

© 2021 by Zoë Richter. All rights reserved.

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

BY

ZOË RICHTER

THESIS

Submitted in partial fulfillment of the requirements  
for the degree of Master of Science in Nuclear, Plasma, Radiological Engineering  
in the Graduate College of the  
University of Illinois at Urbana-Champaign, 2021

Urbana, Illinois

Master's Committee:

Professor Kathryn D. Huff  
Dr. Madicken Munk

# 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 changes 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 2 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 rudimentary 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.

# Acknowledgments

I'd like to thank my advisor, Dr. Kathryn Huff, for offering her knowledge and support through these trying times and uncertainties. I would also like to thank Dr. Madicken Munk, whose insight and experience was invaluable. To Nathan Ryan, my tireless reviewer: thank you for all of your hard work. I would like to thank everyone in the Advanced Reactors and Fuel Cycles group, past and present, for giving me their time, aid, and experience: Amanda Bachmann, Dr. Andrei Rykhlevskii, Ansh Chaube, Greg Westphal, Gwendolyn Chee, Mehmet Turkmen, Roberto Fairhurst, Sam Dotson, and Sun Myung Park.

Thank you to my family, for always believing in me; Trinket, for loving hugs; and Sara, without whom nothing in this project would have a good name.

This work is supported by the Nuclear Regulatory Commission Fellowship Program.

# Table of Contents

<b>List of Tables . . . . .</b>	<b>vi</b>
<b>List of Figures . . . . .</b>	<b>vii</b>
<b>Chapter 1 Introduction . . . . .</b>	<b>1</b>
1.1 Motivation . . . . .	1
1.2 Objectives . . . . .	2
1.3 Background . . . . .	3
1.3.1 The High Temperature Gas Cooled Reactor: Beginnings and Concepts . . . . .	3
1.3.2 Earliest Operational HTGRs . . . . .	4
<b>Chapter 2 Literature Review . . . . .</b>	<b>8</b>
2.1 Computational Modeling and Software . . . . .	8
2.1.1 Serpent . . . . .	8
2.1.2 MCNP and BEAU . . . . .	9
2.1.3 Fuel Modeling . . . . .	10
2.2 Modern HTGRs . . . . .	10
2.2.1 PBMR . . . . .	10
2.2.2 Next Generation Nuclear Plant (NGNP) . . . . .	13
2.2.3 X-100 . . . . .	13
2.2.4 HTR-10 . . . . .	13
<b>Chapter 3 Methodology . . . . .</b>	<b>15</b>
3.1 Modeling Particle Dispersal . . . . .	15
3.2 Run Parameters and Conditions . . . . .	15
3.3 Burnup and Depletion Methodology . . . . .	16
3.4 Sangamon200 . . . . .	18
3.5 Sangamon20 . . . . .	20
3.5.1 Inner Core Volume Determination . . . . .	20
3.5.2 Graphite Reflector Thickness Determination . . . . .	23
3.6 Fuel Composition . . . . .	23
3.7 Heterogenization Tests . . . . .	24
3.8 Reactor Sensitivity to Pebble Locations and Symmetry . . . . .	25
<b>Chapter 4 Results . . . . .</b>	<b>27</b>
4.1 Fuel Isotopic Compositions . . . . .	27
4.2 Full-Core Control Model . . . . .	34
4.3 Effect of Homogenization . . . . .	44
4.4 Shuffling and Symmetry Tests . . . . .	58
4.4.1 Effects of Symmetry Assumption . . . . .	58
4.4.2 Effects of Pebble Shuffling . . . . .	60

<b>Chapter 5 Conclusion</b>	62
5.1 Summary and Discussion	62
5.2 Future Work	63
<b>Chapter 6 Appendix</b>	65
6.1 Appendix A: Symmetry Test	65
6.2 Appendix B: Shuffle Test	76
<b>References</b>	89

# List of Tables

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 . . . . .	7
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 . . . . .	7
3.1	Reactor Parameters . . . . .	16
3.2	Pebble Parameters . . . . .	16
3.3	Particles Parameters . . . . .	17
3.4	Reactor Parameters . . . . .	18
3.5	Shuffle Test Run Schemes . . . . .	26
4.1	Symmetry Run Summary . . . . .	58
4.2	Shuffling Run Summary . . . . .	61

# List of Figures

1.1	Side-View of Daniels et. al. (1955) Reactor Concept, from [6]	3
1.2	Diagram of Coolant Flow in Daniels et. al. (1955) Concept, from [6]	4
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).	12
3.1	Pebble Zones	17
3.2	TRISO Particle Layers	18
3.3	Detector Placement Inside Reflector in Sangamon200 and Sangamon20	19
3.4	Curve of possible height and radii that satisfy the volume requirements imposed by packing fraction(s) $\eta_{pf}$	23
3.5	Geometry of the Single-Pebble Burnup Calculation for Sangamon20	24
3.6	Symmetry Test Run Layouts	25
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)	27
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)	28
4.2	Evolution of Safety Relevant Isotopic Concentrations in Pebbles of Sangamon20 over Six Six-Month Passes	30
4.2	Evolution of Safety Relevant Isotopic Concentrations in Pebbles of Sangamon20 over Six Six-Month Passes (cont.)	31
4.2	Evolution of Safety Relevant Isotopic Concentrations in Pebbles of Sangamon20 over Six Six-Month Passes (cont.)	32
4.2	Evolution of Certain Isotopic Concentrations in Pebbles over Six Six-Month Passes (cont.)	33
4.3	Geometry Cross Sections and Thermal Flux(cold color map) and Fission Rate (hot color map) Meshes for the Control Model of Sangamon20	35
4.4	Radial Thermal and Fast Flux Profiles along the X-Axis at the Mid-Plane in Sangamon20: Homogenized Pebbles	36
4.5	Axial Thermal and Fast Flux Profiles at the Centerline of Sangamon20: Homogenized Pebbles	37
4.6	Thermal Flux in xy Plane	38
4.7	Fast Flux in xy Plane	39
4.8	Core Spectrum	40
4.9	Reflector Spectrum	41
4.10	Fresh Pebble Spectrum	42
4.11	Six-Pass Pebble Spectrum	43
4.12	Coolant Spectrum	44
4.13	Full Core Using Heterogenized Pebbles	45

4.14 Radial Thermal and Fast Flux Profiles Along the X-Axis at the Mid-Plane in Sangamon20: Heterogenized Pebbles . . . . .	46
4.15 Axial Thermal and Fast Flux Profiles along the Centerline in Sangamon20: Heterogenized Pebbles . . . . .	47
4.16 Thermal Flux in xy Plane in Sangamon20: Heterogenized Pebbles . . . . .	48
4.17 Fast Flux in xy Plane in Sangamon20: Heterogenized Pebbles . . . . .	49
4.18 Lethargy Adjusted Neutron Flux Energy Spectra: Core Using Heterogenized Pebbles . . . . .	50
4.18 Lethargy Adjusted Neutron Flux Energy Spectra: Core Using Heterogenized Pebbles (cont.) . . . . .	51
4.18 Lethargy Adjusted Neutron Flux Energy Spectra: Core Using Heterogenized Pebbles (cont.) . . . . .	52
4.19 Relative Difference in Radial Thermal and Fast Flux Profiles Between Cores Using Homogenized and Heterogenized Pebbles . . . . .	53
4.19 Relative Difference in Radial Thermal and Fast Flux Profiles Between Cores Using Homogenized and Heterogenized Pebbles (cont.) . . . . .	54
4.20 Relative Difference in Lethargy Adjusted Neutron Flux Energy Spectra Between Cores using Homogenized and Heterogenized Pebbles . . . . .	55
4.20 Relative Difference in Lethargy Adjusted Neutron Flux Energy Spectra Between Cores using Homogenized and Heterogenized Pebbles (cont.) . . . . .	56
4.20 Relative Difference in Lethargy Adjusted Neutron Flux Energy Spectra Between Cores using Homogenized and Heterogenized Pebbles (cont.) . . . . .	57
4.21 Sensitivity Analysis: 0° - 60° . . . . .	59
4.22 An Image Generated by Subtracting 4.21b from 4.3b. . . . .	60
 6.1 Sensitivity Analysis: 60° - 120° . . . . .	66
6.2 An Image Generated by Subtracting 6.1b from 4.3b. . . . .	67
6.3 Sensitivity Analysis: 120° - 180° . . . . .	68
6.4 An Image Generated by Subtracting 6.3b from 4.3b. . . . .	69
6.5 Sensitivity Analysis: 180° - 240° . . . . .	70
6.6 An Image Generated by Subtracting 6.5b from 4.3b. . . . .	71
6.7 Sensitivity Analysis: 240° - 300° . . . . .	72
6.8 An Image Generated by Subtracting 6.7b from 4.3b. . . . .	73
6.9 Sensitivity Analysis: 300° - 360° . . . . .	74
6.10 An Image Generated by Subtracting 6.9b from 4.3b. . . . .	75
6.11 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 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. . . . .	76
6.12 Shuffle Analysis: Run 1 . . . . .	77
6.13 An Image Generated by Subtracting 6.12b from 4.3b. . . . .	78
6.14 Shuffle Analysis: Run 2 . . . . .	79
6.15 An Image Generated by Subtracting 6.14b from 4.3b. . . . .	80
6.16 Shuffle Analysis: Run 3 . . . . .	81
6.17 An Image Generated by Subtracting 6.16b from 4.3b. . . . .	82
6.18 Shuffle Analysis: Run 4 . . . . .	83
6.19 An Image Generated by Subtracting 6.18b from 4.3b. . . . .	84
6.20 Shuffle Analysis: Run 5 . . . . .	85
6.21 An Image Generated by Subtracting 6.20b from 4.3b. . . . .	86
6.22 Shuffle Analysis: Run 6 . . . . .	87
6.23 An Image Generated by Subtracting 6.22b from 4.3b. . . . .	88

# 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

# 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. While nuclear technology is currently in use across the world, many of these reactors are older, and facing closure as their licenses run out. 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.

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). TRISO-based pebble-type fuels in particular can be refueled online, which reduces the need for planned shutdowns.

Beyond HTGRs, another reactor class of interest is the Small Modular Reactor (SMR). These reactors are smaller than the conventional LWR seen in the USA today. So-called Small Modular Reactors, or 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 modular 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 used a pebble-bed high-temperature gas-cooled SMR as a starting point and modeled a 200MWth reactor based on existing designs. We call this 200MWth reactor the Sangamon200. A smaller 20MWth design — Sangamon20 — was created by scaling down the Sangamon200 model. The 20MWth model, hereafter referred to as Sangamon20, is a highly simplified design for use in future testing and analysis. This model is simplified to provide a foundation for testing and analyzing 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. Sangamon20 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. A series of simulations running the Sangamon20 model while utilizing a symmetry condition are analyzed in this work. 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).

Previous work in pebble bed reactors would use 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.

## 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 and reactors. 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 — the project terminated in one form or another before it is 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 in thermal designs. 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].

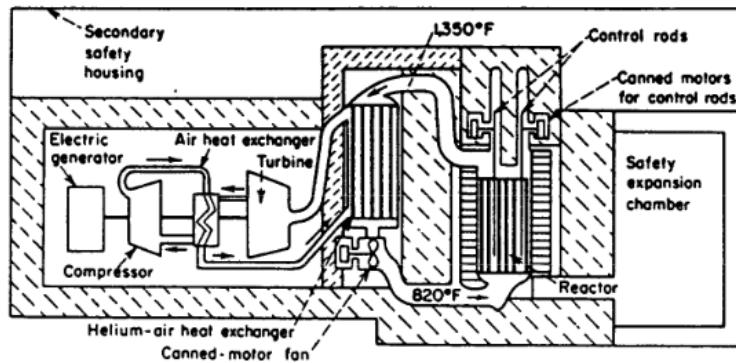


Figure 1.1: Side-View of Daniels et. al. (1955) Reactor Concept, from [6]

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

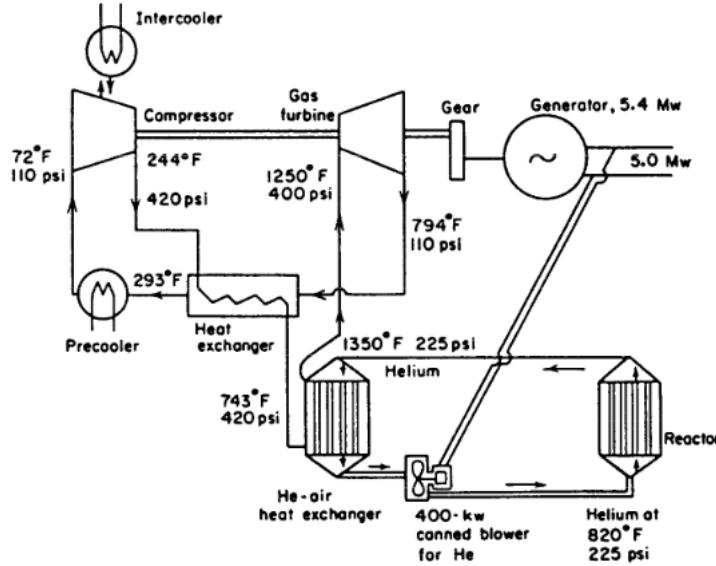


Figure 1.2: Diagram of Coolant Flow in Daniels et al. (1955) Concept, from [6]

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: the AVR, from Germany; Dragon, operating in the UK; and Peach Bottom 1, in the US; came online in the 1960s [7]. The following sections discuss these three early reactors and the impact of knowledge and experience gained during their operation.

#### 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' 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 stationed 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. 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: 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 [ $\frac{Bq}{m^3}$ ]
$\Sigma$ Fission noble gas	$4.6 \times 10^{08}$
$^3H$	$3.7 \times 10^{07}$
$^{14}C$	$1.9 \times 10^{07}$
$^{137}Cs$	$3.0 \times 10^{02}$
$^{131}I$	$5.2 \times 10^{02}$
$^{110m}Ag$	$4.9 \times 10^{01}$
$^{90}Sr$	$2.0 \times 10^{02}$
$^{60}Co$	$1.0 \times 10^{01}$

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

# **Chapter 2**

## **Literature Review**

### **2.1 Computational Modeling and Software**

The sections 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. The last section (see section 2.2) includes a description of the Pebble Bed Molten salt Reactor (PBMR), Next Generation Nuclear Plant (NGNP), Xe-100, and HTR-10 reactors along with some 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. While this sort of information is theoretically possible for a human to create, it is not practical for any significant amount of pebbles. To not only 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 ( see [12]) 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. 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. 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 and BEAU

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. Its creators dubbed the version of MCNP that used the sampling algorithm as MCNP-BALL. After testing by performing isotopic inventory and criticality calculations the MCNP-BALL code results were accurate to 0.2%. The work developing MCNP-BALL also answered a weakness in core simulation due related to difficulties in modeling reactors with a so-called "double-heterogeneity" — having two or more types of pebble in a single reactor [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. 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  $k_{eff}$ . 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].

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`. `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 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 reactor. Assuming a uniformly mixed core, the closeness of the different burnup compositions in the lattice provide a fairly good estimation of the true core.

### 2.1.3 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 author 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 Atomic 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].

## 2.2 Modern HTGRs

The following discusses more recent HTGR designs, which are the inspiration for Sangamon200 and Sangamon20.

### 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 model underwent development and testing. An early version using MCNP5 simplified the fuel by assuming an equilibrium pebble enrichment of 9.6 wt%. It also uses 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 defines 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.

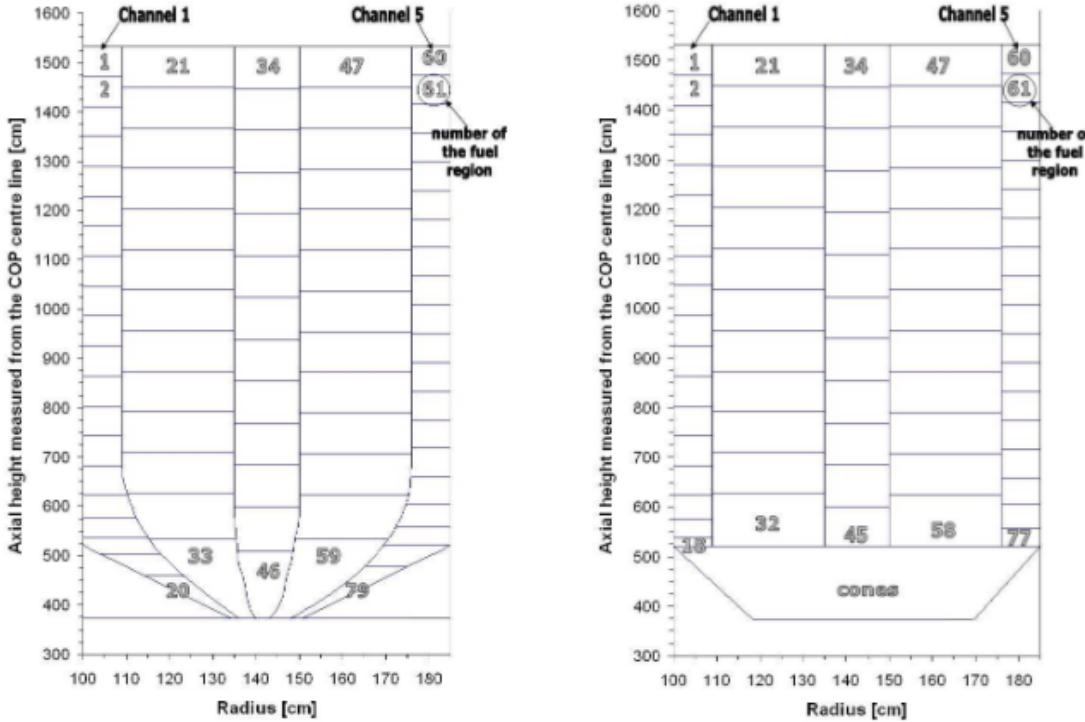


Figure 2.1: Diagram of fuel regions in an equilibrium core model, reproduced from [18]. Axial fuel zones defined for use in MCNP model validation (right) against a previous VSOP model (left).

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  $99,000 \frac{MWD}{T}$ , random 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  $18.66 \frac{MW}{m^3}$  from  $11.32 \frac{MW}{m^3}$  [20]. Of note, 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. 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  $3.0 \text{ [cm]}$  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 ( $\sigma$  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].

# Chapter 3

## Methodology

This chapter introduces Sangamon20, a scale-down of Sangamon200, a 200MWth design 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

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  $\eta_{pf}$ , 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 the particle center (in x,y,z coordinates), the particle radius, and the name of the particle type, to associate it with the "pbed" card (see [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. Below, Table 3.1 gives the run parameters for each Serpent model.

See [34] for all input files.

Table 3.1: Reactor Parameters

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

### 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 six, 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, see 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.

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

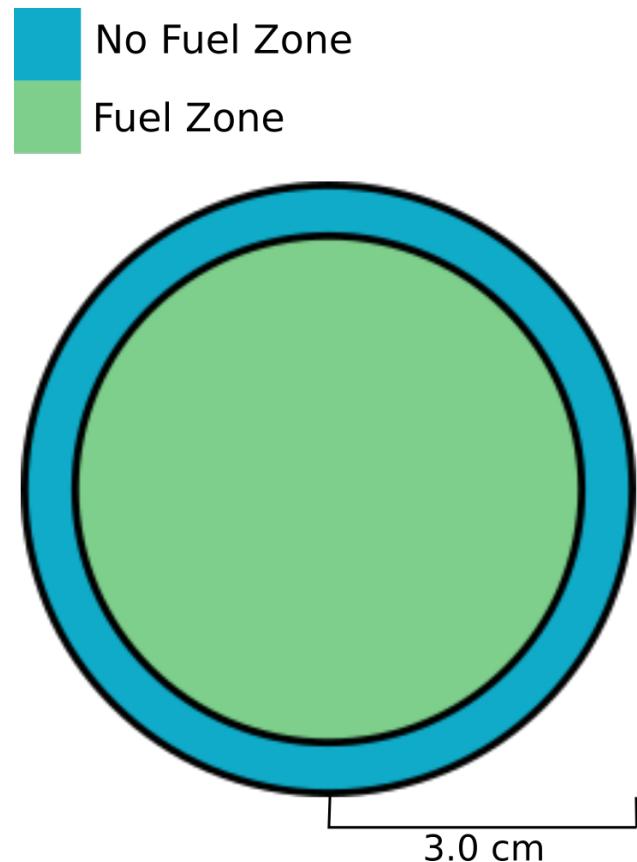


Figure 3.1: Pebble Zones

Table 3.3: Particles 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

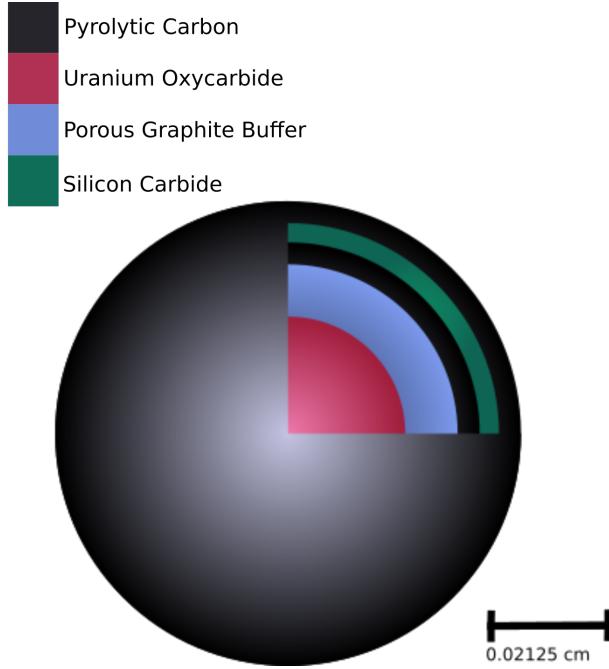


Figure 3.2: TRISO Particle Layers

### 3.4 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.

Table 3.4: Reactor Parameters

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

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 3.3, tracks the outward neutron current. When determining the appropriate reflector thickness in Sangamon20, this current is used as an upper boundary and reference point — i.e., 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 Sangamon200's to protect the RPV.

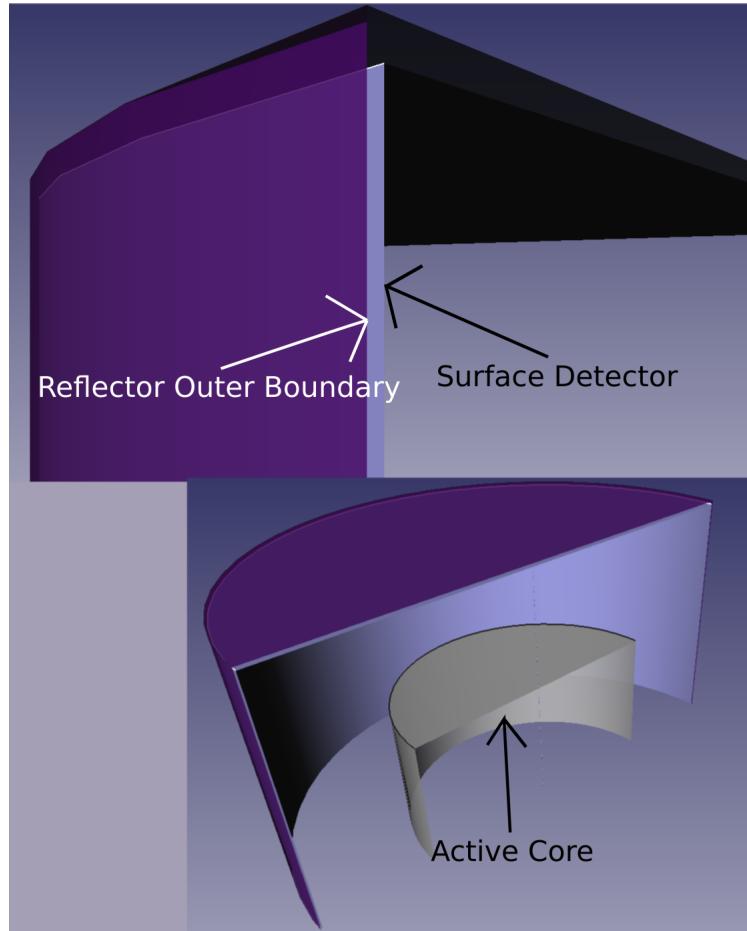


Figure 3.3: Detector Placement Inside Reflector in Sangamon200 and Sangamon20

In Figure 3.3, the graphite reflector outer boundary (dark purple) is shown, with the surface detector 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 fluence 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

$$\begin{aligned} J^+ &= \text{outward neutron current } \left[ \frac{\#}{cm^2 s} \right] \\ J_s^+ &= \text{surface unadjusted outward neutron current } \left[ \frac{\#}{s} \right] \\ S_d &= \text{detector surface area } [cm^2] \end{aligned} \quad (3.2)$$

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

## 3.5 Sangamon20

Sangamon20 is a 20 MWth helium-cooled pebble bed reactor, fueled with 19.75% enriched uranium oxycarbide. While the capacity 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 work, but in order to be certain that this volume would hold the mass of fuel sufficient, a simple calculation was carried out, in the following section.

### 3.5.1 Inner Core Volume Determination

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

To calculate the mass of fuel in Sangamon200:

$$M_{f,200} = \frac{4}{3} \pi r_u^3 \rho_u n_T n_{p,200} \quad (3.3)$$

where

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

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

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

$n_T$  = number of TRISO particles in one pebble

$n_p$  = number of pebbles in Sangamon200 (3.4)

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

$$M_{f,20} = \frac{P}{\rho_p} = 181818.18 [g] \quad (3.5)$$

where

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

$P$  = Thermal power of Sangamon20 [kW]

$\rho_p$  = Sangamon20's power density [ $\frac{kW}{g}$ ] (3.6)

Equation 3.3 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:

$$n_{p,20} = \frac{M_{f,20}}{\frac{4}{3}r_u^3 n_T \rho_u} \quad (3.7)$$

where

$$\begin{aligned}
 n_{p,20} &= \text{number of pebbles in Sangamon20 [-]} \\
 M_{f,20} &= \text{total mass of UCO in Sangamon20 [g]} \\
 r_u &= \text{radius of a UCO kernel [cm]} \\
 n_T &= \text{number of TRISO particles in a single pebble [-]} \\
 \rho_u &= \text{density of UCO } [\frac{\text{g}}{\text{cm}^3}] \tag{3.8}
 \end{aligned}$$

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

$$V_{c,20} = \frac{n_{p,20} \frac{4}{3} \pi r_p^3}{\eta_{pf}} \tag{3.9}$$

where

$$\begin{aligned}
 V_{c,20} &= \text{volume of the active core in Sangamon20 } [\text{cm}^3] \\
 n_{p,20} &= \text{number of pebbles in Sangamon20 [-]} \\
 r_p &= \text{radius of a pebble [cm]} \\
 \eta_{pf} &= \text{packing fraction [-]} \tag{3.10}
 \end{aligned}$$

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.

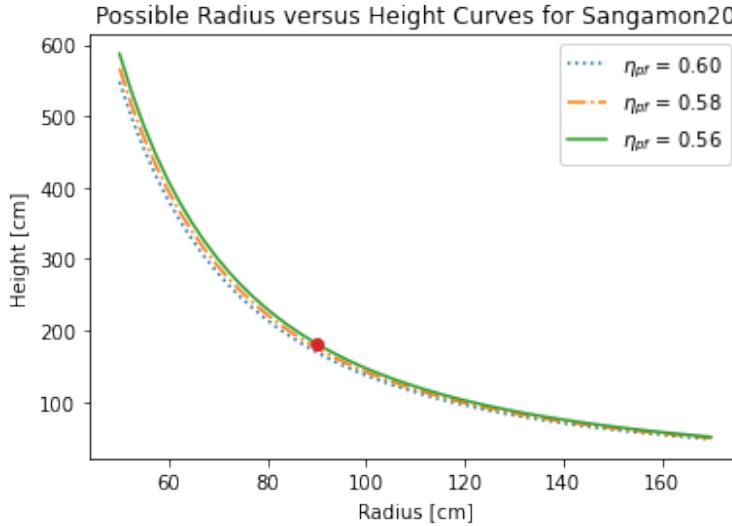


Figure 3.4: Curve of possible height and radii that satisfy the volume requirements imposed by packing fraction(s)  $\eta_{pf}$

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 a flat shape is logically inconvenient, Sangamon20 is the former. The point indicated in 3.4 shows the radius and height selected for Sangamon20 - a radius of 90 [cm], and a height of 180 [cm].

