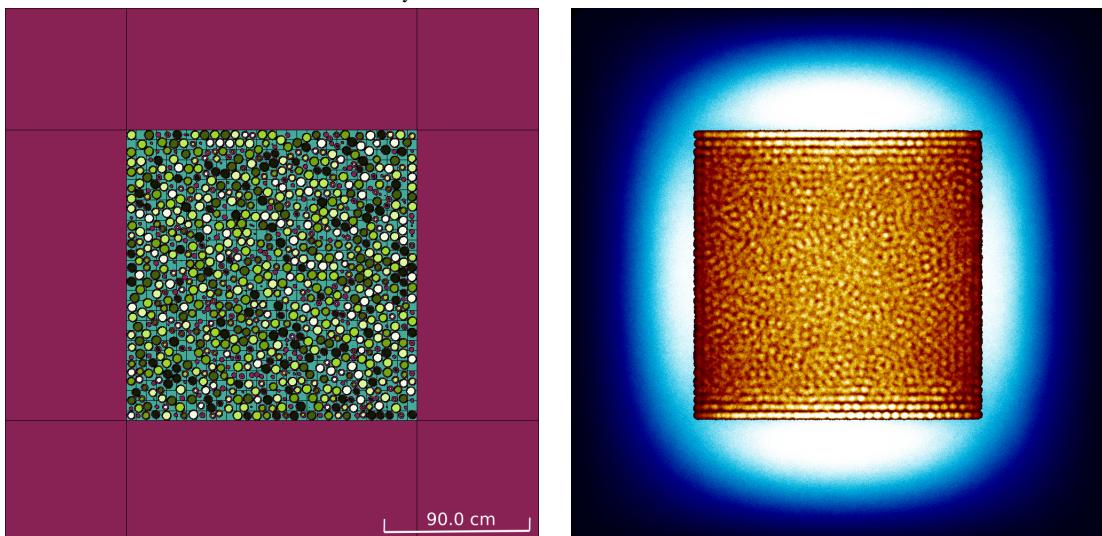
Figure 4.3 shows a cross section of the core geometry at the origin (the midplane, the center of which is the point (0, 0, 0)) in the xy and xz planes (Sub-Figures 4.3a and 4.3c, respectively) and provides a mesh of the fission rate and thermal flux in the xy and xz planes (Sub-Figures 4.3b and 4.3d, respectively). Both of these integrate over z and y, respectively, to produce a 2D image. The value of k_{eff} was 1.041 ± 0.00054 .

Figure 4.3e is accurate for all cross sections of reactor geometry. In homogenized simulations, the shades of green represent the material blend forming the center of the pebble at a given burnup. For heterogenized simulations, these same shades represent the TRISO particle kernel at a particular burnup.



(a) Radial Cross Section at $y=0$

(b) Radial Mesh



(c) Axial Cross Section at $z=0$

(d) Axial Mesh

Graphite

Helium

Fresh

Burnt

(e) Legend for 4.3a and 4.3c

Figure 4.3: Geometry Cross Sections (left) and Thermal Flux(cold color map) and Fission Rate (hot color map) Meshes (right) for the Control Model of Sangamon20

Figure 4.3b shows bands of concentric rings around the outer edges of the active core. These bands suggest

that the outermost areas of the core are regions of high fission activity relative to the center, which is at odds with what most might expect from the neutronics behavior in a cylindrical reactor. Certainly the pebbles are physically forming rings at the outer edges, and their placement becomes less structured toward the center. However, the high intensities seen in this outer region in the mesh figures are unindicative of a total flux profile showing the same. Recall that Serpent integrates over the z direction to produce a 2D plot of the xy plane. For a cylinder, the distance in z each point integrates over is the same - the height of the reactor. However, points at the outermost regions are integrating in a volume composed more of pebbles - and therefore fissile material - than the center, where more space filled with coolant. The outer regions are more regularly packed with pebbles - and therefore have less coolant than the center - because the dispersal routine (and the grow and shake algorithm) naturally cause the pebbles to line up along the reactor boundary. Lattice arrangements wouldn't have this feature because these methods ignore core boundaries.

In Figure 4.3d we can see a similar banding effect on the top and bottom edge of the core region, but not on the sides. No hot-spots on the edges because Figure 4.3d is in the xz plane, and integrates over y. However, for a cylinder, the distance integrated over is not the same at all points. At the centerline, the distance is simply the diameter. However, as you move towards the edge, the distance integrated over approaches zero. So, while these plots can help provide some insight into the core, one must be very careful to keep this uneven integration in mind when interpreting them.

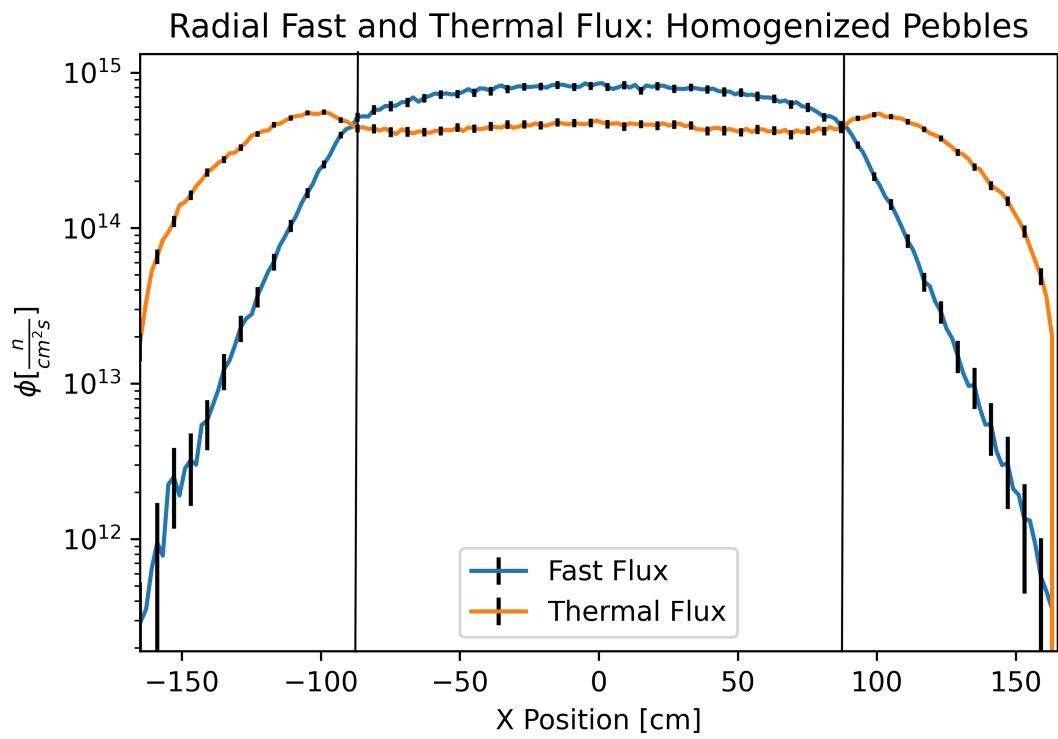


Figure 4.4: Radial Thermal and Fast Flux Profiles along the X-Axis at the Mid-Plane in the Homogenized-Pebble Sangamon20. Black vertical lines at ± 90 cm show the inner reflector boundary.

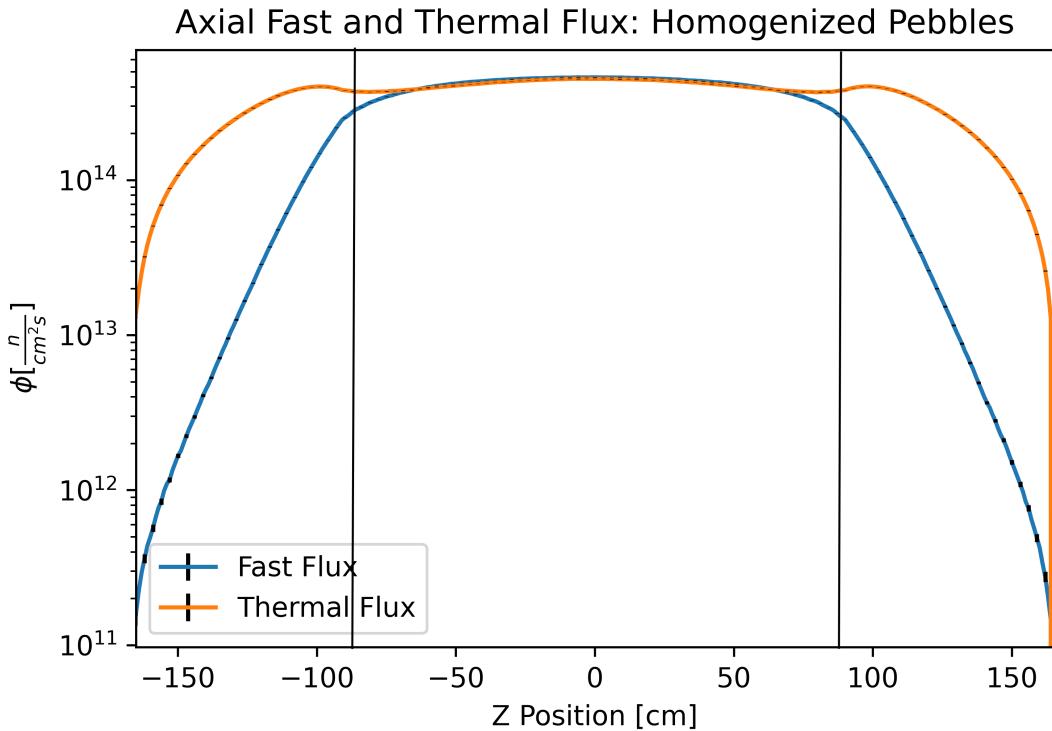


Figure 4.5: Axial Thermal and Fast Flux Profiles along the X-Axis at the Mid-Plane in the Homogenized-Pebble Sangamon20. Black vertical lines at ± 90 cm show the inner reflector boundary.

Figures 4.4 and 4.5 provide the fast and thermal flux profiles in Sangamon20 at the axial and radial (x-direction) centerlines, respectively. For the radial flux, a detector in the xy plane was used, which had finite bin sizes in x and y, and spanned the whole height of the reactor in the z direction. For the axial fluxes, the bins were finite in z and spanned the entire diameter of the core. Normally, these two figures would be subject to the same unequal bin sizing that affected Figure 4.3. To counteract this, the axial fluxes (Figure 4.5) are multiplied by the ratio of the radial detector bin volume to the axial detector bin volume, as follows:

$$\phi_{axial,adjusted} = \phi_{axial,unadjusted} \frac{V_{radial}}{V_{axial}} \quad (4.1)$$

where

$$\phi_{axial,adjusted} = \text{detector bin-size adjusted flux } \left[\frac{\#}{cm^2 s} \right]$$

$$\phi_{axial,unadjusted} = \text{unadjusted axial flux } \left[\frac{\#}{s} \right]$$

$$V_{radial} = \text{radial detector bin volume } [cm^3]$$

$$V_{axial} = \text{axial detector bin volume } [cm^3]$$

Both axially and radially, the thermal flux sees a 'bump', which peaks approximately 10 cm into the reflector, at 100 cm. These are the highest peaks in the thermal flux, with the second highest thermal flux being at the center line. For the fast flux profile we see a flattened peak in the active core (-90.0 cm to 90 cm). Fast flux rapidly decreases in the reflector as fast neutrons down scatter in the graphite. Both Figures 4.4 and 4.5 show that while the radial banding seen in the fission rate mesh profiles are of high intensity, the flux peaks are elsewhere.

In addition to centerline fast and thermal flux profiles, Figures 4.7 and 4.6 provide the fast and thermal flux profiles in the xy plane.

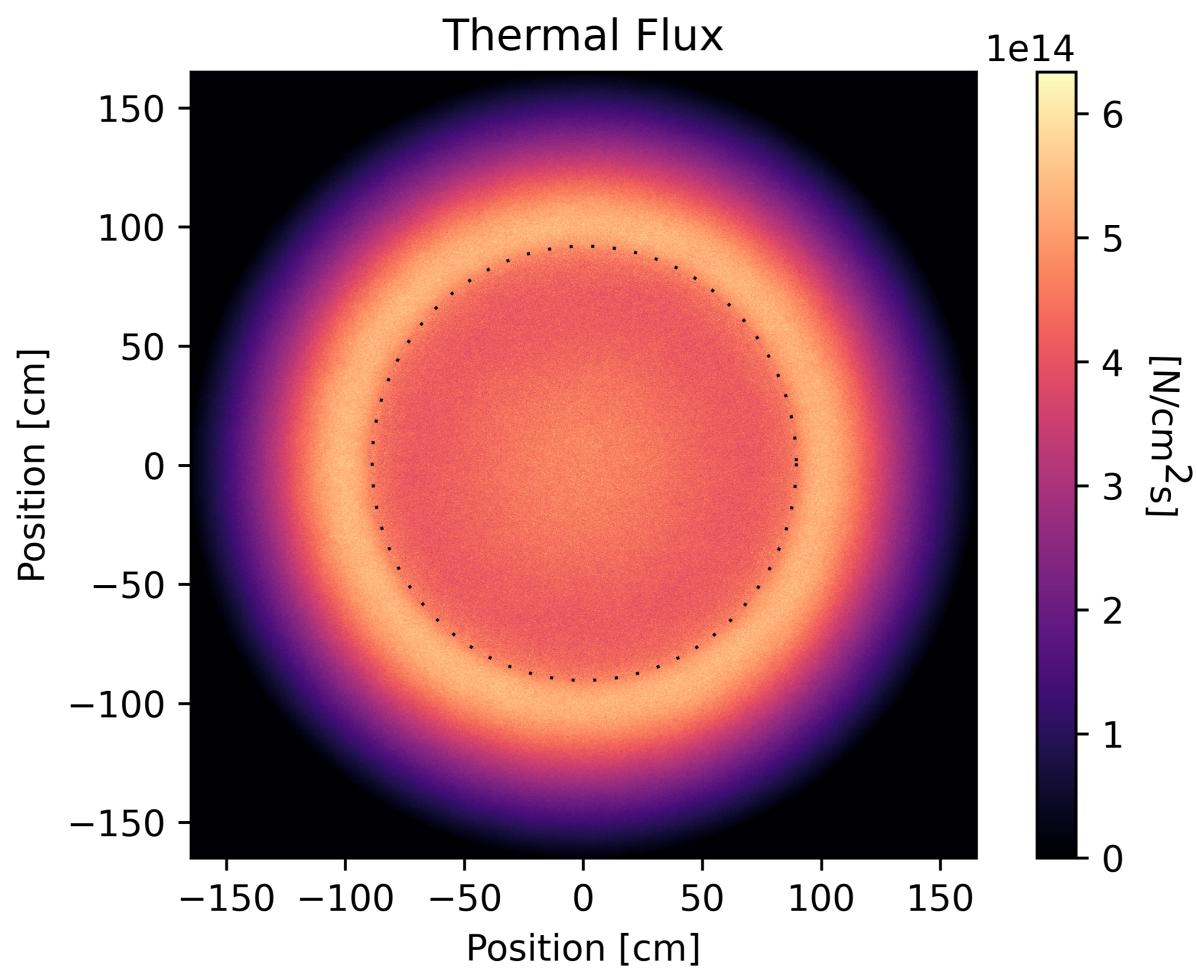


Figure 4.6: Thermal Flux in xy Plane

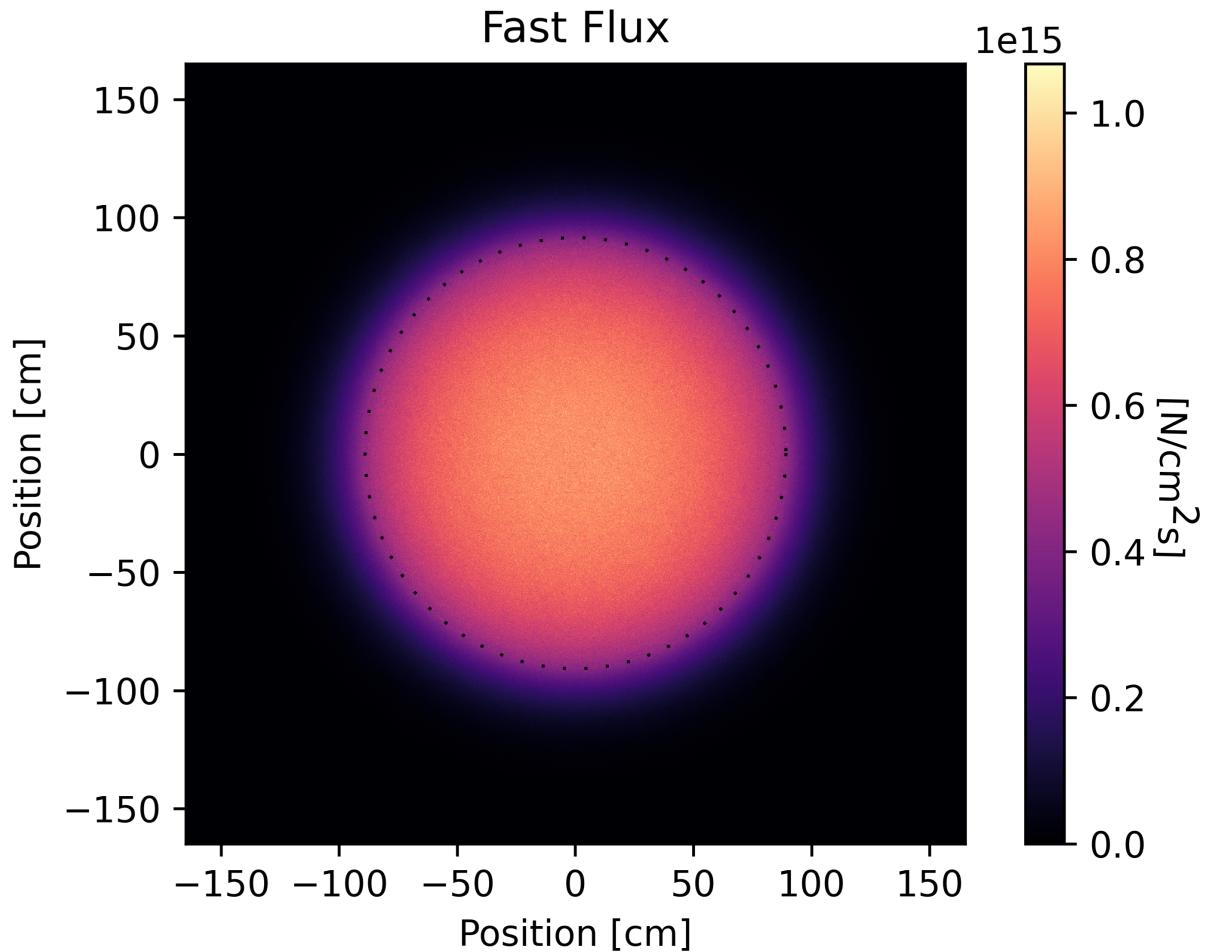


Figure 4.7: Fast Flux in xy Plane

A slight banding pattern on the active core's edge exists — primarily in the fast, rather than thermal, flux — but with less intensity than the fission rate banding. In the thermal flux, we see that the peak in 4.4 continues in a circular pattern surrounding the active core, approximately 10 cm into the graphite reflector. The steep drop-off in fast flux once within the outer reflector, meanwhile, is clearer in 4.7. Once again, Figure 4.7 and Figure 4.6 show that while the banding morphology may be present in the fission rate profile (and do cause a slight increase relative to the region immediately surrounding it) it does not cause concentric spikes in the flux profiles. It is suspected that the banding pattern is less prevalent in the thermal flux because the banded region is directly next to the reflector, which has a smoothing effect.

Figures 4.8 through 4.12 gives the energy spectra in the reflector, coolant, overall core, and a randomly selected fresh and sixth-pass pebble. The results are per unit lethargy and use the Tripoli 315-group energy structure [41] to set energy bin boundaries. This group structure was chosen not only because there were a sufficient number of bins

to provide the desired fidelity, but also because the highest fidelity regions (smallest bin size) in the spectrum were in the lower energy values, which is of greater interest to a thermal spectrum reactor.

