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AN INVESTIGATION INTO GAS-COOLED FAST SPECTRUM NUCLEAR REACTOR MODELLING SOFTWARE

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ABSTRACT

As the Earth's population continues to grow at an ever-increasing rate, the demand for electricity grows with it. Meeting the electrical power demands of tomorrow will require a safe, reliable, and sustainable source of energy. Additionally, a growing portion of the world is supportive of protecting the environment through the reduction of carbon emissions. Consequently, an energy source is more desirable if it minimizes its contribution to worldwide carbon emissions. Fortunately, nuclear power satisfies all of those requirements, as well as being a proven technology that can be economically viable. And while current nuclear reactors are certainly capable of supplying energy in the future, research continues in the nuclear industry toward innovation and improvement. One such type of improved reactor design under research is the gas-cooled fast spectrum reactor. With inherent safety features, increased thermal efficiency, and vastly improved fuel utilization, gas-cooled fast reactors may be a better option than current designs. Studying this reactor type could help advance the nuclear industry, but in order to do that, researchers must have access to accurate modelling software. Software such as MC2-3, as well as the NEAMS Workbench, which combines a number of nuclear codes including MC2-3, can aid in this process. However, they must be proven accurate first. The research discussed in this paper investigated the ability of MC2-3 and the NEAMS Workbench to model a GFR design by comparing these code outputs to those of a previous experiment and another reactor physics code, Serpent. It concluded that both MC2-3 and the NEAMS Workbench were capable of accurately modelling a GFR design, provided that the assumptions made in the modelling process do not cause significant deviation from the actual reactor design.

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Chapter 1

Introduction

As of 2015, there were 99 commercially operated nuclear reactors producing power in the United States of America.[1] These reactors were responsible for approximately 19% of the total energy produced in the United States, as well as 58% of the total carbon-free energy produced.[1] Worldwide, nuclear reactors produced approximately 11% of the total energy and 31% of the carbon-free energy in the same year.[1] In a world with an increasing population and energy demand, nuclear power has the opportunity and ability to safely provide reliable, consistent baseload electrical power for consumption around the world. Nuclear power currently occupies a unique role in the energy portfolios of countries that have access to it. It provides clean, consistent, economically sustainable energy, largely independent of environmental conditions. It does not suffer many of the drawbacks that other clean energy sources experience. Unlike wind and solar, nuclear power operates consistently, regardless of weather conditions. Additionally, nuclear features the ability to grow through the construction and operation of new power plants, which is not easily accomplished in the case of hydroelectric power. However, the implementation of nuclear power is not immune to its own unique drawbacks and difficulties.

First and foremost, the primary concern of any nuclear plant is safety. Protection of the plant operators, surrounding public, and environment must all be guaranteed. This is evidenced by the extreme risk-averse nature of the nuclear industry as a whole, as well as the degree to which nuclear power plants are designed to handle design and environmentally based accident scenarios. This can be seen in the infamous nuclear accidents that have occurred to nuclear power plants throughout the existence of commercial nuclear power. In the case of the Three Mile Island accident, the meltdown caused by a component malfunction was contained by reactor safety mechanisms and no radioactive material was released to the public.[2] Following the Three Mile Island incident, much more stringent protocols regarding operation and component redundancies were implemented to prevent a similar accident from occurring again. In the case of the Chernobyl meltdown, the reactor design was exclusive to the USSR due to the inherent dangers associated with the RBMK design. Reactors of that type were retrofitted following the disaster in order to remove the risk of another RBMK reactor meltdown. Finally, the Fukushima accident was caused by a natural disaster beyond what the plant was designed to endure. As a result, safety guidelines were reinforced for nuclear reactor designs and currently operating plants. Additionally, though there was a significant release of radioactive material from the Fukushima Daiichi plant, no deaths or instances of radiation sickness have been reported. This is largely a result of governmental precautions and safety protocols that were successfully implemented.