### 3.5.2 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, 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 3.3.

## 3.6 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.

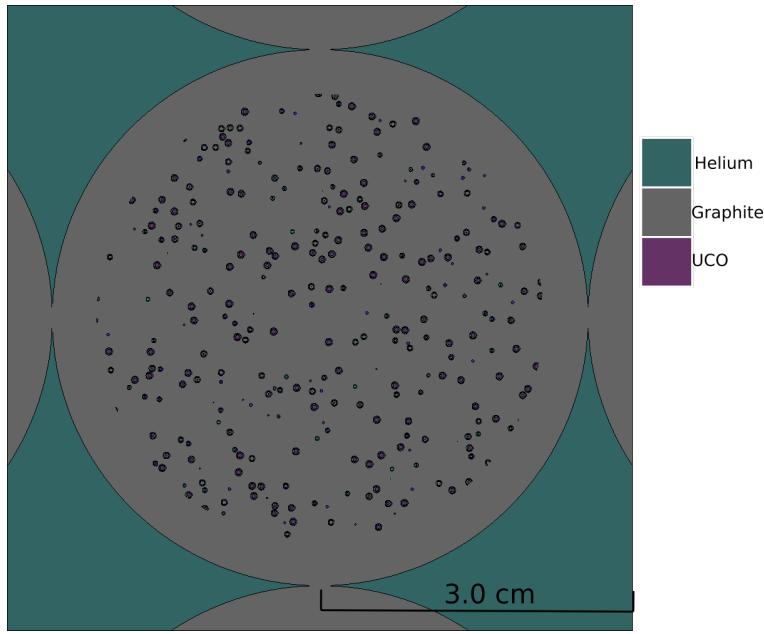


Figure 3.5: Geometry of the Single-Pebble Burnup Calculation for Sangamon20

Figure 3.5 above 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 below.

### 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

Due to the random nature of pebble locations, it is 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 the reactor, 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 section subsection 4.4.2). The second analyzed the effects of utilizing a symmetry simplification, in order to improve computational speed (see ??) 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 3.6. In each test, all other parameters remain the same.

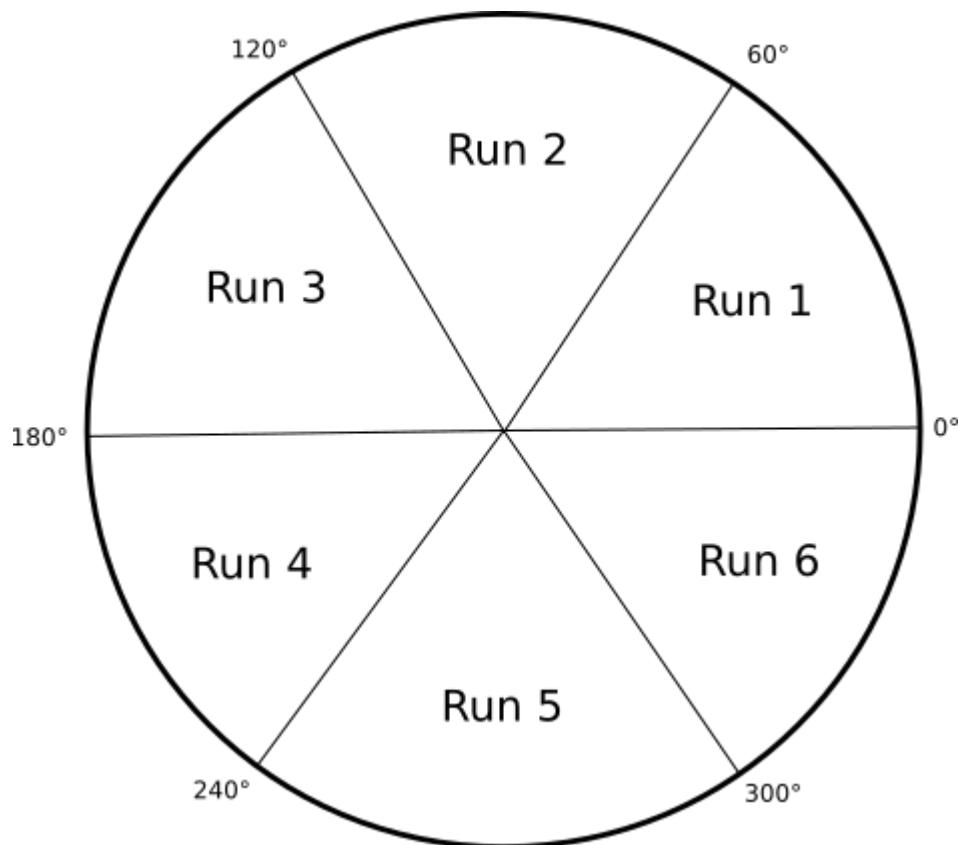


Figure 3.6: Symmetry Test Run Layouts

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 down the line. The other four tests follow in this same pattern, as shown in 3.5.

Table 3.5: Shuffle Test Run Schemes

Original Fuel Position in Control	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 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. The following section section 4.2, covers the results of the basic control model. The final sections — dedicated to homogenization section 4.3, symmetry subsection 4.4.1, and shuffling subsection 4.4.2 — compare them to the control.

#### 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.

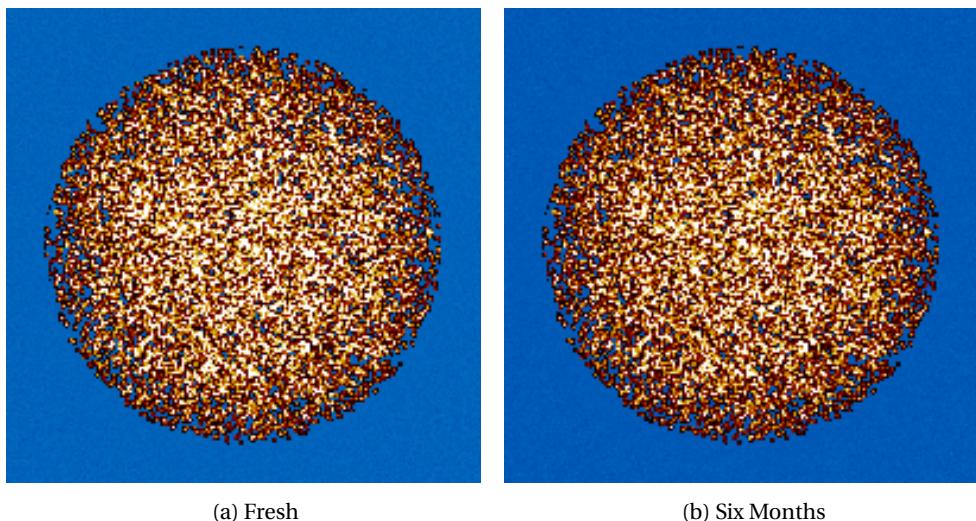


Figure 4.1: Serpent-generated mesh figures of the fission rate (hot color map) and thermal flux (cold color map) for the representative single-pebble at each depletion step. A cold color map is from shades of whitish-blue (high) to blackish-blue (low) while the hot color map is from a whitish-yellow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

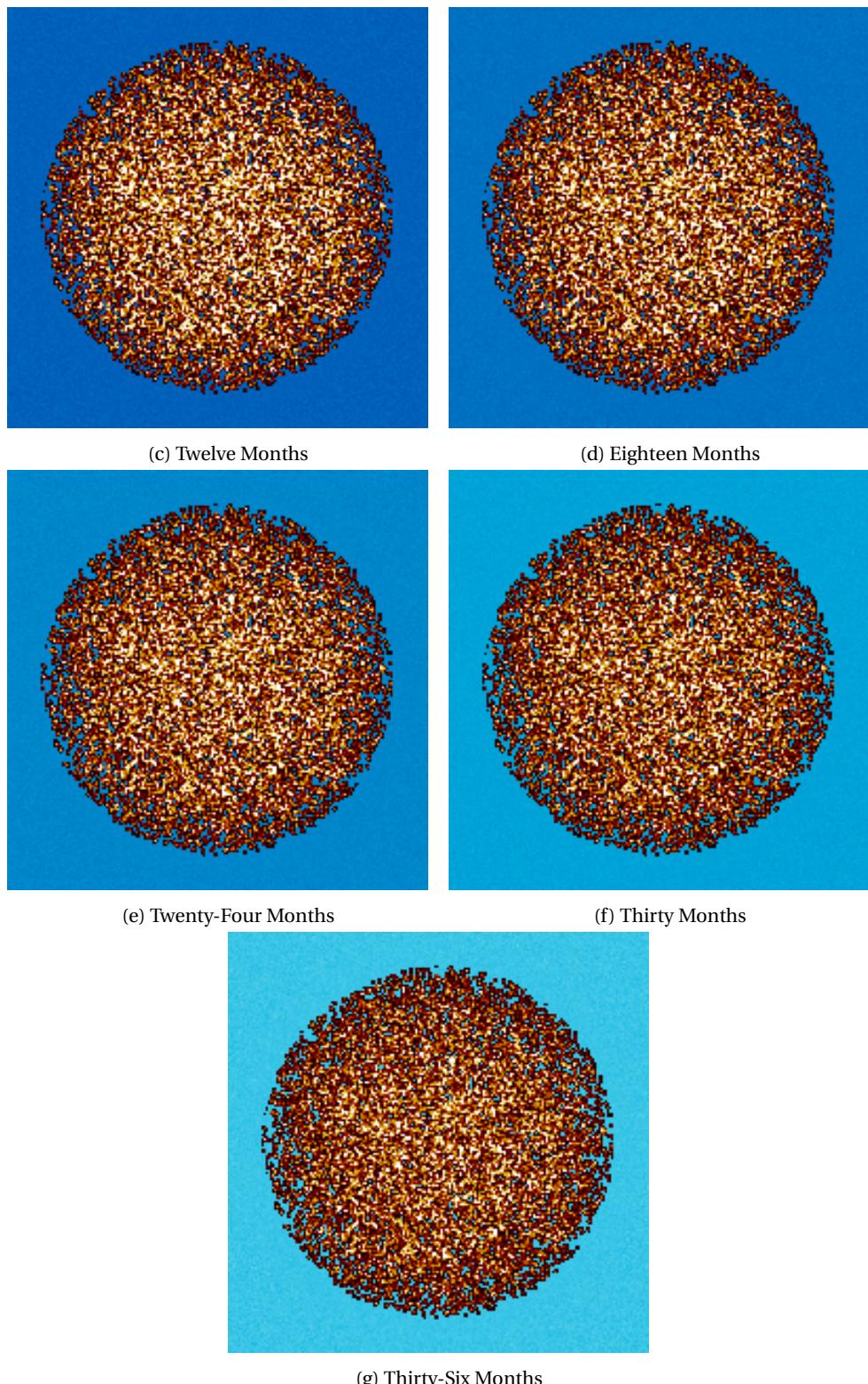
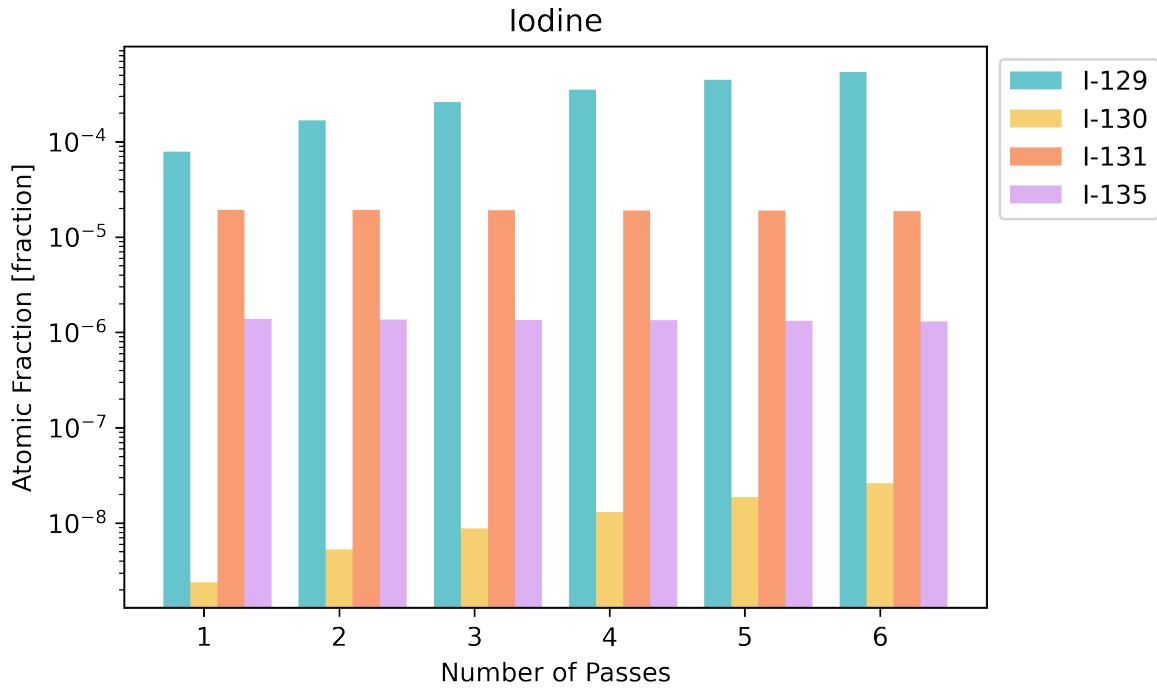


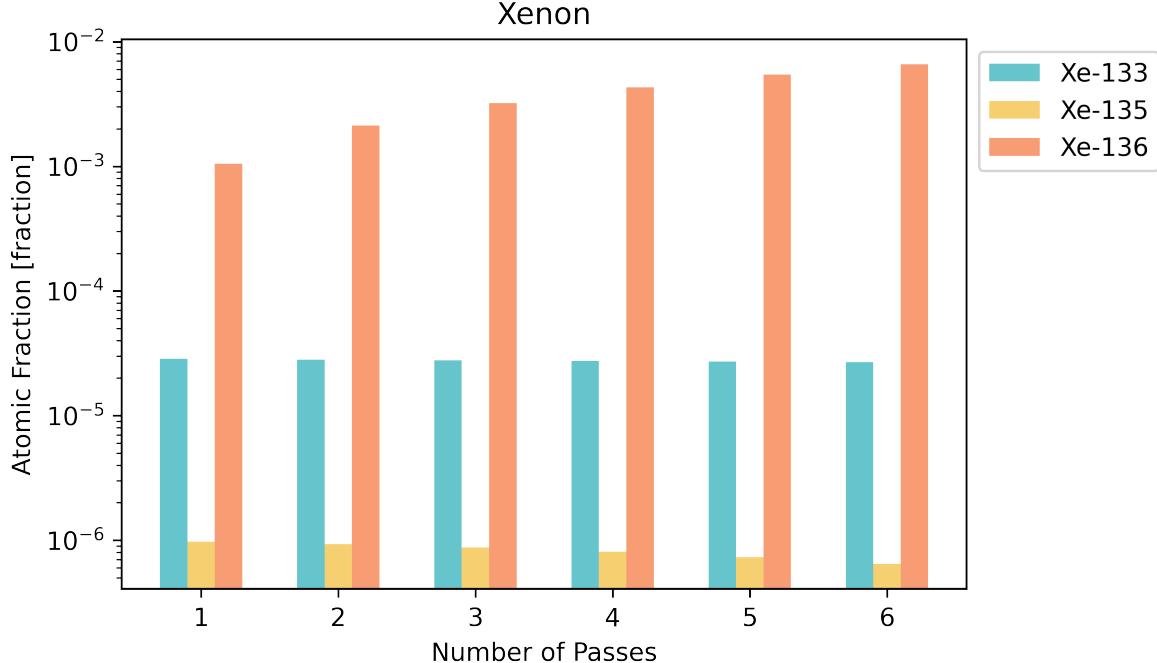
Figure 4.1: Serpent-generated mesh figures of the fission rate (hot color map) and thermal flux (cold color map) for the representative single-pebble at each depletion step. A cold color map is from shades of whitish-blue (high) to blackish-blue (low) while the hot color map is from a whitish-yellow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

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 discussed 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.

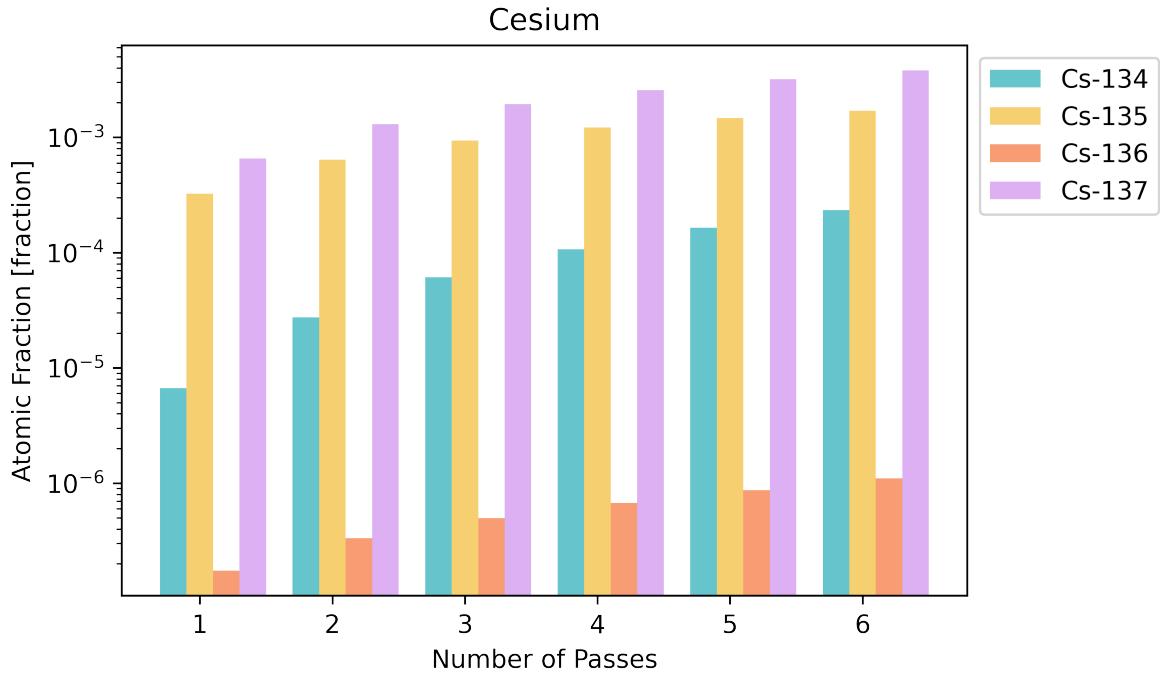


(a) Iodine isotope buildup with each pass

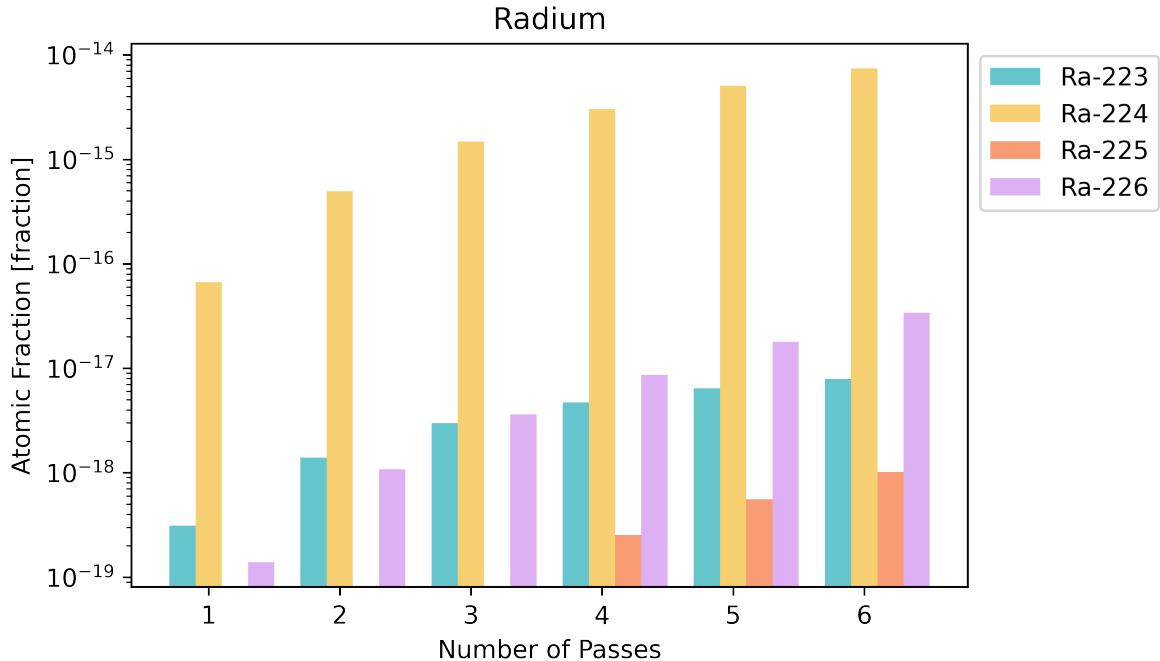


(b) Xenon isotope buildup with each pass

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.)

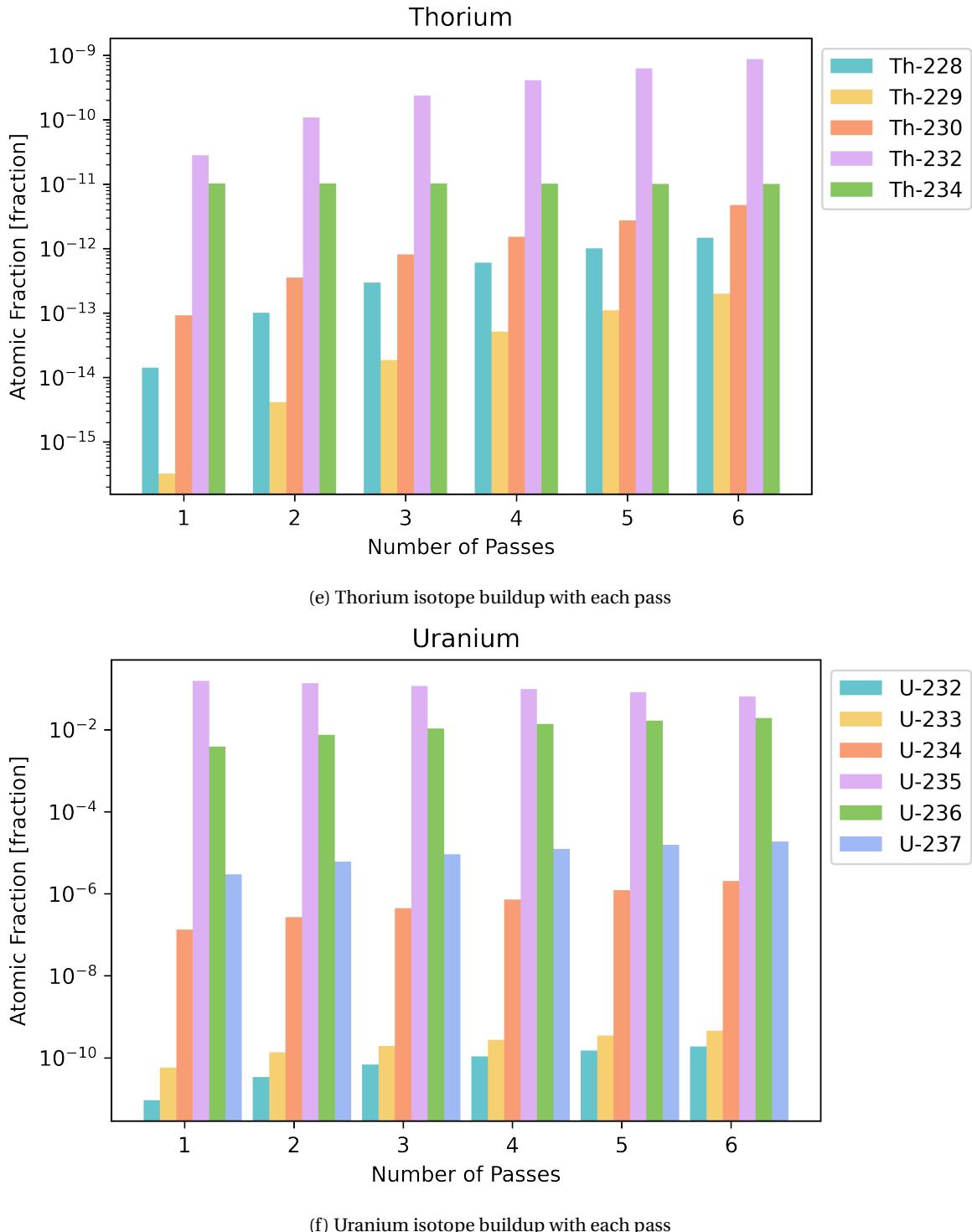
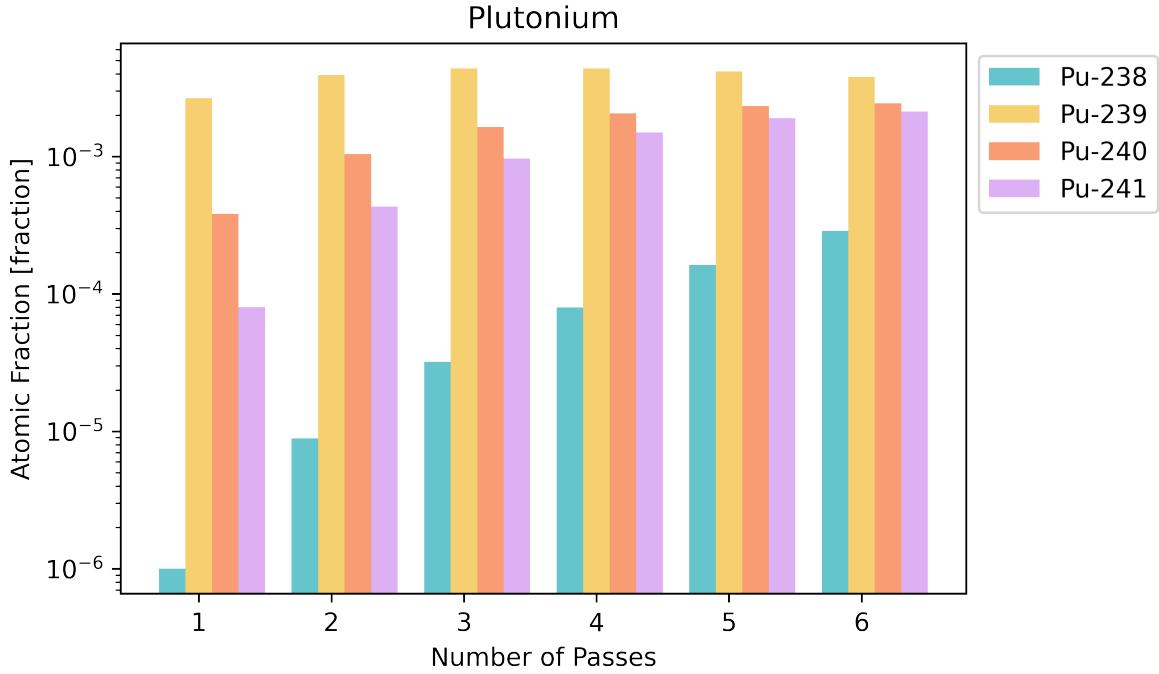


Figure 4.2: Evolution of Safety Relevant Isotopic Concentrations in Pebbles of Sangamon20 over Six Six-Month Passes (cont.)



(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.