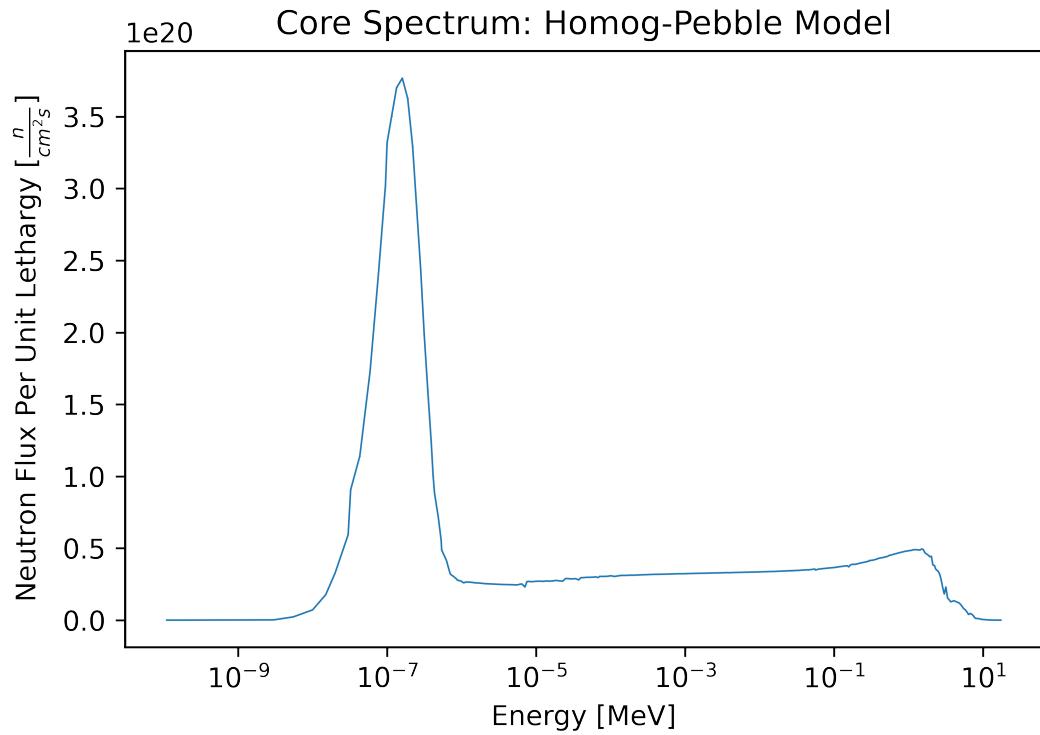


Figure 4.8: Lethargy Adjusted Neutron Flux Energy Spectrum in the Whole-Core for the Homogenized-Pebble Sangamon20

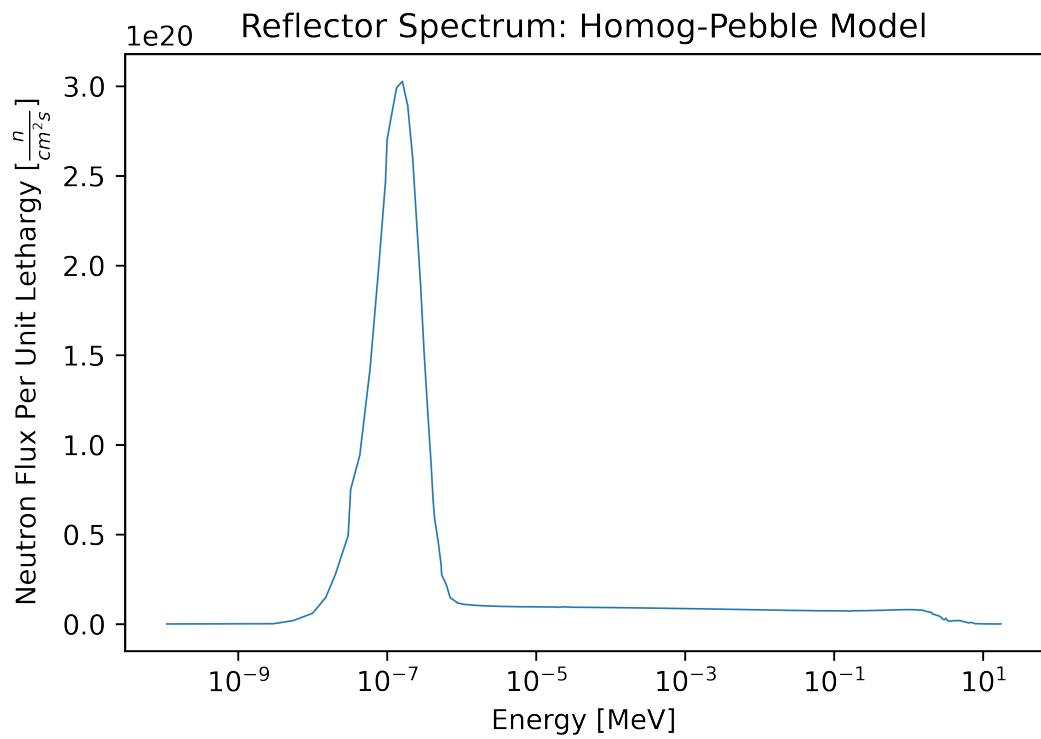


Figure 4.9: Lethargy Adjusted Neutron Flux Energy Spectrum in the Reflector for the Homogenized-Pebble Sangamon20

The thermal peak of the whole-core and reflector both occur around 10×10^{-7} MeV, which is also the energy of neutrons most-responsible for fission. The thermalization of neutrons in the reflector dominates the spectrum in Figure 4.8, indicated by the high magnitude of the thermal peak in the reflector and core and their similar shape.

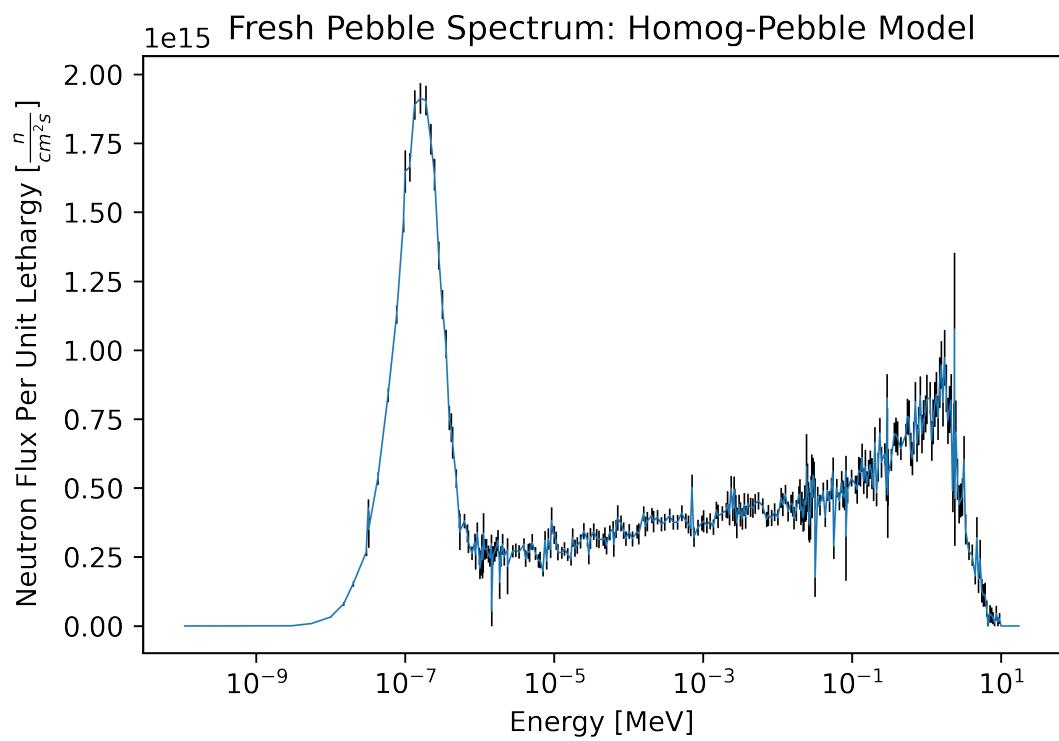


Figure 4.10: Lethargy Adjusted Neutron Flux Energy Spectrum in a Fresh Pebble for the Homogenized-Pebble Sangamon20

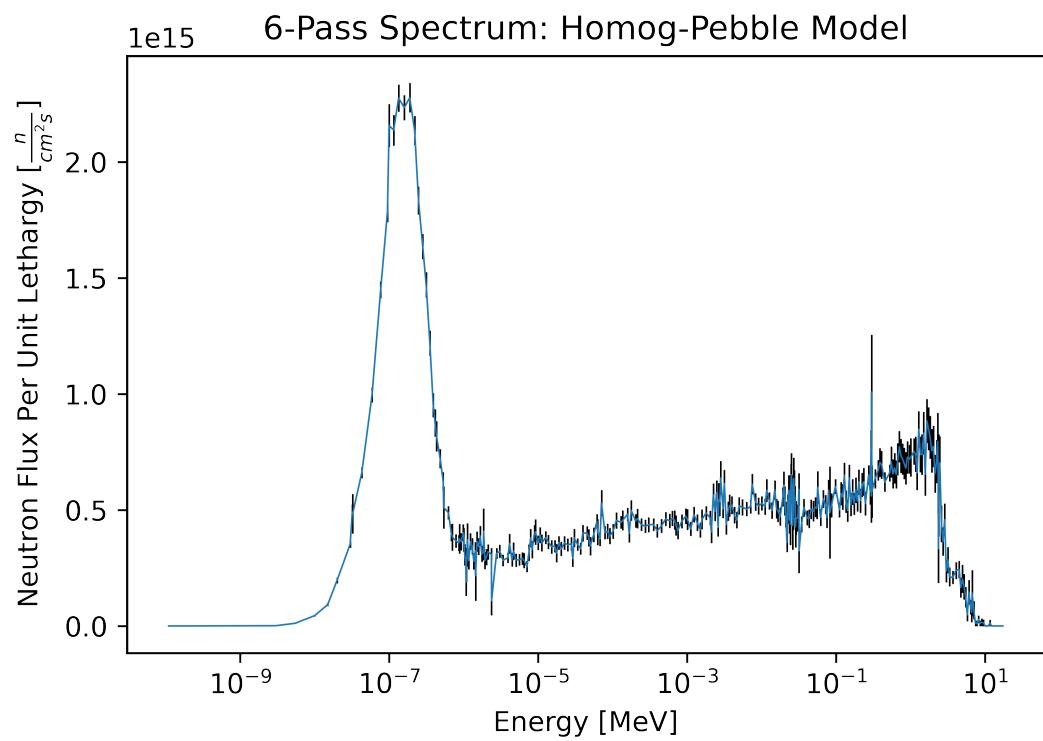


Figure 4.11: Lethargy Adjusted Neutron Flux Energy Spectrum in a Six-Pass Pebble for the Homogenized-Pebble Sangamon20

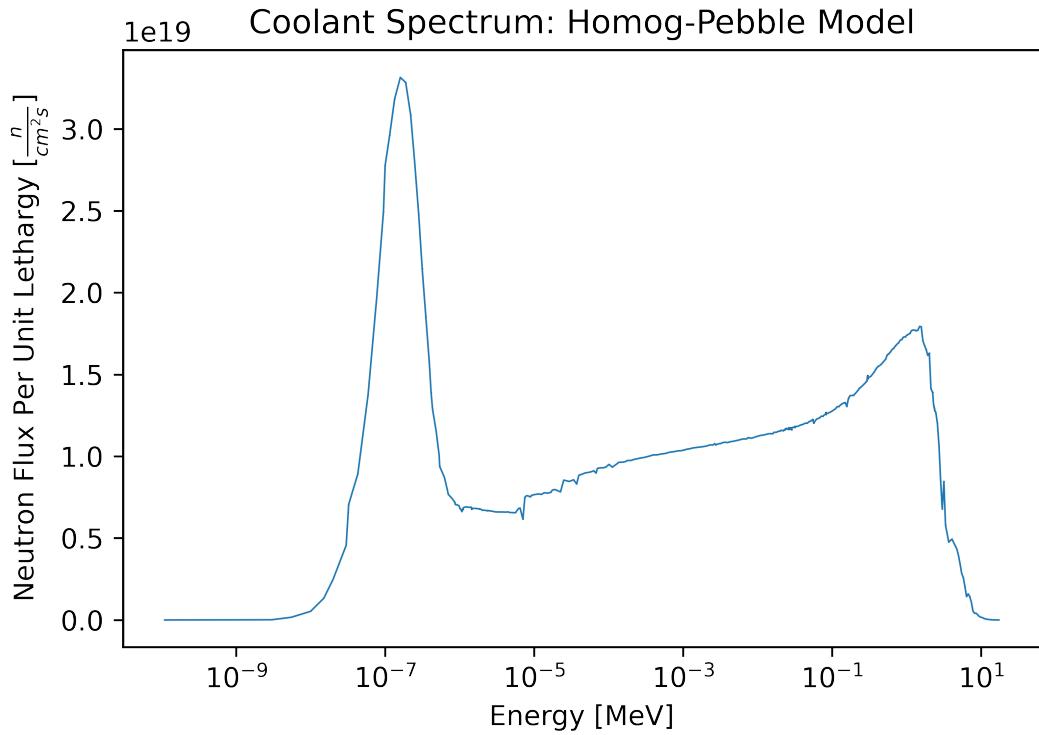


Figure 4.12: Lethargy Adjusted Neutron Flux Energy Spectrum in the Coolant for the Homogenized-Pebble Sangamon20

The spectra for a randomly selected fresh and sixth-pass pebble are subject to the highest uncertainty of all the provided spectra in Figures 4.8 through 4.12, as a single pebble has a relatively small bin size, which means fewer particles contribute to the tally regions. However, if coupled with the coolant spectra, Figure 4.12, they provide a clearer look at the flux energy spectrum in the active core region. We can see that, while the thermal energy of the fresh and six-pass pebbles are similar in shape and magnitude, the magnitude of the faster groups differ considerably.

4.3 Effect of Homogenization

The results discussed previously use the assumption of a pebble that has the TRISO particles homogenized and blended with the rest of the pebble matrix in the region containing fuel. However, homogenization can cause under-predictions of k-eff as much as 5-6% [42]. To test the impact of homogenization on Sangamon20, the heterogenization tests were performed. These tests use an otherwise identical Sangamon20 model with explicitly modeled TRISO particles. As a reminder, the isotopic compositions come from the same burnup simulation. As such, the isotopic compositions between the homogenized and heterogenized simulations are identical.

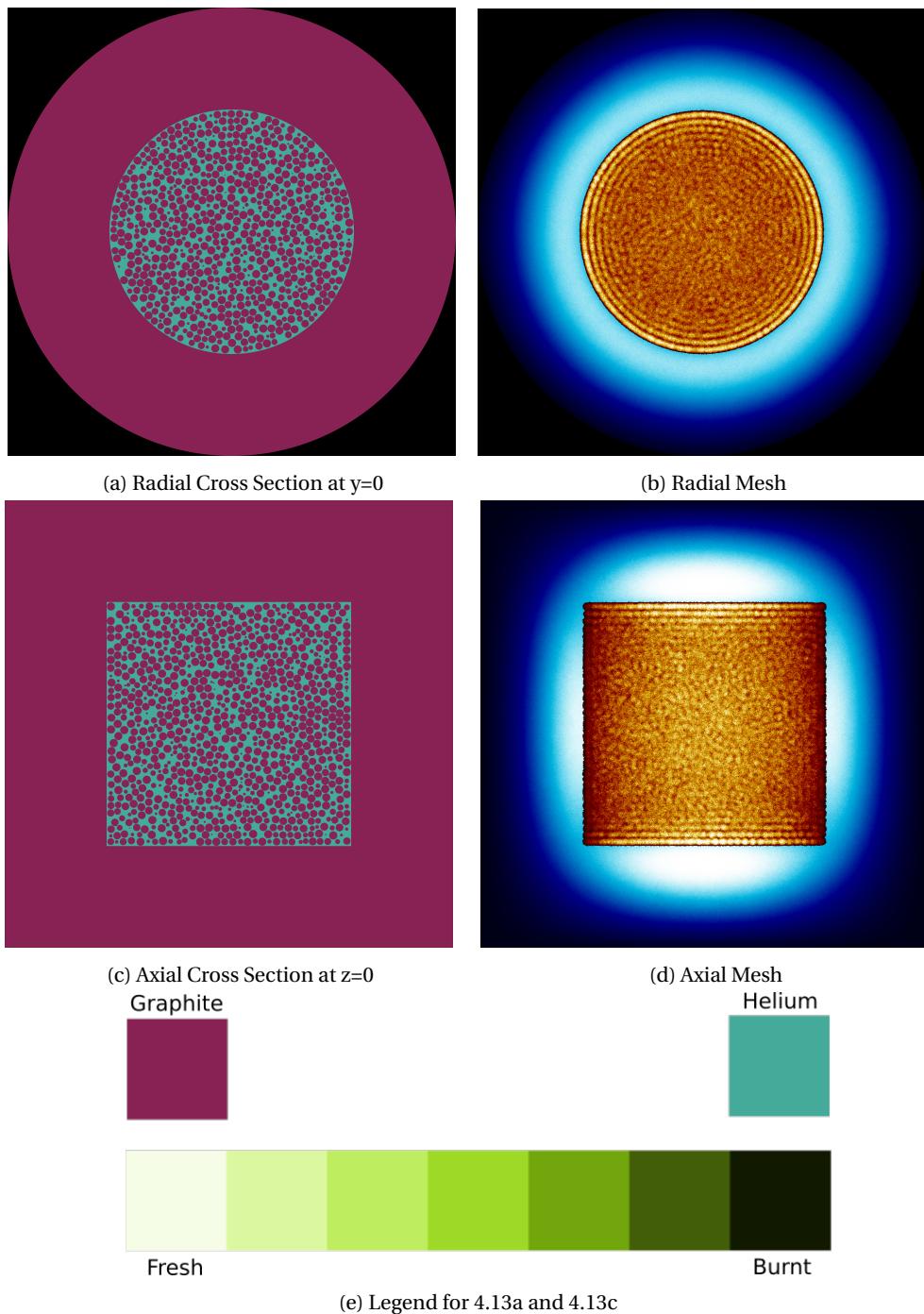


Figure 4.13: Full Core Using Heterogenized Pebbles

The heterogenized-TRISO model reported a k_{eff} of 1.087 ± 0.00032 . This is significantly higher than the k_{eff} reported for the control (homogenized-TRISO) model — only 1.041 ± 0.00054 . In agreement with [42], this is a difference of 4.23%.

Overall, the mesh result for the heterogenization test fission rate is much the same - the banding patterns are

still present, if slightly less defined. While Figure 4.13 best serves as a qualitative visualization aid, Figures 4.14, 4.15, 4.16, and 4.17 support this in a more quantitative manner. These figures give the shape and magnitude of the fluxes, which 4.13 cannot.

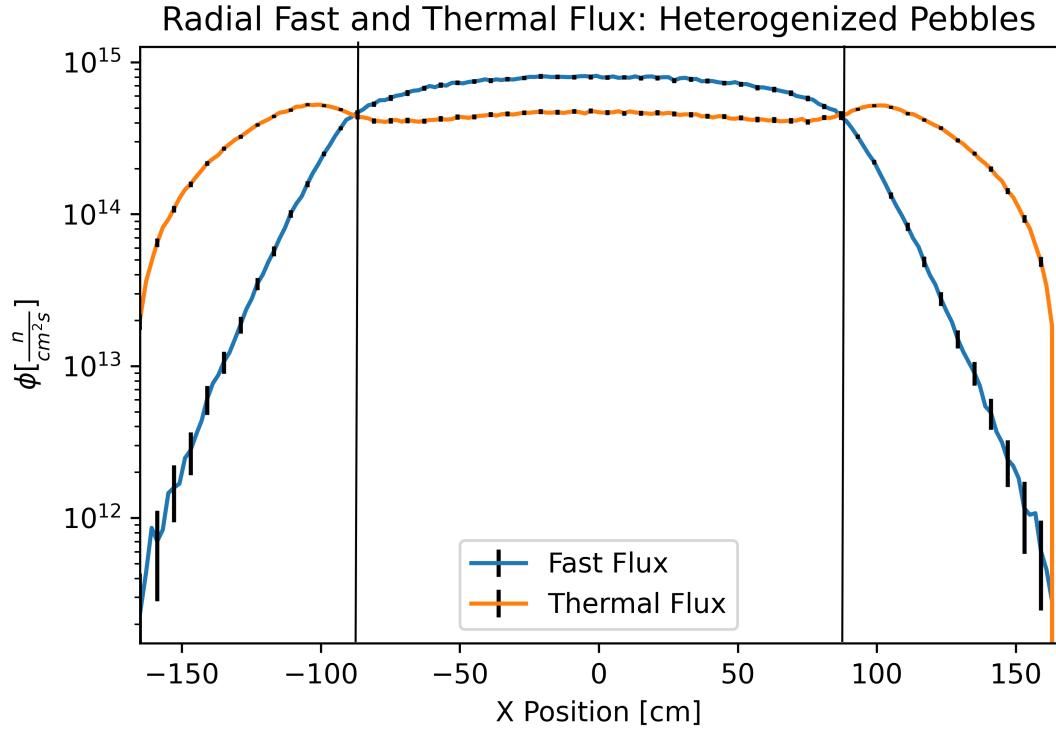


Figure 4.14: Radial Thermal and Fast Flux Profiles along the X-Axis at the Mid-Plane in the Heterogenized-Pebble Sangamon20. Black vertical lines at ± 90 cm show the inner reflector boundary.

Compared with the homogenized Sangamon20, the heterogenized core reports a slightly lower neutron current at the outer edge of the reflector, at $5.718 \times 10^{11} \pm 5.032 \times 10^{08}$, an absolute difference of approximately 2.00×10^{09} , which corresponds to a relative difference of 0.35%. The heterogenized model otherwise shows a similar flux profile to the homogenized model (see Figure 4.23), and experiences a similar level of uncertainty in the outer edges of the reflector for the fast flux profiles, likely due to the significant thermalization of neutrons by that point in the reflector — which results in fewer fast neutrons contributing to outer region tallies.

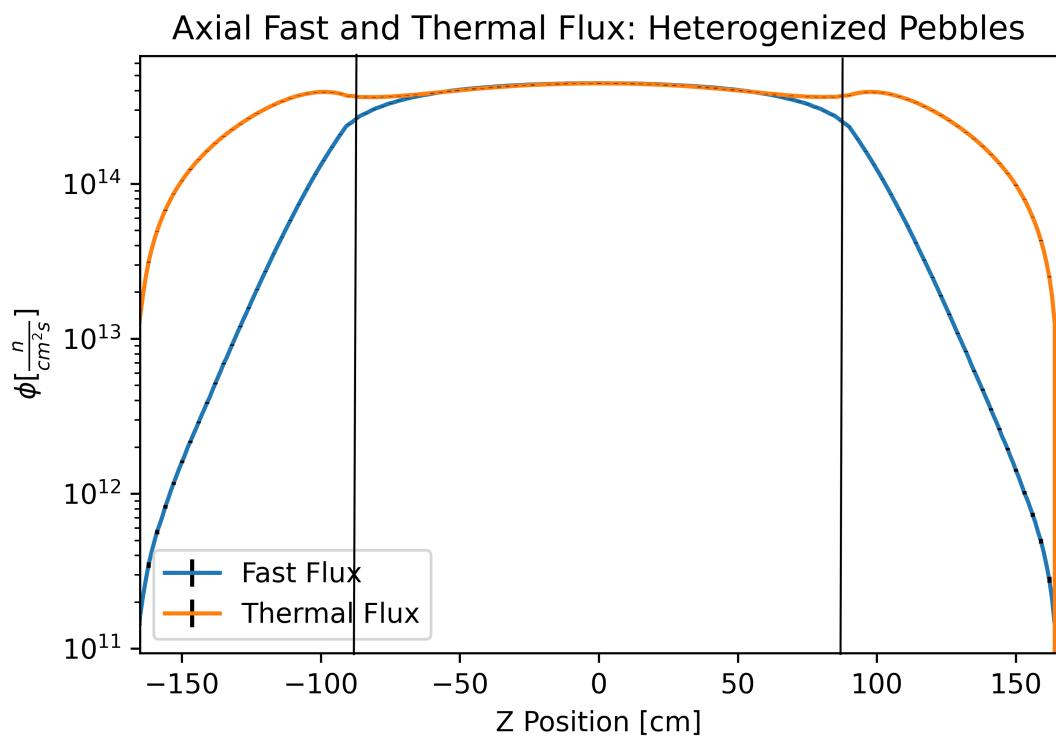


Figure 4.15: Axial Thermal and Fast Flux Profiles along the X-Axis at the Mid-Plane in the Heterogenized-Pebble Sangamon20. Black vertical lines at ± 90 cm show the inner reflector boundary.