These accidents, though few in number, have reinforced widespread public concern over the nuclear power industry as a whole. In the United States, this has resulted in the main obstacles to nuclear power being public opinion and policy based. In the last 20 years, there has been only one nuclear reactor brought online in the entire country, Unit 2 at the Watts Bar Nuclear Generating Station. However, despite the lull in nuclear power plant construction in recent years, the nuclear industry remains committed to designing safer and more efficient reactors for the future.

Much of the current research in the nuclear power industry concerns a number of alternative nuclear reactor systems referred to as generation IV reactors.[3,4,5] Generation IV nuclear reactor designs are supported and encouraged by the Generation IV International Forum (GIF), which is an international cooperative with the expressed goal of encouraging and supporting the development of the next generation of nuclear reactors.[3,5,6] There is a total of six different reactor types that comprise generation IV reactors, each designed with goals of enhanced safety, sustainability, as well as economic and operational efficiency.[4-8] The six reactor types include very high temperature reactors (VHTR), molten salt reactors (MSR), supercritical water reactors (SCWR), gas-cooled fast reactors (GFR), sodium-cooled fast reactors (SFR), and lead-cooled fast reactors (LFR).[5,6] The motivation behind the interest in development and possible future use of alternate nuclear reactors is that each type of generation IV reactor can provide various unique advantages over standard light water reactors. Despite this, many of the generation IV reactor designs are still in the early stages of research and development. There is still a long way to go until any of these alternative reactor designs will be built for commercial operation.

Statement of Problem

Aside from the specific technical design challenges associated with each of the six, independent reactor designs set forth by the Generation IV International Forum, there are several other challenges that each reactor type will have to face prior to the actual construction of a functioning commercial reactor.

One of these challenges involves the ability to accurately simulate a basic reactor core in a computer program. While there is a plethora of reactor simulation programs available in the nuclear industry, many are designed with a specific purpose in mind. Thus, many of these programs are only valid under a specific set of conditions and corresponding assumptions. Before any computer simulation software can be used for design purposes, safety calculations, or operational analysis, it must first be demonstrated that the software is valid under applicable conditions. Therefore, any software must first undergo an adequate amount of testing before it can be used in the design process. This testing requires running the code for a series of benchmark examples pertaining to the design scenario and comparing the results to those of another nuclear code that has been previously shown to be accurate. Alternatively, the code under examination can model a situation present in an experimental test reactor and compare the outputs to experimentally measured quantities. Ideally, a nuclear code being investigated will be able to be verified by both an alternative program and an experimental test reactor.

A second, non-design related obstacle to the alternative reactor development process is the construction, operation, and analysis of a test reactor that obeys the design specifications of the specific reactor type. While comparing a nuclear code analysis to that of another, verified program may be satisfactory justification for using a new program (or an existing program for a new purpose), it is not enough verification for a reactor design construction license. Before any of the generation IV reactor types will be able to be licensed and built, their basic principles and operation characteristics will have to be demonstrated in an experimental test reactor. This can be an expensive and time-consuming process, and often serves to complicate the development of new nuclear reactor designs.

Purpose of Research

Due to the wide variety and diversity of the alternative reactor designs supported by the Generation IV International Forum, the research summarized in this paper will pertain to gas-cooled fast spectrum nuclear reactors. Specifically, it will be investigating the accuracy and predictive capabilities of two nuclear reactor programs, Serpent and MC^2-3. Serpent is a continuous-energy Monte Carlo reactor physics burnup calculation code, while MC^2-3 is a multigroup cross section generation code for fast reactor analysis.[9,10,11] Both programs will be used to model a gas-cooled fast breeder reactor experiment previously carried out at the Argonne National Laboratory (ANL) ZPR-9 critical facility. The outputs of both codes will be compared to one another, as well as to the full-scale measurements and calculations from the ZPR-9 facility. The relative effectiveness and accuracy of Serpent and MC^2-3 codes will then be analyzed and discussed.

Additionally, the research discussed in this paper will include a demonstration of the Nuclear Energy Advanced Modelling and Simulation (NEAMS) Workbench as it is used to create the input files for a series of Argonne Reactor Computation (ARC) nuclear codes. The ARC code in question is MC^2-3. The NEAMS Workbench will also model the ZPR-9 facility experiment, and the results from the Workbench-generated MC^2-3 input will be considered alongside the Serpent and MC^2-3 (without the NEAMS Workbench) results.