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 ( $9.28 \times 10^{-12}$ ) and sixth ( $1.9 \times 10^{-10}$ ) cycle. While the atomic fraction doesn't reach an equilibrium, the rate at which it increases each cycle is steady - increasing by  $4.02 \times 10^{-11}$ ,  $4.2 \times 10^{-11}$ , and  $3.9 \times 10^{-11}$  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).

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

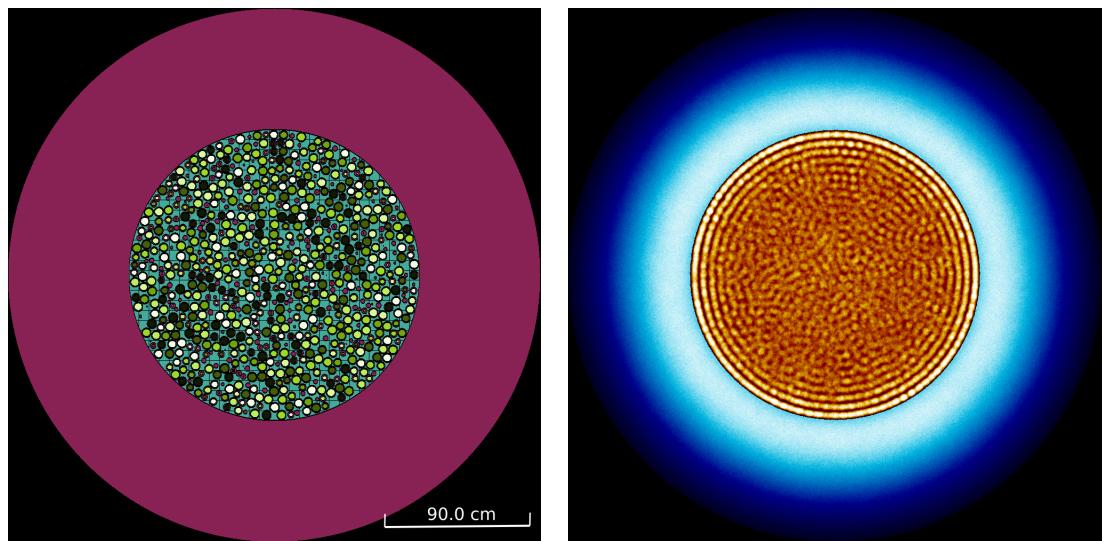
the fuel, and the only isotope reported in Figure 4.2b to increase, owing to its long half life. Each cycle increases  $^{136}Xe$  content by 0.0011, beginning at a concentration of 0.00105 in the first cycle and ending at 0.0066 after the sixth. Isotopes of iodine form a smaller portion of fission products 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  $7.38 \times 10^{-5}$  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  $9.99 \times 10^{-20}$ ) for the first three passes.  $^{224}Ra$  far outweighs the other reported isotopes of radium, with an atomic fraction of  $7.46 \times 10^{-15}$  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  $8.80 \times 10^{-10}$  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

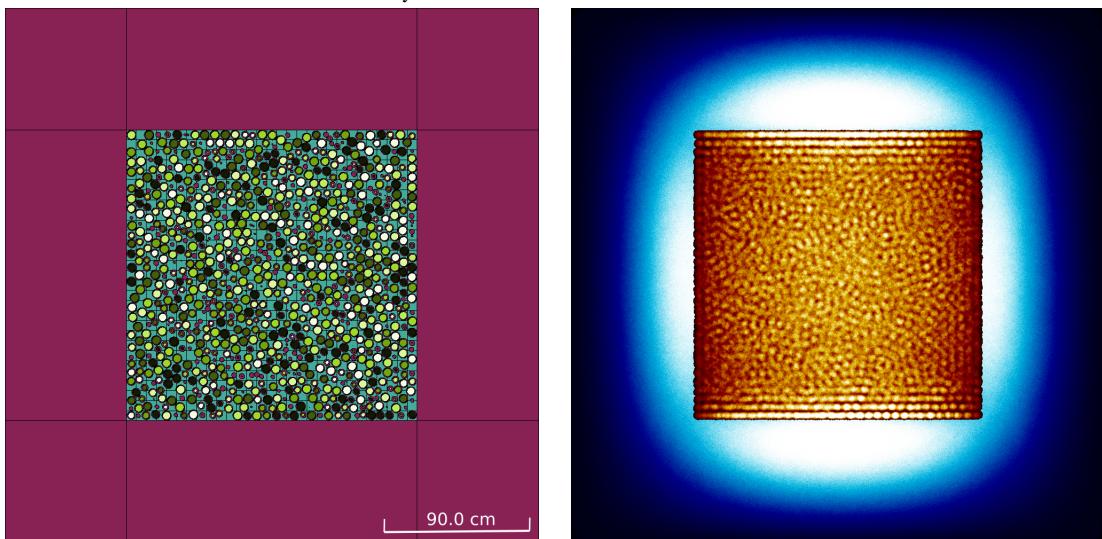
Figure 4.3 shows a cross section of the core geometry at the origin (the midplane, the center of which is the point (0, 0, 0) ) in the xy and xz planes (Sub-Figures a and c, respectively) and provides a mesh of the fission rate and thermal flux in the xy and xz planes (Sub-Figures b and d, respectively). Both of these integrate over z and y, respectively, to produce a 2D image. The value of  $k_{eff}$  was  $1.04077 \pm 0.00054$ .

Figure 4.13e 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 and Thermal Flux(cold color map) and Fission Rate (hot color map) Meshes for the Control Model of Sangamon20

The mesh in 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.

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.

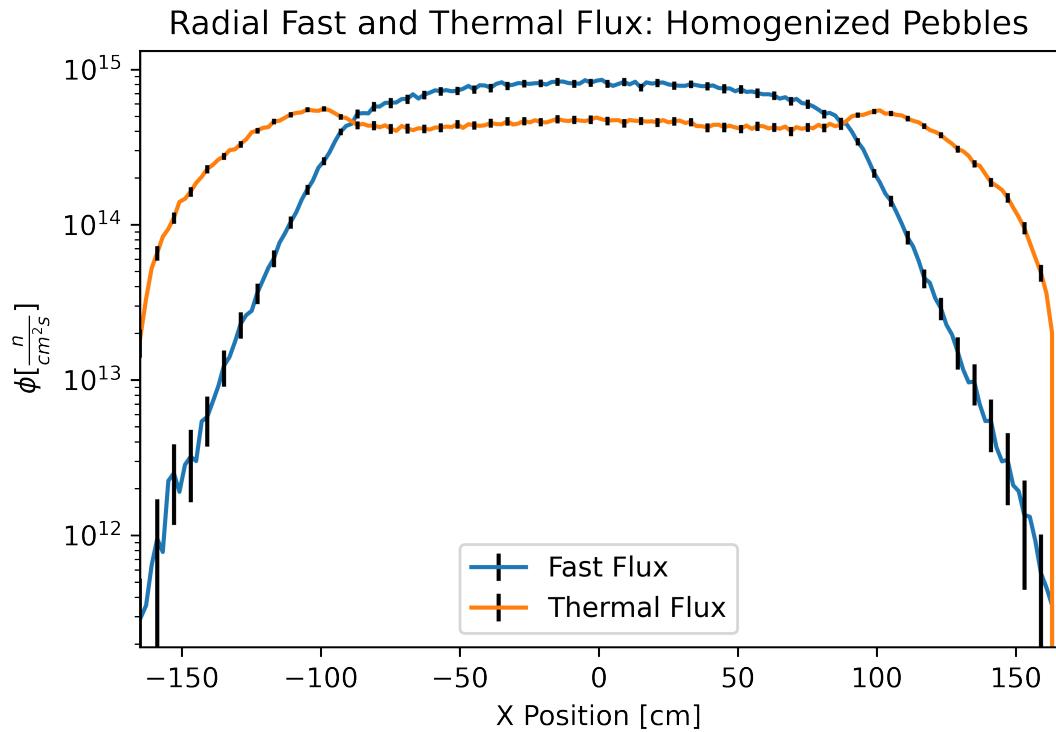


Figure 4.4: Radial Thermal and Fast Flux Profiles along the X-Axis at the Mid-Plane in Sangamon20: Homogenized Pebbles

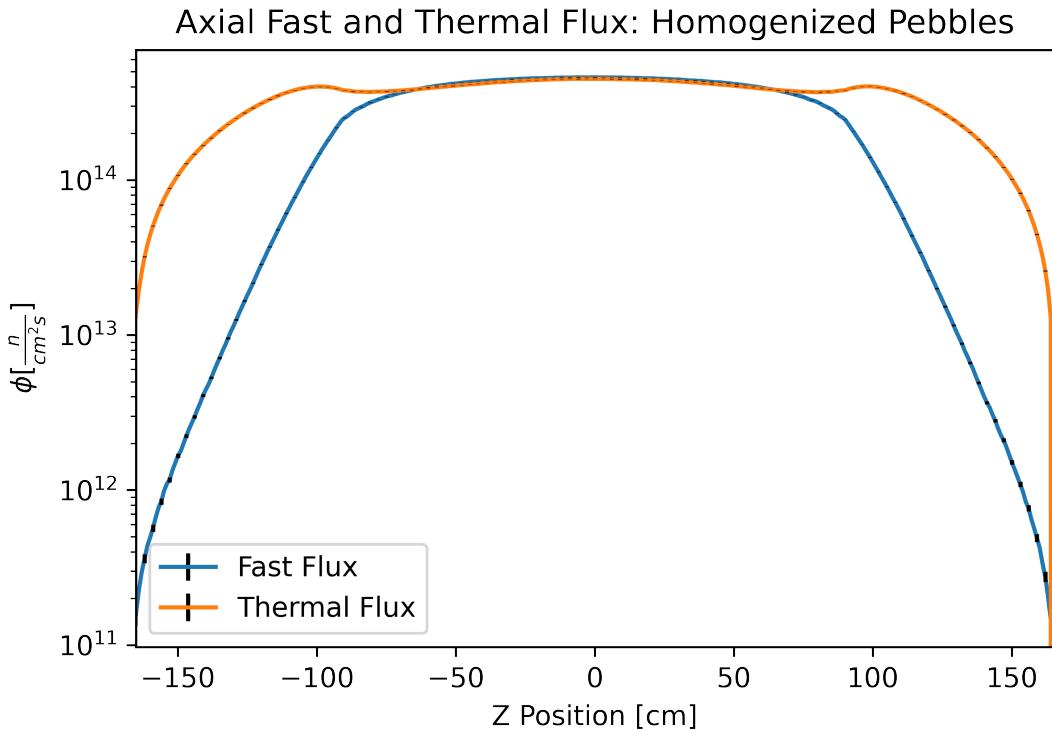


Figure 4.5: Axial Thermal and Fast Flux Profiles at the Centerline of Sangamon20: Homogenized Pebbles

Figures 4.4 and 4.5 provide the fast and thermal flux profiles in Sangamon20 at the axial and radial (x-direction) centerlines, respectively. 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. Detector bins span the entirety of the height of the reactor.

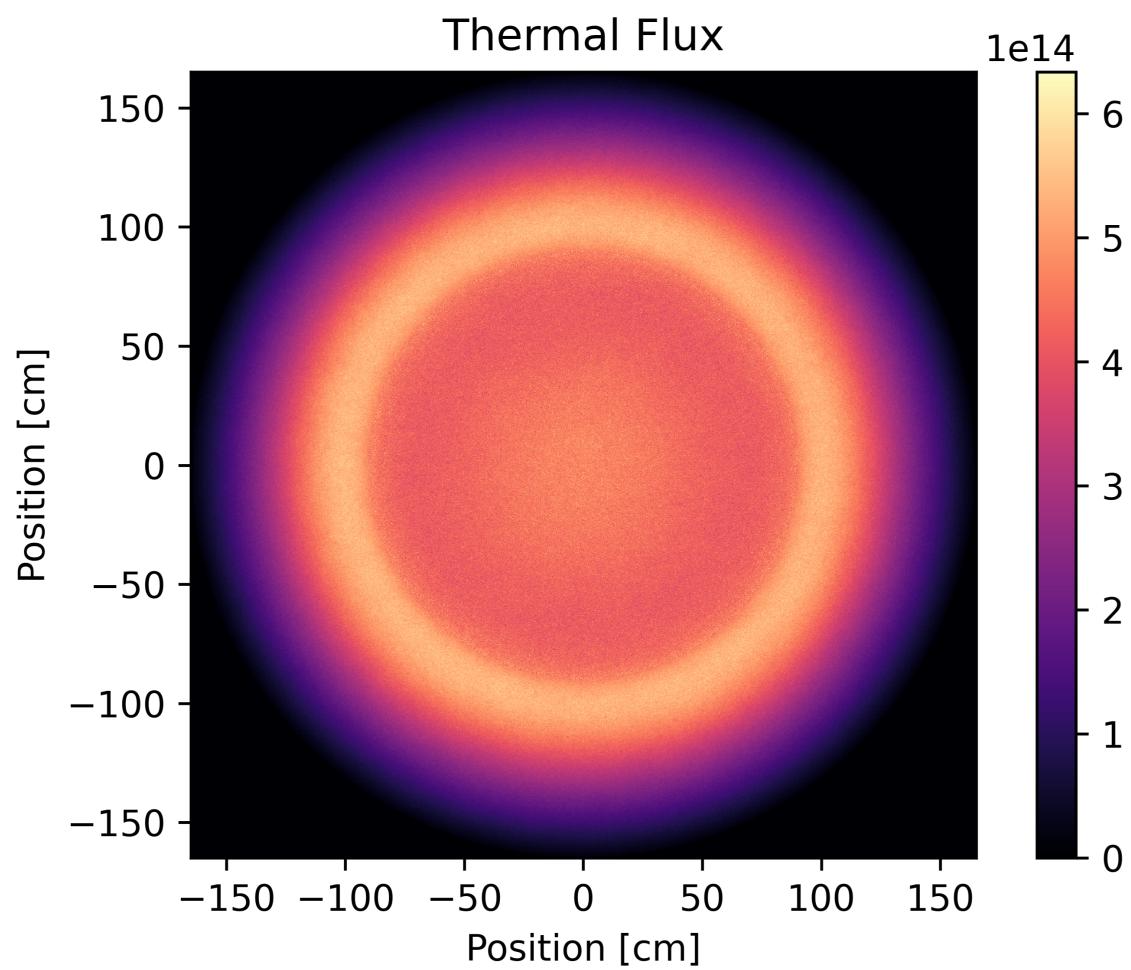


Figure 4.6: Thermal Flux in xy Plane

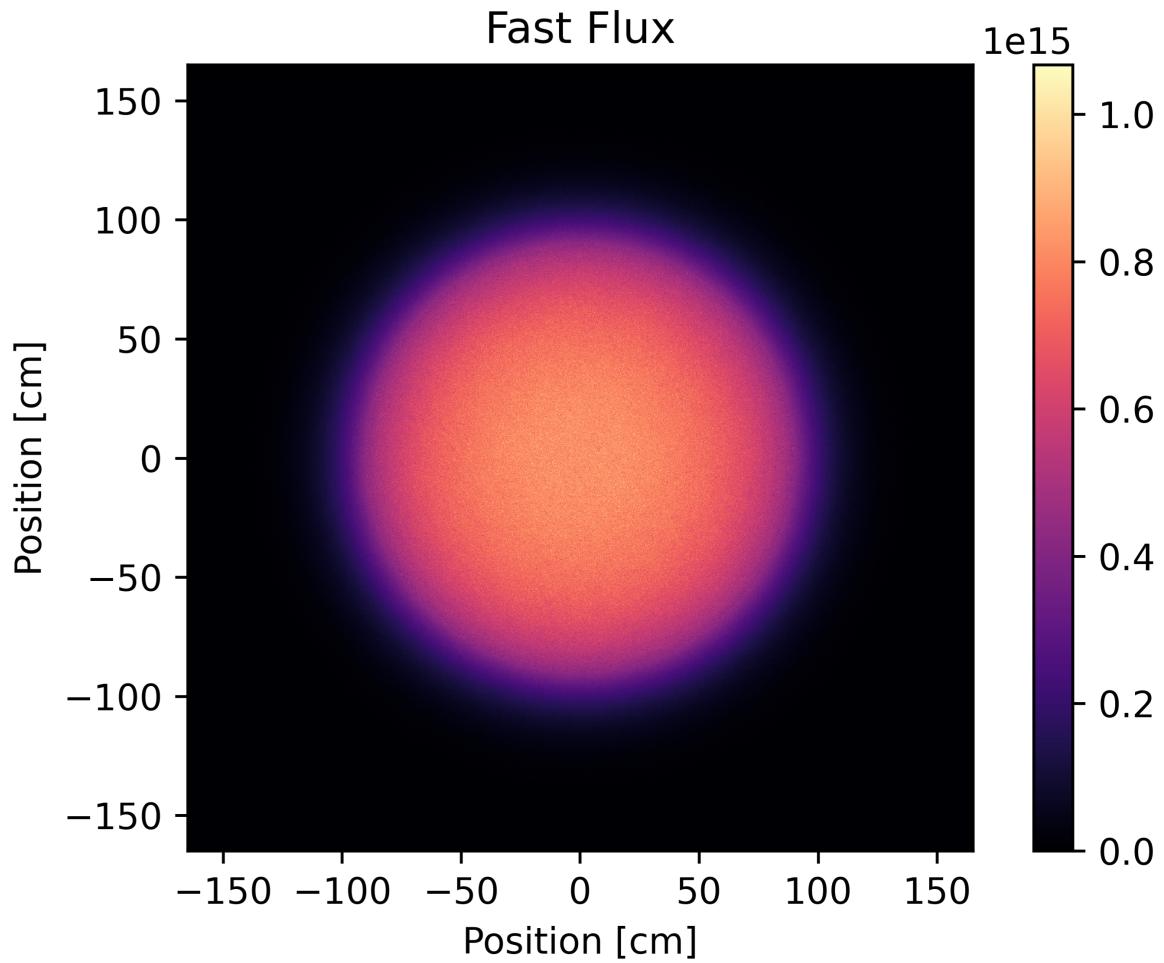


Figure 4.7: Fast Flux in xy Plane

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 it is directly next to the reflector, which has a smoothing effect.

Below, Figure 4.18 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.

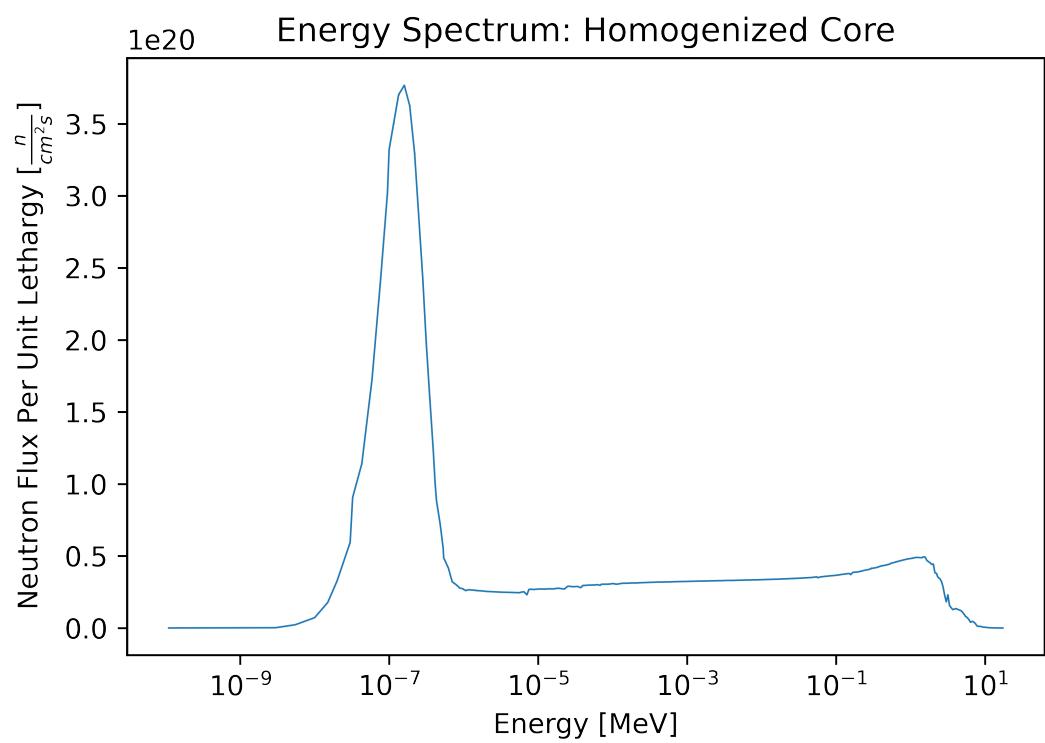


Figure 4.8: Core Spectrum

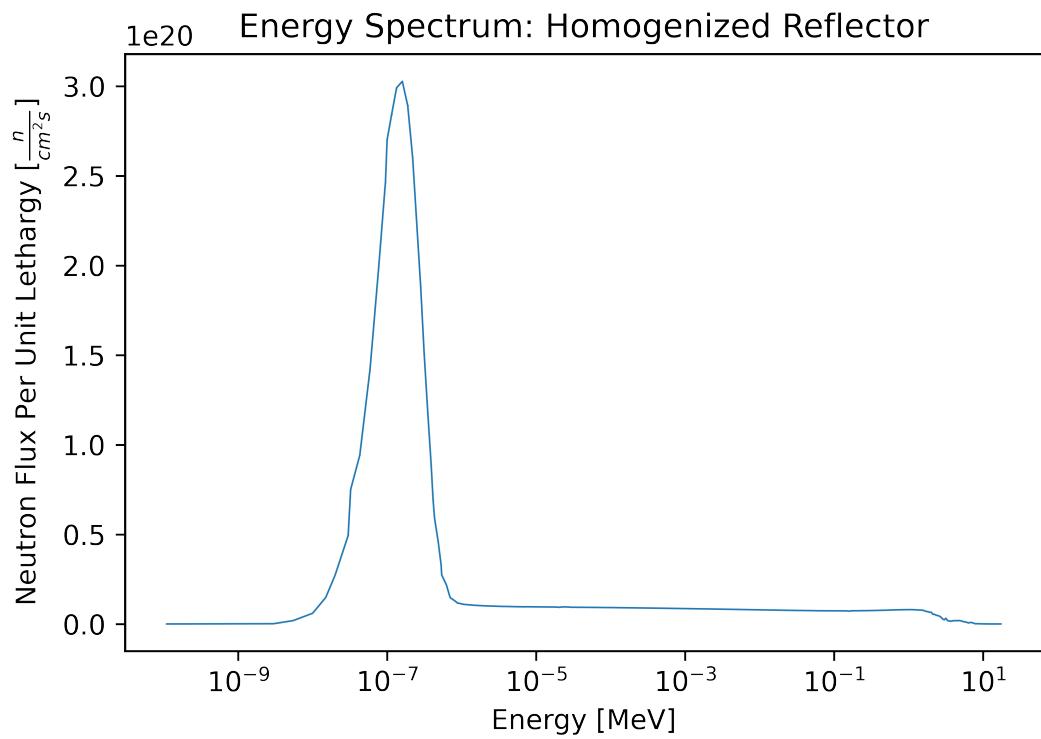


Figure 4.9: Reflector Spectrum

The thermal peak of the whole-core and reflector both occur around  $10 \times 10^{-7}$  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.

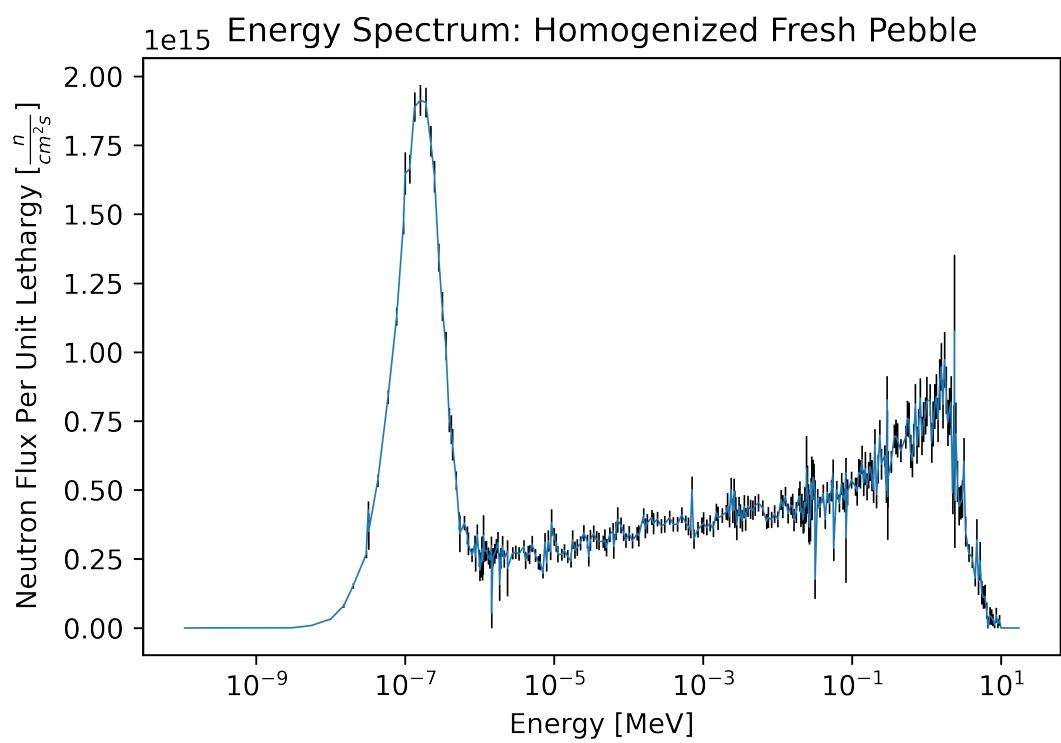


Figure 4.10: Fresh Pebble Spectrum

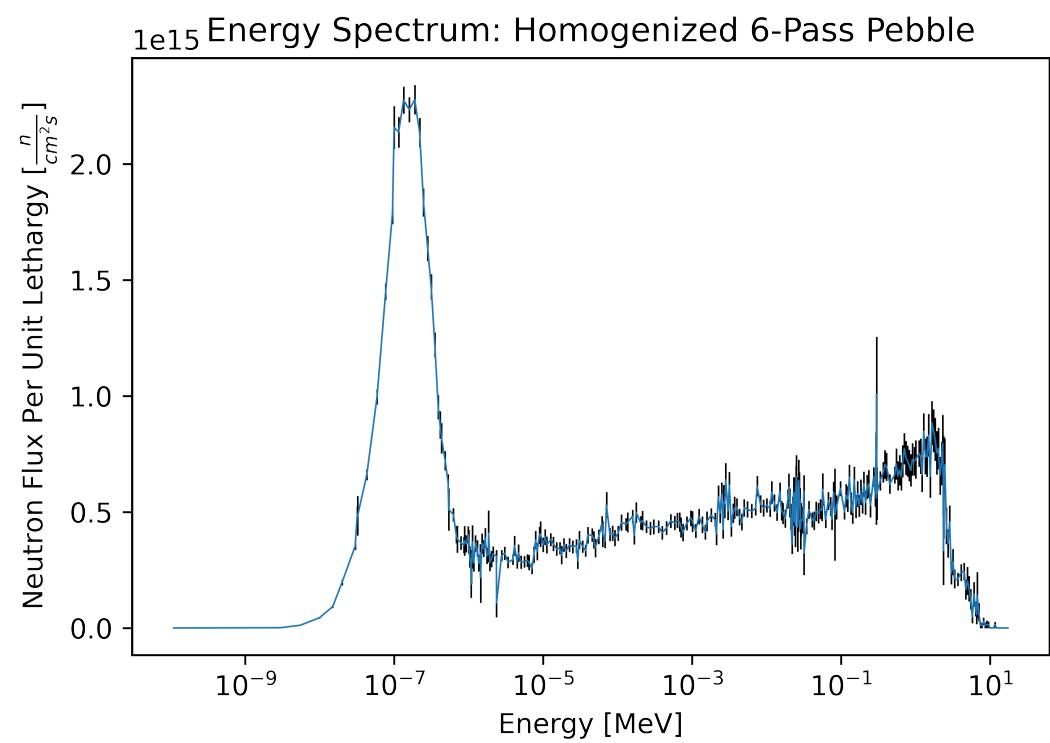


Figure 4.11: Six-Pass Pebble Spectrum

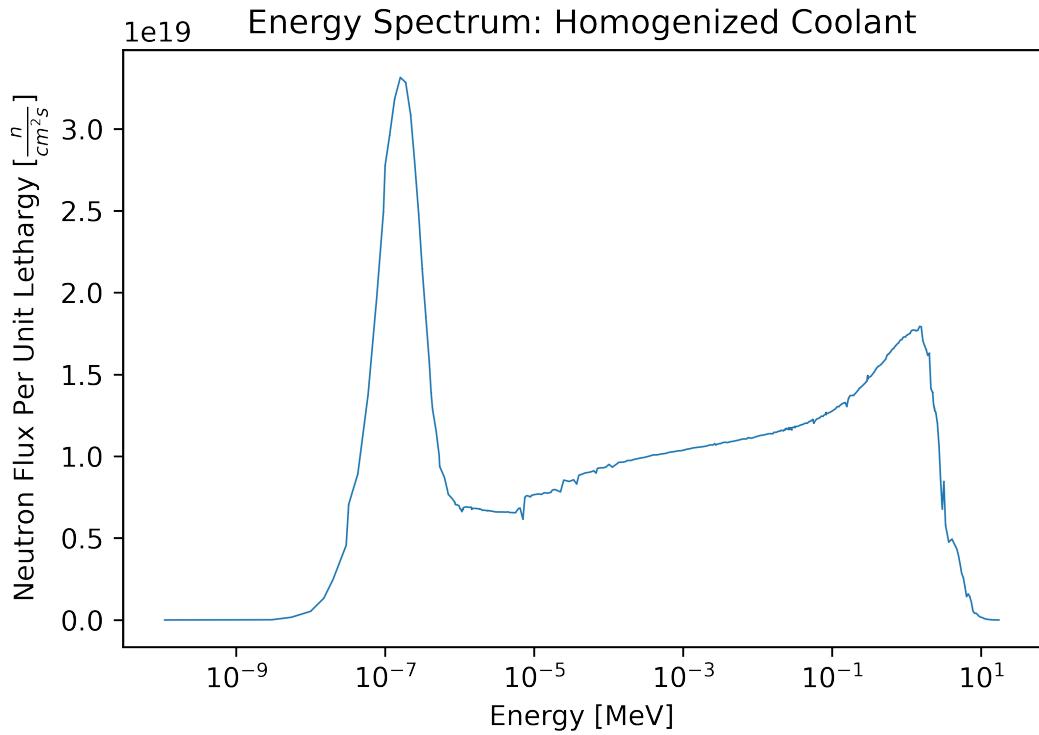


Figure 4.12: Coolant Spectrum

The spectra for a randomly selected fresh and sixth-pass pebble are subject to the highest uncertainty of all the provided spectra in Figure 4.18, as a single pebble is a relatively small bin. 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 higher energy range differs 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]. And so, this test uses an otherwise identical model with explicit TRISO particles to investigate the effect of homogenization. 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.