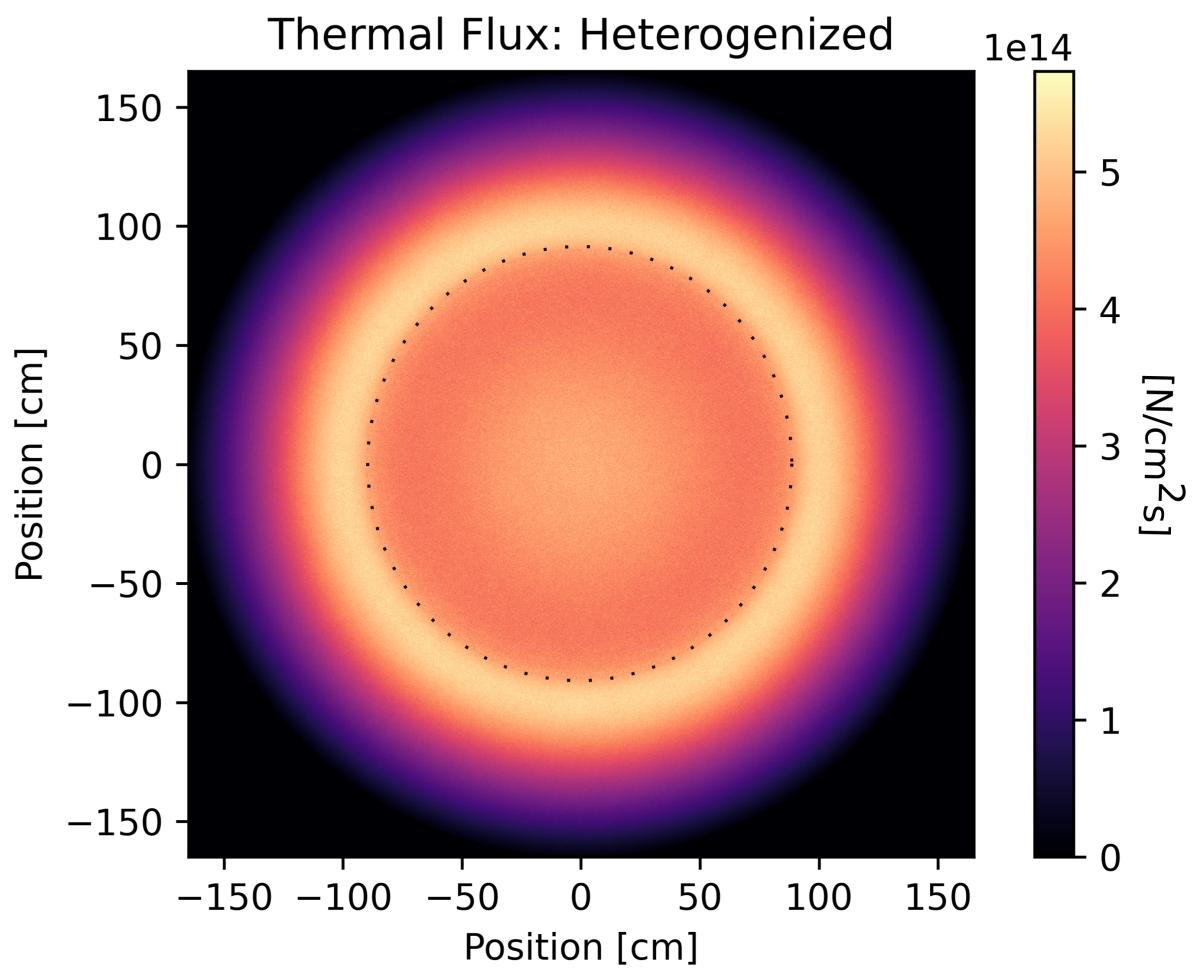


Figure 4.16: Thermal Flux in xy Plane in Sangamon20: Heterogenized Pebbles

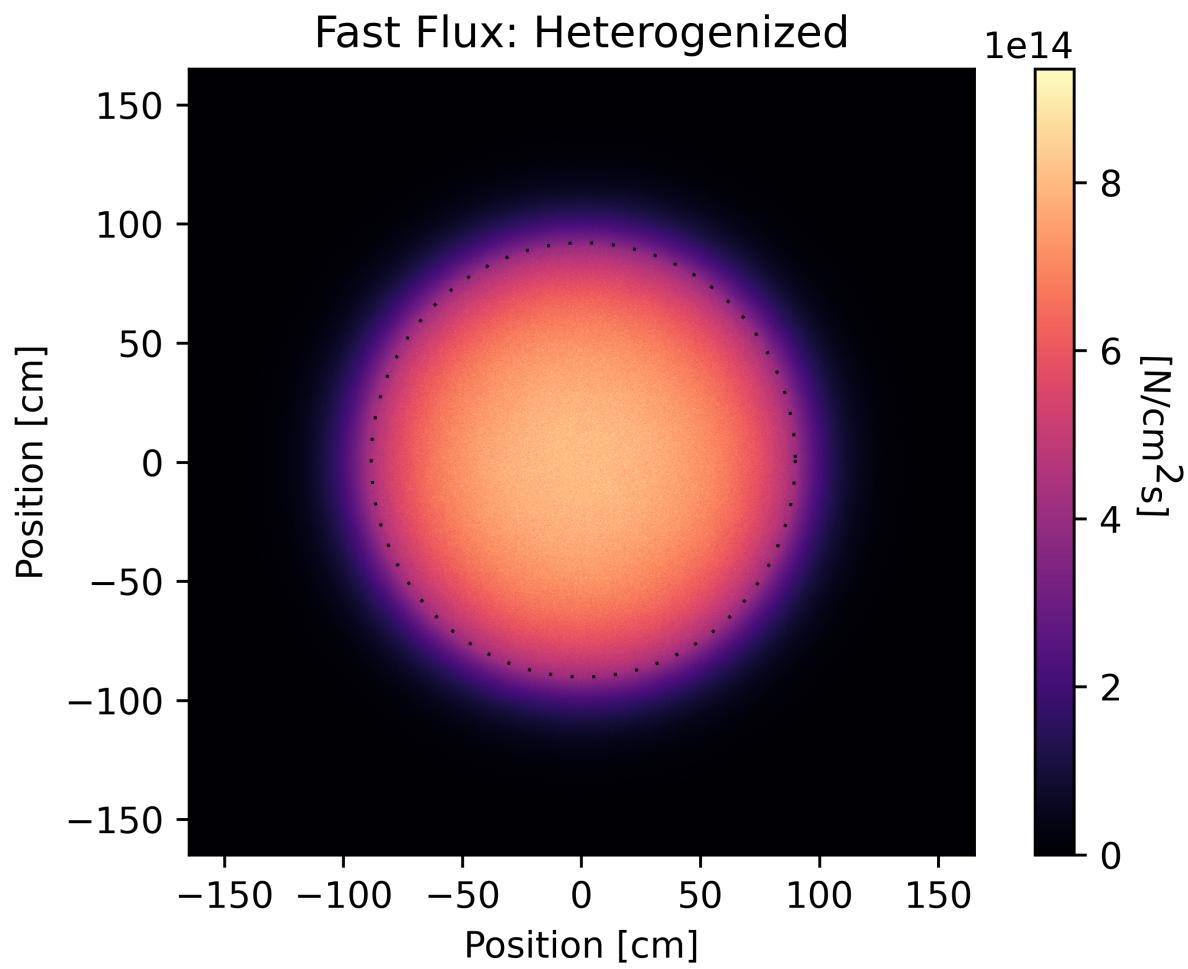


Figure 4.17: Fast Flux in xy Plane in Sangamon20: Heterogenized Pebbles

Compared with Figures 4.16 and 4.17, the edge pebble bands are much less distinct. This is because the homogenized pebbles have the fissile material spread over the entirety of the 2.5 cm radius fueled center. The heterogenized pebbles, meanwhile, may have the same number of fissile atoms, but the concentrate the regions capable of fission in the TRISO kernel. The rest of the pebble consists of its graphite matrix.

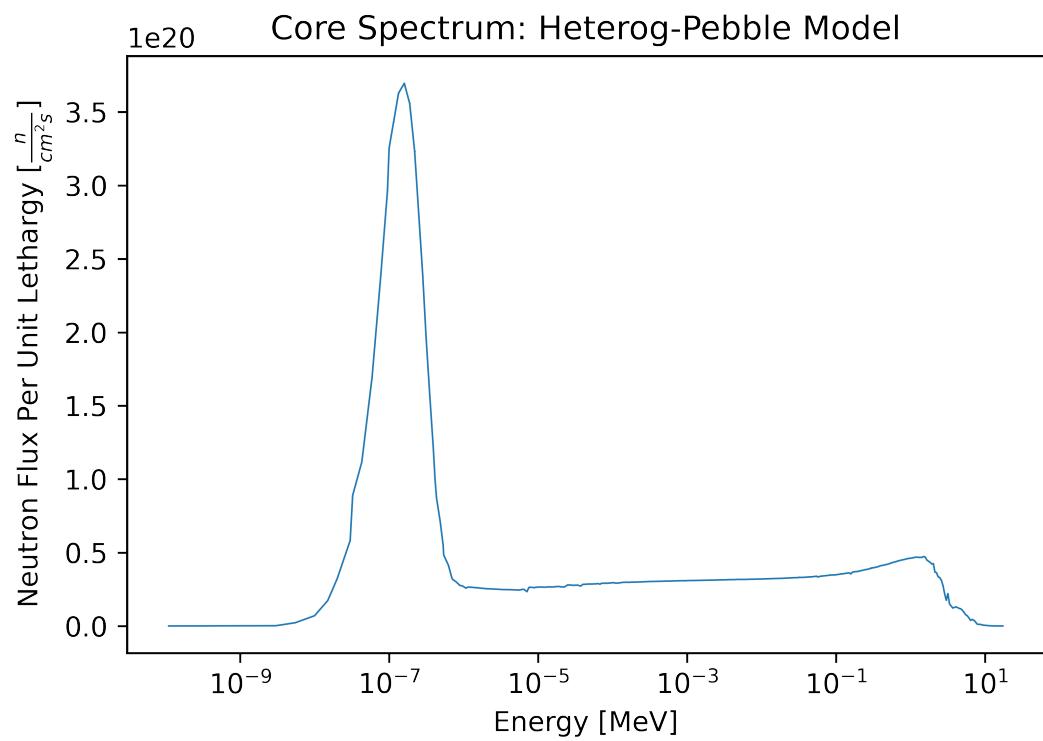


Figure 4.18: Lethargy Adjusted Neutron Flux Energy Spectrum in the Whole-Core for the Heterogenized-Pebble Sangamon20

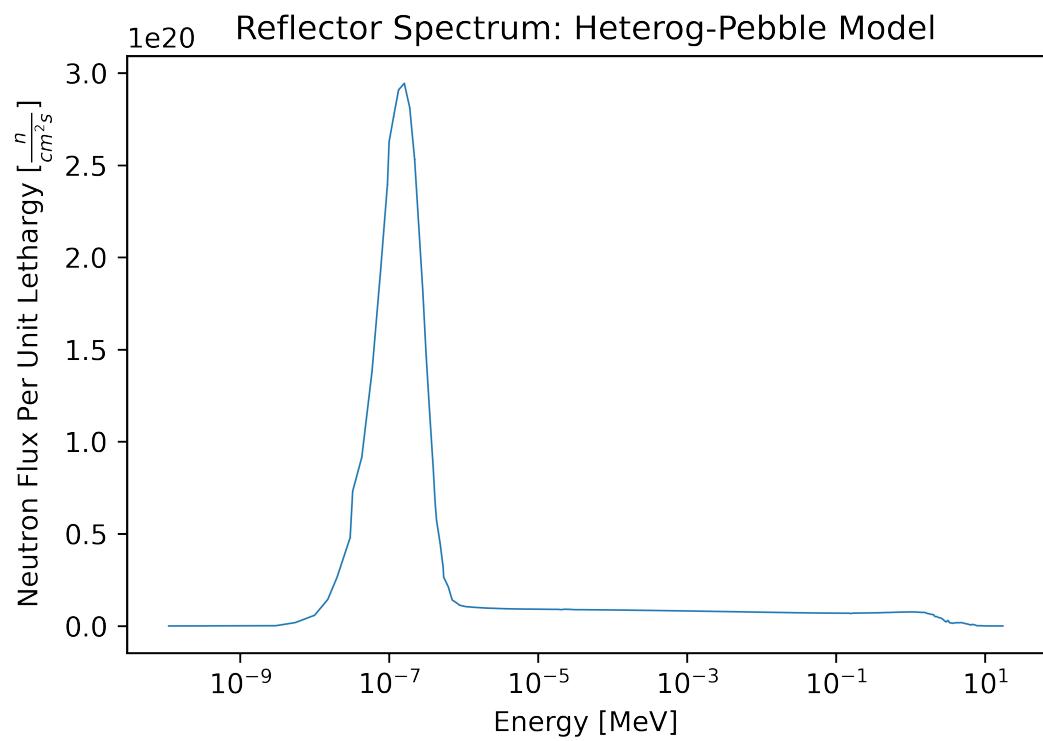


Figure 4.19: Lethargy Adjusted Neutron Flux Energy Spectrum in the Reflector for the Homogenized-Pebble Sangamon20

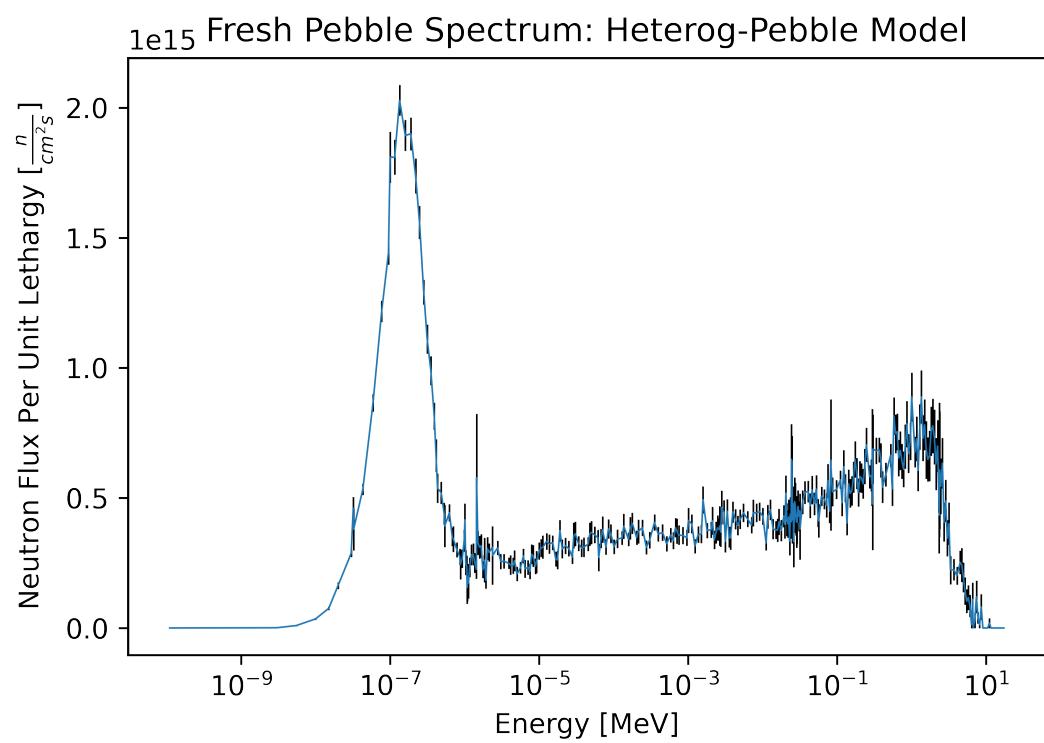


Figure 4.20: Lethargy Adjusted Neutron Flux Energy Spectrum in a Fresh Pebble for the Heterogenized-Pebble Sangamon20

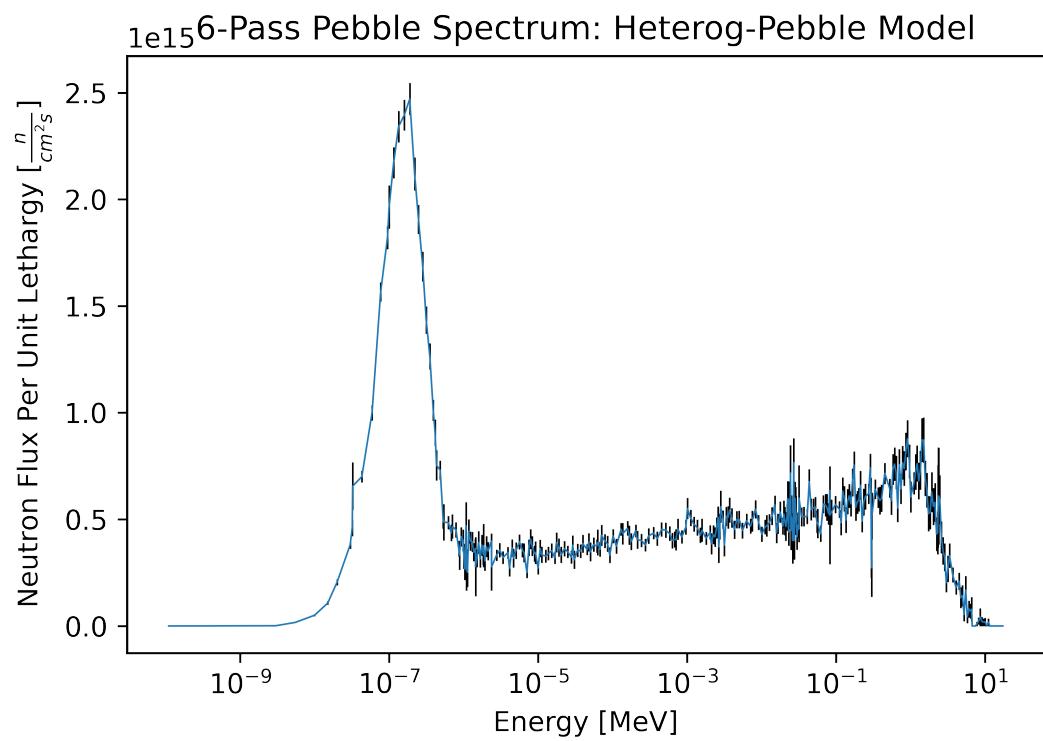


Figure 4.21: Lethargy Adjusted Neutron Flux Energy Spectrum in a Six-Pass Pebble for the Homogenized-Pebble Sangamon2

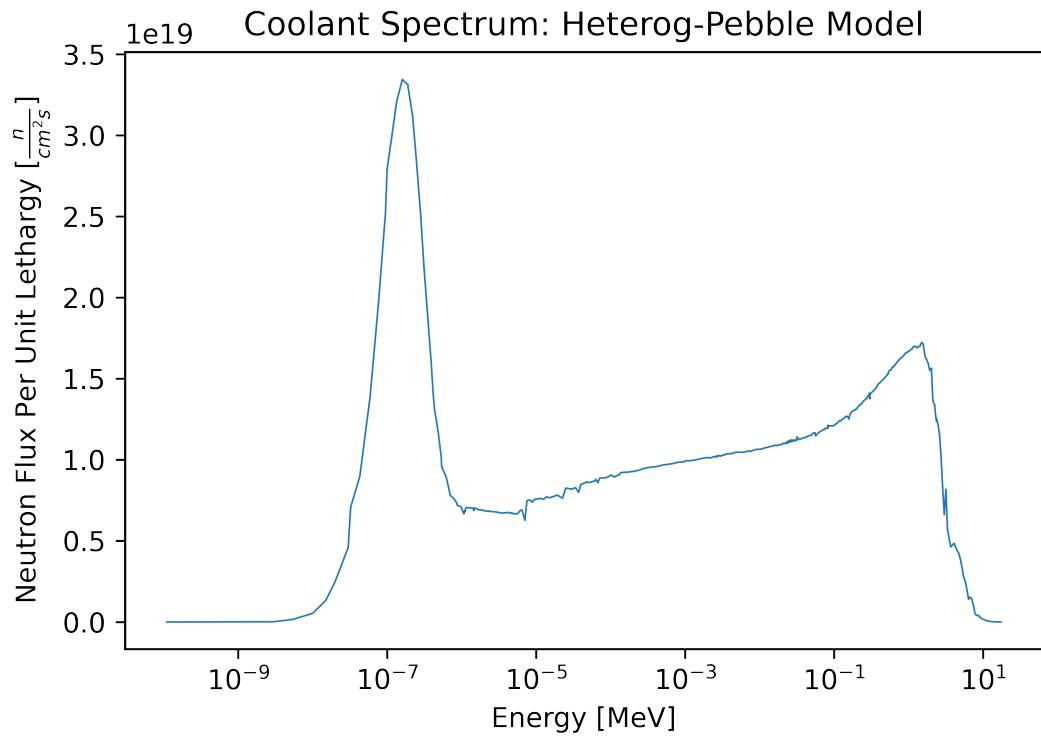


Figure 4.22: Lethargy Adjusted Neutron Flux Energy Spectrum in the Coolant for the Homogenized-Pebble Sangamon20