Chapter 2

Review of Literature

History of Nuclear Power

The theoretical concept of a nuclear chain reaction, of which all commercial nuclear reactors are based upon, was first hypothesized by Leo Szilard in 1933.[2] Then, five years later in 1938, when Otto Hahn and Fritz Strassmann proved that nuclear fission was possible, it became clear that Szilard's chain reaction hypothesis was theoretically viable.[2] This discovery also prompted the first confirmation of Albert Einstein's theorized relationship between mass and energy, as calculated by Lise Meitner.[2]

After the discovery of nuclear fission, scientists around the world began to recognize the possibilities of a controlled, self-sustaining nuclear reaction. This led Enrico Fermi and a team of scientists to design and build the first nuclear reactor, located at the University of Chicago. They named it Chicago Pile-1. After just a few months, in December 1942, they succeeded in creating the world's first self-sustaining nuclear reaction.[2] Thus, just 4 years after nuclear fission was discovered, the nuclear age had begun.

Due to the ongoing nature of World War II, the vast majority of research into the newly established nuclear industry involved the development of an atomic weapon for American use.[2] This research was carried out in secret, under the code name *Manhattan Project*. While the immensely destructive results of the *Manhattan Project* are well known, it nonetheless played a crucial role in the development of the nuclear industry and allowed for many technological achievements that greatly benefit society today.

Following the conclusion of World War II, much of the work in the nuclear industry centered around the development of nuclear power for peaceful purposes. These peaceful purposes primarily involved the development of commercial nuclear power reactors. The earliest nuclear reactors were based on a breeder reactor concept, which creates more fissionable material through operation than it consumes.[2] The first reactor of this design was the Experimental Breeder Reactor I (EBR-1), which was approved by the newly created Atomic Energy Commission (AEC) and built in the late 1940s.[2] EBR-1 was constructed in Idaho, at the site that would become Idaho National Laboratory (INL). It generated the first electricity in December 1951.[2] In the following years, the first commercial nuclear plant was built in Shippingport, Pennsylvania. It reached full power in 1957.[2] This first commercial plant was a light-water reactor (LWR).[2] The LWR design was selected due to the advancements in LWR design technology that was fueled by the United States Navy research into reactors for submarine and aircraft carrier use.

After the Shippingport reactor proved nuclear power was a viable option for commercial power production, the private power industry in America became much more interested and involved in the development of commercial nuclear power.[2] This resulted in an American boom in nuclear power throughout the 1960s and early 1970s.[2] Nuclear power was an environmentally-friendly and economical feasible source of electricity for the entire nation. This time period and the years immediately following it were when the vast majority of the 99 currently operating American nuclear power plants were constructed.[2] Following the example set forth by Shippingport, all of these commercial reactors were of the LWR design. However, growth in the commercial nuclear industry began to slow in the late 1970s and 1980s, due to a variety of factors. One such factor was the decrease in demand for electrical power.[2] Another was a rise in public concern over reactor safety and nuclear waste disposal.[2] This increase in concern was largely due to the two major nuclear power plant meltdowns of the time, Three Mile Island in 1979 and Chernobyl in 1986. These developments in the nuclear industry led to stricter regulations for nuclear reactors and a greater emphasis being placed on safety in reactor design and operation.

In the years following the US development of commercial reactors, nuclear power managed to spread to over 30 countries around the world.[2] Worldwide research into nuclear science, as well as government programs such as Atoms for Peace were responsible for this spread of commercial nuclear power. Throughout its relatively brief history, nuclear science and research has led to great improvements in many aspects of human society worldwide and will continue to do so for years to come.