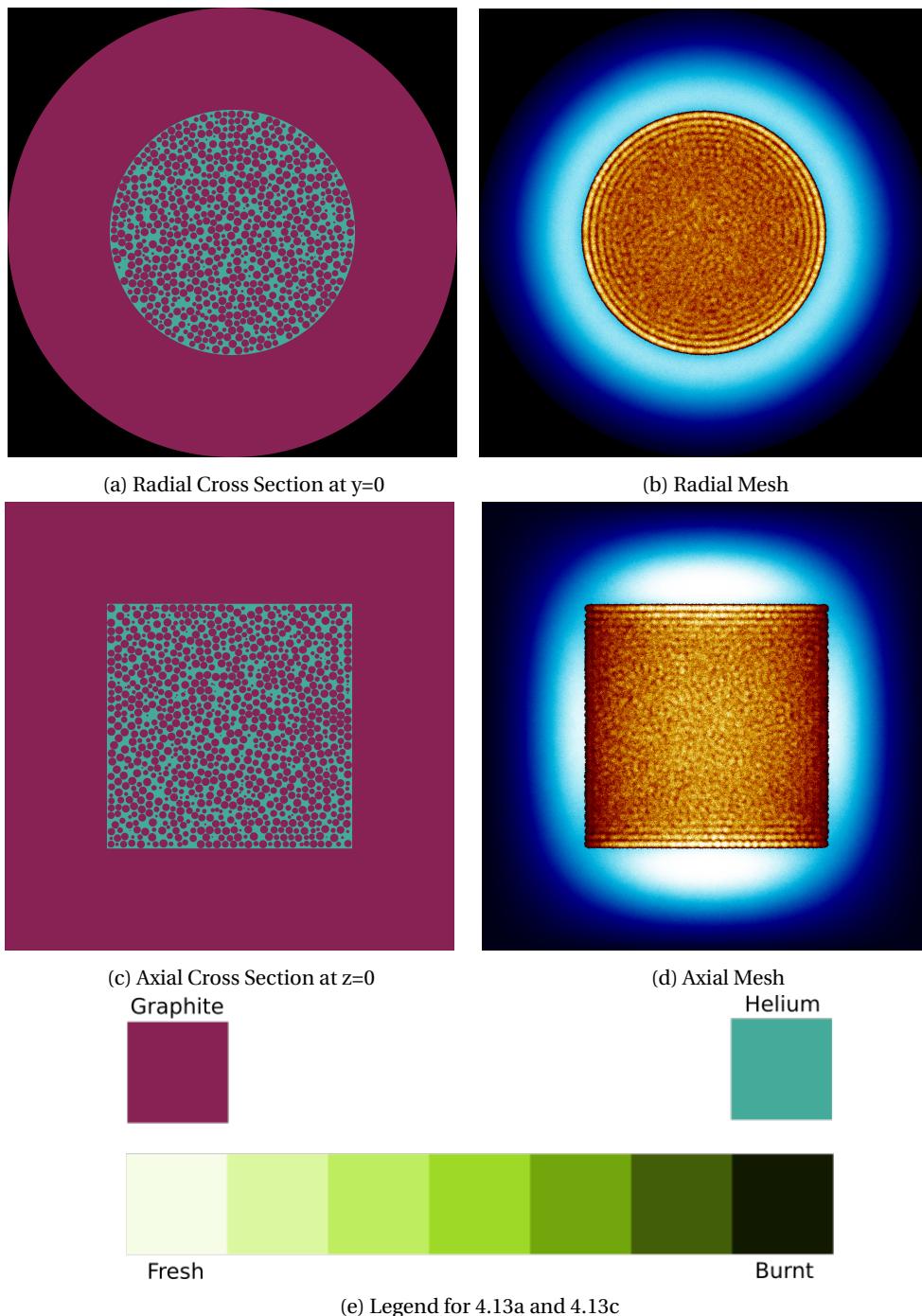


Figure 4.13: Full Core Using Heterogenized Pebbles

In agreement with [42], the heterogenized version reported a  $k_{\text{eff}}$  of  $1.087 \pm 0.00032$ , compared with the homogenized's  $1.041 \pm 0.00054$ , a difference of 4.23%.

Overall, the mesh result for the 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. It gives the shape and magnitude of the fluxes, which 4.13 cannot.

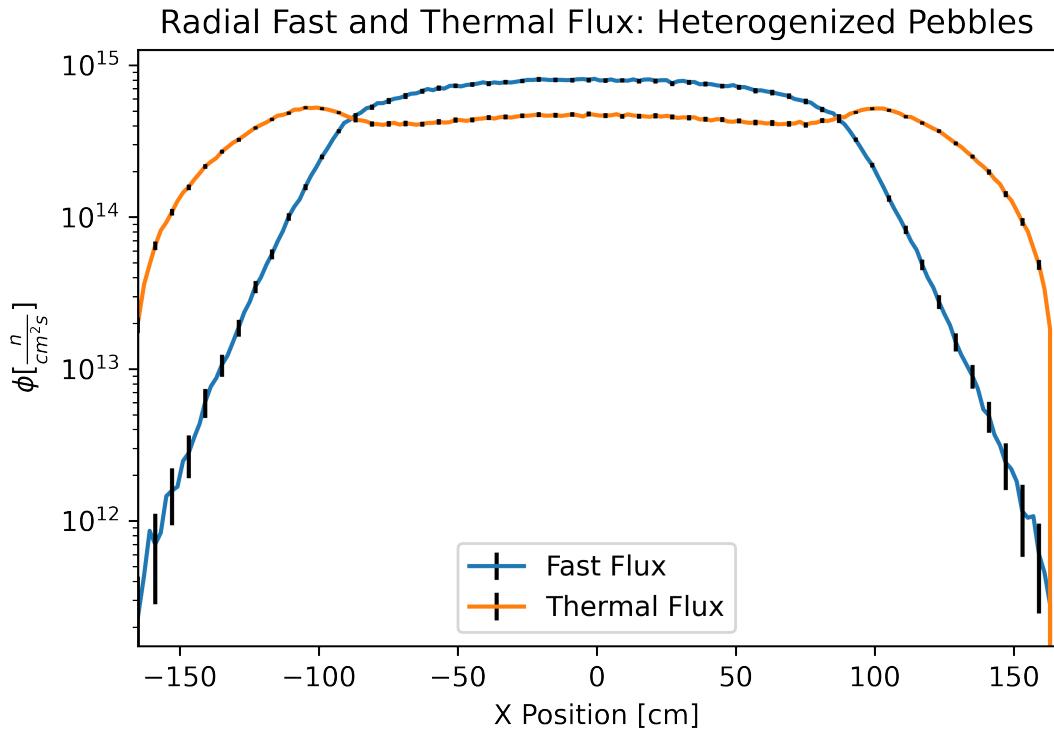


Figure 4.14: Radial Thermal and Fast Flux Profiles Along the X-Axis at the Mid-Plane in Sangamon20: Heterogenized Pebbles

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  $2.00 \times 10^{09}$ . The heterogenized model otherwise shows a similar flux profile to the homogenized model (see Figure 4.19), 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.

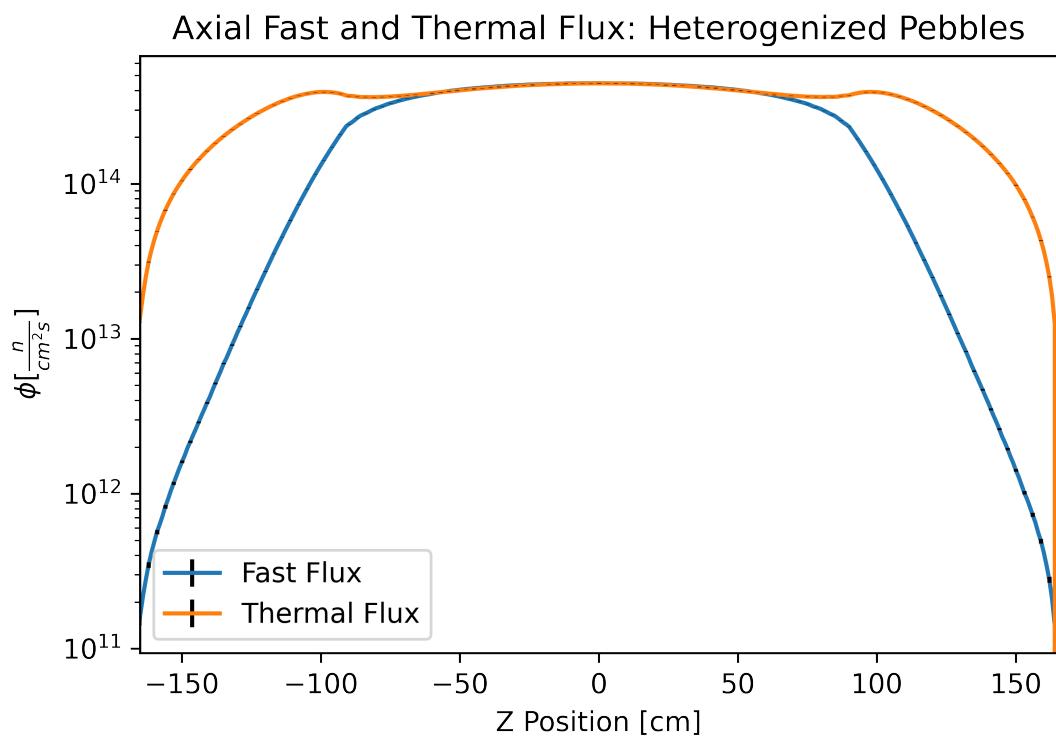


Figure 4.15: Axial Thermal and Fast Flux Profiles along the Centerline in Sangamon20: Heterogenized Pebbles

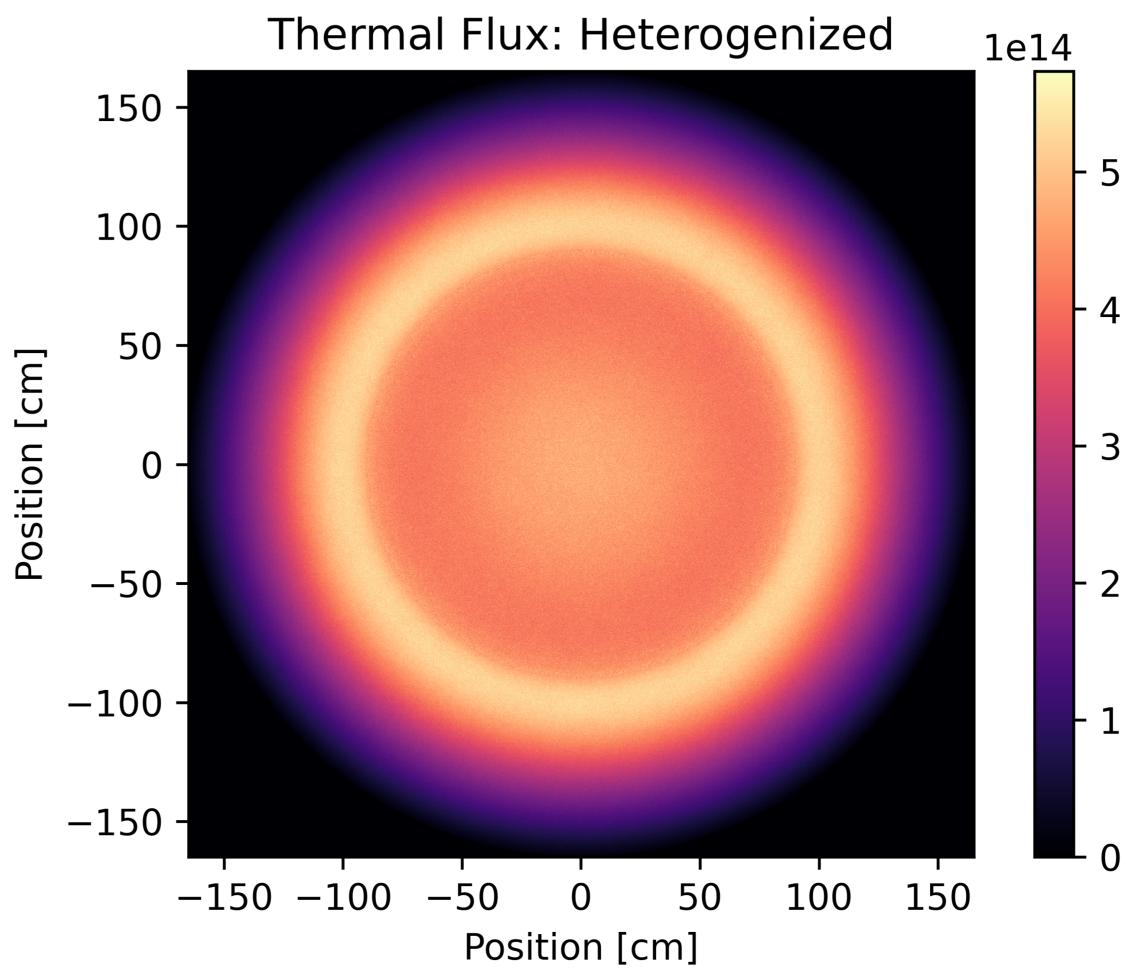


Figure 4.16: Thermal Flux in  $xy$  Plane in Sangamon20: Heterogenized Pebbles

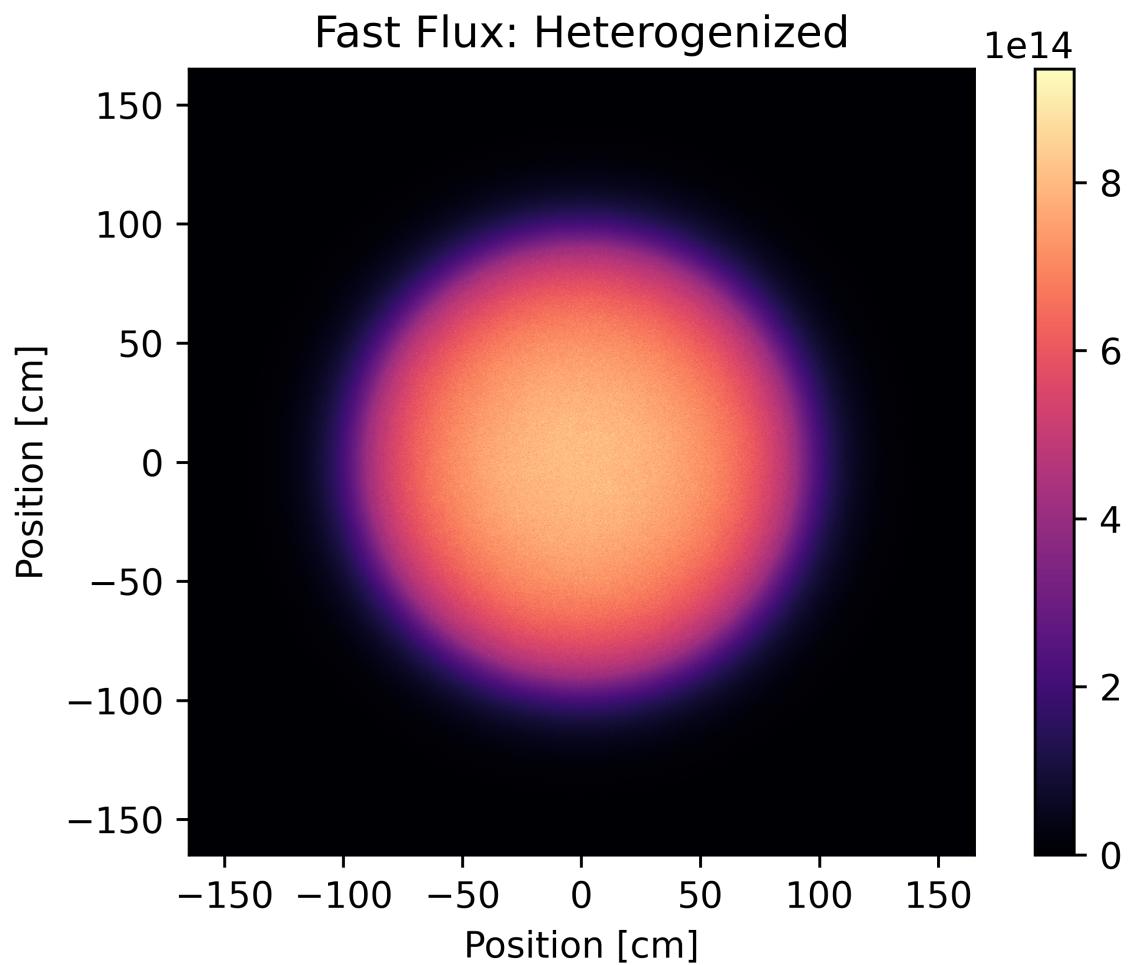
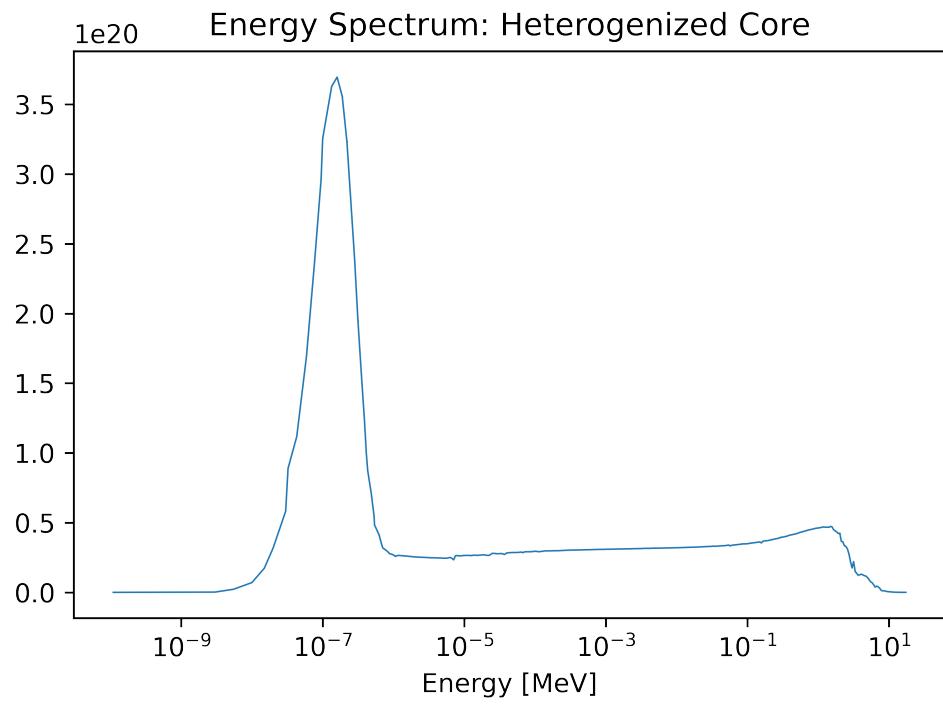


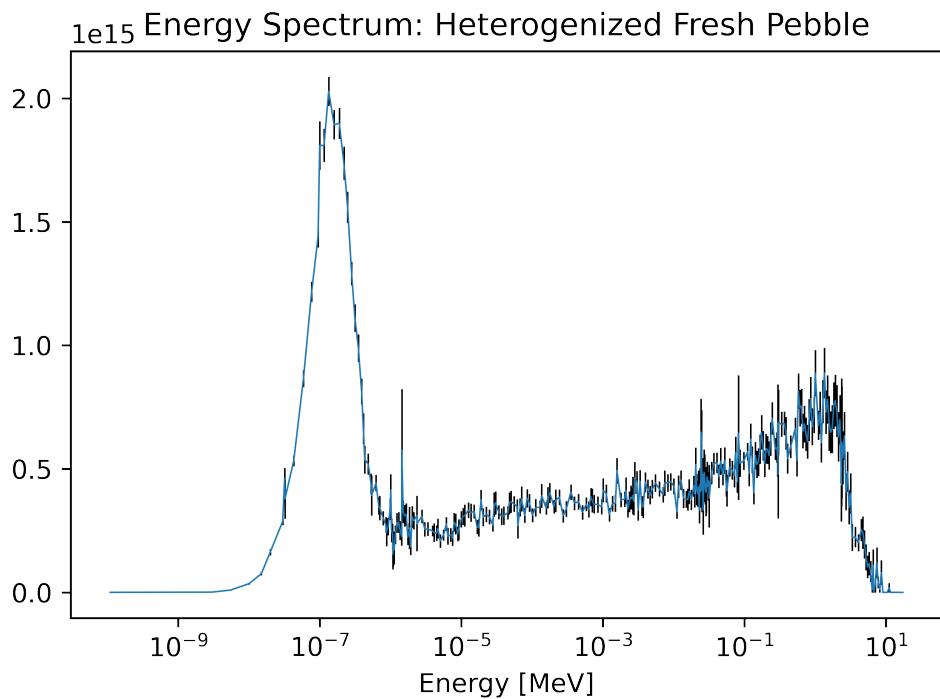
Figure 4.17: Fast Flux in xy Plane in Sangamon20: Heterogenized Pebbles

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.

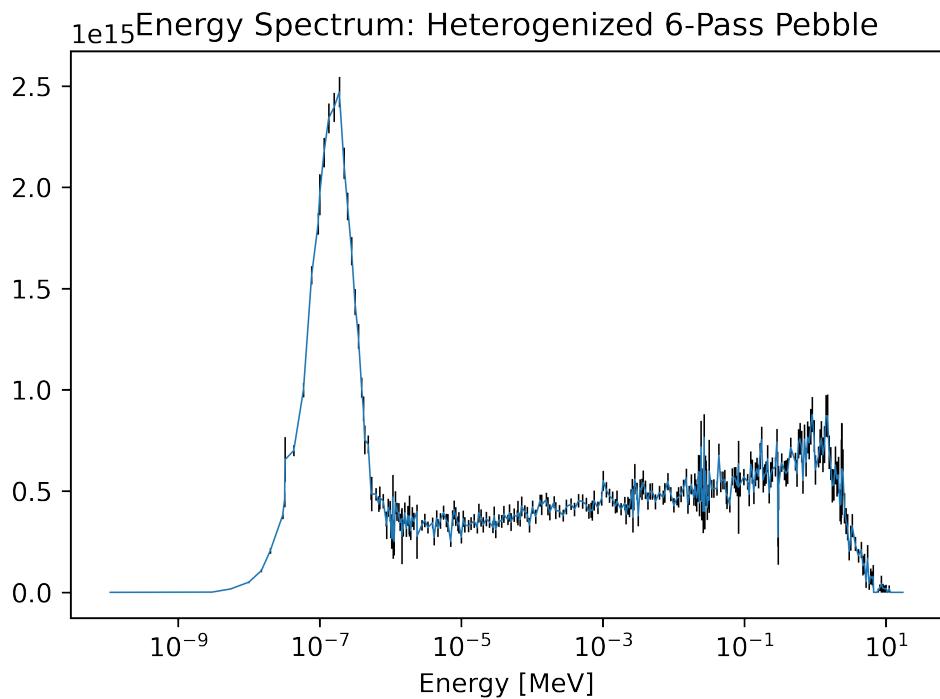


(a) Core Spectrum

Figure 4.18: Lethargy Adjusted Neutron Flux Energy Spectra: Core Using Heterogenized Pebbles

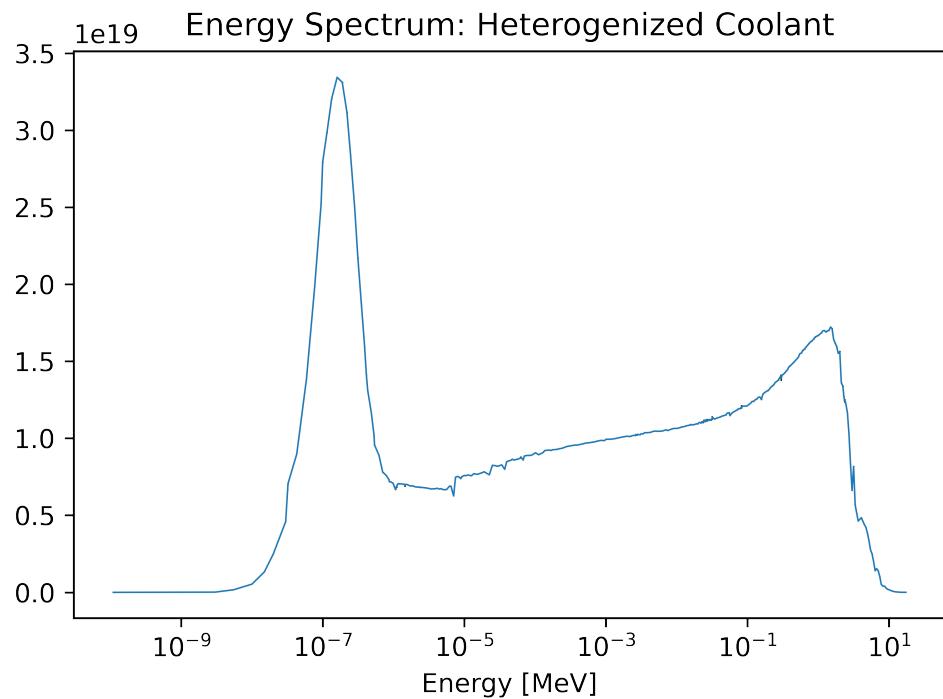


(b) Fresh Pebble Spectrum

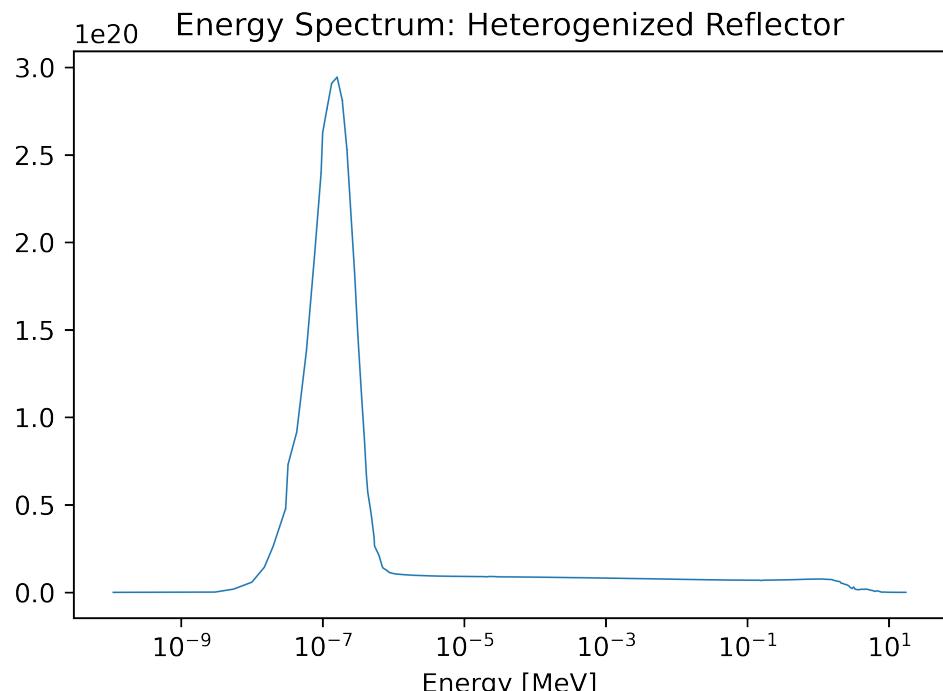


(c) Six-Pass Pebble Spectrum

Figure 4.18: Lethargy Adjusted Neutron Flux Energy Spectra: Core Using Heterogenized Pebbles (cont.)