The spectra for the Sangamon20 core using heterogenized TRISO particles are shown in Figures 4.18 through 4.22, much like the flux profiles, are of a similar morphology. In order to better examine the differences between the homogenized and heterogenized versions, Figures 4.23 and 4.24 plot the simple relative difference for all spectra, and the radial fast and thermal profiles. The relative difference calculation used the following:

$$\Delta i = \frac{i_{\text{homogenized}} - i_{\text{heterogenized}}}{i_{\text{heterogenized}}} \quad (4.2)$$

where

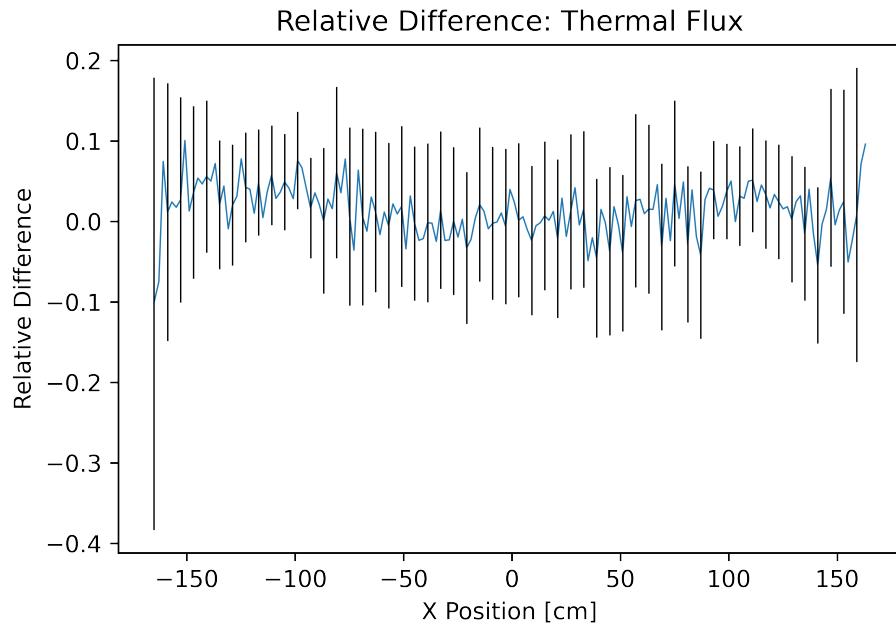
Δi = relative difference for parameter i between homogenized and heterogenized model

$i_{\text{homogenized}}$ = homogenized parameter i

$i_{\text{heterogenized}}$ = heterogenized parameter i

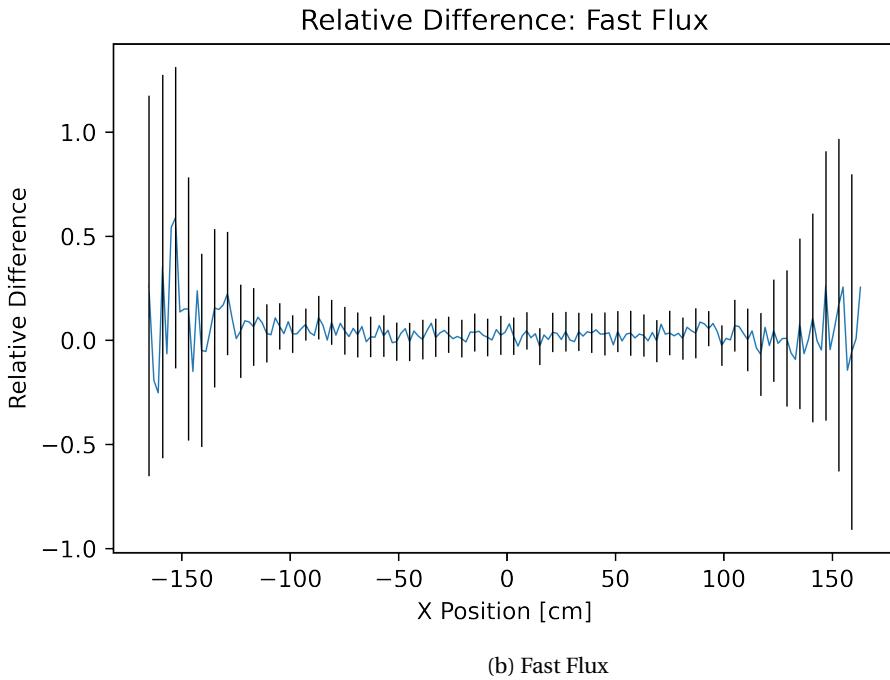
(4.3)

And error calculation followed simple error propagation rules [43].



(a) Thermal Flux

Figure 4.23: Relative Difference in Radial Thermal and Fast Flux Profiles Between Cores Using Homogenized and Heterogenized Pebbles

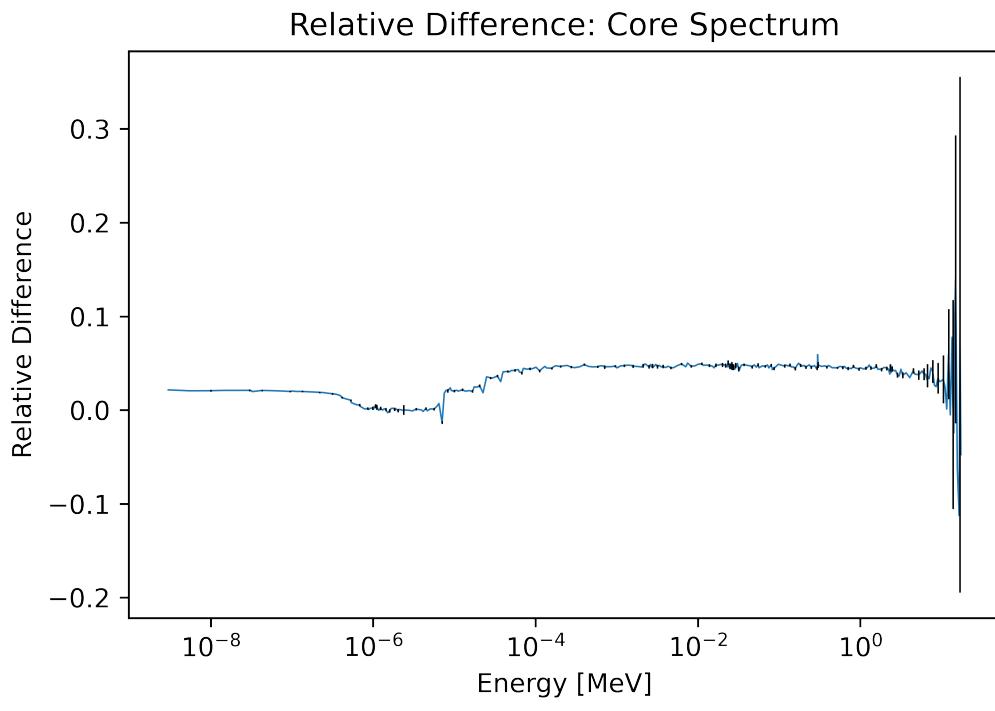


(b) Fast Flux

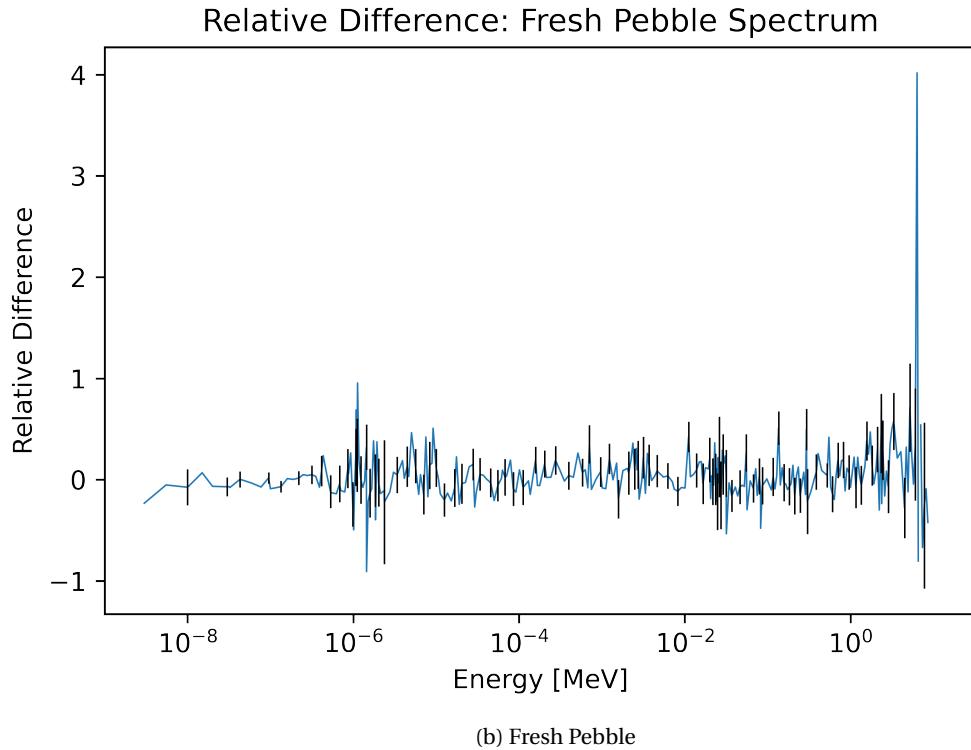
Figure 4.23: Relative Difference in Radial Thermal and Fast Flux Profiles Between Cores Using Homogenized and Heterogenized Pebbles (cont.)

The relative difference in the thermal flux is generally between $\pm 10\%$ for the entire span of the reactor. However, once one accounts for error, it is entirely possible that these differences are wholly accounted for with error alone. The magnitude of the error is fairly constant — except at the edges, where it is much larger. For the fast flux spectrum, the active core region containing the fuel pebbles has a similarly low range of $\pm 10 - 20\%$ relative difference, which is once again accounted for by error. The error on the outer edges in the fast flux plot is much greater than that in the thermal flux, but this is to be expected — as said before, the reflector causes significant thermalization of neutrons entering it, and this means that there are fewer fast neutrons in the reflector to contribute to tallies.

For both the thermal and fast flux profiles, error only worsens on the outermost edges. Overall, Figures 4.23a and 4.23b suggest that the homogenized simulation is slightly over-predicting the magnitude of the flux; however, given the size of the error, these differences do not exist with certainty.

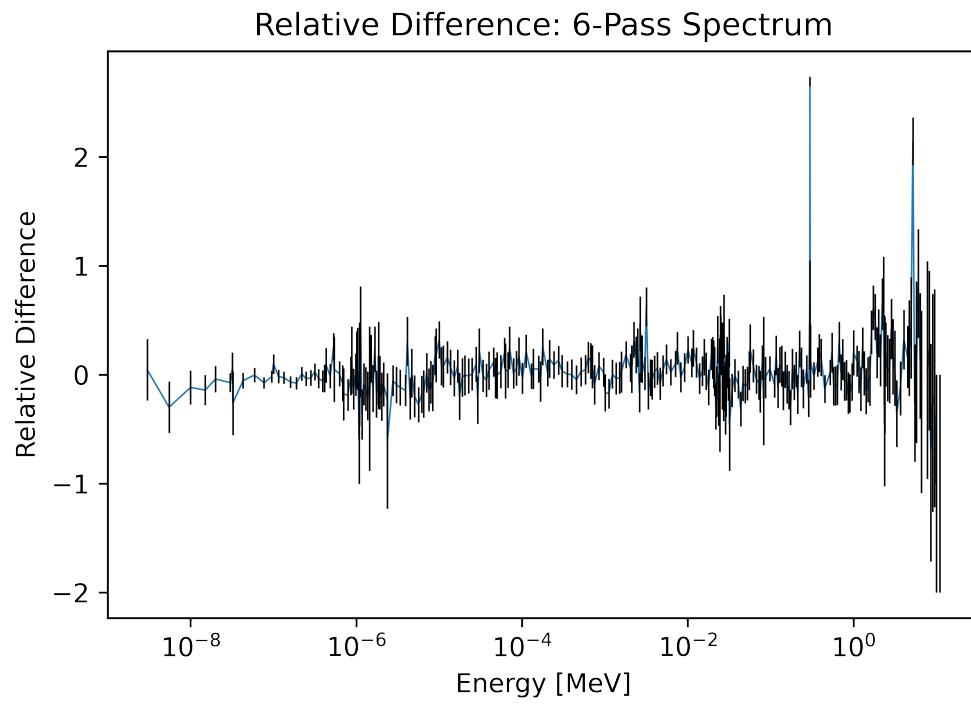


(a) Core

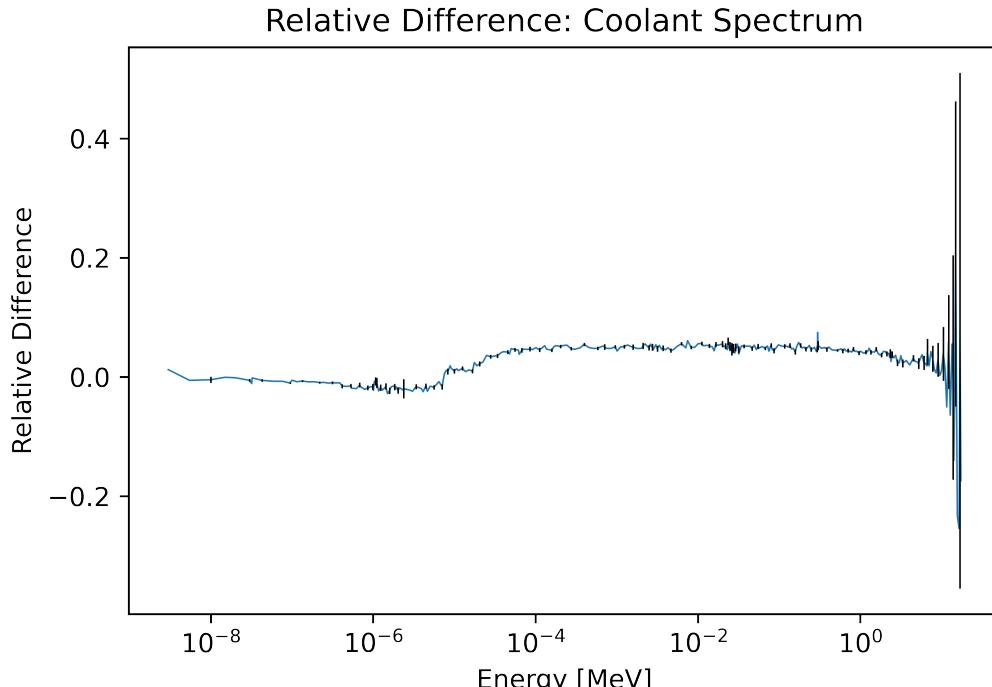


(b) Fresh Pebble

Figure 4.24: Relative Difference in Lethargy Adjusted Neutron Flux Energy Spectra Between Cores using Homogenized and Heterogenized Pebbles



(c) Six-Pass Pebble



(d) Coolant

Figure 4.24: Relative Difference in Lethargy Adjusted Neutron Flux Energy Spectra Between Cores using Homogenized and Heterogenized Pebbles (cont.)

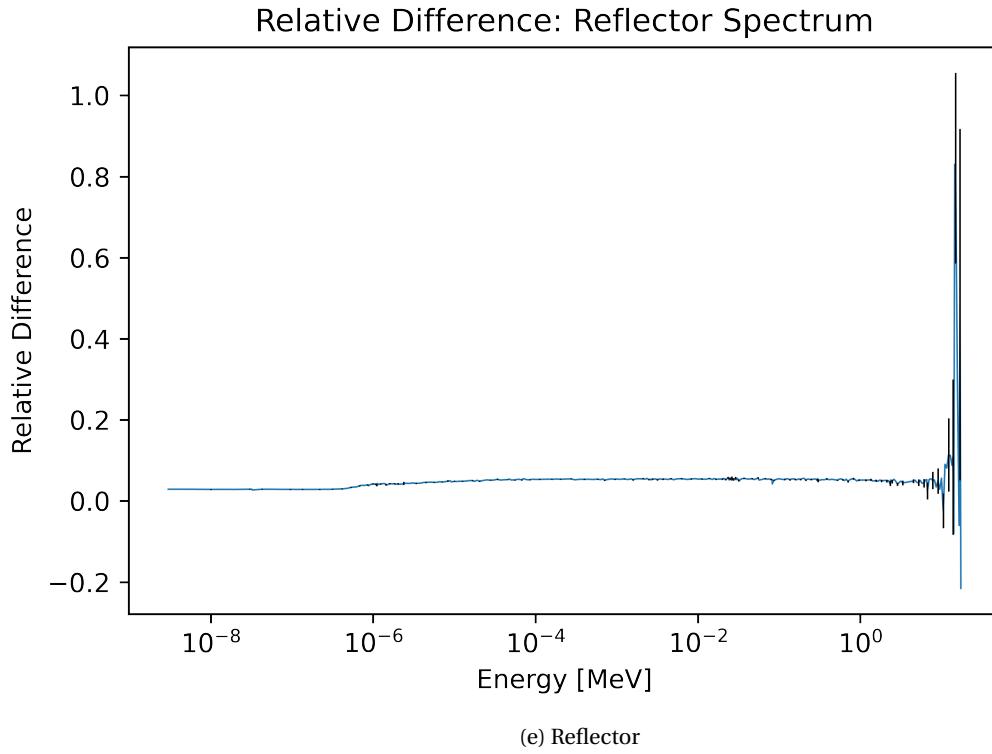


Figure 4.24: Relative Difference in Lethargy Adjusted Neutron Flux Energy Spectra Between Cores using Homogenized and Heterogenized Pebbles (cont.)

Overall, the homogenized model is over-predicting the thermal peak compared with heterogenized in the core spectra by 5%. Around 10×10^{-6} MeV, just after the thermal peak, the two spectra agree before diverging again, this time with a slightly greater disagreement. Unlike Figure 4.23, error alone leaves the relative differences seen in Figure 4.24 unaccounted for (with the exception of the highest neutron energy ranges).

The coolant spectra differed after the thermal peak in a magnitude and shape matching the differences in core spectra. Unlike the core, however, the coolant has much closer agreement at lower energy levels, including at the thermal peak. The reflector shows a slight over estimation for the homogeneous spectra, which is consistent for all but the highest energy levels.

It is in the pebble spectra that we see the most dramatic disagreement. Around the thermal peak, in both Figures 4.24b and 4.24c (note the change in y-axis scale compared to others in Figures 4.18, 4.19, and 4.22), the relative difference spikes; though the error is still substantial in this region compared with the peaks in the relative difference. Between 10×10^{-7} and 5×10^{-2} , the differences are minimal and likely accounted for by noise or error. Between 10×10^{-2} and 10×10^{-1} , the difference has a slight blip, which may be indicative of a fission product with a resonance around this region.

The most dramatic peaks occur in the sixth-pass pebble at 0.2995 MeV, at which point the homogenized reactor is over-predicting the lethargy-adjusted neutron flux by a factor of 2.69. Both the fresh and sixth-pass spectra have another peak at higher energy levels - fresh peaks at 6.3763 MeV, while the sixth-pass spectra has its second peak at 5.2205 MeV. One possibility is that the ^{235}U in the pebble is more likely to undergo fission in a homogenized pebble, which disperses the ^{235}U atoms in what is almost pure graphite.

4.4 Shuffling and Symmetry Tests

Two additional studies look at the effects of assuming a one-sixth core symmetry, and the effects of changing the fuel composition in each pebble, effectively shuffling the pebbles without re-generating their location. All tests use the homogenized pebble assumption as a base.

4.4.1 Effects of Symmetry Assumption

Overall, the effects of using a one-sixth core symmetry were minimal. For both Table 4.1 and Table 4.2, the relative difference between k_{eff} and J^+ are calculated between the value provided in the table, and the same parameter in the Sangamon20 control model (see section 4.2).

Run	k_{eff}	$k_{eff} \% \Delta$	$J^+ [\frac{n}{cm^2 s}]$	$J^+ \% \Delta$
Run 1	1.03990 ± 0.00055	0.0836%	$5.921 \times 10^{11} \pm 8.704 \times 10^{08}$	0.626%
Run 2	1.03979 ± 0.00050	0.0942%	$5.884 \times 10^{11} \pm 8.296 \times 10^{08}$	0.010%
Run 3	1.04150 ± 0.00054	0.0701%	$5.908 \times 10^{11} \pm 7.444 \times 10^{08}$	0.392%
Run 4	1.03927 ± 0.00057	0.144%	$5.910 \times 10^{11} \pm 8.687 \times 10^{08}$	0.425%
Run 5	1.04154 ± 0.00054	0.0740%	$5.884 \times 10^{11} \pm 8.885 \times 10^{08}$	0.010%
Run 6	1.04047 ± 0.00050	0.0288%	$5.888 \times 10^{11} \pm 8.478 \times 10^{08}$	0.057%

Table 4.1: Symmetry Run Summary

Figure 6.22 provides cross-sections of the geometry, and fission rate/thermal flux meshes for the one-sixth core symmetry test. The fission rate mesh naturally exhibits a six-part repeating pattern, and still shows the banding patterns on the outer edges.