Alternative Nuclear Reactor Systems

The principles pertaining to reactor safety (for the surrounding public, reactor personnel, and the environment), efficiency, and economic viability are central to the entire commercial nuclear industry.[5,12] Thus, any nuclear reactor design or modification must enhance the ability of the nuclear industry to meet these principles. Regardless of the status of the American commercial nuclear industry, nuclear power continues to grow and contribute to power production around the world. Therefore, research and development of nuclear reactors has continued relatively undiminished since the conception of commercial nuclear power.[5,12] This research can be evidenced by the consistent improvement in reactor safety and efficiency since the first commercial plants were built in the 1950s. While many researchers are committed to the overall improvement of the current nuclear fleet, either through improved fuel utilization, safety features, or other means, many researchers are devoted to designing fundamentally different reactor types.

The vast majority of the focus on alternative reactor designs today is centered around a series of reactor designs that are referred to as Generation IV Advanced Reactors.[3,4,5] These are reactors that vary in basic design principles from the most prevalent reactor type utilized in the world today, the light-water moderated reactor. The primary motivation for the deviation from an LWR design is that alternative reactors can be utilized for different purposes or provide performance improvements to current designs. Current commercial power plants can be improved with respect to thermal efficiency, waste generation, inherent safety risks, and fuel utilization.[4-6,8,12] Generation IV reactors seek to improve upon most or all of these factors. According to Piyush Sabharwall et al. "advanced reactor development under GIF seeks to achieve:[7]

1. Sustainability via optimal resource utilization and waste minimization;
2. Economic viability by establishing clear life cycle cost advantages and comparable financial risk relative to other energy sources;
3. Safety and reliability through passive and inherent safety systems that minimize the likelihood for core damage and eliminate the need for offsite emergency response; and
4. High proliferation resistance"

The proposed alternative reactor designs have the potential to provide much more variety and versatility to the commercial nuclear power industry, which could allow the nuclear industry to play a more significant role in the world today.

The Generation IV International Forum, which supports the research and development of these advanced reactor designs, has selected six basic designs for further investigation.[5,6] The six Generation IV Advanced Reactor designs are as follows:[5,6]

1. Very High Temperature Reactors (VHTR)
2. Molten Salt Reactors (MSR)
3. Supercritical Water Reactors (SCWR)
4. Sodium-Cooled Fast Reactors (SFR)
5. Lead-Cooled Fast Reactors (LFR)
6. Gas-Cooled Fast Reactors (GFR)

Very High Temperature Reactors

The primary advantage of the VHTR concept is that it operates, as the name suggest, at a significantly higher temperature than a standard LWR.[3,5-7] The typical Pressurized Water Reactor (PWR), the most common type of LWR, operates with typical coolant outlet temperatures below 350°C. Proposed VHTRs can operate with coolant temperatures as high as 1000°C. This temperature allows for the VHTR and the direct Brayton gas-turbine cycle that it utilizes to achieve efficiencies of approximately 55%.[5,6] 55% is a sharp increase from the average efficiencies of current LWRs, which are below 40%.[5,6]

The basic VHTR design consists of a graphite-moderated core that is cooled with pressurized helium.[3,5-7] It is intended to operate with a once-through uranium fuel cycle.[3,5,6] Due to the quantity of graphite incorporated throughout the reactor core, the VHTR design operates with a thermal neutron spectrum.[3,5-7] Figure 1 shows the basic design for the VHTR reactor type if it were used to produce process heat for hydrogen production. However, the hydrogen production plant in Figure 1 could be replaced with a steam-powered turbine and generator if electricity generation was the purpose of the nuclear plant.