(d) Coolant Spectrum



(e) Reflector Spectrum

Figure 4.18: Lethargy Adjusted Neutron Flux Energy Spectra: Core Using Heterogenized Pebbles (cont.)

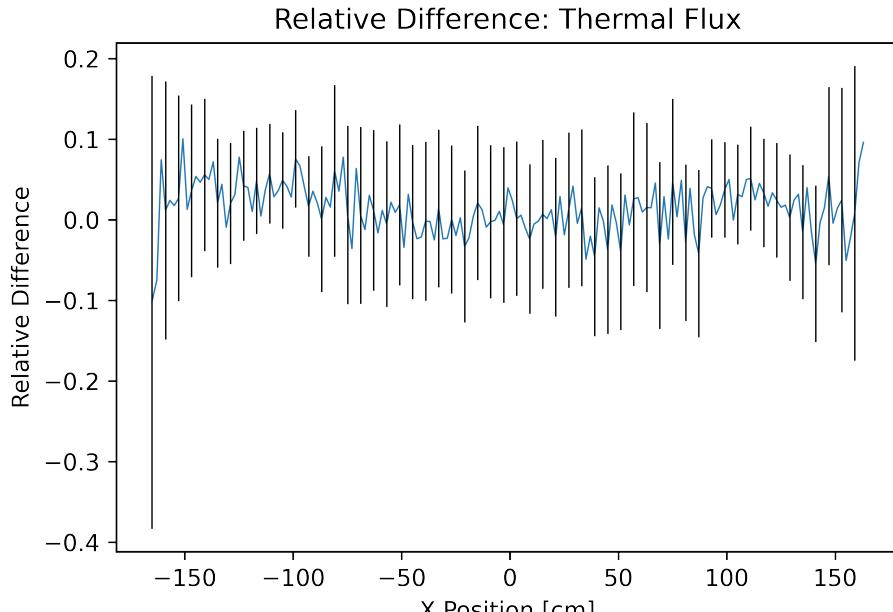
The heterogenized spectra, much like the flux profiles, are of a similar morphology. In order to better examine the differences between the homogenized and heterogenized versions, Figures 4.19 and 4.20 plot the simple relative difference for all spectra, and the radial fast and thermal profiles. The relative difference calculation used the following:

$$\Delta i = \frac{i_{\text{homogenized}} - i_{\text{heterogenized}}}{i_{\text{heterogenized}}} \quad (4.1)$$

where

$$\begin{aligned} \Delta i &= \text{relative difference for parameter } i \text{ between homogenized and heterogenized model} \\ i_{\text{homogenized}} &= \text{homogenized parameter } i \\ i_{\text{heterogenized}} &= \text{heterogenized parameter } i \end{aligned} \quad (4.2)$$

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



(a) Thermal Flux

Figure 4.19: Relative Difference in Radial Thermal and Fast Flux Profiles Between Cores Using Homogenized and Heterogenized Pebbles

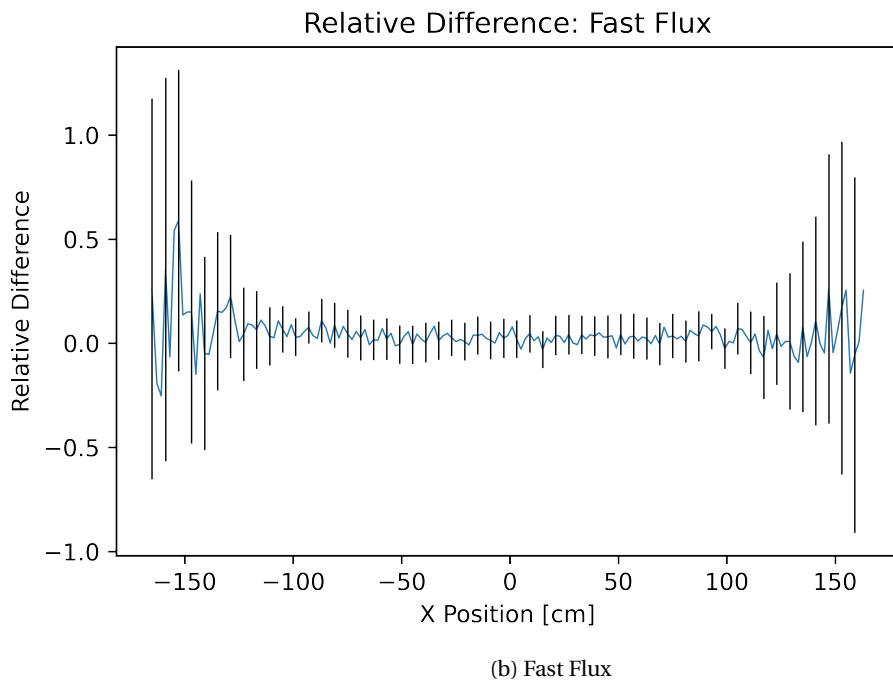
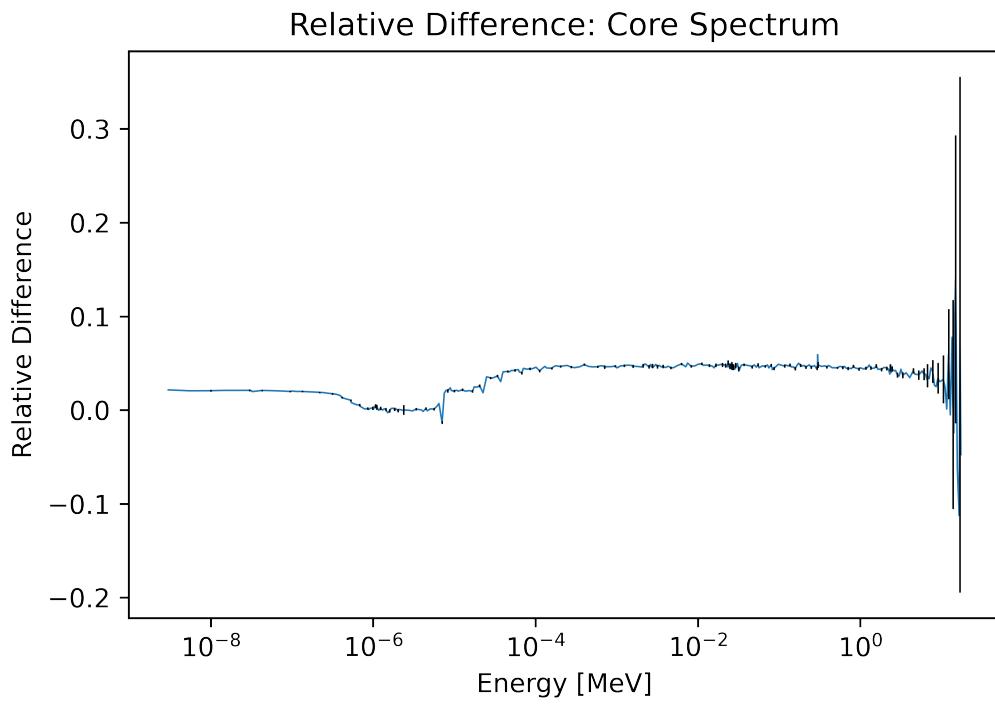
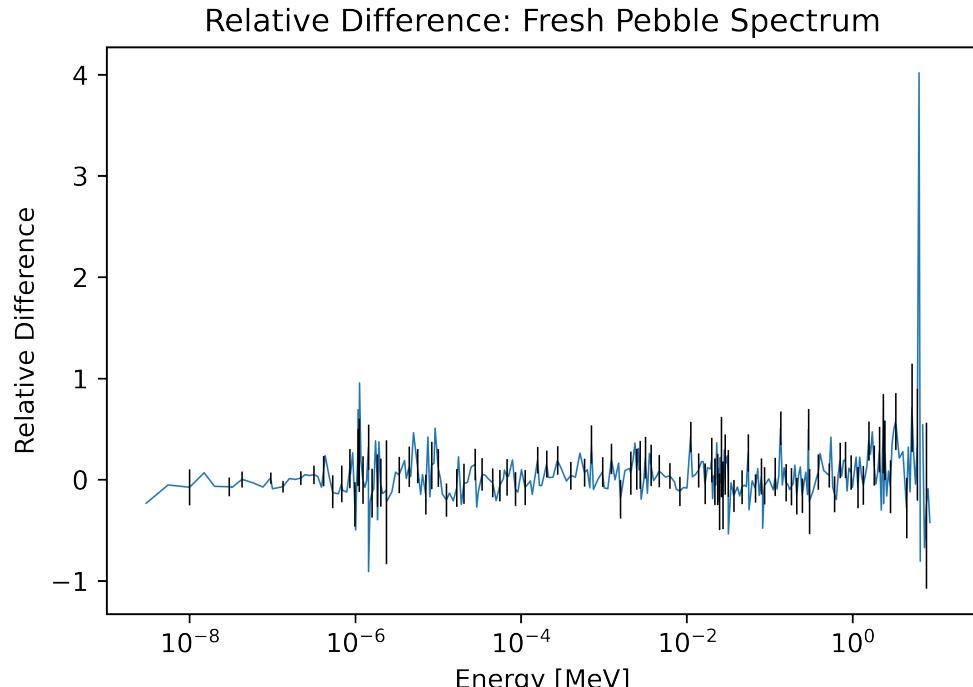


Figure 4.19: Relative Difference in Radial Thermal and Fast Flux Profiles Between Cores Using Homogenized and Heterogenized Pebbles (cont.)

For both the thermal and flux profiles, error only worsens on the outermost edges. Overall, Figures 4.19a and 4.19b 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.

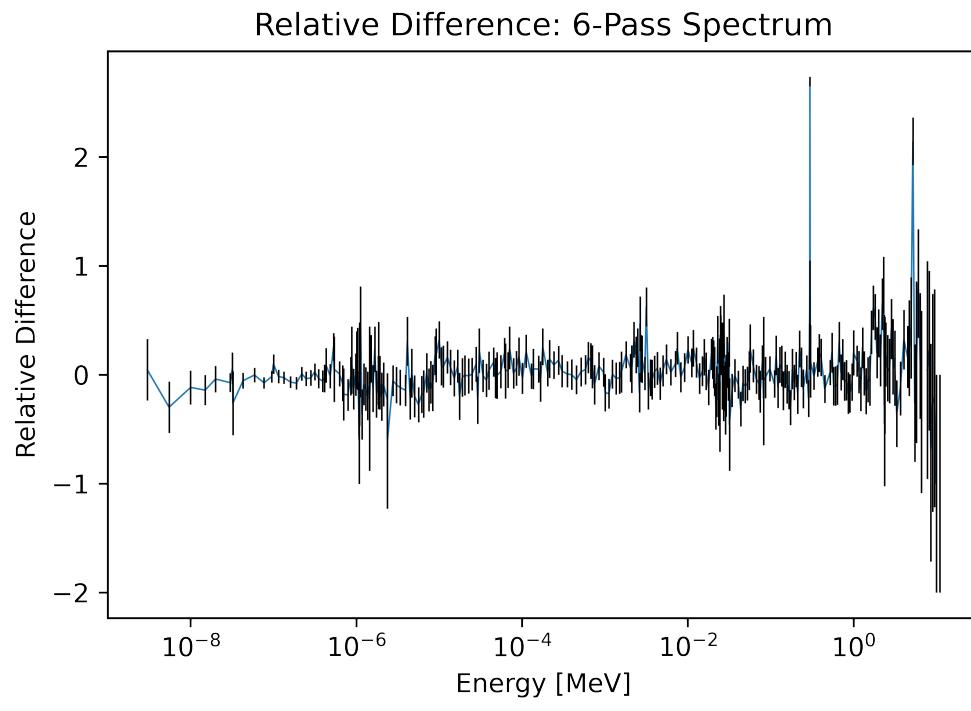


(a) Core

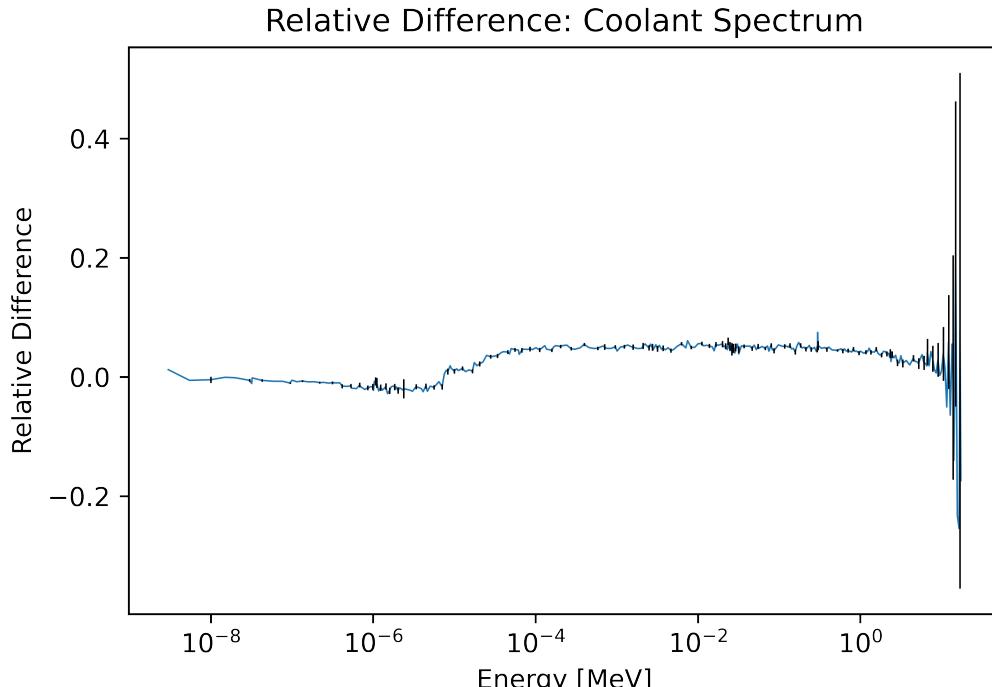


(b) Fresh Pebble

Figure 4.20: Relative Difference in Lethargy Adjusted Neutron Flux Energy Spectra Between Cores using Homogenized and Heterogenized Pebbles



(c) Six-Pass Pebble



(d) Coolant

Figure 4.20: Relative Difference in Lethargy Adjusted Neutron Flux Energy Spectra Between Cores using Homogenized and Heterogenized Pebbles (cont.)

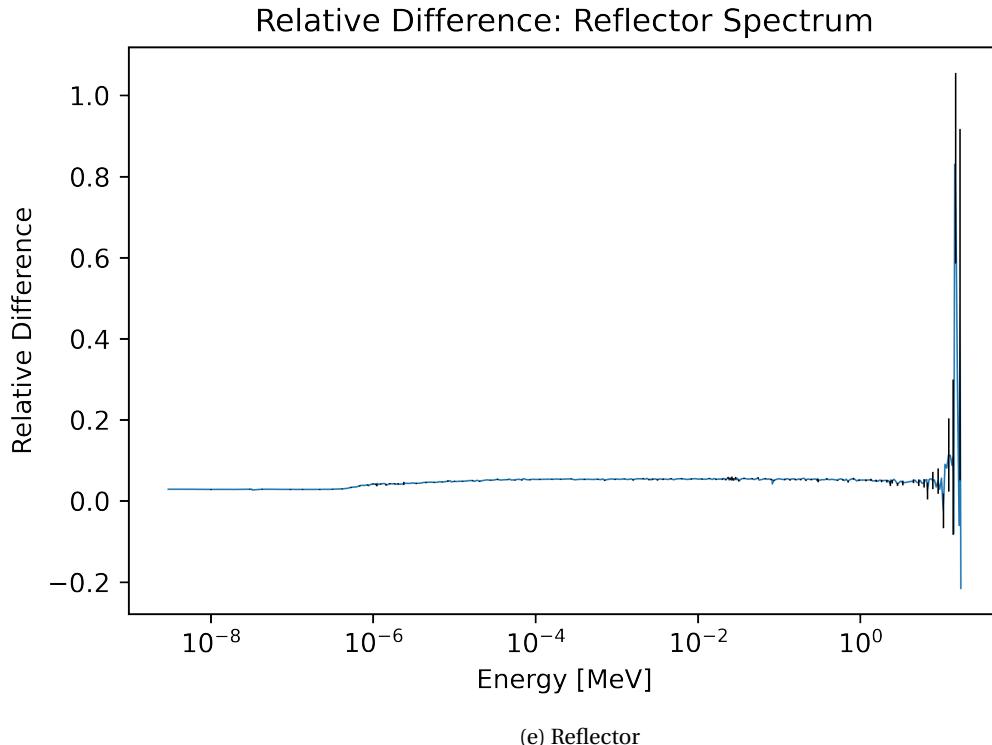


Figure 4.20: Relative Difference in Lethargy Adjusted Neutron Flux Energy Spectra Between Cores using Homogenized and Heterogenized Pebbles (cont.)

Overall, the homogenized model is over-predicting the thermal peak compared with heterogenized in the core spectra by 5%. Around  $10 \times 10^{-6}$  MeV, just after the thermal peak, the two spectra agree before diverging again, this time with a slightly greater disagreement. Unlike Figure 4.19, error alone leaves the relative differences seen in Figure 4.20 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 4.20b and 4.20c, the relative difference spikes; though the error is still substantial in this region compared with the peaks in the relative difference. Between  $10 \times 10^{-7}$  and  $5 \times 10^{-2}$ , the differences are minimal and likely accounted for by noise or error. Between  $10 \times 10^{-2}$  and  $10 \times 10^{-1}$ , 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.

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

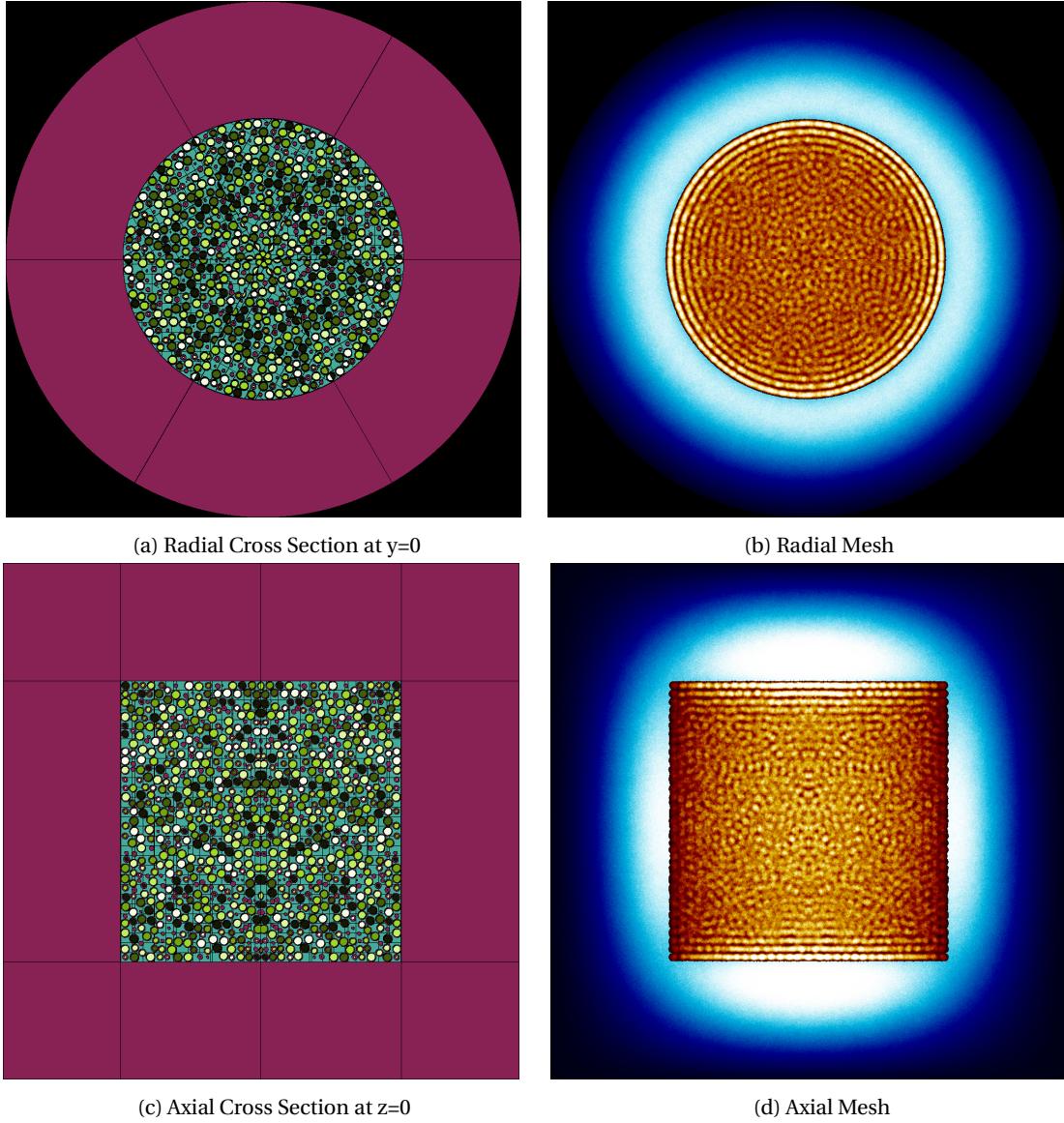


Figure 4.21: Sensitivity Analysis:  $0^\circ - 60^\circ$

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 4.22 by subtracting the radial meshes for the control (Figure 4.3b) and first symmetry test (Figure 4.21b).

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 4.22 are not a gradient, but

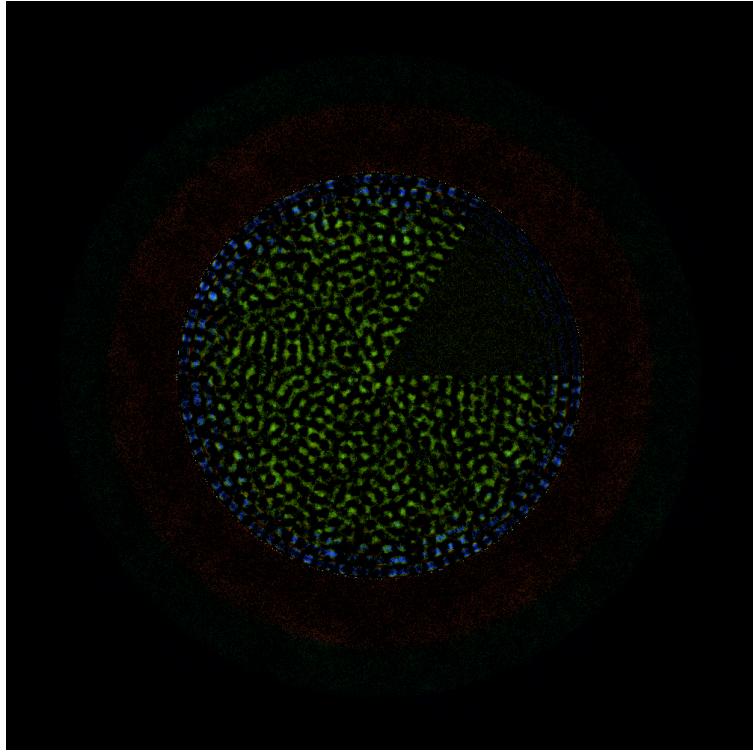


Figure 4.22: An Image Generated by Subtracting 4.21b from 4.3b.

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.

#### 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 reassigned 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. This shuffling happened several times (recall 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	$1.03994 \pm 0.00054$	0.0797%	$5.897 \times 10^{11} \pm 8.668 \times 10^{08}$	0.626%
Run 2	$1.03999 \pm 0.00055$	0.0749%	$5.902 \times 10^{11} \pm 8.086 \times 10^{08}$	0.295%
Run 3	$1.04002 \pm 0.00053$	0.0721%	$5.896 \times 10^{11} \pm 8.490 \times 10^{08}$	0.192%
Run 4	$1.04103 \pm 0.00057$	0.0249%	$5.884 \times 10^{11} \pm 9.355 \times 10^{08}$	0.013%
Run 5	$1.03960 \pm 0.00053$	0.112%	$5.904 \times 10^{11} \pm 8.443 \times 10^{08}$	0.329%
Run 6	$1.04014 \pm 0.00057$	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.

# 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 0.65% 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 . Additionally, otherwise-identical models with a well-mixed core and different dispersal of pebbles differ between 0.63% and 0.013% in the outward current at the outer reflector edge with an average of 0.28%, and between 0.12% 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 reactor designs beyond Sangamon20, 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.

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  $1 \times 10^{-04}$  [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 4.19b) 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 4.19a), so the thermal neutron current is also similar.

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 acrfullotto 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.

## 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.

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 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 isotropics. From there, an exploration of the resulting source term, compared to a simpler model especially, could provide insight on the accuracy of fuel composition data required to accurately determine source term and accident consequences.

The current core is not thermodynamically optimal, and future work could adjust the height-diameter ratio, provided it follows the volume requirements outlined in Figure 3.4. As the current design is slightly supercritical, there should be room to shift to a slightly less critical shape that is more thermally beneficial. If a slight excess reactivity exists at this point, 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. Alternatively, one could explore the addition of neutron-absorber pebbles to handle excess reactivity.