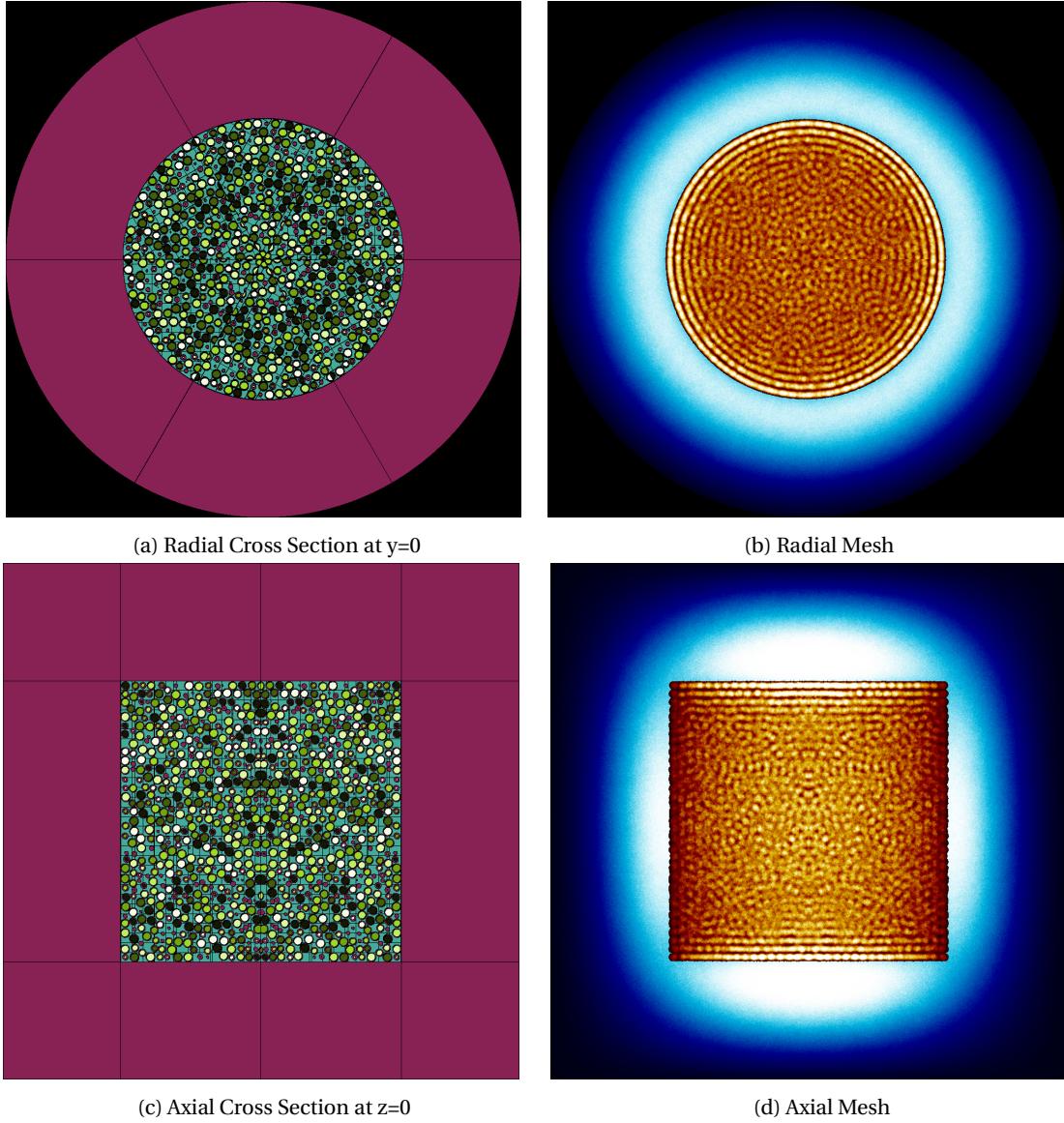


Figure 4.25: Sensitivity Analysis: $\frac{1}{6}$ Symmetry Using the Portion of the Core Between $0^\circ - 60^\circ$

One point of interest is the degree to which the region from 0 to 60 degrees matches the same region in the control fission rate mesh. An image subtraction program generated Figure 4.26 by subtracting the radial meshes for the control (Figure 4.3b) and first symmetry test (Figure 4.25b).

Within the region between 0 and 60 degrees, the two meshes are almost identical, pixel for pixel. While this might be unsurprising in the center of this region, the perfect match towards the edges of it are less so. As a reminder, the symmetry tests all use a one-sixth symmetry, and a periodic boundary condition, i.e., if a neutron leaves the slice on one side, it re-enters the slice on the other. In effect, the edges of the 0 to 60 degree slice in the symmetry test are seeing entirely different materials, compared with the control. The edges in 4.26 are not a gradient, but

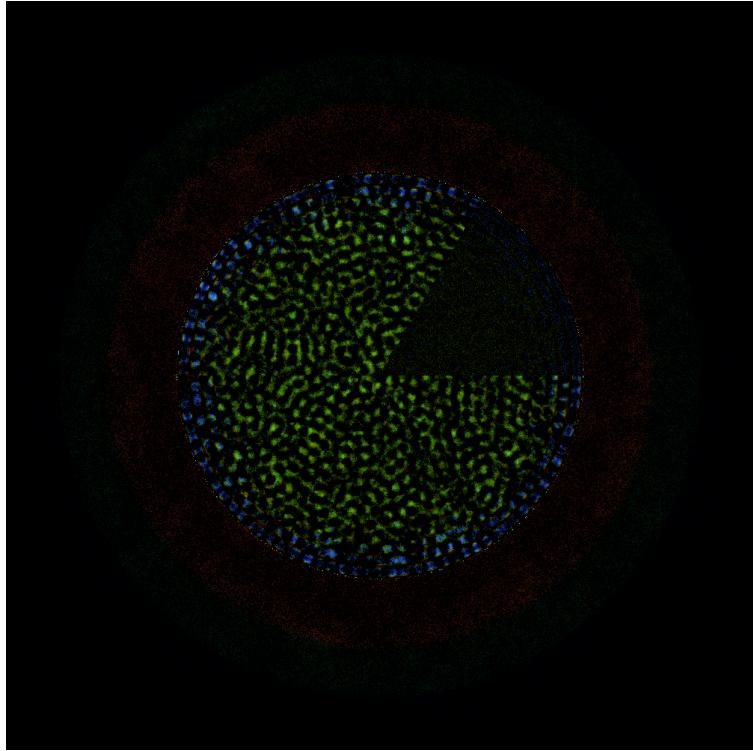


Figure 4.26: An Image Generated by Subtracting 4.25b from 4.3b.

rather a hard line, which may suggest that with proper mixing nearest-neighbor pebbles have a relatively lesser impact on core parameters. However, note that Sangamon20 uses only fuel pebbles, and this observation may be false in a reactor design using, for example, absorber pebbles containing something such as boron, or inert pebbles at the edge to protect the reflector. For the full results of all symmetry tests, see section 6.2.

4.4.2 Effects of Pebble Shuffling

The final test on the effects of changes to core modeling is another test of consistency between similar HTGR designs with a different pebble configurations. Rather than re-generate the pebble locations several times, the 'shuffling' test simply reassigns each pebble with a different fuel composition (creating a new input file). For example, the pebbles that were once fresh are now first-pass, the first pass pebbles are now second-pass, and so on. The manual shuffling followed the process outlined in section 3.8, Table 3.5, and the results of this test are in Table 4.2.

Run	k_{eff}	$k_{eff} \%\Delta$	$J^+ [\frac{n}{cm^2 s}]$	$J^+ \%\Delta$
Run 1	1.03994 ± 0.00054	0.0797%	$5.897 \times 10^{11} \pm 8.668 \times 10^{08}$	0.211%
Run 2	1.03999 ± 0.00055	0.0749%	$5.902 \times 10^{11} \pm 8.086 \times 10^{08}$	0.295%
Run 3	1.04002 ± 0.00053	0.0721%	$5.896 \times 10^{11} \pm 8.490 \times 10^{08}$	0.192%
Run 4	1.04103 ± 0.00057	0.0249%	$5.884 \times 10^{11} \pm 9.355 \times 10^{08}$	0.013%
Run 5	1.03960 ± 0.00053	0.112%	$5.904 \times 10^{11} \pm 8.443 \times 10^{08}$	0.329%
Run 6	1.04014 ± 0.00057	0.0605%	$5.898 \times 10^{11} \pm 7.726 \times 10^{08}$	0.227%

Table 4.2: Shuffling Run Summary

Overall, much like the symmetry test, re-mixing the pebbles had little effect on overall results. Likely, provided the pebbles are sufficiently mixed, and no 'pockets' of like pebbles exist, designs that are otherwise identical should provide similar results. For all geometry cross-sections and thermal flux/fission rate mesh images, and the results of image difference for each run, see section 6.3.

Chapter 5

Conclusion

This chapter provides a synopsis of this work. The first section gives a general summary of the results from the heterogenization section 4.3, symmetry (see subsection 4.4.1) and shuffling (see subsection 4.4.2) and discussion. The second, and final, section covers suggested future work

5.1 Summary and Discussion

Previous work in HTGR pebble-bed modeling noted that the specific lattice arrangement used had little effect [15], [14], [42]. The pebble-shuffling and symmetry tests support this observation in regards to a random arrangement of the pebbles.

The symmetry test showed that for minimal banding — areas of like pebbles creating streaks and rings once reflected — the difference between a full core model and one using symmetry to simplify is between 0.63% and 0.01% in the outward neutron current with an average of 0.25%, and between 0.15% and 0.03% for k_{eff} with an average of 0.082%. Additionally, otherwise-identical models with a well-mixed core and different dispersal of pebbles differ between 0.33% and 0.013% in the outward current at the outer reflector edge with an average of 0.21%, and between 0.11% and 0.025% in k_{eff} with an average of 0.072%.

This is greater than the uncertainty of either the outward current or k_{eff} , which are about 0.14% and 0.05% for the symmetry assumption, respectively, and 0.14% and 0.05% in the shuffling test, respectively, in the uppermost ranges of error, but less than or equal to the uncertainty in the lower ranges. For other pebble bed gas reactors, this suggests that one does not need to re-create the same reactor over and over with slightly different pebble arrangements in order to accurately characterize a core. However, this may not remain true if the random pebble arrangement happens to cause similar pebble burnups to "lump" together, as shown by the upper ranges of error — especially in the symmetry test — being greater than error alone in some runs.

The heterogenization tests highlight the need for an accurate representation of TRISO particles. While the overall differences between the fast and thermal flux profiles are within error, the homogenized pebbles will under-predict k_{eff} by more than 4.0%, while over-predicting the magnitude of the neutron energy lethargy-adjusted flux core

spectrum by as much as 5.0% at energies greater than 1×10^{-04} [MeV]. The most dramatic changes to spectra are within the pebbles themselves, where high-energy neutron peaks are over-estimated in the fresh and sixth-pass pebbles by a factor of 2-4. However, the total outward neutron current, used to gauge the effectiveness of the reflector, differed by only 0.349%. This is likely because the reflector is thick enough to minimize fast neutron leakage, which prevents the fast flux changes (see Figure 4.23b) in the active core from affecting the outer regions of the reflector. The thermal flux isn't changed to a degree unexplained by error (see Figure 4.23a), so the thermal neutron contribution to outward neutron current should be similar to that in the control as well.

For isotopic inventories, most isotopes either increased or decreased at a uniform rate with each pass through the core. However, some isotopes, such as ^{239}Pu , reach a peak concentration in MOL, and subsequently decline. When choosing a multi-pass cycle over an Once Through Then Out (OTTO) fuel cycle, it is important to remember this behavior in the case of fuel failure that may require ejecting a pebble before its final pass. This behavior also means that the pebble dust that accumulates in the reactor core and gas circulation loops will likely have a higher ^{239}Pu concentration than in spent fuel pebbles, as all pebble burnup states will contribute to the dust.

5.2 Future Work

The symmetry test showed that, with random mixing, simplifying the simulation by approximating the whole-core with a $\frac{1}{6}$ slice had minimal effects on the current and k_{eff} . However, the 'banding' and petal-like pebble patterns this symmetry creates highlights a potential issue, however unlikely. What if the random pebble dispersal happens to lump a number of the same or similar burnup pebbles together? How would this affect a whole core model, or one using symmetry? Future work could explore the effects of pebble 'lumping', such as the size of pebble-lump needed before it causes a noticeable effect, and what magnitude of effect can be expected.

Additionally, this design used an infinite lattice of like pebbles in the depletion model to arrive at an equilibrium composition. It is possible to improve the accuracy of the equilibrium composition by using other methods. By tracking compositions over time in the actual core, as opposed to an infinite lattice, or splitting the core into axial layers to track the pebble isotopic inventory as a function of the number of passes and current height in the core. This would provide higher-fidelity, time-dependent data on pebble isotopes. From there, an exploration of the resulting source term based on models of varying fidelity could provide insight on the accuracy of fuel composition data required to accurately determine source term and accident consequences.

The current design is slightly supercritical, and one could explore adding in an additional "half-pass" — i.e., half of the sixth-pass pebbles go for a seventh pass, and the other half replaced with fresh pebbles. This change would mean that there are half as many fresh pebbles in the core as there are currently, and the 7th pass pebbles,

as they continue to burn in the core, would build up a higher concentration of neutron poisons and other fission products. This would likely change the magnitude of the fast flux — though it likely wouldn't change the overall shape — and it would have an effect on the coolant and whole-core energy spectra, likely shifting it to lower energy ranges. Alternatively, one could explore the addition of neutron-absorber pebbles to handle excess reactivity.

Finally, the pebble dispersal method used here does not account for gravity, which would make the pebbles settle closer together. Without using a core that has a diameter which is an integer multiple of the pebble diameter, it is not possible to get a perfect close-pack arrangement (shaking a vessel will help achieve closer packing, but this is not possible here). One could simulate the effects of gravity by dispersing the pebbles over a volume with a slightly shorter height, instead of the full height. One could also split the core into axial layers, and apply a packing fraction equal to the theoretical maximum at the bottom-most layers, and reduce packing fraction as one moves up through the layers. This would require careful tracking of the number of pebbles in each layer if the entire core uses a target number of fuel pebbles, but may provide a better estimate of pebble behavior in a system that does not otherwise incorporate gravity. However, it is important to note that at a packing fraction of around 0.58, the model is already approaching the theoretical maximum packing fraction, so the difference this would make may be minimal. At the same time, as pointed out in [14], even small changes to packing fraction and pebble arrangement may have a significant impact in small, low-leakage systems (such as a well-reflected SMR or microreactor), which is why exploring the effect the aforementioned changes may have could be important, even if the pebble arrangement doesn't appear to change much.

Chapter 6

Appendices

6.1 Image Difference and RGB Color

To help explain the color difference plots later in the Appendix, it may be helpful to go into further depth on RGB (red, green, blue) based colors and how the individual values correspond to colors when mixed.

In the RGB color format, values for red, green, and blue can range from 0 to 255. The higher the value for a color, the more of it is present in the resulting color. If the values for red, green, and blue are the same, then the resulting color is a shade of grey. If all values are set to their maximum, 255, then the result is pure white. If all values are 0, then the result is pure black. In general, colors with low RGB values are darker than ones with greater RGB values.

To understand why the differences in the active core are in green (see Figure 6.5 for an example), it is useful to revisit color theory and complementary colors. The fission rate meshes are shown in a hot color map, which ranges in color from an almost-white shade of yellow, to very dark browns. In between these maximum and minimum shades are varying shades of yellow, orange, and brown. To create a shade of yellow in RGB format, one uses a large amount of red and green. To create the sort of almost-white yellow, one simply takes the base yellow, with large amounts of red and green, and increases the blue value (which, as described before, will transition the color to a lighter shade as all three RGB values approach the maximum of 255). To move from yellow to an orangey-brown, one shifts the green value down. Lowering red and green while keeping blue at a low value produces the darkest shades of brown seen in the color map.

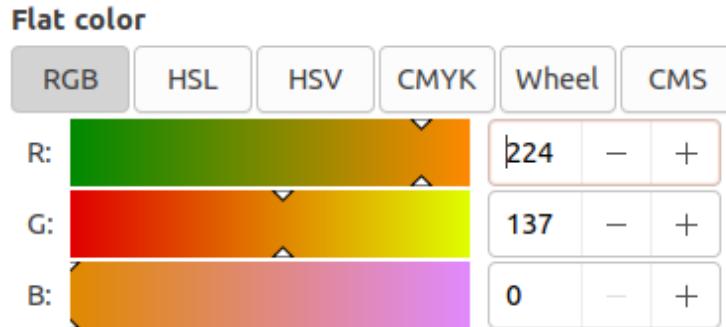


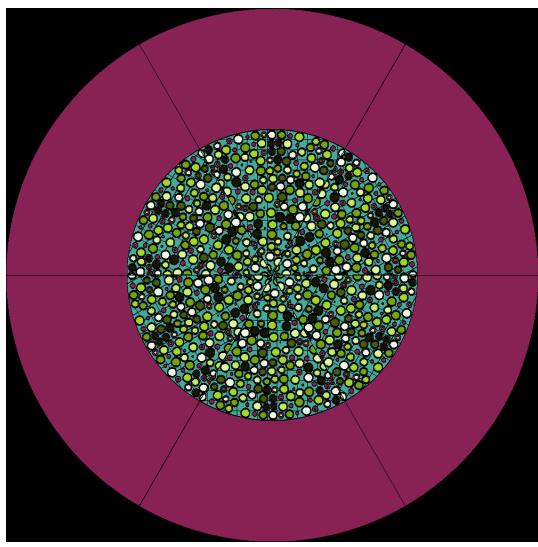
Figure 6.1: An example of RGB values. If the value for red and blue are held constant, shifting the value for green up or down shifts the resulting color along the color gradient to the left of the green value, which ranges from red to yellow. The arrows on the green gradient indicate what the current color is. As one can see, moving the slider to the right - increasing the value of green - will make the color more yellow, while moving it to the left, or decreasing the green level, will shift it towards orange and red.

Figure 6.1 gives an example of selecting a color using RGB values. Image difference works by subtracting the RGB values from each other - for example, subtracting (200, 150, 50) from (100, 200, 75) results in (100, 50, 25). Absolute values are used because negative values don't exist in RGB colors. So, when two colors which have contrasting values of green, and similar values of red and blue, the result is, of course, a shade of green. The image difference results in the "banded" regions at the outermost edges of the active core shift to blue from green simply because in the original images this region is already in the yellow to white color range, and so the only RGB value that changes is blue.

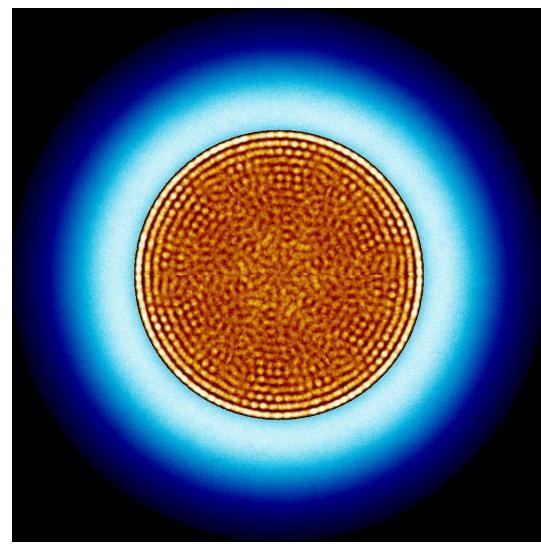
One can image the two extremes that an image difference could give - pure black, or RGB (0, 0, 0) means the two images were identical at that particular pixel. Meanwhile, pure white — (255, 255, 255) — is the greatest possible difference that could exist. Therefore, when interpreting the image difference results in Appendix A and Appendix B, it is important to keep in mind that the specific *color* the differences are shown in — usually green, but also blue or, rarely, red — are far less important than how bright, or intense, these colors are.

6.2 Appendix A: Symmetry Test

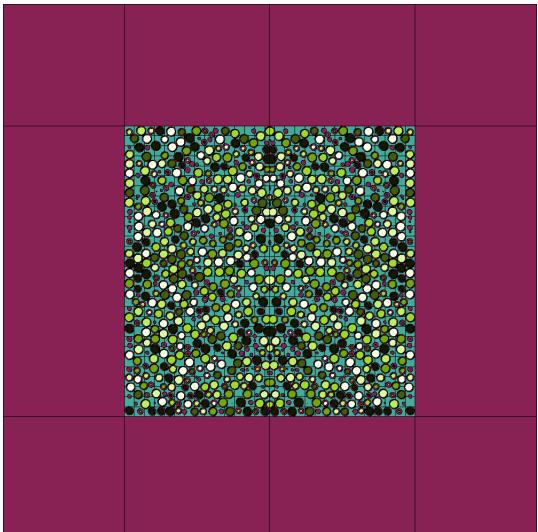
Appendix A contains the geometry cross sections, fission rate/thermal flux meshes, and image difference results from the other symmetry tests, corresponding to Run 2 through Run 5 in Figure 3.6. These symmetry test use an otherwise identical core model and set of run parameters (see section 3.2) for the Sangamon20 core model. Image difference for each run compares to the Sangamon20 control model results.