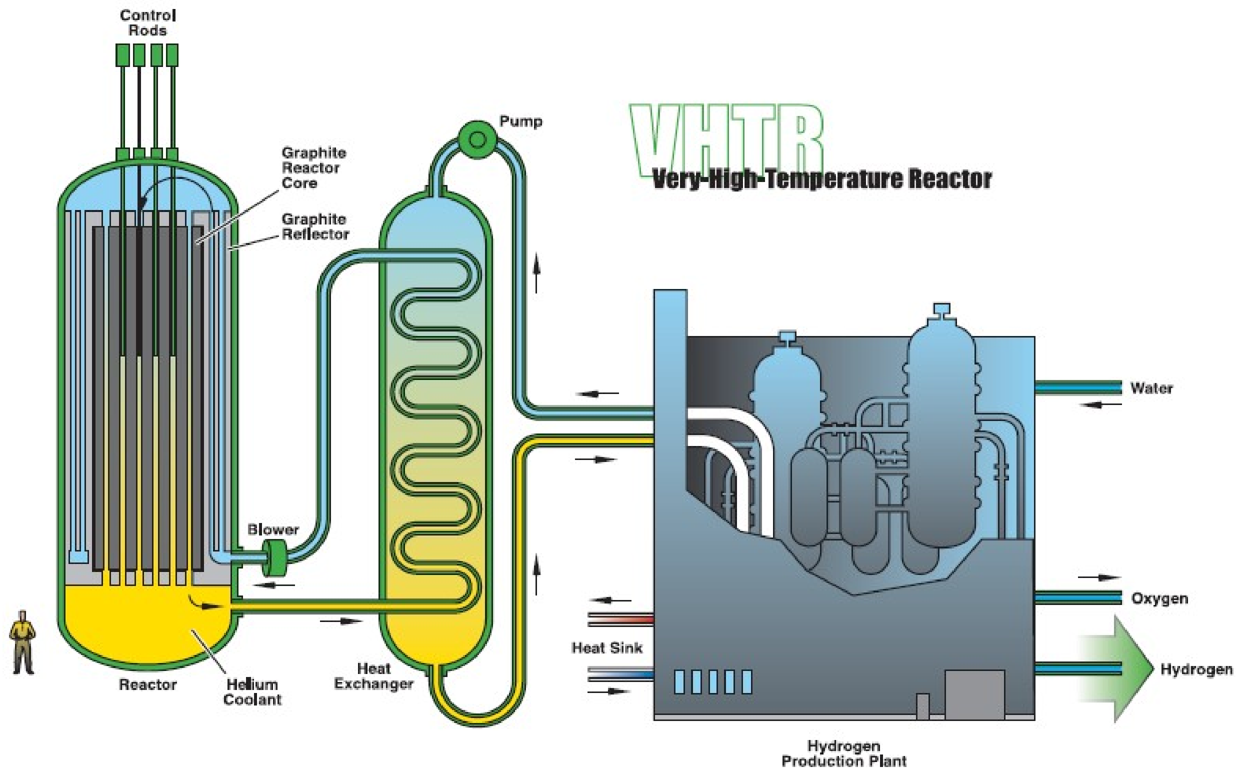

Figure 1: Diagram of a VHTR System[5,6]

Molten Salt Reactors

The MSR generation IV design significantly diverges from current commercial reactors by utilizing a completely liquid fuel that continuously circulates inside the reactor core. As it circulates, the fuel passes through graphite channels, which serve to thermalize the resulting neutron spectrum.[5] The fuel itself consists of sodium, zirconium, and uranium fluorides in the form of a molten salt solution.[5] A summarized diagram of the MSR design can be seen in Figure 2, complete with secondary and tertiary coolant cycles utilized for electricity generation.

The primary advantage of the MSR design is in its vastly improved fuel utilization.[5] Because the liquid fuel form allows for varied feed composition and the design itself allows for the burning of actinides, no fuel fabrication is required and a full actinide recycle fuel cycle is possible.[5,13,14] This means that the MSR design can effectively operate with a closed fuel cycle.