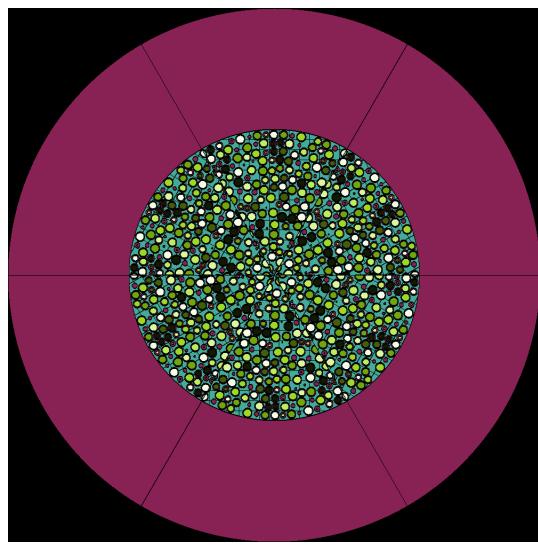
Finally, the pebble dispersal method used here does not account for gravity, which would make the pebbles settle closer together. Without using a core that has a diameter which is an integer multiple of the pebble diameter, it is not possible to get a perfect close-pack arrangement (shaking a vessel 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.

# **Chapter 6**

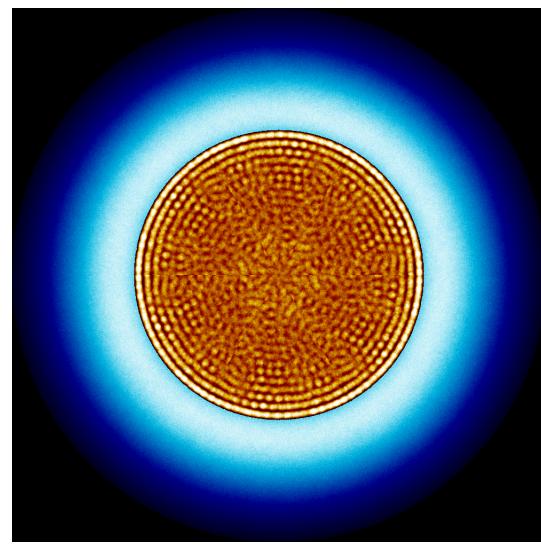
## **Appendix**

### **6.1 Appendix A: Symmetry Test**

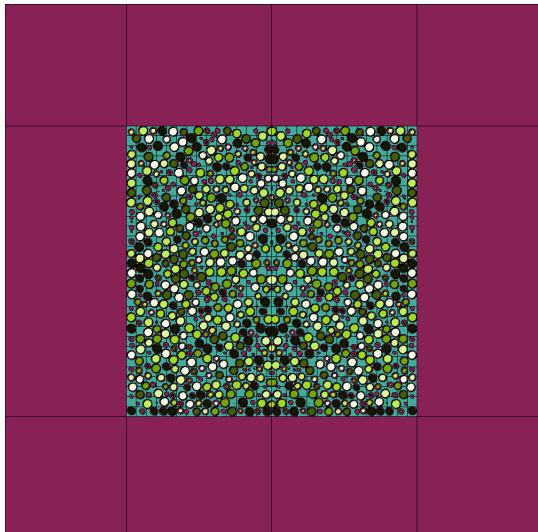
Appendix A contains the geometry cross sections, fission rate/thermal flux meshes, and image difference results from the other symmetry tests.



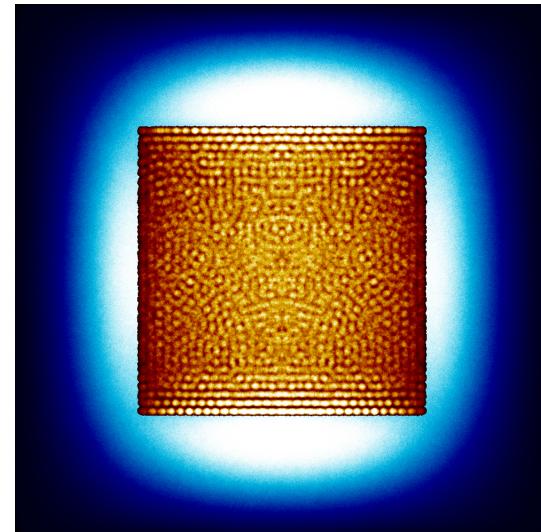
(a) Radial Cross Section at  $y=0$



(b) Radial Mesh



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



(d) Axial Mesh

Figure 6.1: Sensitivity Analysis:  $60^\circ - 120^\circ$

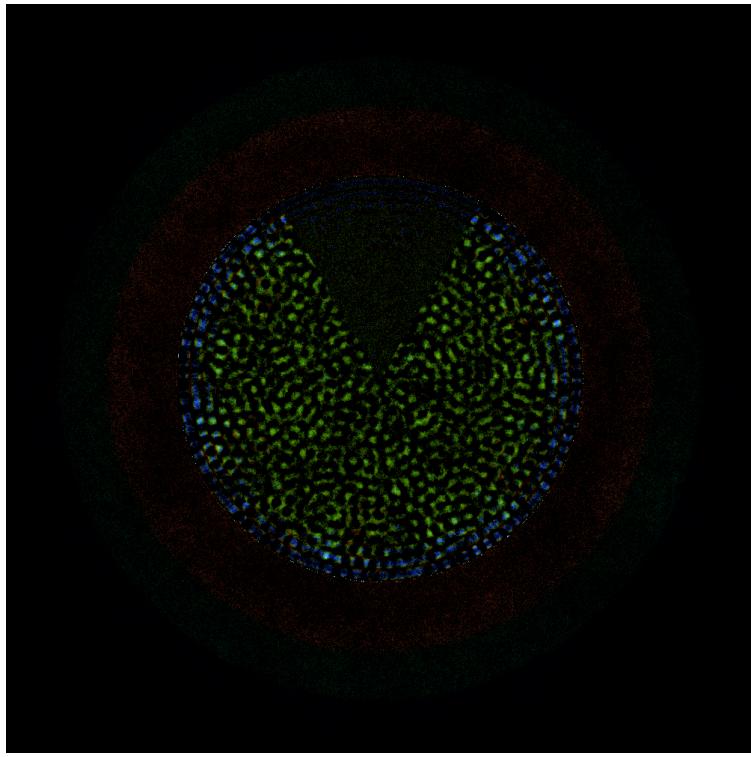
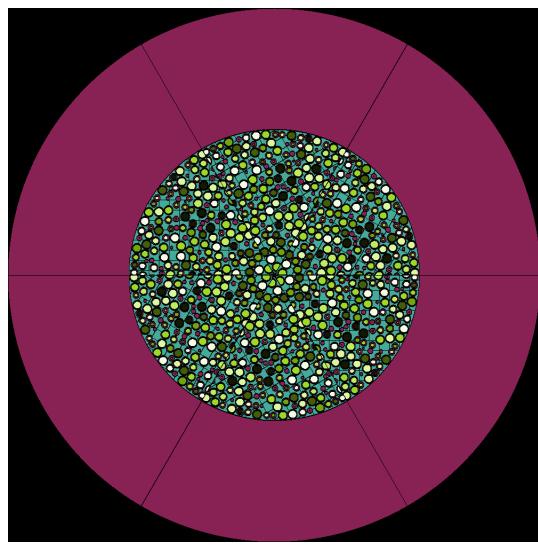
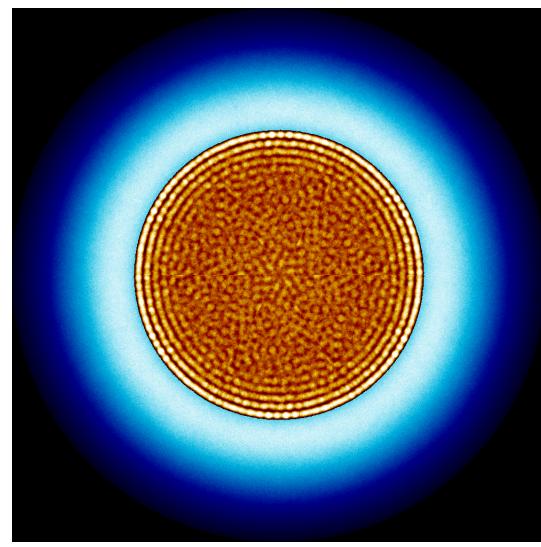


Figure 6.2: An Image Generated by Subtracting 6.1b from 4.3b.

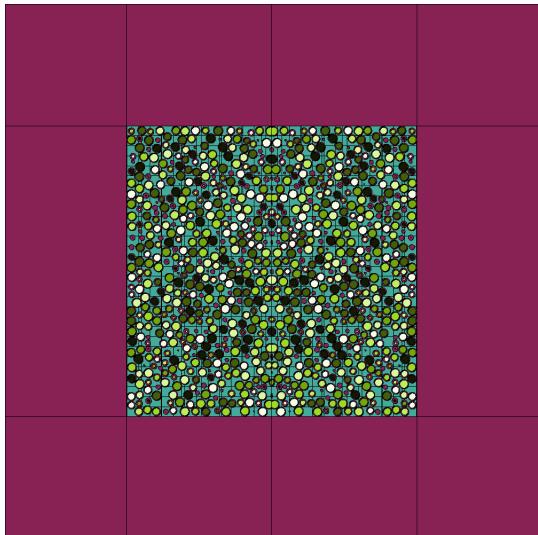
Figure ?? provides fission rate and thermal flux visualization meshes for the symmetry test using the 60 - 120 degree slice. Figure 6.2 is the result of using image-difference between the control's full-core radial mesh and the symmetry test's mesh.



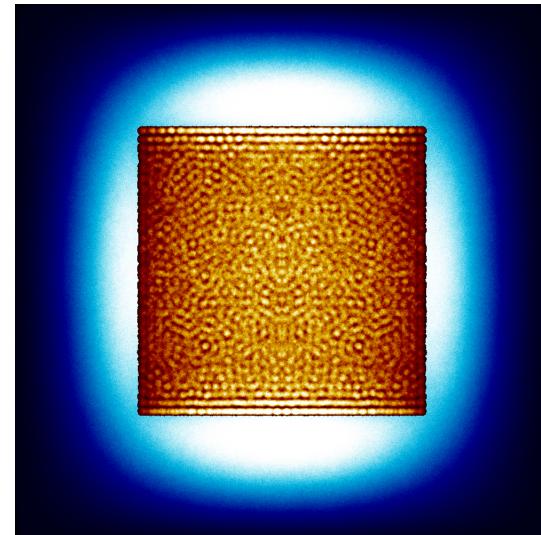
(a) Radial Cross Section at  $y=0$



(b) Radial Mesh



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



(d) Axial Mesh

Figure 6.3: Sensitivity Analysis:  $120^\circ - 180^\circ$

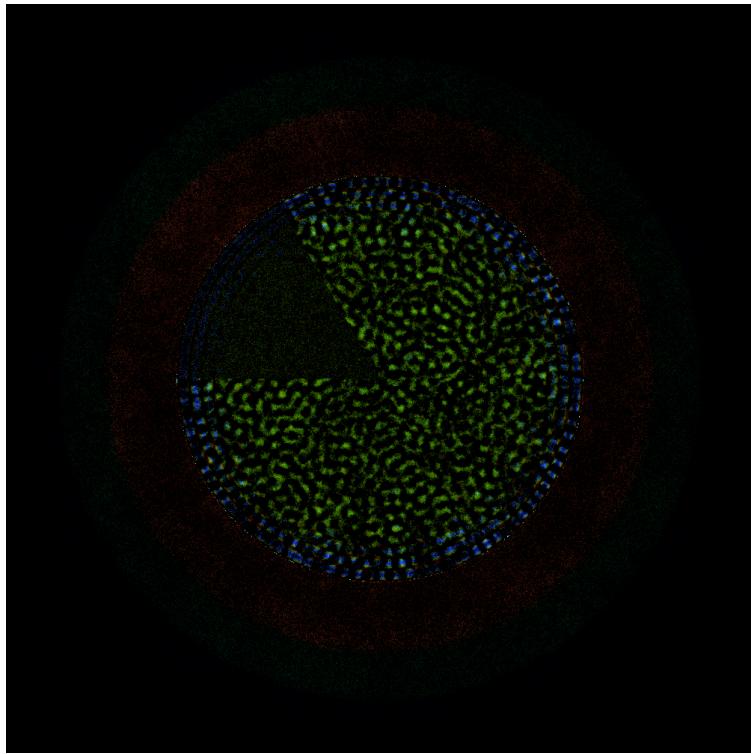
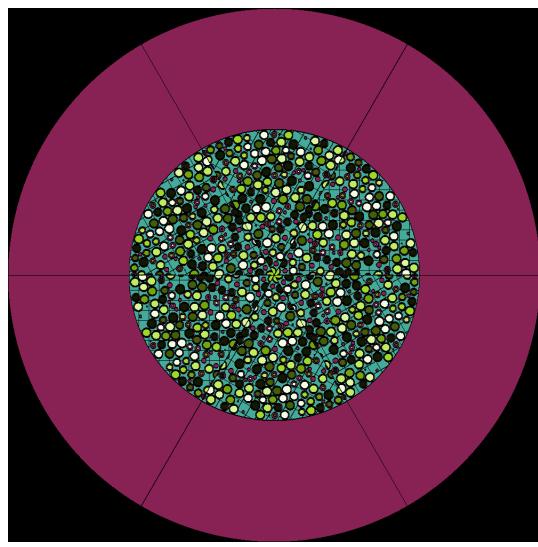
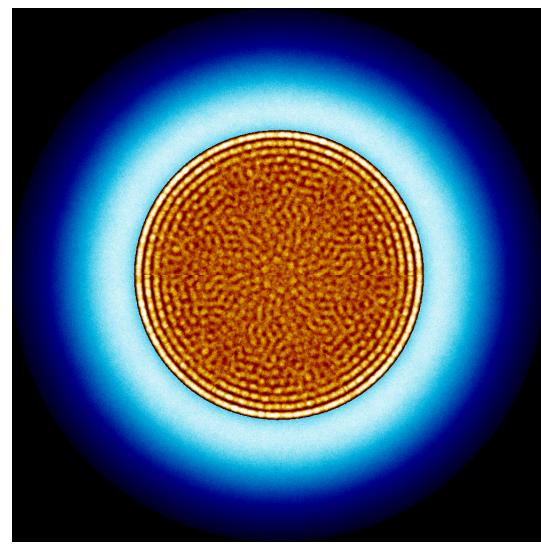


Figure 6.4: An Image Generated by Subtracting 6.3b from 4.3b.

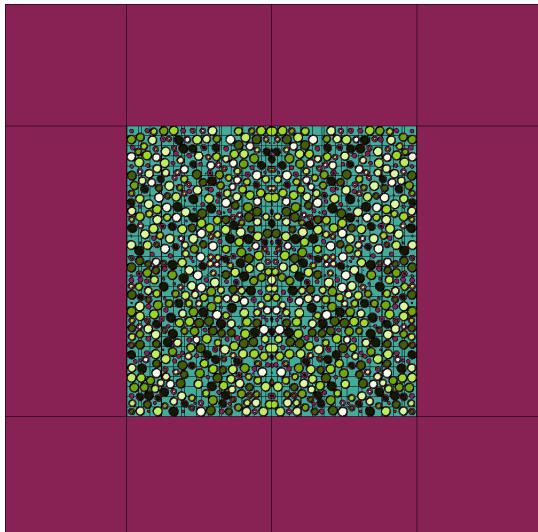
Figure 6.3 provides fission rate and thermal flux visualization meshes for the symmetry test using the 120 - 180 degree slice. Figure 6.4 is the result of using image-difference between the control's full-core radial mesh and the symmetry test's mesh.



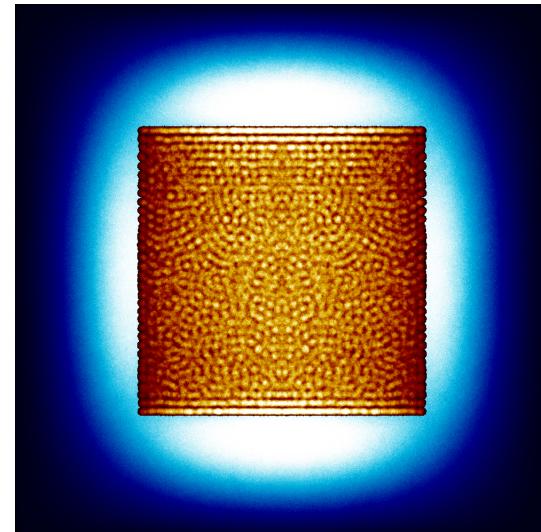
(a) Radial Cross Section at  $y=0$



(b) Radial Mesh



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



(d) Axial Mesh

Figure 6.5: Sensitivity Analysis:  $180^\circ - 240^\circ$

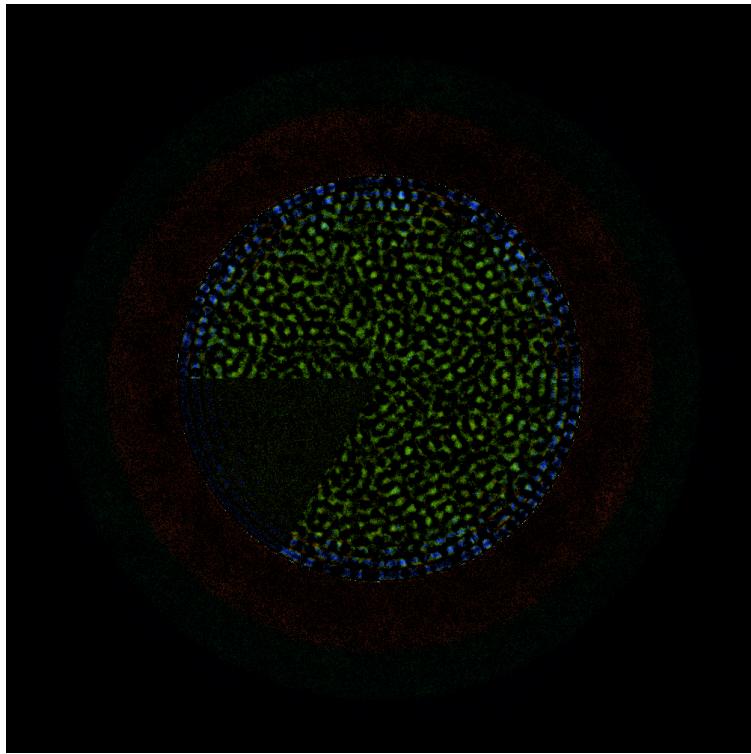
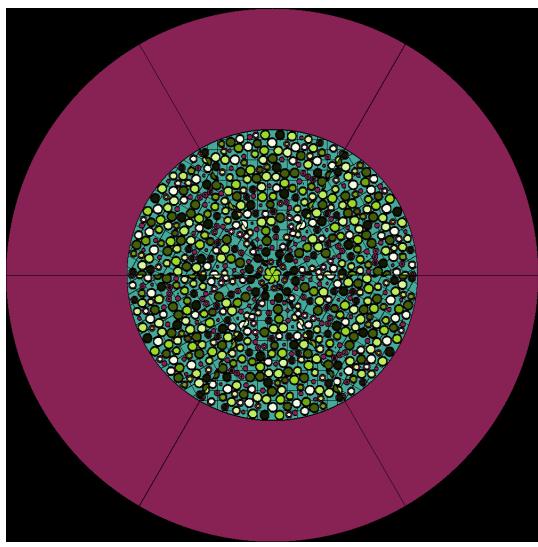
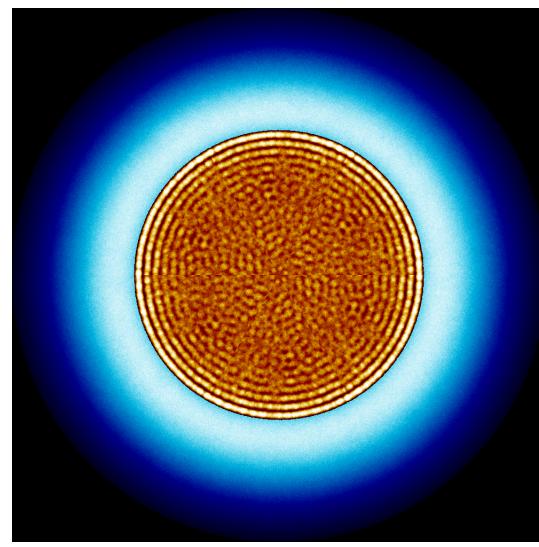


Figure 6.6: An Image Generated by Subtracting 6.5b from 4.3b.

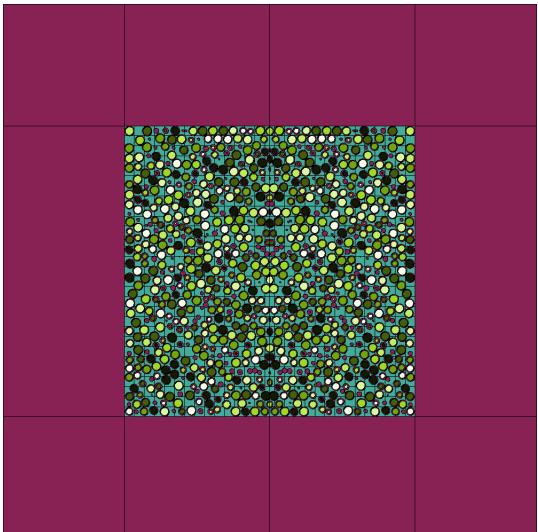
Figure 6.5 provides fission rate and thermal flux visualization meshes for the symmetry test using the 180 - 240 degree slice. Figure 6.6 is the result of using image-difference between the control's full-core radial mesh and the symmetry test's mesh.



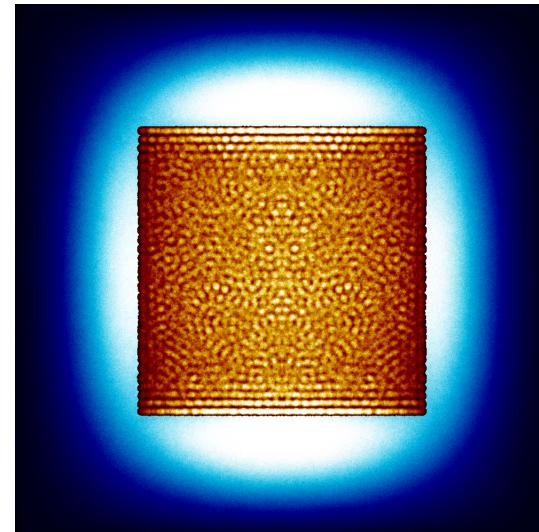
(a) Radial Cross Section at  $y=0$



(b) Radial Mesh



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



(d) Axial Mesh

Figure 6.7: Sensitivity Analysis:  $240^\circ - 300^\circ$

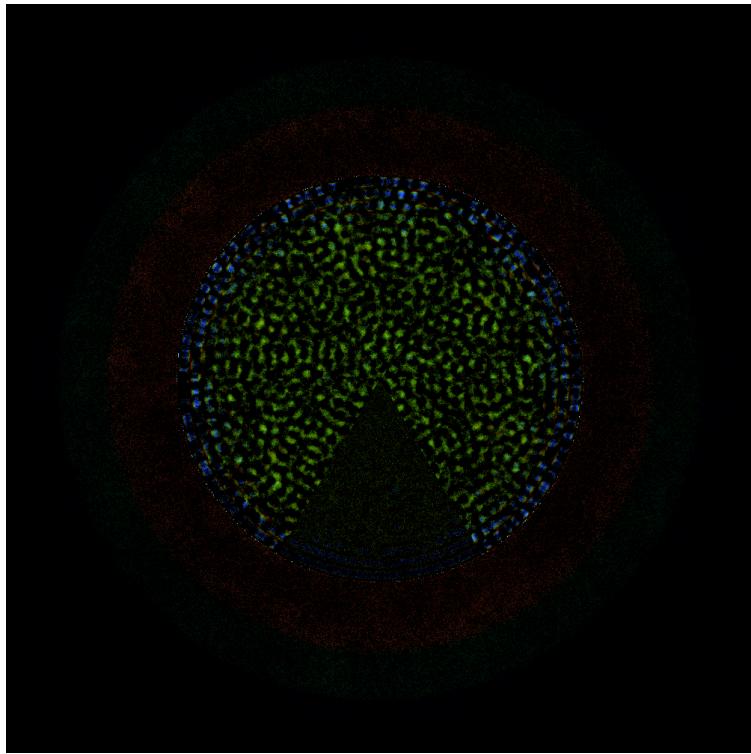
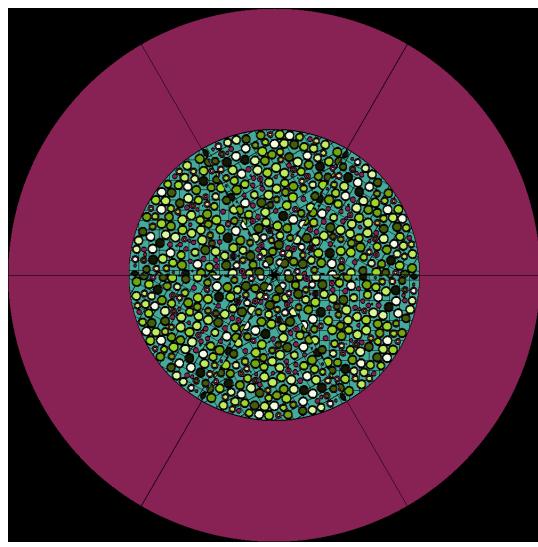
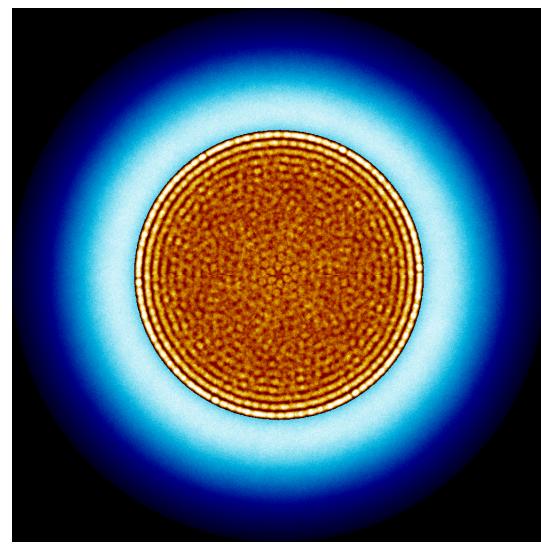


Figure 6.8: An Image Generated by Subtracting 6.7b from 4.3b.

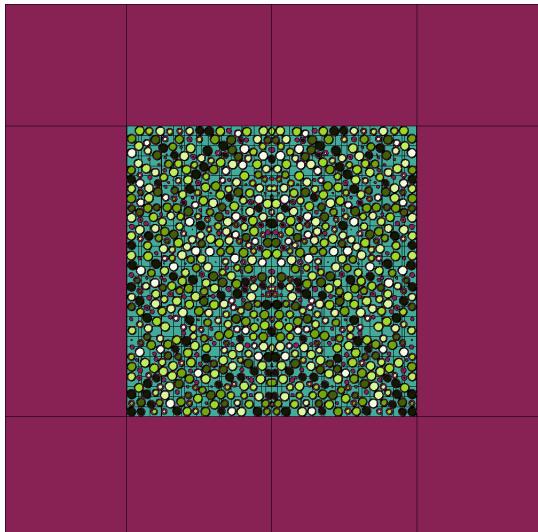
Figure 6.7 provides fission rate and thermal flux visualization meshes for the symmetry test using the 240 - 300 degree slice. Figure 6.8 is the result of using image-difference between the control's full-core radial mesh and the symmetry test's mesh.