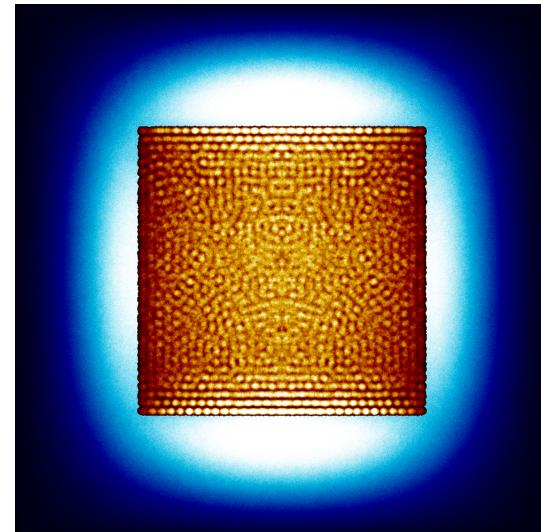
(a) Radial Cross Section at $y=0$



(b) Radial Mesh



(c) Axial Cross Section at $z=0$



(d) Axial Mesh

Figure 6.2: Sensitivity Analysis: $\frac{1}{6}$ Symmetry Using the Portion of the Core Between $60^\circ - 120^\circ$

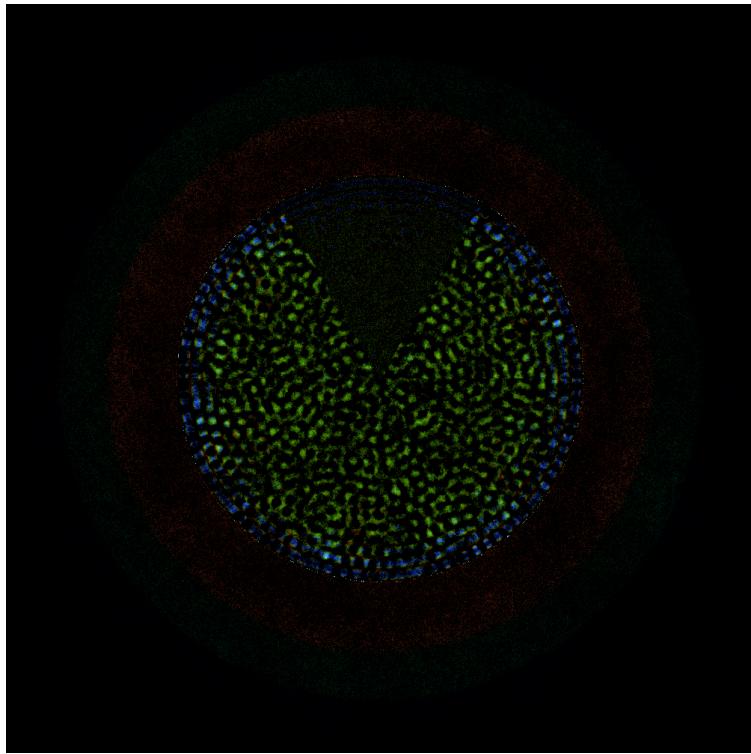
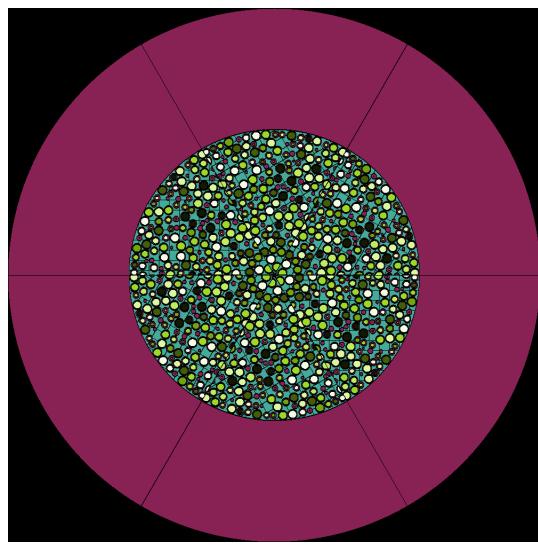
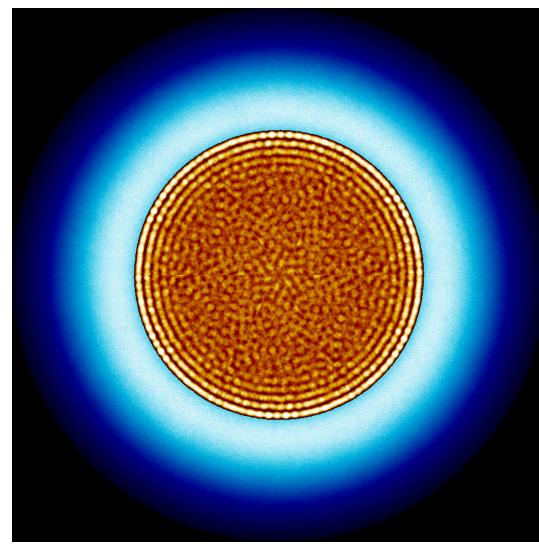


Figure 6.3: An Image Generated by Subtracting 6.2b from 4.3b.

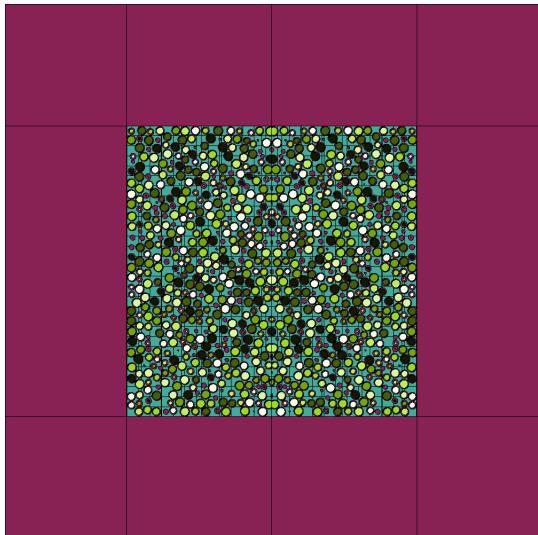
Figure ?? provides fission rate and thermal flux visualization meshes for the symmetry test using the 60 - 120 degree slice. Figure 6.3 is the result of using image-difference between the control's full-core radial mesh and the symmetry test's mesh.



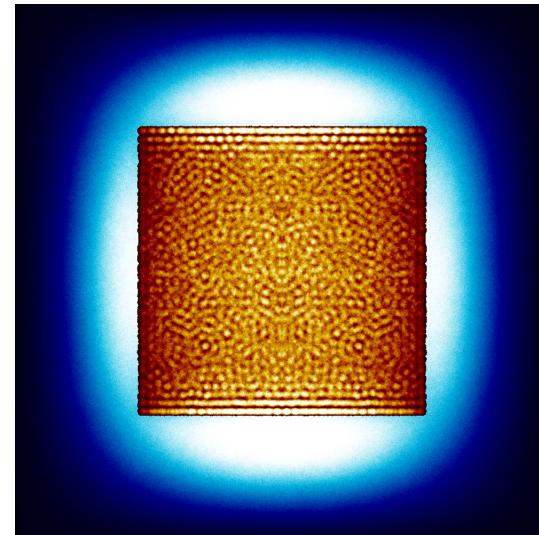
(a) Radial Cross Section at $y=0$



(b) Radial Mesh



(c) Axial Cross Section at $z=0$



(d) Axial Mesh

Figure 6.4: Sensitivity Analysis: $\frac{1}{6}$ Symmetry Using the Portion of the Core Between $120^\circ - 180^\circ$

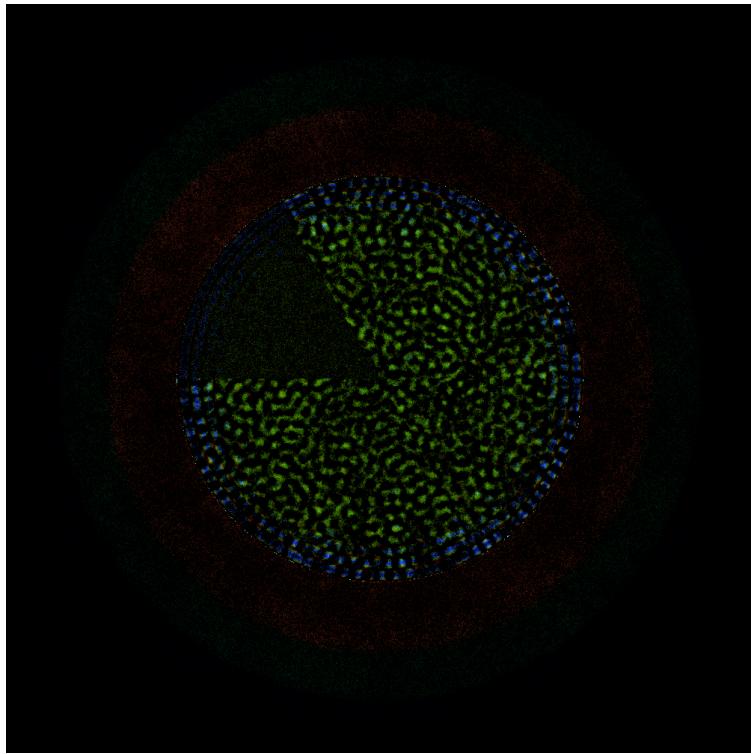
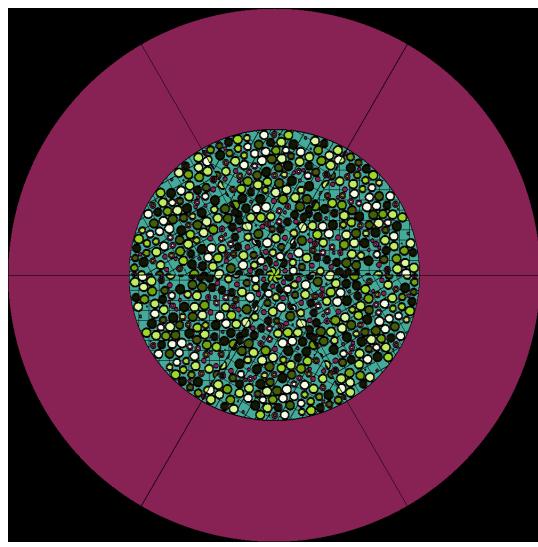
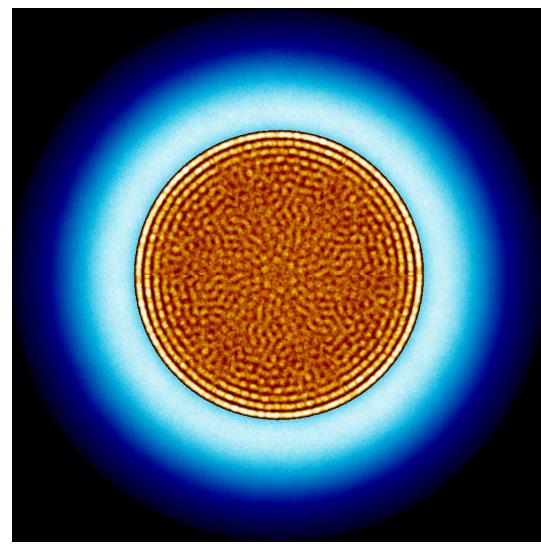


Figure 6.5: An Image Generated by Subtracting 6.4b from 4.3b.

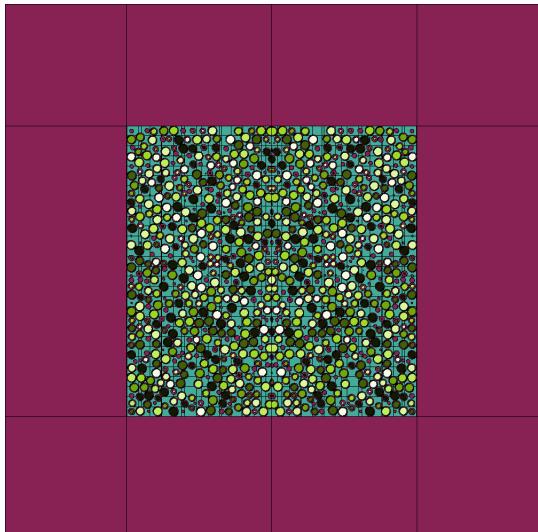
Figure 6.4 provides fission rate and thermal flux visualization meshes for the symmetry test using the 120 - 180 degree slice. Figure 6.5 is the result of using image-difference between the control's full-core radial mesh and the symmetry test's mesh.



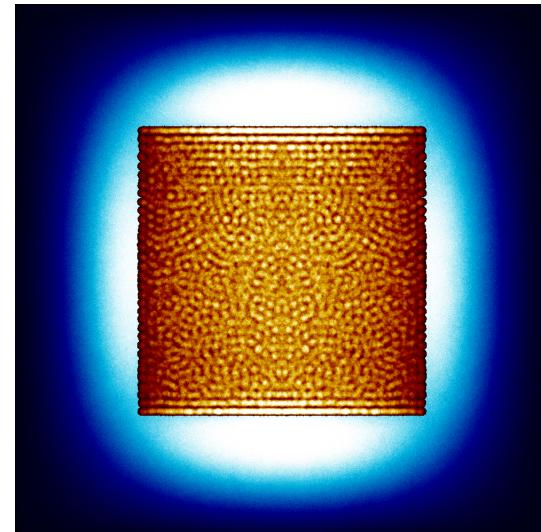
(a) Radial Cross Section at $y=0$



(b) Radial Mesh



(c) Axial Cross Section at $z=0$



(d) Axial Mesh

Figure 6.6: Sensitivity Analysis: $\frac{1}{6}$ Symmetry Using the Portion of the Core Between $180^\circ - 240^\circ$

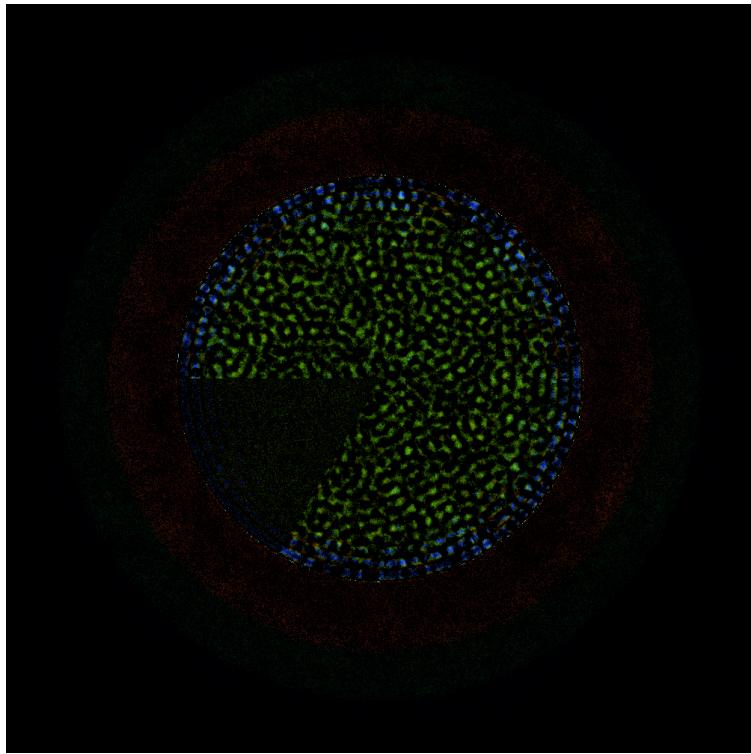
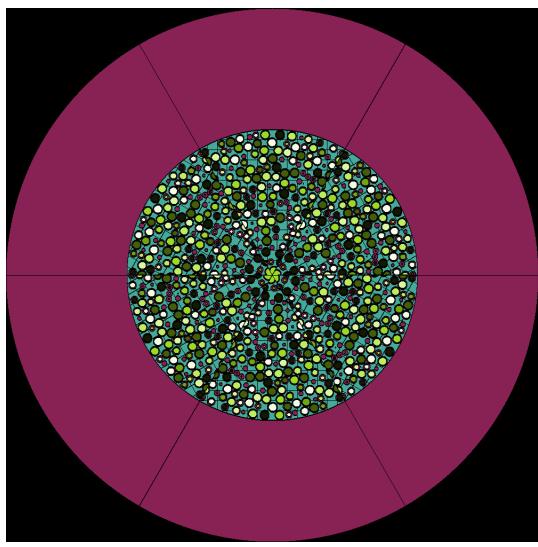
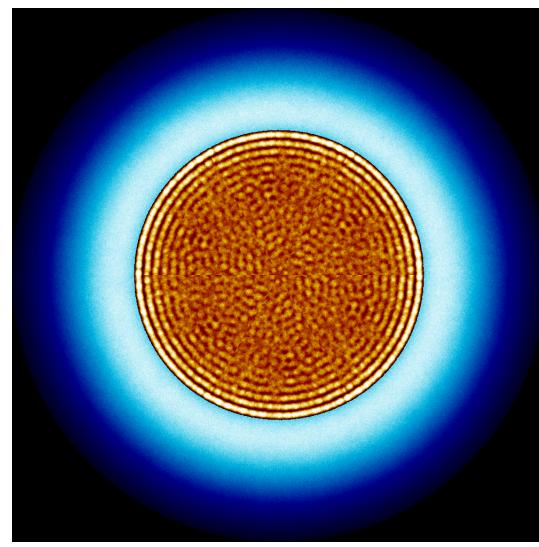


Figure 6.7: An Image Generated by Subtracting 6.6b from 4.3b.

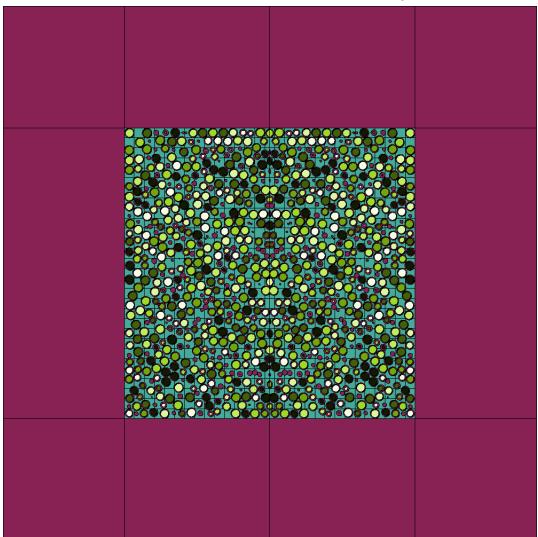
Figure 6.6 provides fission rate and thermal flux visualization meshes for the symmetry test using the 180 - 240 degree slice. Figure 6.7 is the result of using image-difference between the control's full-core radial mesh and the symmetry test's mesh.



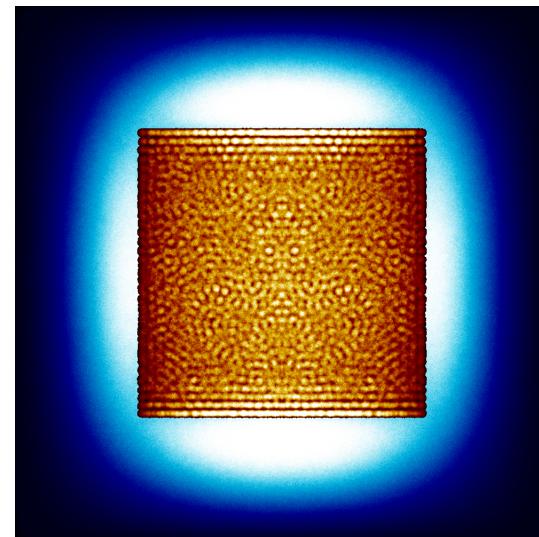
(a) Radial Cross Section at $y=0$



(b) Radial Mesh



(c) Axial Cross Section at $z=0$



(d) Axial Mesh

Figure 6.8: Sensitivity Analysis: $\frac{1}{6}$ Symmetry Using the Portion of the Core Between $240^\circ - 300^\circ$

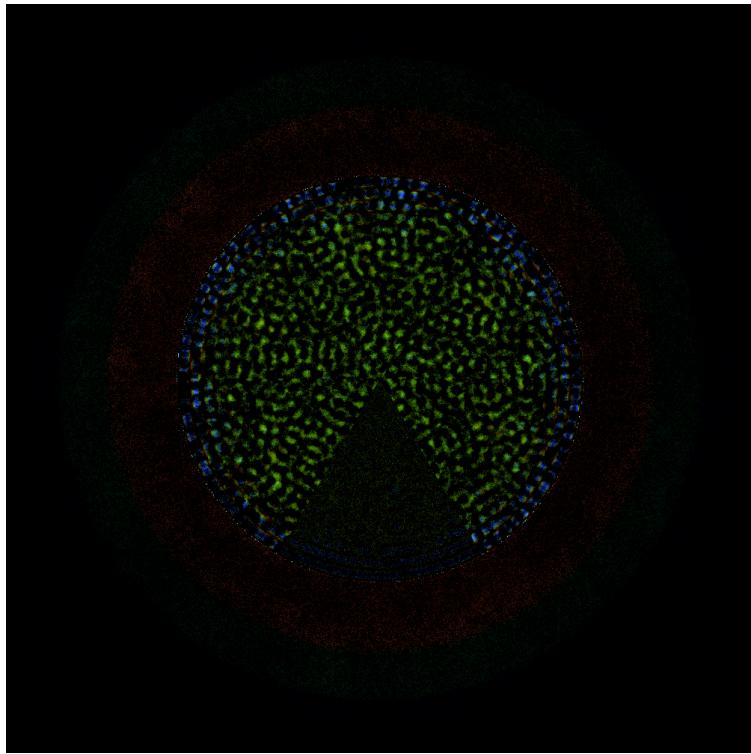
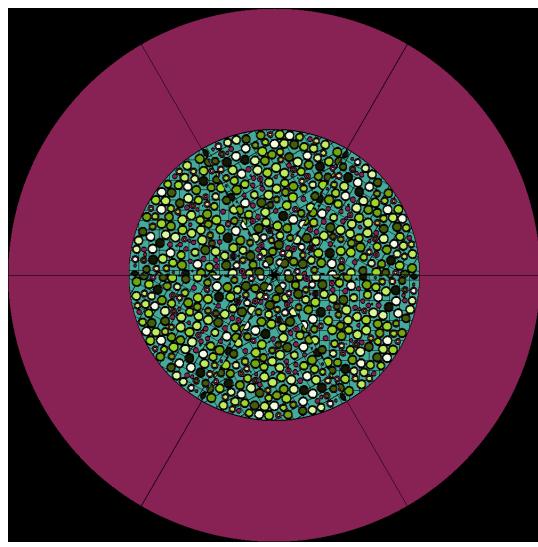
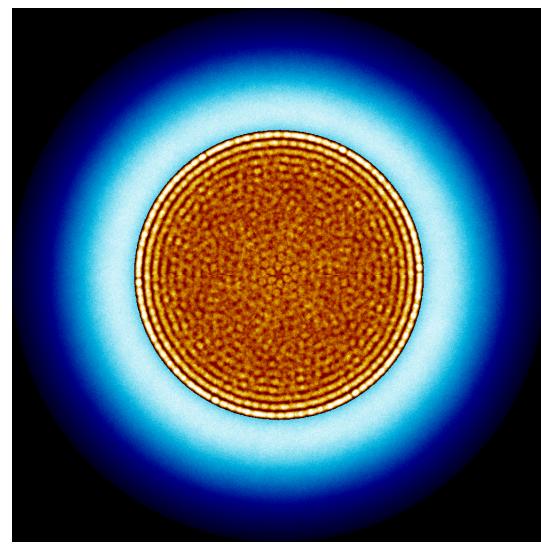


Figure 6.9: An Image Generated by Subtracting 6.8b from 4.3b.