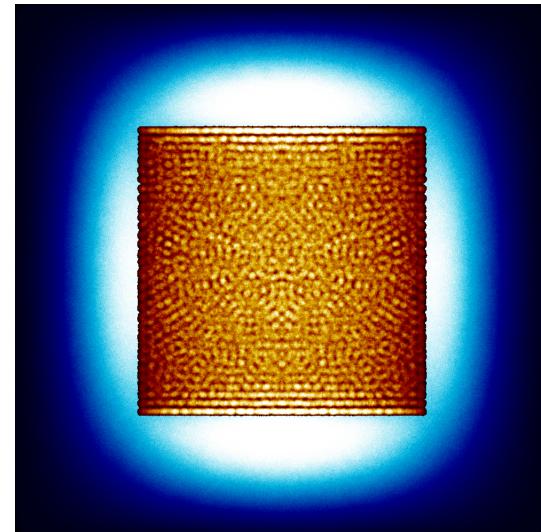
(a) Radial Cross Section at  $y=0$



(b) Radial Mesh



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



(d) Axial Mesh

Figure 6.9: Sensitivity Analysis:  $300^\circ - 360^\circ$

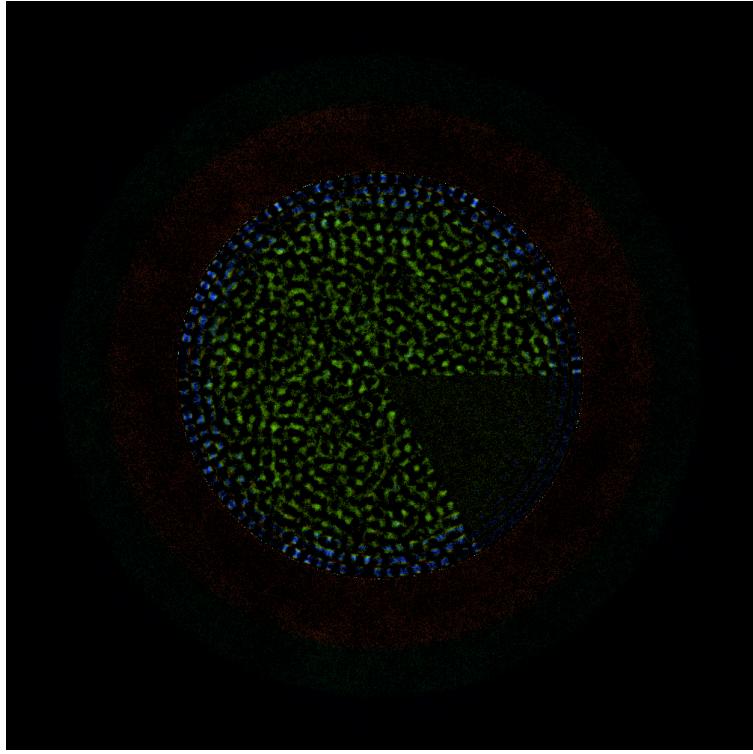


Figure 6.10: An Image Generated by Subtracting 6.9b from 4.3b.

Figure 6.9 provides fission rate and thermal flux visualization meshes for the symmetry test using the 300 - 360 degree slice. Figure 6.10 is the result of using image-difference between the control's full-core radial mesh and the symmetry test's mesh.

To help explain the color difference plots, 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, it is useful to further describe basic 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.

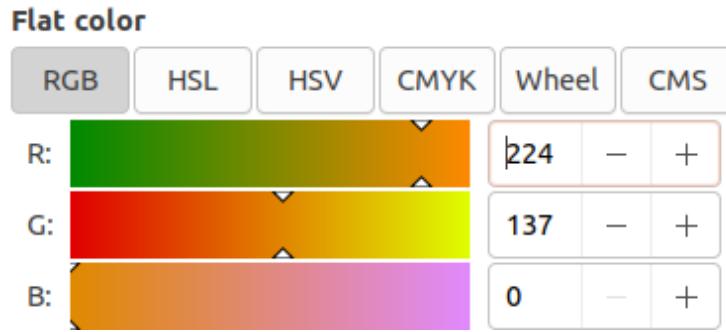


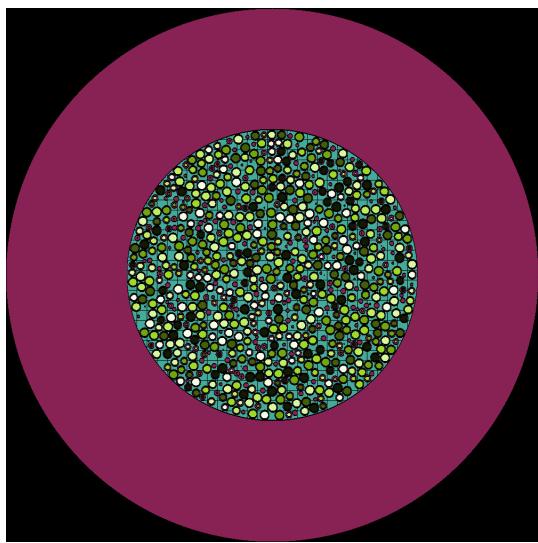
Figure 6.11: An example of RGB values. If the value for red and blue are held constant, shifting the value for green up or down shifts the resulting color along the color gradient to the left of the green value, which ranges from red to yellow. The arrows on the green gradient indicate what the current 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 6.11 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.

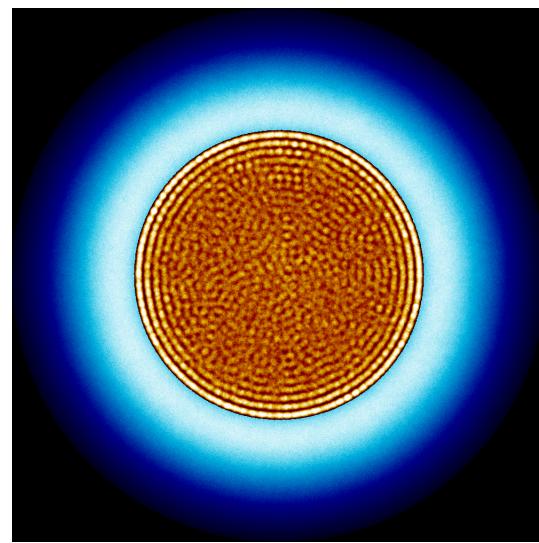
In each of the image differences, the section used to approximate the entire core (for example, the section from 60 to 120 degrees in Figure 6.2). Is very dark, which indicates that this region has little to no difference from the full-core control mesh.

## 6.2 Appendix B: Shuffle Test

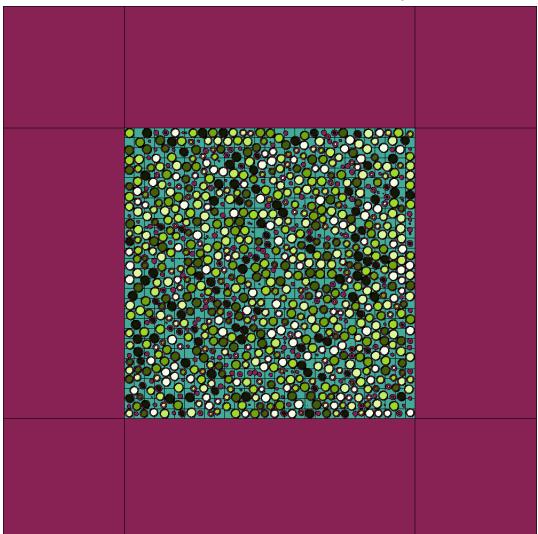
Appendix B contains the geometry cross sections, fission rate/thermal flux meshes, and image difference results from the shuffling tests.



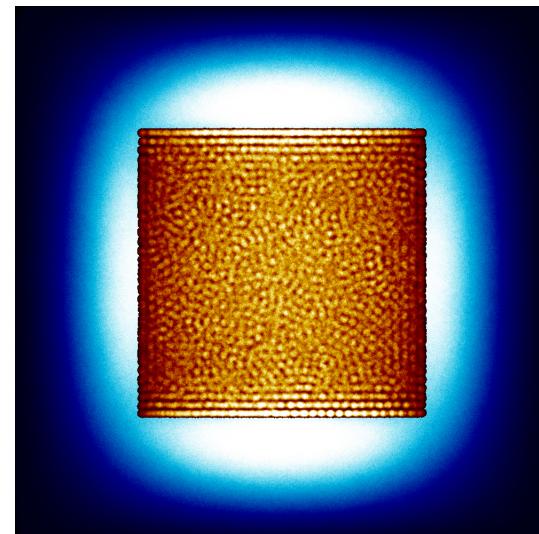
(a) Radial Cross Section at  $y=0$



(b) Radial Mesh



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



(d) Axial Mesh

Figure 6.12: Shuffle Analysis: Run 1

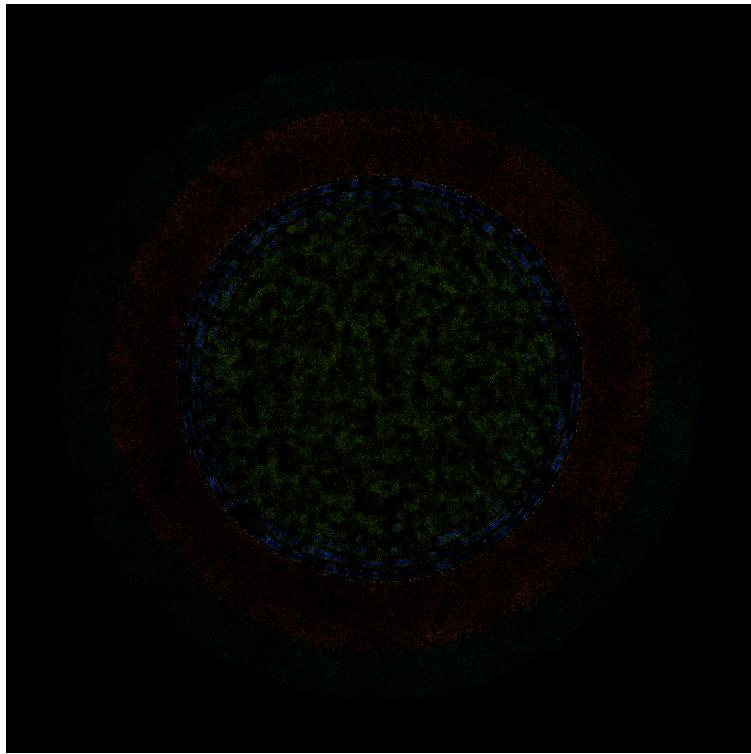
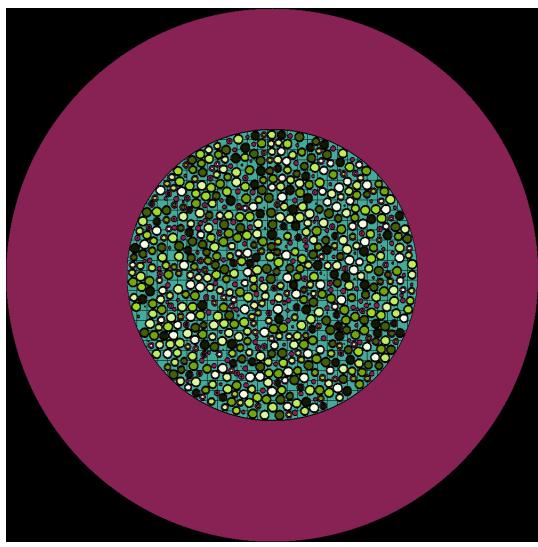
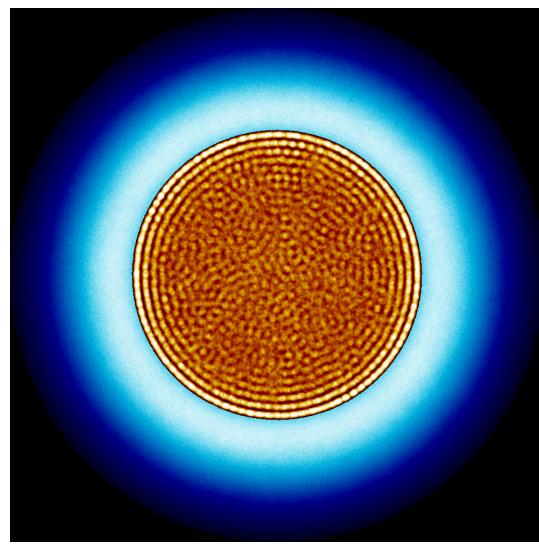


Figure 6.13: An Image Generated by Subtracting 6.12b from 4.3b.

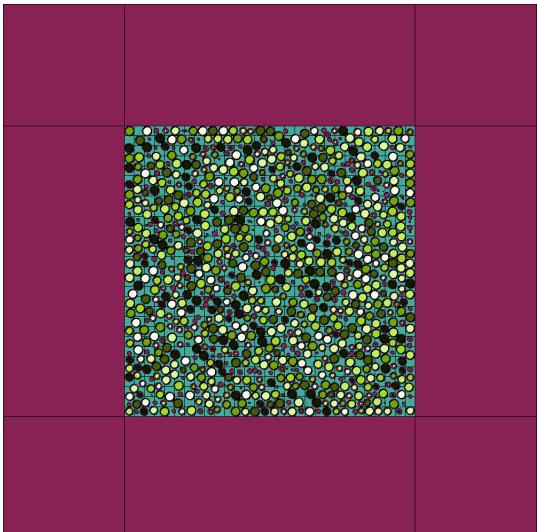
Figure 6.12 provides the thermal flux and fission rate meshes and geometric cross sections axially and radially. Figure 6.13 is the result of the image difference between the full core control mesh and Figure 6.12b.



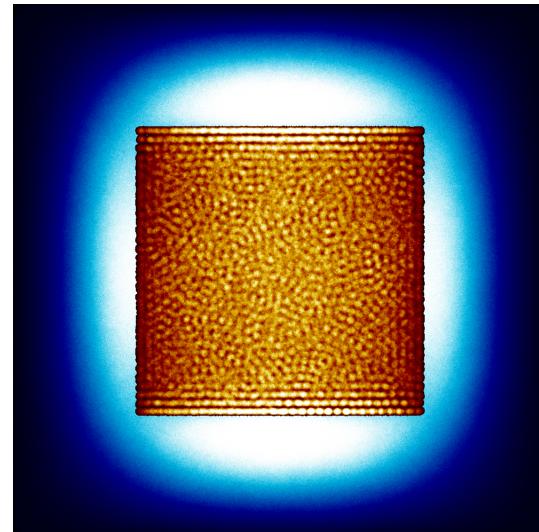
(a) Radial Cross Section at  $y=0$



(b) Radial Mesh



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



(d) Axial Mesh

Figure 6.14: Shuffle Analysis: Run 2

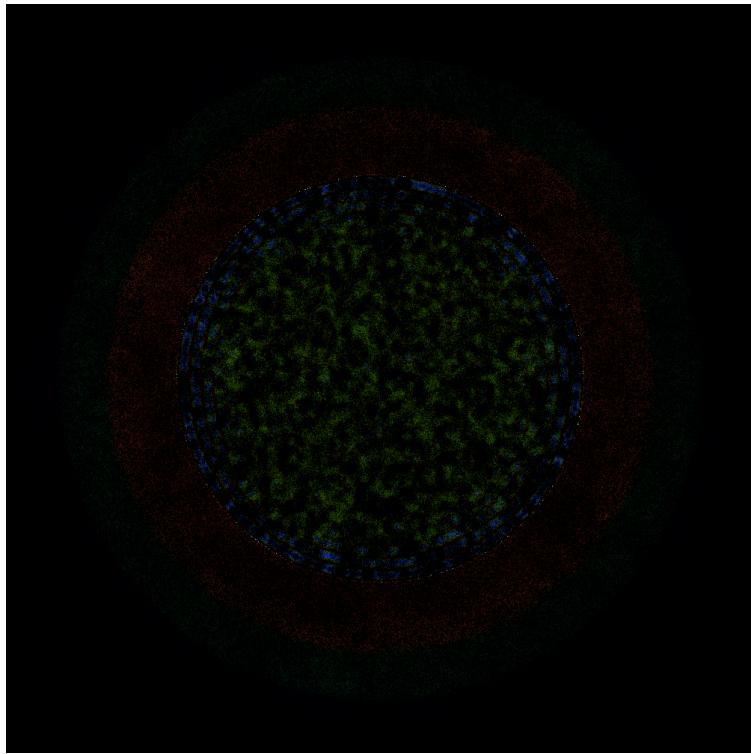
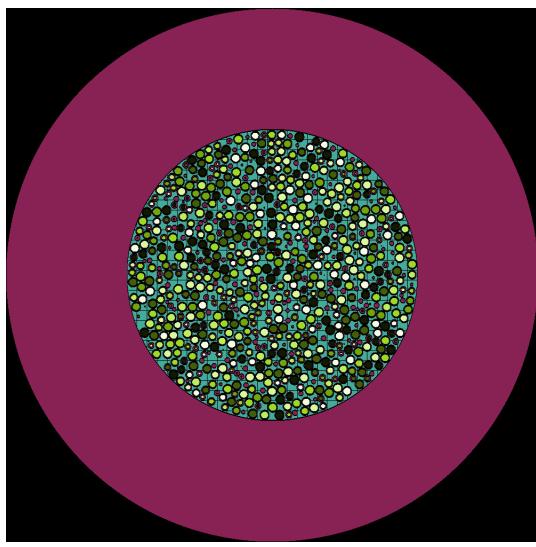
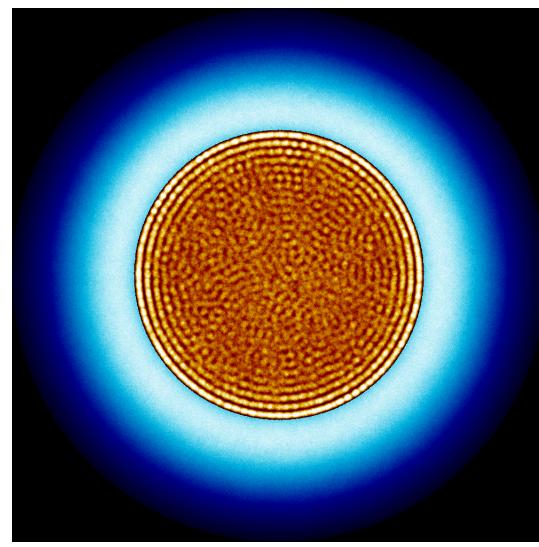


Figure 6.15: An Image Generated by Subtracting 6.14b from 4.3b.

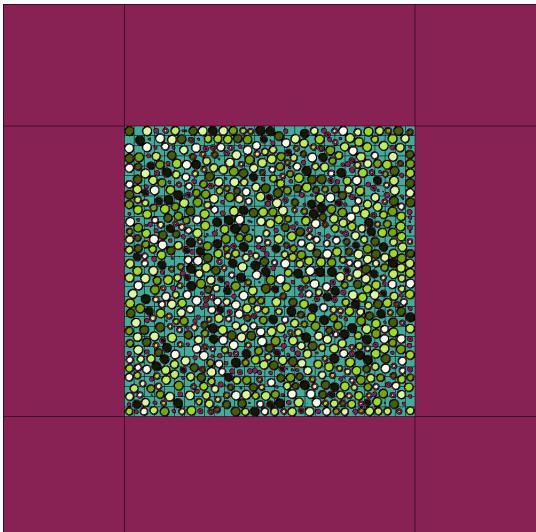
Figure 6.14 provides the thermal flux and fission rate meshes and geometric cross sections axially and radially. Figure 6.15 is the result of the image difference between the full core control mesh and Figure 6.14b.



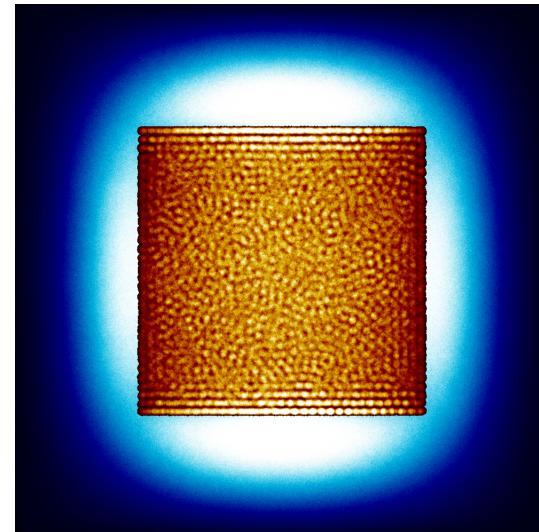
(a) Radial Cross Section at  $y=0$



(b) Radial Mesh



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



(d) Axial Mesh

Figure 6.16: Shuffle Analysis: Run 3

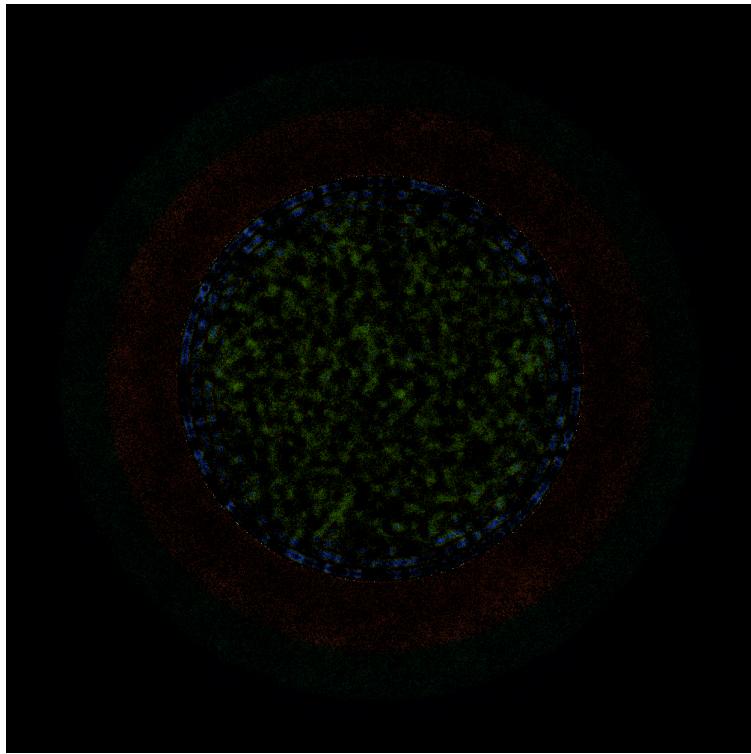
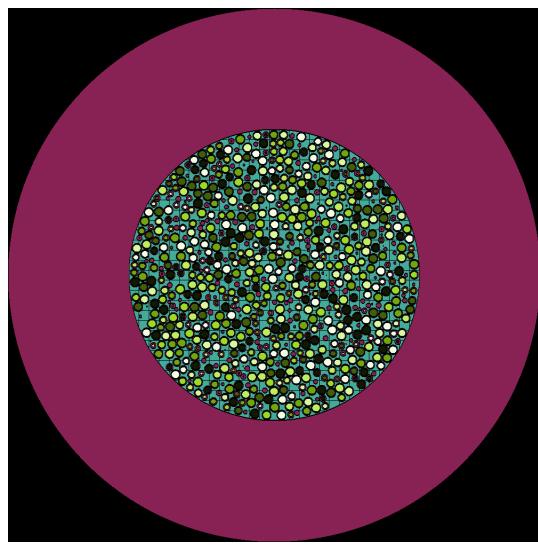
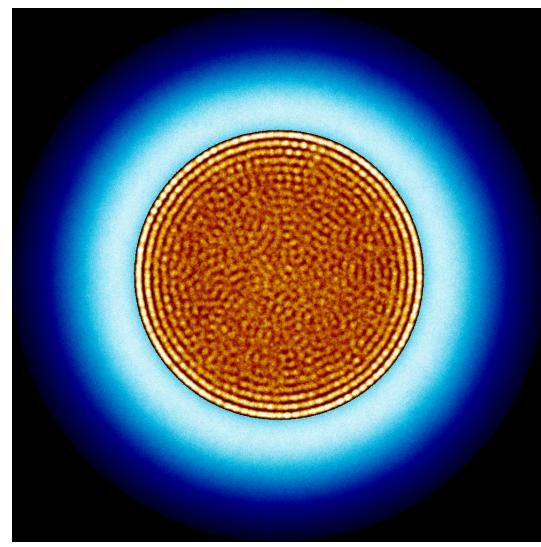


Figure 6.17: An Image Generated by Subtracting 6.16b from 4.3b.

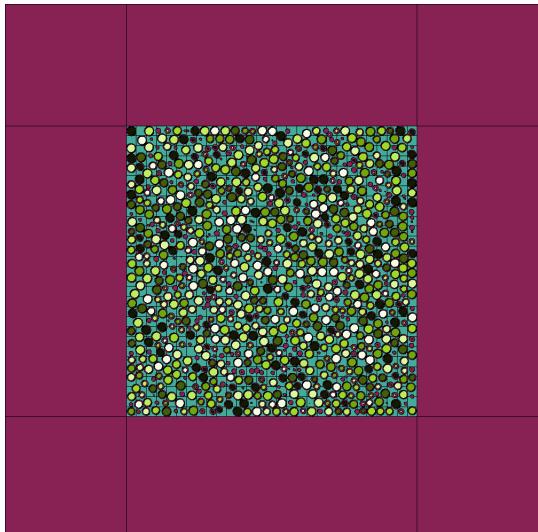
Figure 6.16 provides the thermal flux and fission rate meshes and geometric cross sections axially and radially. Figure 6.17 is the result of the image difference between the full core control mesh and Figure 6.16b.



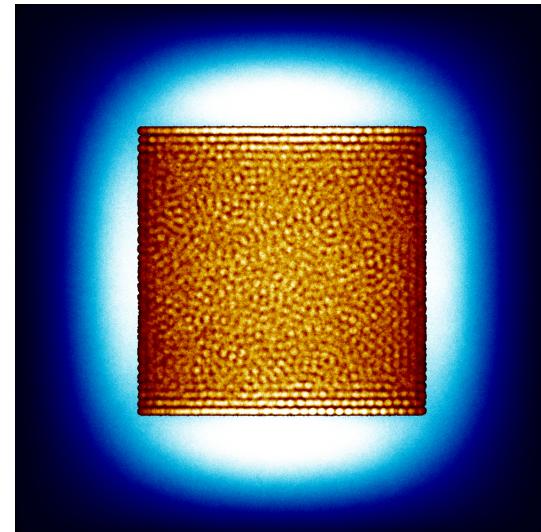
(a) Radial Cross Section at  $y=0$



(b) Radial Mesh



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



(d) Axial Mesh

Figure 6.18: Shuffle Analysis: Run 4

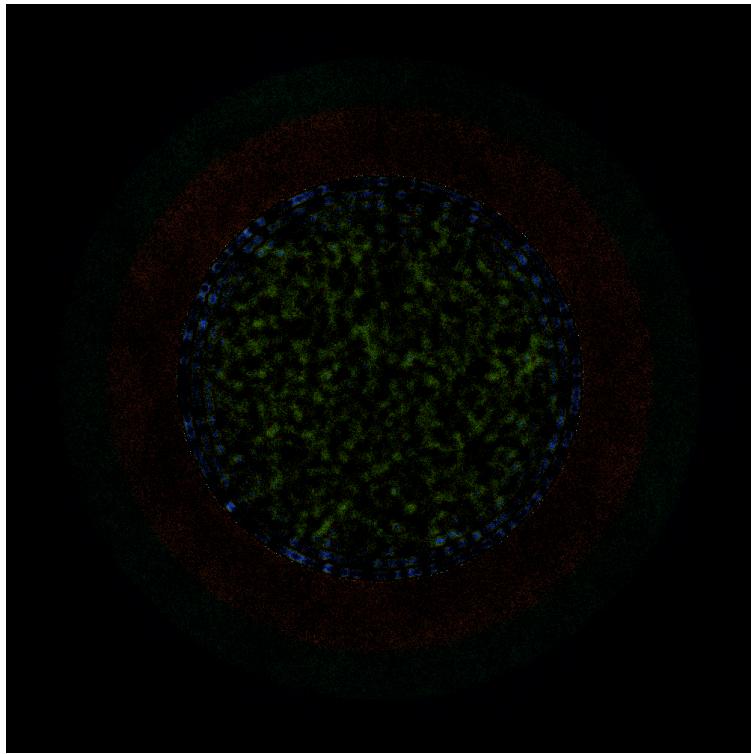
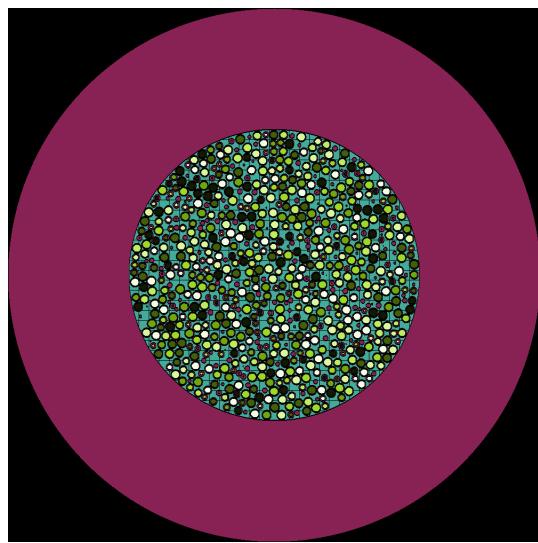
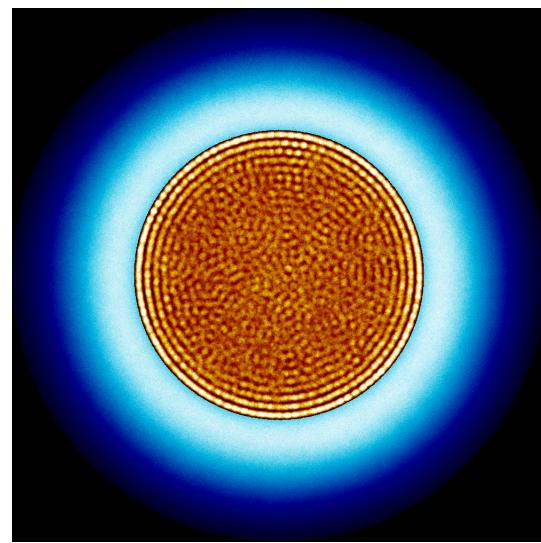


Figure 6.19: An Image Generated by Subtracting 6.18b from 4.3b.

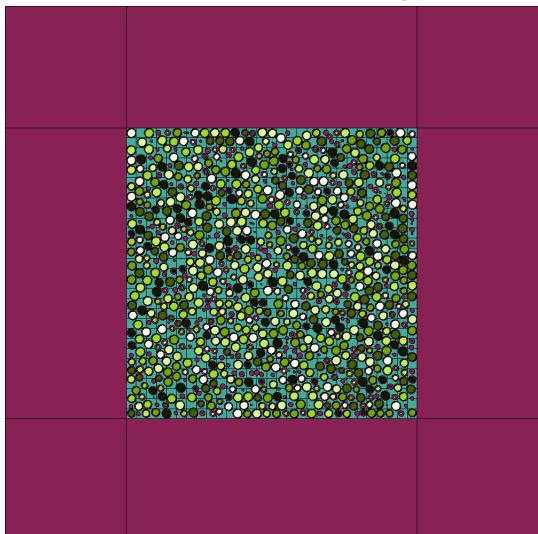
Figure 6.18 provides the thermal flux and fission rate meshes and geometric cross sections axially and radially. Figure 6.19 is the result of the image difference between the full core control mesh and Figure 6.18b.



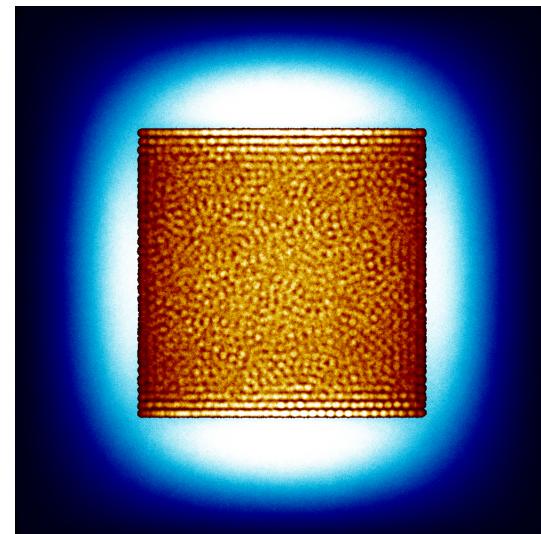
(a) Radial Cross Section at  $y=0$



(b) Radial Mesh



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



(d) Axial Mesh

Figure 6.20: Shuffle Analysis: Run 5

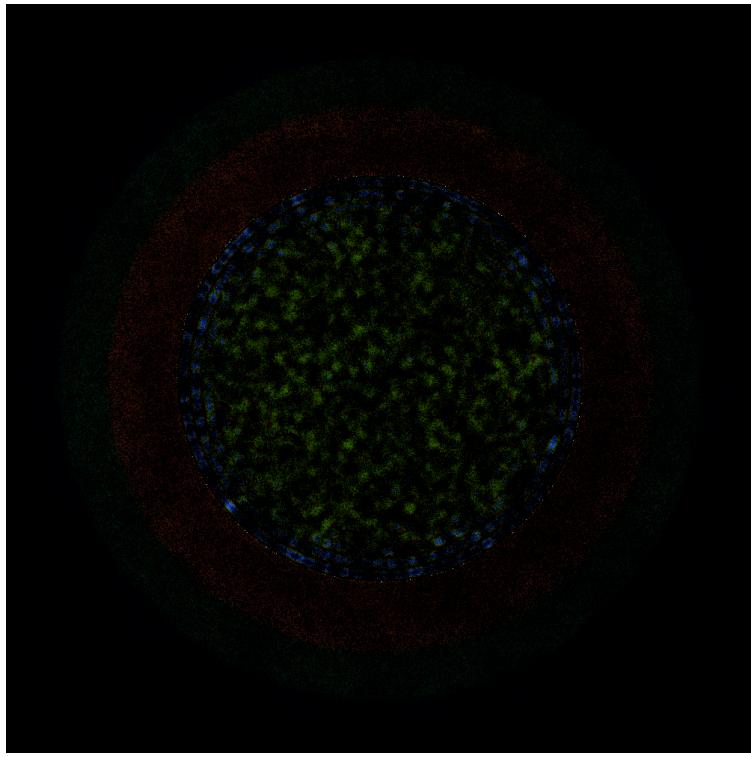
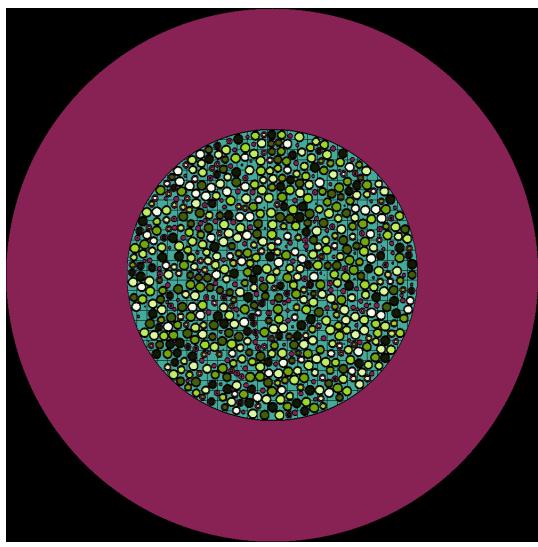
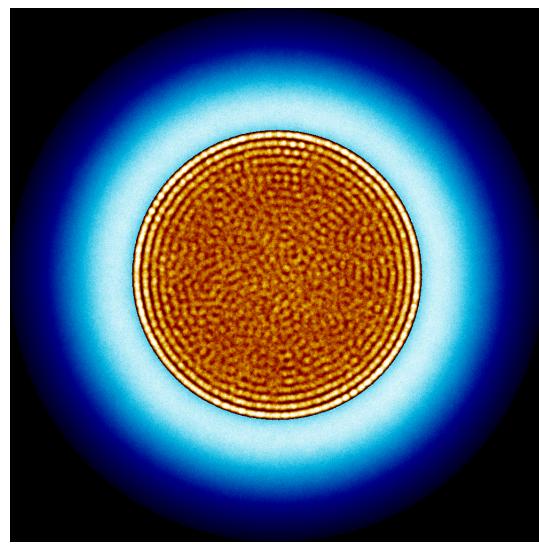


Figure 6.21: An Image Generated by Subtracting 6.20b from 4.3b.

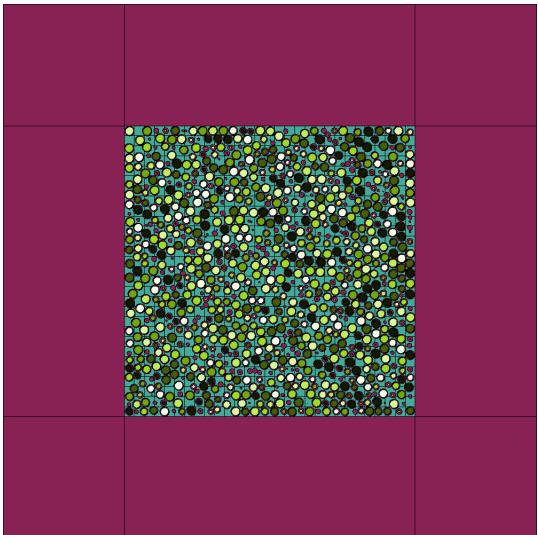
Figure 6.20 provides the thermal flux and fission rate meshes and geometric cross sections axially and radially. Figure 6.21 is the result of the image difference between the full core control mesh and Figure 6.20b.



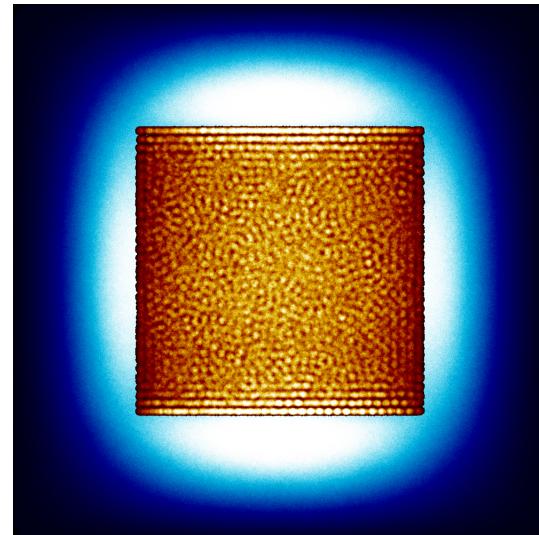
(a) Radial Cross Section at  $y=0$



(b) Radial Mesh



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



(d) Axial Mesh

Figure 6.22: Shuffle Analysis: Run 6

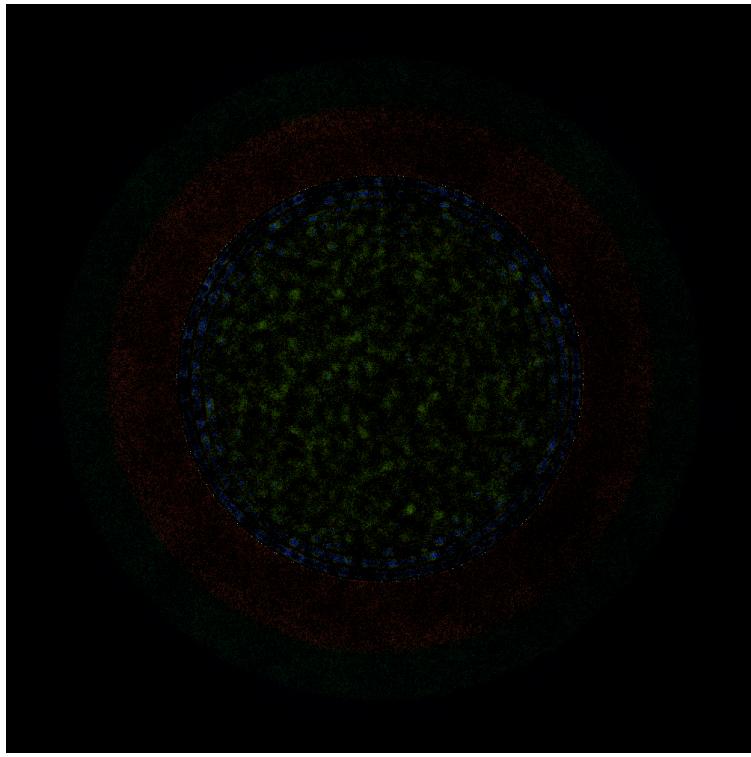


Figure 6.23: An Image Generated by Subtracting 6.22b from 4.3b.

Figure 6.1 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 there is a smaller difference caused by the shuffling tests overall. The small differences in this particular test would most likely indicate that the core is well-mixed, i.e., that each bin in the vertical direction, along the z axis, has each of the 7 fuel compositions represented equally. In theory, if certain regions were highlighted in bright green, it would indicate regions that are poorly mixed.

# References

- [1] Z. Richter, "Isotopic fuel compositions in sangamon20 and sangamon200 models," type: dataset. [Online]. Available: <https://zenodo.org/record/5501385>
- [2] H. Reutler and G. H. Lohnert, "Advantages of going modular in HTRs," vol. 78, no. 2, pp. 129–136. [Online]. Available: <http://www.sciencedirect.com/science/article/pii/002954938490298X>
- [3] P. J. Venter, M. N. Mitchell, and F. Fortier, "PBMR REACTOR DESIGN AND DEVELOPMENT," p. 15.
- [4] Pebble bed modular reactor SOC ltd. [Online]. Available: <http://www.pbmrv.co.za/index2.asp?Content=129>
- [5] B. Harlan, "X-energy xe-100 reactor initial NRC meeting," xe-100 Reactor initial NRC meeting. [Online]. Available: <https://adamswebsearch2.nrc.gov/webSearch2/main.jsp?AccessionNumber=ML18253A109>
- [6] M. T. Simnad, "The early history of high-temperature helium gas-cooled nuclear power reactors," vol. 16, no. 1, pp. 25–32. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/036054429190084Y>
- [7] J. M. Beck and L. F. Pincock, "High temperature gas-cooled reactors lessons learned applicable to the next generation nuclear plant," p. 78.
- [8] Peach bottom - unit 1. [Online]. Available: <https://www.nrc.gov/info-finder/decommissioning/power-reactor/peach-bottom-atomic-power-station-unit.html>
- [9] "Results of experiments at the AVR reactor," vol. 121, no. 2, pp. 143–153, publisher: North-Holland. [Online]. Available: <https://www.sciencedirect.com.proxy2.library.illinois.edu/science/article/pii/002954939090099J>
- [10] A. T. Cisneros, "Pebble bed reactors design optimization methods and their application to the pebble bed fluoride salt cooled high temperature reactor (PB-FHR)." [Online]. Available: <http://gradworks.umi.com/36/16/3616613.html>
- [11] Serpent - a monte carlo reactor physics burnup calculation code. [Online]. Available: <http://montecarlo.vtt.fi/>
- [12] F. Bostelmann, H. R. Hammer, J. Ortensi, G. Strydom, K. Velkov, and W. Zwermann, "Criticality calculations of the very high temperature reactor critical assembly benchmark with serpent and SCALE/KENO-VI," vol. 90, pp. 343–352. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0306454915300177>
- [13] I. MURATA, A. TAKAHASHI, T. MORI, and M. NAKAGAWA, "New sampling method in continuous energy monte carlo calculation for pebble bed reactors," vol. 34, no. 8, pp. 734–744, publisher: Taylor & Francis \_eprint: <https://doi.org/10.1080/18811248.1997.9733737>. [Online]. Available: <https://doi.org/10.1080/18811248.1997.9733737>
- [14] Z. Karriem, C. Stoker, and F. Reitsma, "MCNP modelling of HTGR pebble-type fuel," in *Advanced Monte Carlo for Radiation Physics, Particle Transport Simulation and Applications*, A. Kling, F. J. C. Baräo, M. Nakagawa, L. Távora, and P. Vaz, Eds. Springer, pp. 841–846.
- [15] M. Türkmen and Çolak, "Effect of pebble packing on neutron spectrum and the isotopic composition of HTGR fuel," vol. 46, pp. 29–36. [Online]. Available: <https://www.sciencedirect.com/science/article/pii/S0306454912000953>

- [16] C. J. Hamilton, N. D. Holder, V. H. Pierce, and M. W. Robertson, "HTGR spent fuel composition and fuel element block flow." [Online]. Available: <https://www.osti.gov/biblio/7157851>
- [17] H.-C. Kim, S. Y. Kim, J. K. Kim, and J. M. Noh, "Monte carlo benchmark calculations for 400mwth PBMR core," p. 5.
- [18] F. Albornoz and S. Korochinsky, "MCNP modelling of the PBMR equilibrium core," p. 11.
- [19] "Criticality and burnup analyses of a PBMR-400 full core using monte carlo calculation method," vol. 38, no. 2, pp. 298–301, publisher: Pergamon. [Online]. Available: <http://www.sciencedirect.com/science/article/pii/S0306454910003828>
- [20] F. Reitsma, W. R. Joubert, A. M. Ougouag, and H. D. Gougar, "INVESTIGATION OF THE POWER PEAKING IN THE PBMER PEBBLE- BED REACTOR," p. 13.
- [21] Areva modular reactor selected for NGNP development - world nuclear news. [Online]. Available: [https://www.world-nuclear-news.org/NN-Areva\\_modular\\_reactor\\_selected\\_for\\_NGNP\\_development-1502124.html](https://www.world-nuclear-news.org/NN-Areva_modular_reactor_selected_for_NGNP_development-1502124.html)
- [22] INL. Basis for NGNP reactor design down-selection. [Online]. Available: <https://inldigitallibrary.inl.gov/sites/sti/sti/5223031.pdf>
- [23] T.K.Kim, W.S. Yang, T.A. Taiwo, and H.S. Khalil, "Whole-core depletion studies in support of fuel specification for the next generation nuclear plant (NGNP) core." [Online]. Available: <https://publications.anl.gov/anlpubs/2004/11/51497.pdf>
- [24] N. Agnihotri and E. Mulder. An intrinsically safe generation IV reactor. [Online]. Available: <http://digitaleditions.nuclearplantjournal.com/SO17/24/>
- [25] G. W. Helmreich, J. D. Hunn, J. W. McMurray, R. D. Hunt, B. C. Jolly, M. P. Trammell, D. R. Brown, B. J. Blamer, T. J. Reif, and H. T. Kim, "Year one summary of x-energy pebble fuel development at ORNL." [Online]. Available: <https://www.osti.gov/biblio/1376502>
- [26] H.-C. Kim, S.-Y. Kim, C.-H. Shin, J.-K. Kim, and J.-M. Noh, "Monte carlo benchmark calculations for HTR-10 initial core," pp. 5–6, publisher: Korean Nuclear Society. [Online]. Available: <https://www.koreascience.or.kr/article/CFKO200533239312837.page>
- [27] D. She, F. Xie, F. Li, S. Liu, and K. Wang, "EXPLICIT MODELLING OF DOUBLE-HETEROGENEOUS PEBBLE-BED REACTORS WITH THE RMC CODE," p. 12.
- [28] S. Liu, Z. Li, K. Wang, Q. Cheng, and D. She, "Random geometry capability in RMC code for explicit analysis of polytype particle/pebble and applications to HTR-10 benchmark," vol. 111, pp. 41–49. [Online]. Available: [https://www.sciencedirect.com/science/article/pii/S0306454917302724](http://www.sciencedirect.com/science/article/pii/S0306454917302724)
- [29] B. Harlan, "ANS xe 100 overview 2017." [Online]. Available: [http://local.ans.org/dc/wp-content/uploads/2014/01/ANS\\_Xe-100-Overview\\_04052017.pdf](http://local.ans.org/dc/wp-content/uploads/2014/01/ANS_Xe-100-Overview_04052017.pdf)
- [30] J. Leppänen. Serpent – a continuous-energy monte CarloReactor physics burnup calculation code. [Online]. Available: [http://montecarlo.vtt.fi/download/Serpent\\_manual.pdf](http://montecarlo.vtt.fi/download/Serpent_manual.pdf)
- [31] G. van Rossum and F. L. Drake, "Python reference manual," p. 196.
- [32] C. R. Harris, K. J. Millman, S. J. van der Walt, R. Gommers, P. Virtanen, D. Cournapeau, E. Wieser, J. Taylor, S. Berg, N. J. Smith, R. Kern, M. Picus, S. Hoyer, M. H. van Kerkwijk, M. Brett, A. Haldane, J. F. del Río, M. Wiebe, P. Peterson, P. Gérard-Marchant, K. Sheppard, T. Reddy, W. Weckesser, H. Abbasi, C. Gohlke, and T. E. Oliphant, "Array programming with NumPy," vol. 585, no. 7825, pp. 357–362, bandiera\_abtest: a Cc\_license\_type: cc\_by Cg\_type: Nature Research Journals Number: 7825 Primary\_atype: Reviews Publisher: Nature Publishing Group Subject\_term: Computational neuroscience;Computational science;Computer science;Software;Solar physics Subject\_term\_id: computational-neuroscience;computational-science;computer-science;software;solar-physics. [Online]. Available: <https://www.nature.com/articles/s41586-020-2649-2>

- [33] A. Scopatz, P. K. Romano, P. P. H. Wilson, and K. D. Huff, "PyNE: Python for nuclear engineering," in *Transactions of the American Nuclear Society*, ser. Reactor Physics: General—I, vol. 107. American Nuclear Society, pp. 985–987. [Online]. Available: <http://epubs.ans.org/?a=14978>
- [34] Z. M. Richter, R. Fairhurst, mehmeturkmen, K. Huff, and S. Dotson, "ZoeRichter/phlox: Symmetry/shuffling/heterog tests." [Online]. Available: <https://zenodo.org/record/5715933>
- [35] S. G. Nagley, C. M. Barnes, D. L. Husser, M. L. Nowlin, and W. C. Richardson, "Fabrication of uranium oxycarbide kernels for HTR fuel," p. 10.
- [36] Accuratus. Silicon carbide SiC material properties. [Online]. Available: <https://www.accuratus.com/silicar.html>
- [37] ESPI Metals. Graphite-pyrolytic grade. [Online]. Available: <https://www.espimetals.com/index.php/technical-data/74-graphite-pyrolytic-grade>
- [38] F. Ho, R. Vollmar, and R. Turner. Graphite design handbook. [Online]. Available: <https://www.osti.gov/servlets/purl/714896/>
- [39] W. Johnson and G. Engle, "Properties of unirradiated fuel element graphites h-451 and TS-1240," pp. GA-A-13 752, 7 283 150. [Online]. Available: <http://www.osti.gov/servlets/purl/7283150-NEjJgM/>
- [40] S. S. Tulluri, "Analysis of random packing of uniform spheres using the monte carlo simulation method," p. 107.
- [41] Tripoli 315-group structure - serpent wiki. [Online]. Available: [https://serpent.vtt.fi/mediawiki/index.php/Tripoli\\_315-group\\_structure](https://serpent.vtt.fi/mediawiki/index.php/Tripoli_315-group_structure)
- [42] F. B. Brown, W. R. Martin, W. Ji, J. L. Conlin, and J. C. Lee, "STOCHASTIC GEOMETRY AND HTGR MODELING WITH MCNP5," p. 13.
- [43] Uncertainties and error propagation. [Online]. Available: <https://www.geol.lsu.edu/jlorenzo/geophysics/uncertainties/Uncertaintiespart2.html>
- [44] Amir Afzali, "High temperature, gas-cooled pebble bed reactor licensing modernization project demonstration," u.S. Department of Energy (DOE) Office of Nuclear Energy Under DOE Idaho Operations Office Contract DE-AC07-0SID14517. [Online]. Available: <https://www.nrc.gov/docs/ML1822/ML18228A779.pdf>
- [45] W. Moe, "Licensing modernization project for advanced reactor technologies: FY 2018 project status report."
- [46] M. El-Genk and T. Schriener. Post-operation radiological source term and dose rate estimates for the scalable Liquid metal-cooled small modular reactor | elsevier enhanced reader. [Online]. Available: <https://reader.elsevier.com/reader/sd/pii/S0306454918300550?token=72A5D70FC4A85A4EF41A5E9256B0B120D6DBE8E80266F7BFD35BB528A887F463F8647F134921742AAE435B0A9D635F61>
- [47] M. B. Richards, "Reaction of nuclear-grade graphite with low concentrations of steam in the helium coolant of an MHTGR," vol. 15, no. 9, pp. 729–739. [Online]. Available: <http://www.sciencedirect.com/science/article/pii/036054429090112F>
- [48] "Accident analysis for nuclear power plants with modular high temperature gas cooled reactors," OCLC: 637106283.
- [49] M. Rainer, "Fission product transport and source terms in HTRs: Experience from AVR pebble bed reactor," vol. 2008.
- [50] E. Eaves, "Can north america's advanced nuclear reactor companies help save the planet?" vol. 73, no. 1, p. 27. [Online]. Available: <http://search.ebscohost.com/login.aspx?direct=true&db=ulh&AN=120392537>
- [51] M. Englert, F. Friess, and M. V. Ramana, "Accident scenarios involving pebble bed high temperature reactors," vol. 25, no. 1, pp. 42–55. [Online]. Available: <https://www.tandfonline.com/doi/full/10.1080/08929882.2017.1275320>

- [52] Y. Brits, F. Botha, H. van Antwerpen, and H.-W. Chi, “A control approach investigation of the xe-100 plant to perform load following within the operational range of 100 – 25 – 100%,” vol. 329, pp. 12–19. [Online]. Available: <http://www.sciencedirect.com/science/article/pii/S0029549317305630>
- [53] M. V. Ramana, “The checkered operational history of high-temperature gas-cooled reactors,” vol. 72, no. 3, pp. 171–179. [Online]. Available: <https://doi.org/10.1080/00963402.2016.1170395>
- [54] Z. Zhang and Y. Sun, “Economic potential of modular reactor nuclear power plants based on the chinese HTR-PM project,” vol. 237, no. 23, pp. 2265–2274. [Online]. Available: <http://www.sciencedirect.com/science/article/pii/S002954930700283X>
- [55] M. Hussain, F Reitsma, M. Subki, and H. Kiuchi, “Advances in small modular reactor technology developments.” [Online]. Available: <http://aris.iaea.org>
- [56] H. G. Hereward, H. R. Paneth, G. C. Laurence, and B. W. Sargent, “Measurement of the diffusion length of thermal neutrons in graphite,” vol. 25a, no. 1, pp. 15–25, publisher: NRC Research Press. [Online]. Available: <https://www.nrcresearchpress.com/doi/abs/10.1139/cjr47a-002>
- [57] E. Mulder, “Reactor physics overview of the xe-100 GEN IV reactor,” NPREG 596 Graduate Seminar.
- [58] R. Nanstad and W. L. Server. Milestone report-08-2011-assessment of thermal annealing-FINAL.pdf. [Online]. Available: <https://www.energy.gov/sites/prod/files/Milestone%20Report-08-2011-Assessment%20of%20Thermal%20Annealing-FINAL.pdf>
- [59] O. K. Chopra and A. S. Rao, “Degradation of LWR core internal materials due to neutron irradiation.” [Online]. Available: <https://www.nrc.gov/docs/ML1027/ML102790482.pdf>
- [60] T. Dudley, O. Tsaoi, and E. Mulder, “THE REACTOR CORE NEUTRONIC MODEL FOR THE PBMR PLANT TRAINING SIMULATOR,” p. 13.
- [61] E. J. Mulder, “Pebble bed reactor with equalised core power distribution inherently safe and simple.” [Online]. Available: <https://juser.fz-juelich.de/record/820874/>
- [62] NASA’s Goddard Institute for Space Studies, “Global surface temperature.” [Online]. Available: <https://climate.nasa.gov/vital-signs/global-temperature>
- [63] L. Lommers and G. Honma, “NGNP high temperature materials white paper.” [Online]. Available: <https://www.osti.gov/biblio/1055953-ngnp-high-temperature-materials-white-paper>
- [64] Cole Gentry. generate random particle or pebble bed files for HTGR calc - discussion forum for serpent users. [Online]. Available: <https://ttuki.vtt.fi/serpent/viewtopic.php?f=3&t=2267&p=6161&hilit=growth+and+shake#p6161>