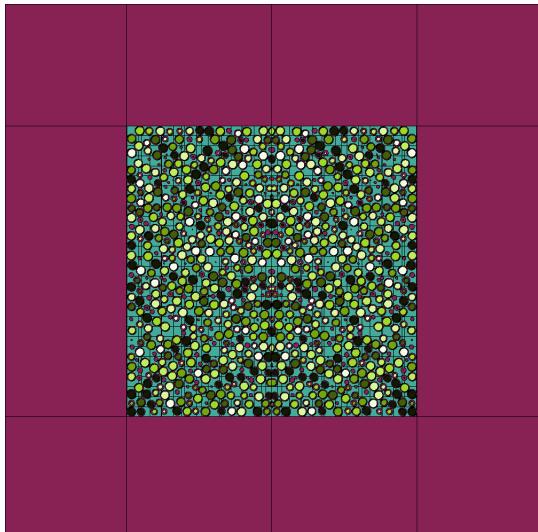
Figure 6.8 provides fission rate and thermal flux visualization meshes for the symmetry test using the 240 - 300 degree slice. Figure 6.9 is the result of using image-difference between the control's full-core radial mesh and the symmetry test's mesh.



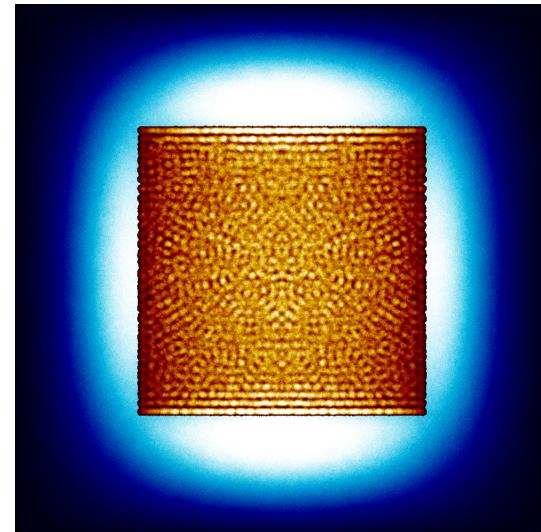
(a) Radial Cross Section at $y=0$



(b) Radial Mesh



(c) Axial Cross Section at $z=0$



(d) Axial Mesh

Figure 6.10: Sensitivity Analysis: $\frac{1}{6}$ Symmetry Using the Portion of the Core Between $300^\circ - 360^\circ$

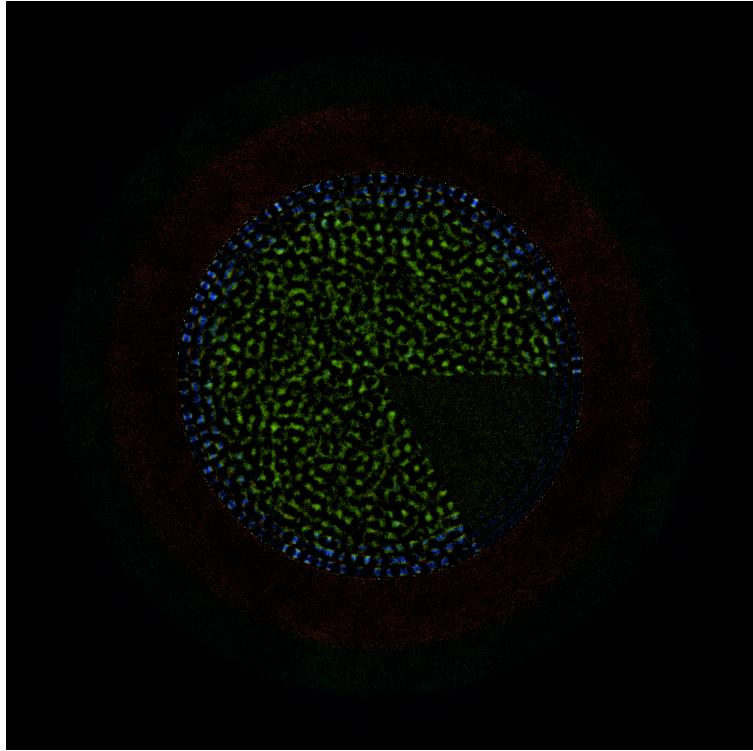


Figure 6.11: An Image Generated by Subtracting 6.10b from 4.3b.

Figure 6.10 provides fission rate and thermal flux visualization meshes for the symmetry test using the 300 - 360 degree slice. Figure 6.11 is the result of using image-difference between the control's full-core radial mesh and the symmetry test's mesh.

In each of the image difference results, the section of the core the symmetry assumption uses — for example, the portion of Figure 6.3 in the sector from 60° - 120° — is very dark. This means that this region has very little difference between it and the same sector on the control model result. The boundaries of these sectors in the image difference are also hard lines, not gradients, which suggests that the neutronics (specifically the fission rate) within and around pebbles closest to the boundary of the sector might not be as significantly impacted by their neighbor pebbles "changing" as expected. The image difference results also show very little difference in the reflector region, which makes sense, as the reflector is uniform. However, this does indicate that there wasn't a local peak in thermal flux due to, say, a mass of fresh pebbles in the representative slice. If there were such a spike, there would likely be repeating regions of brighter "hotspots" in the reflector everywhere *except* the representative sector used in the symmetry assumption.

6.3 Appendix B: Shuffle Test

Appendix B contains the geometry cross sections, fission rate/thermal flux meshes, and image difference results from the shuffling tests (see section 3.8, Table 3.5)

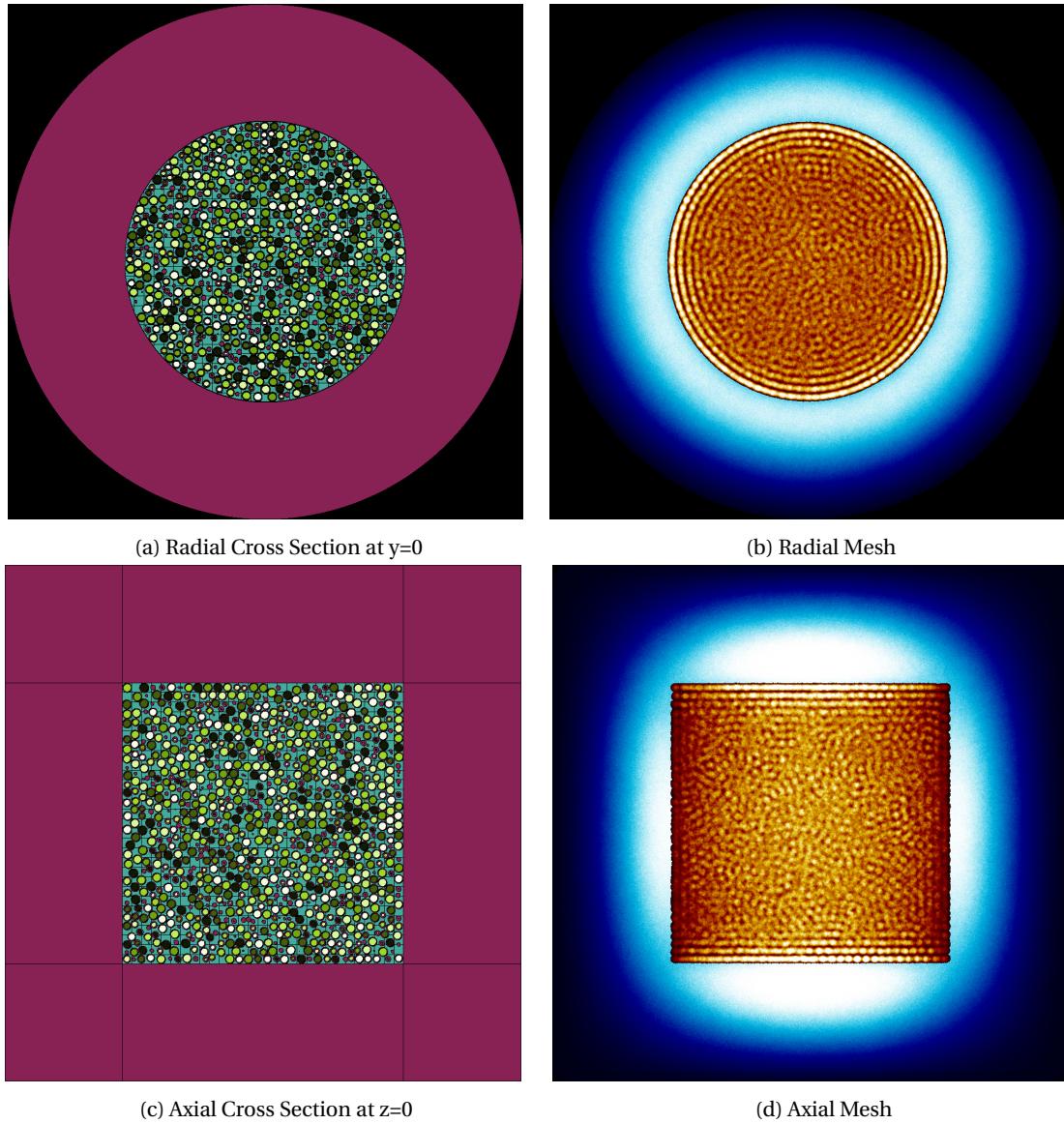


Figure 6.12: Shuffle Analysis: Run 1

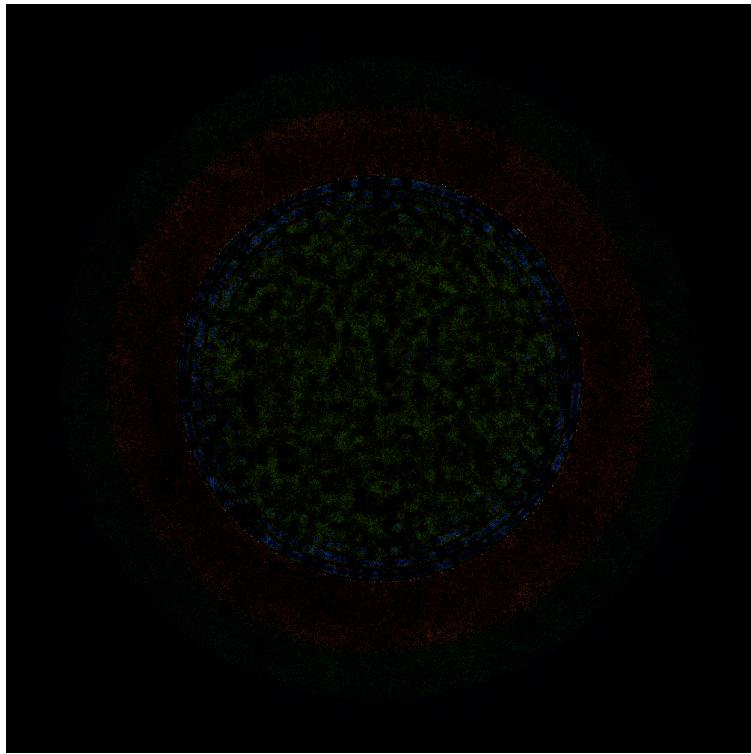
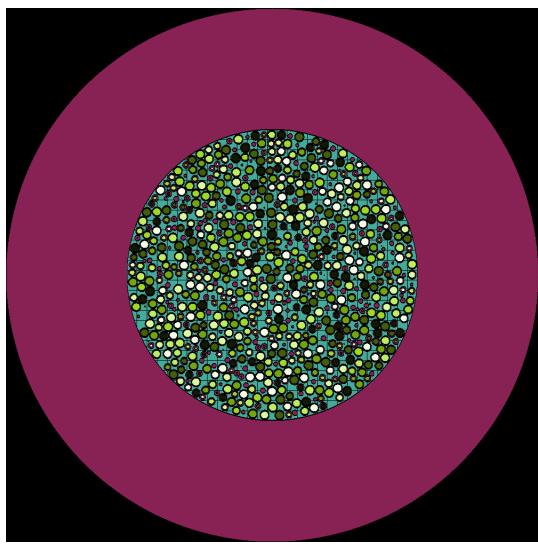
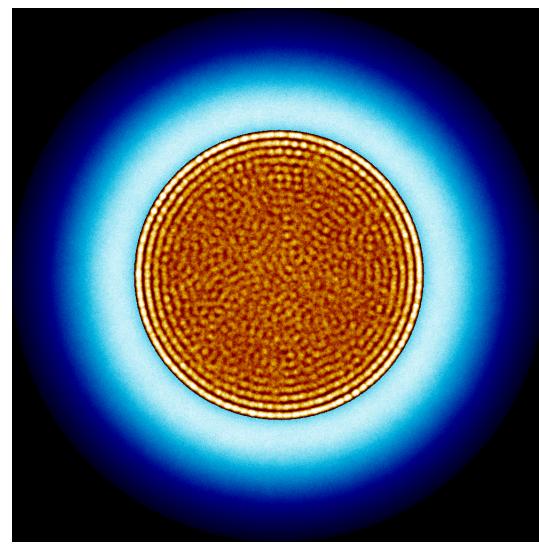


Figure 6.13: An Image Generated by Subtracting 6.12b from 4.3b.

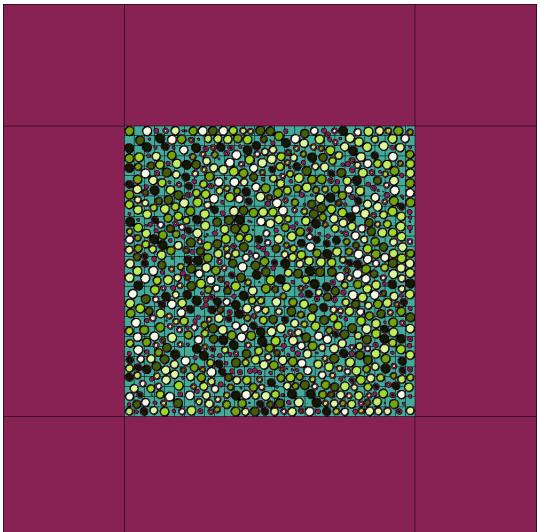
Figure 6.12 provides the thermal flux and fission rate meshes and geometric cross sections axially and radially. Figure 6.13 is the result of the image difference between the full core control mesh and Figure 6.12b.



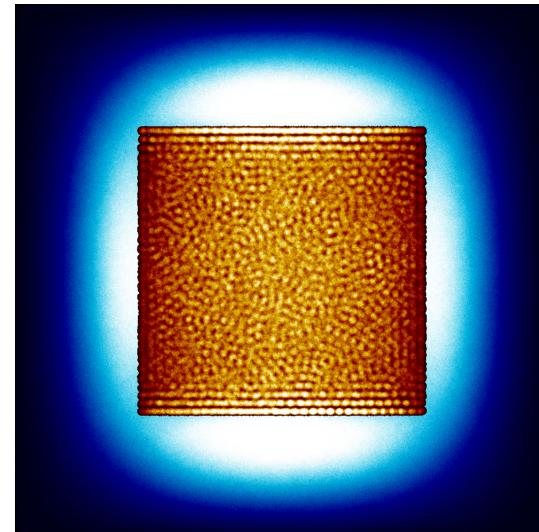
(a) Radial Cross Section at $y=0$



(b) Radial Mesh



(c) Axial Cross Section at $z=0$



(d) Axial Mesh

Figure 6.14: Shuffle Analysis: Run 2

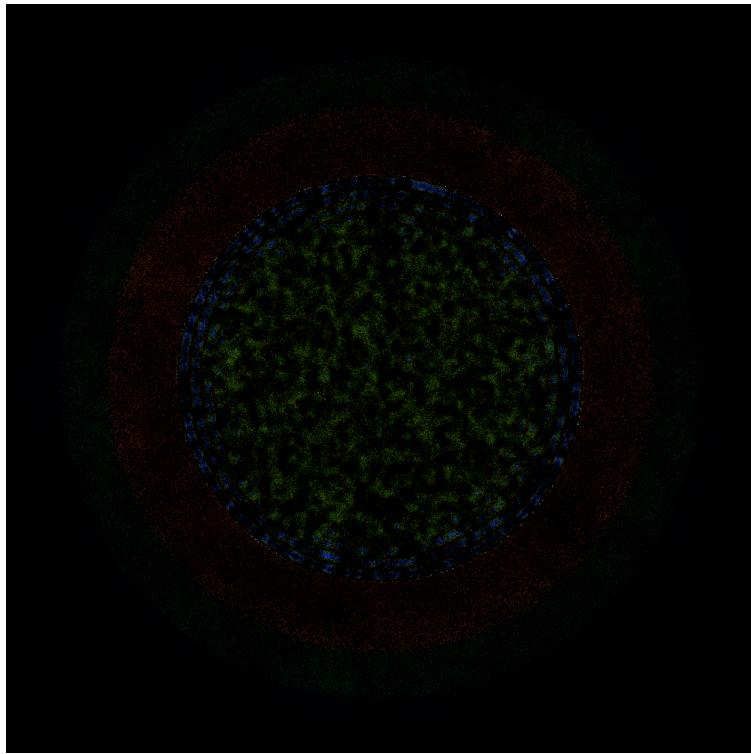
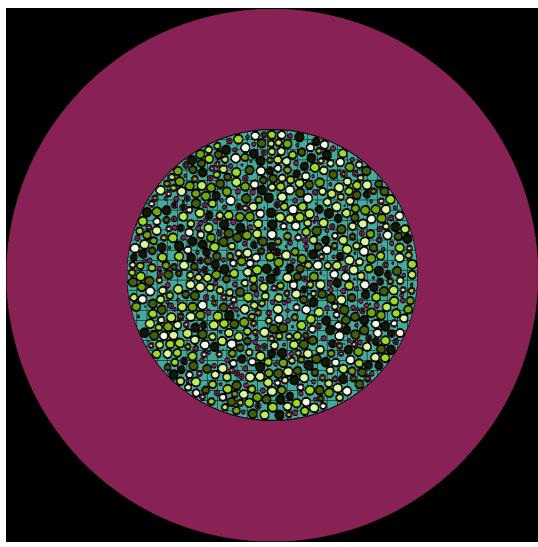
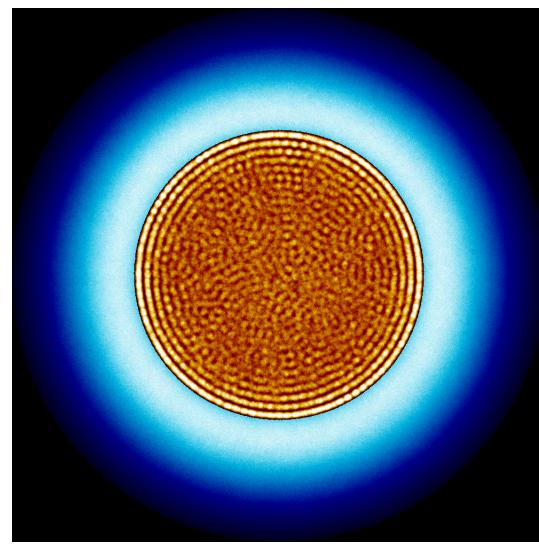


Figure 6.15: An Image Generated by Subtracting 6.14b from 4.3b.

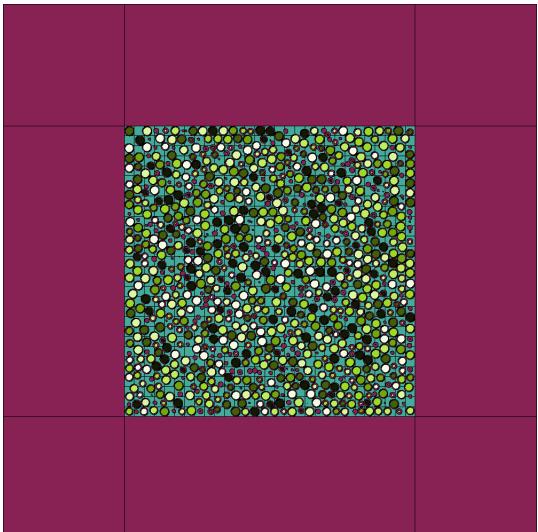
Figure 6.14 provides the thermal flux and fission rate meshes and geometric cross sections axially and radially. Figure 6.15 is the result of the image difference between the full core control mesh and Figure 6.14b.



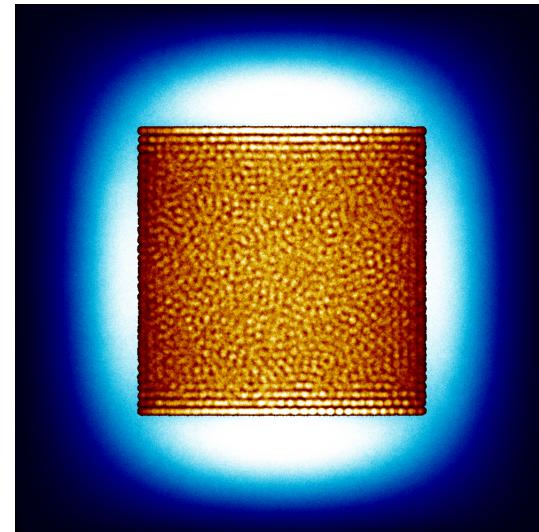
(a) Radial Cross Section at $y=0$



(b) Radial Mesh



(c) Axial Cross Section at $z=0$



(d) Axial Mesh

Figure 6.16: Shuffle Analysis: Run 3

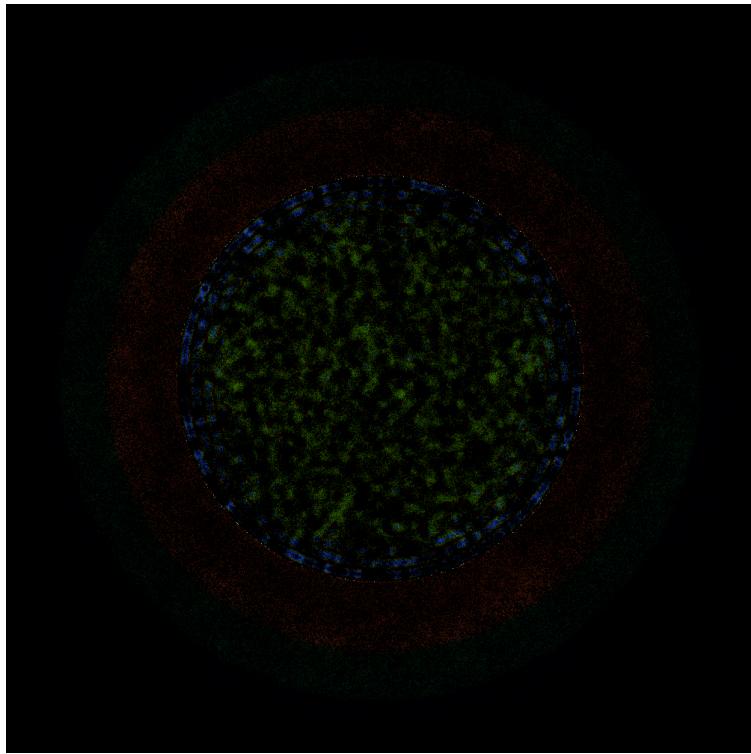
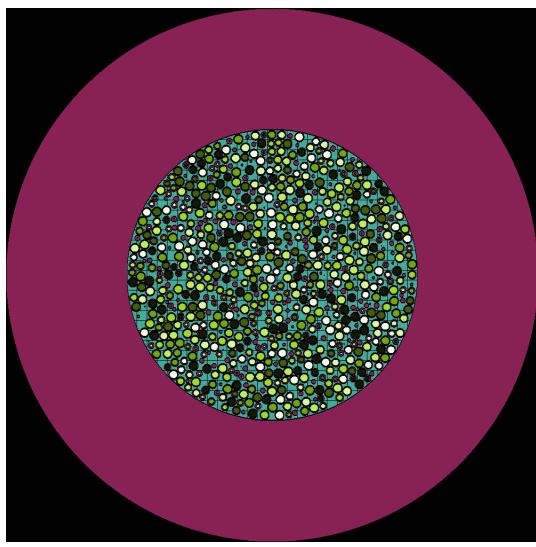
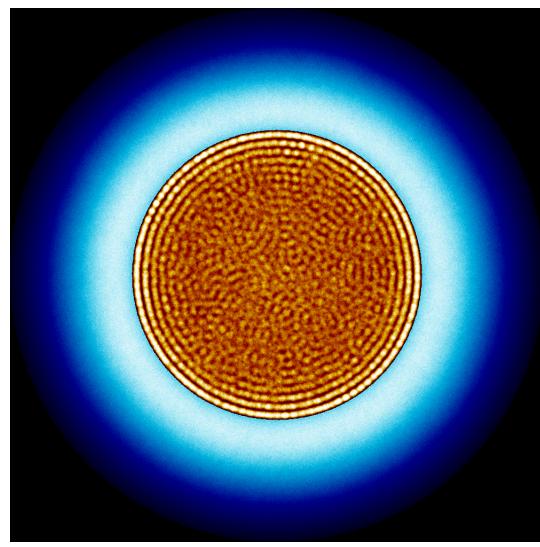


Figure 6.17: An Image Generated by Subtracting 6.16b from 4.3b.

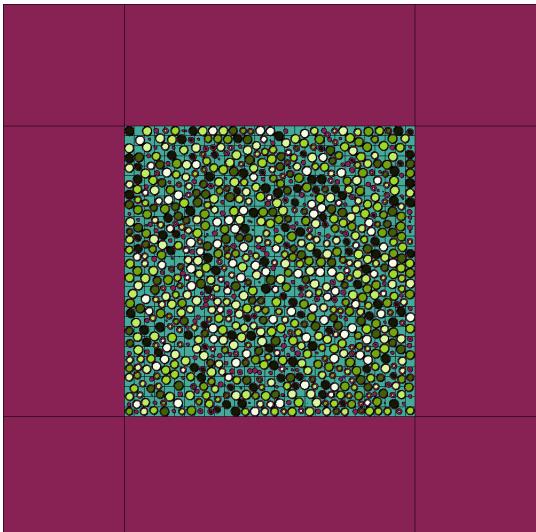
Figure 6.16 provides the thermal flux and fission rate meshes and geometric cross sections axially and radially. Figure 6.17 is the result of the image difference between the full core control mesh and Figure 6.16b.



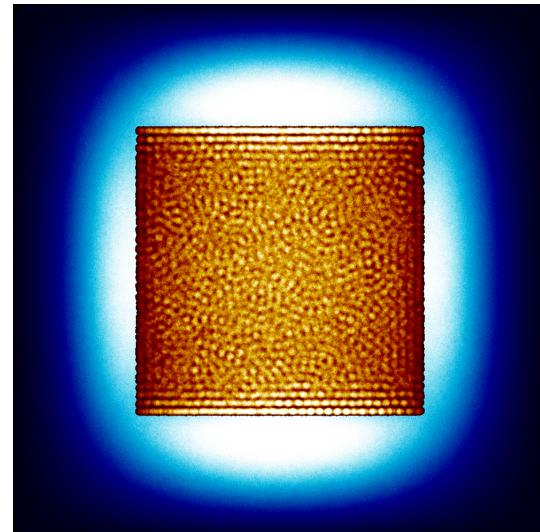
(a) Radial Cross Section at $y=0$



(b) Radial Mesh



(c) Axial Cross Section at $z=0$



(d) Axial Mesh

Figure 6.18: Shuffle Analysis: Run 4

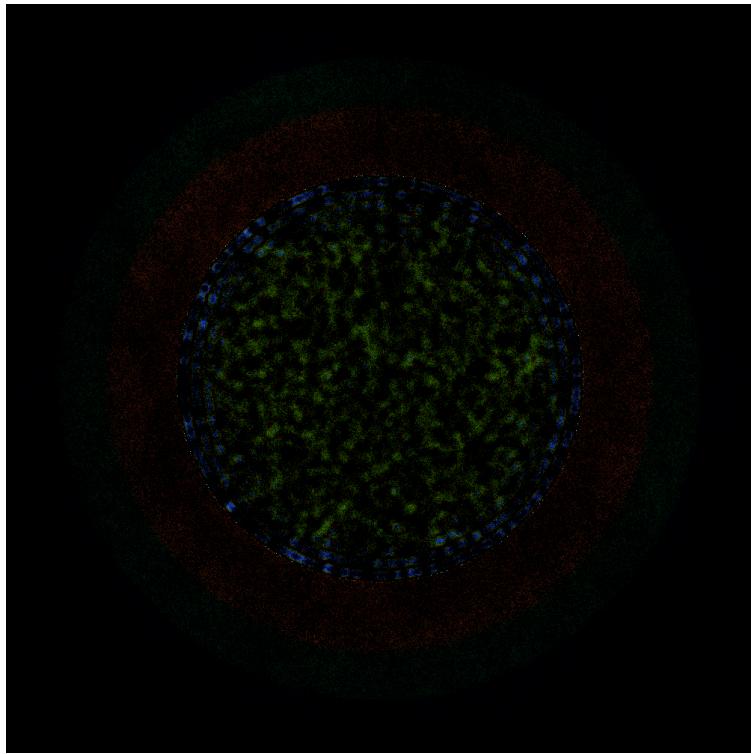
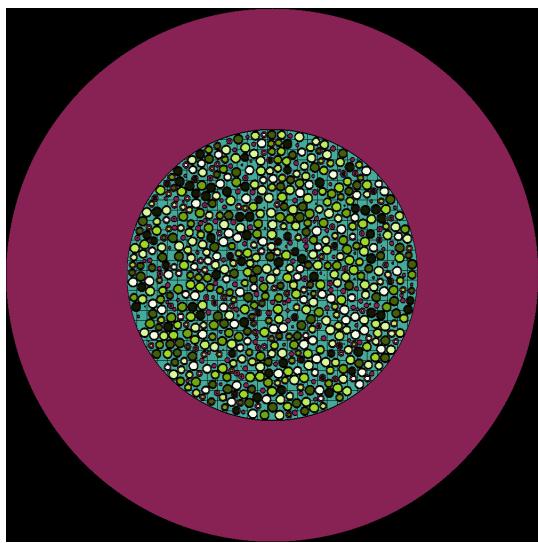
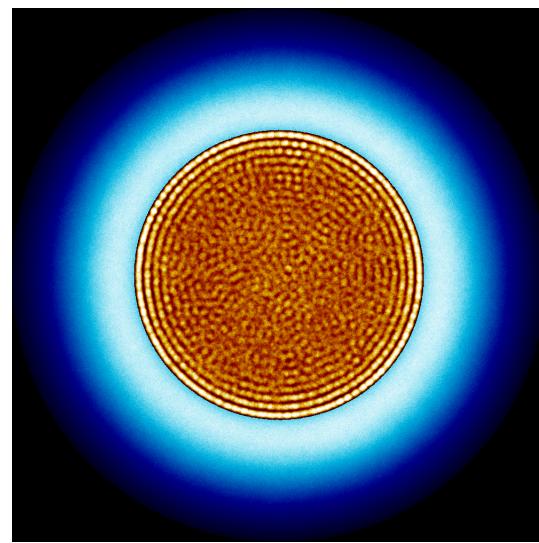


Figure 6.19: An Image Generated by Subtracting 6.18b from 4.3b.

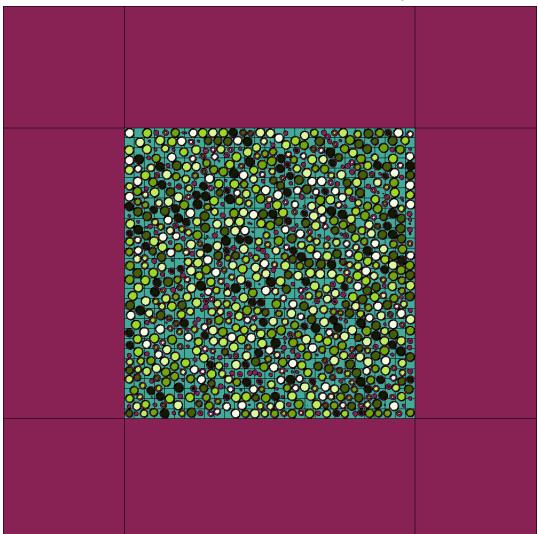
Figure 6.18 provides the thermal flux and fission rate meshes and geometric cross sections axially and radially. Figure 6.19 is the result of the image difference between the full core control mesh and Figure 6.18b.



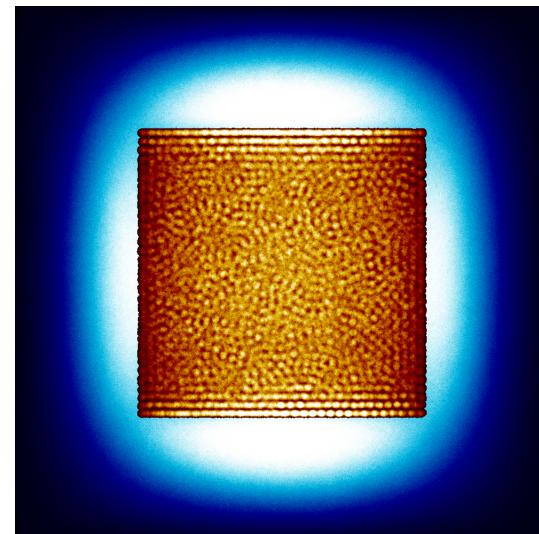
(a) Radial Cross Section at $y=0$



(b) Radial Mesh



(c) Axial Cross Section at $z=0$



(d) Axial Mesh

Figure 6.20: Shuffle Analysis: Run 5

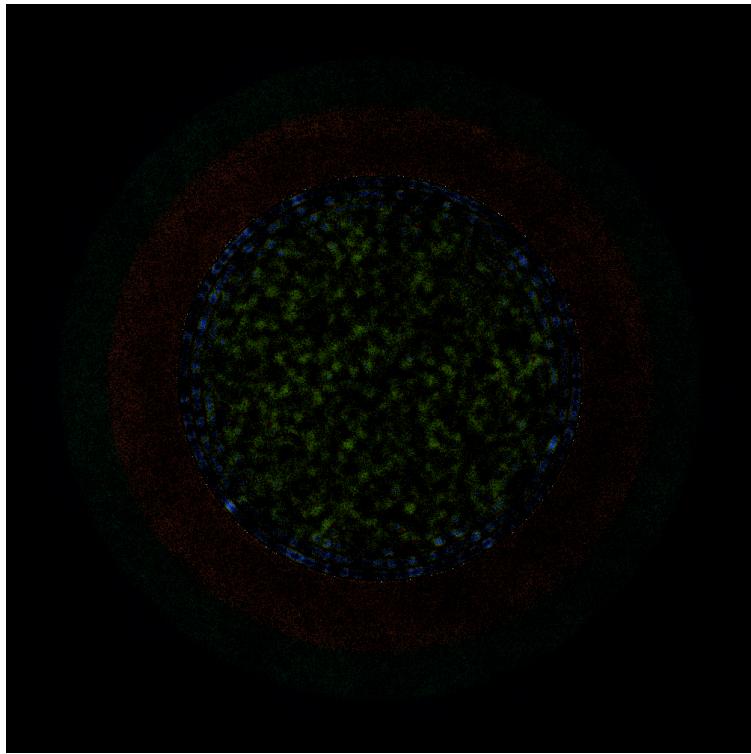
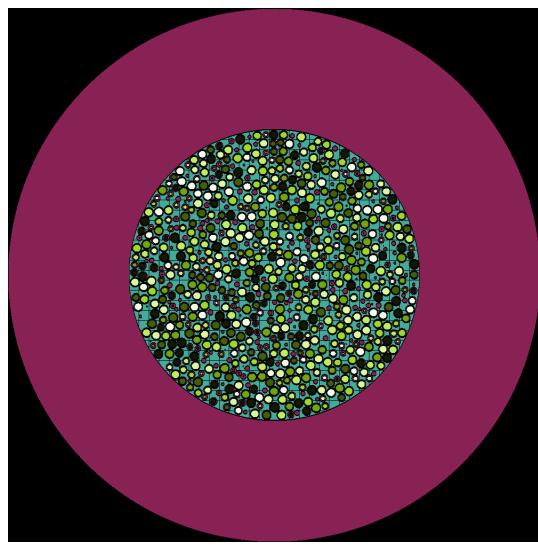
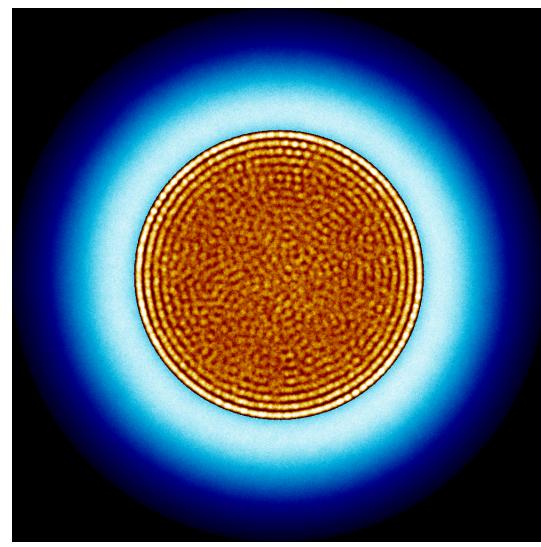


Figure 6.21: An Image Generated by Subtracting 6.20b from 4.3b.

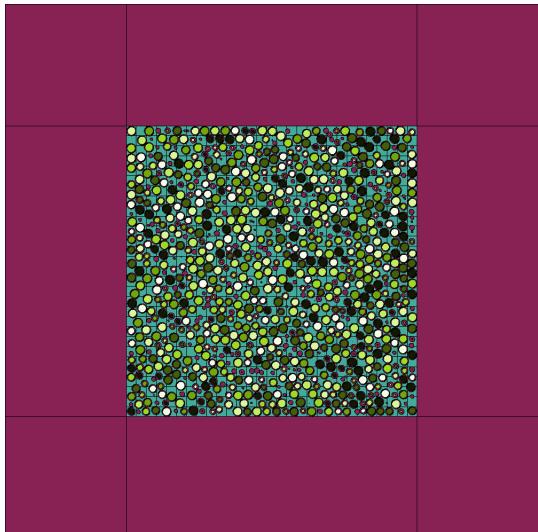
Figure 6.20 provides the thermal flux and fission rate meshes and geometric cross sections axially and radially. Figure 6.21 is the result of the image difference between the full core control mesh and Figure 6.20b.



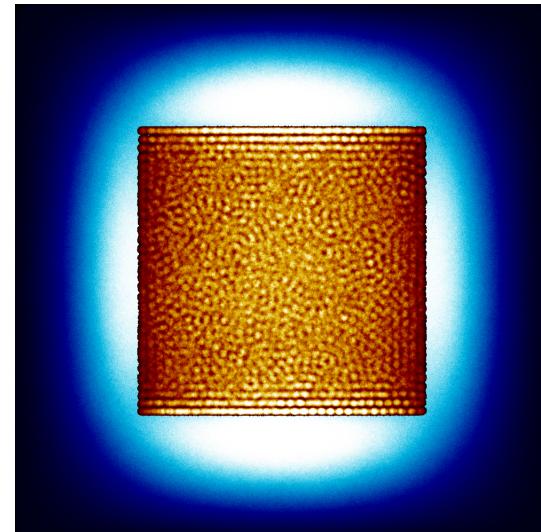
(a) Radial Cross Section at $y=0$



(b) Radial Mesh



(c) Axial Cross Section at $z=0$



(d) Axial Mesh

Figure 6.22: Shuffle Analysis: Run 6

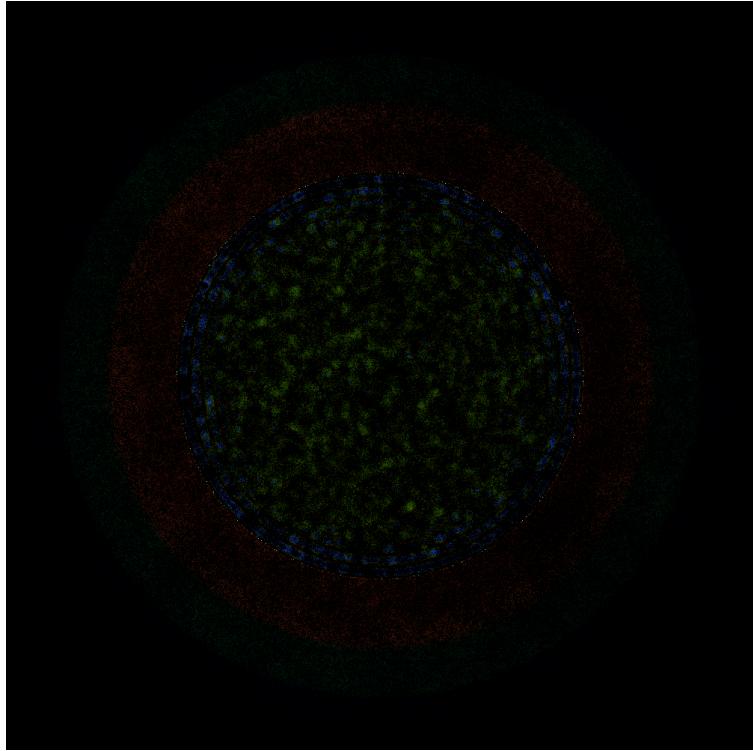


Figure 6.23: An Image Generated by Subtracting 6.22b from 4.3b.

Figure 6.2 provides the thermal flux and fission rate meshes and geometric cross sections axially and radially. Figure 6.23 is the result of the image difference between the full core control mesh and Figure 6.22b.

Comparing the image difference results of Appendix B, the shuffling test, to Appendix A, the symmetry test, shows that the shuffling tests have a weaker effect on the fission rate and thermal flux than the symmetry tests. The small differences in this particular test would most likely indicate that the core is generally well-mixed, i.e., that each bin in the vertical direction, along the z axis, has each of the 7 fuel compositions represented equally.

There are however, a few hotspots, where small regions show a brighter patch of green. The best example of this is in the fourth quadrant of Figure 6.23, near the 270° line. Hotspots such as this could be caused by poor mixing, which would make some pebbles occur in higher concentrations (and then cause a larger difference in the shuffle test, when the same region is now dominated by a different burnup) or by the shuffling putting a different pebble burnup in a region of lower or higher flux. To investigate the source of this, the pebbles in a 10 cm square column (10 cm in x and y, the height of the reactor in z) around the hotspot were found. Table 6.1 shows the count of each pebble burnup.

Table 6.1: Representation of Pebbles by Number of Passes in a 10 cm Square Rectangular Prism Surrounding an Image Difference Hotspot at Approximately x = 11 cm, y = -56 cm

Pebble Pass	Number of Pebbles
Fresh	20
First Pass	12
Second Pass	13
Third Pass	12
Fourth Pass	10
Fifth Pass	14
Sixth Pass	11

When this region was narrowed further, to a 5 cm region, the poor mixing was more dramatic, as seen in Table 6.2.

Table 6.2: Representation of Pebbles by Number of Passes in a 5 cm Square Rectangular Prism Surrounding an Image Difference Hotspot at Approximately x = 11 cm, y = -56 cm

Pebble Pass	Number of Pebbles
Fresh	10
First Pass	3
Second Pass	4
Third Pass	1
Fourth Pass	2
Fifth Pass	2
Sixth Pass	2

In the 10 cm square column, fresh pebbles originally make up 21.7% of all pebbles in the region. In the 5cm square column that is tighter around the hotspot, fresh pebbles make up 41.7% of all pebbles. The hotspot pointed out in Figure 6.23 exists in some degree in Figures 6.13, 6.15, 6.17, 6.19, and 6.21 — it is simply brightest in Figure 6.23 because the shuffle scheme corresponding to this Figure 6.23 replaces fresh pebbles with 6-pass pebbles, which have the greatest disparity in burnup.

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