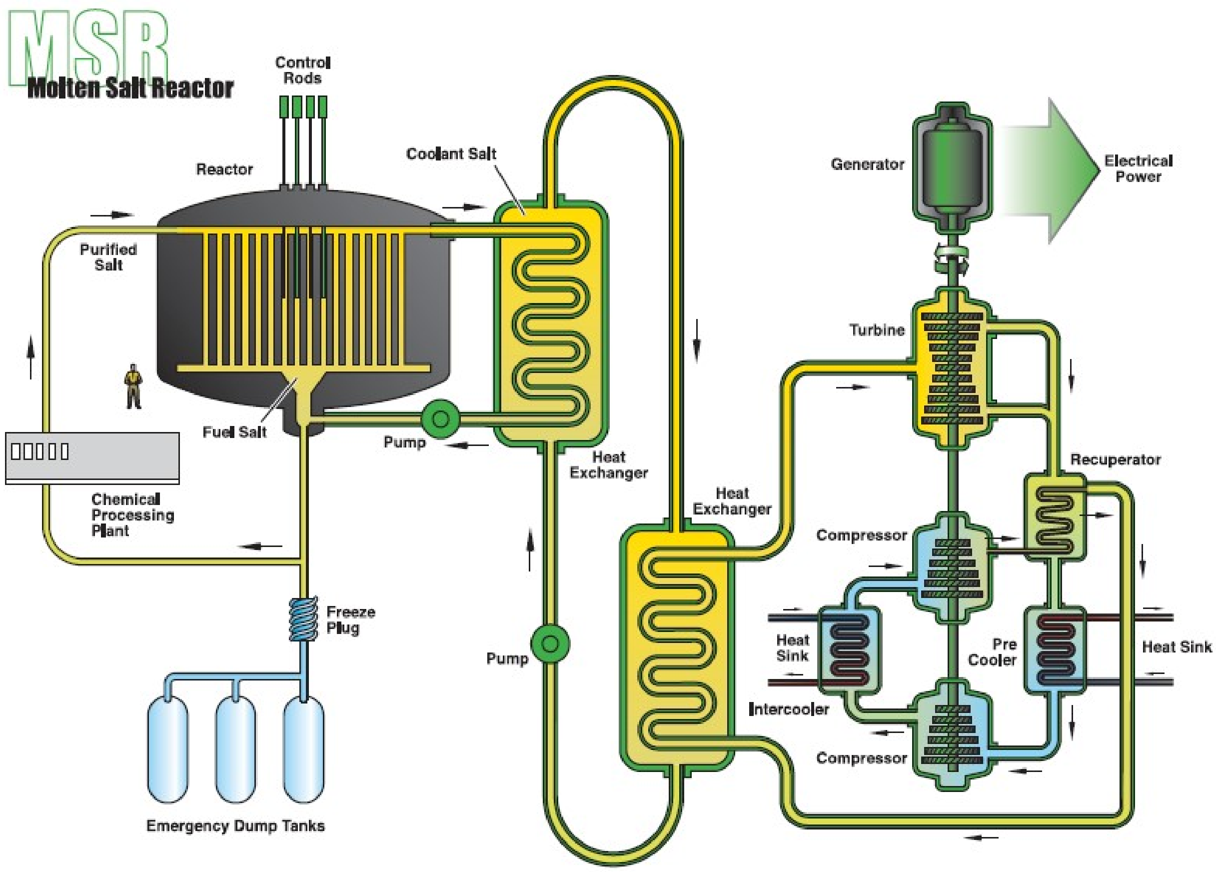

Figure 2: Diagram of an MSR Power Generation System[5]

Supercritical Water Reactors

Similar to current commercial LWRs, the SCWR design utilizes water as a primary coolant. However, unlike commercial LWRs in operation, the SCWR design has the ability to support two different fuel cycle options.[5] The first is a once-through uranium cycle that operates with a thermal neutron cycle.[5] Due to the relatively low density of supercritical water, a separate, independent moderator is necessary for this fuel cycle to be feasible.[5] The second fuel cycle option features a fast neutron spectrum that allows for the use of a full actinide recycle fuel cycle.[5,13,14] This allows for reactor operation with a closed fuel cycle.

The advantages offered by the generation IV SCWR design are dependent on the fuel cycle selected for operation. In the case of the once-through uranium cycle, the increased outlet temperature allows for increased thermal efficiency and an overall balance of plant simplification.[5] This is due to the lack of a phase transition in the primary coolant.[5] The second fuel cycle option offers a greatly improved fuel utilization in addition to the increased thermal efficiency and plant simplification of this design.[5] Figure 3 details a generic plant schematic of an SCWR utilized for electricity generation.

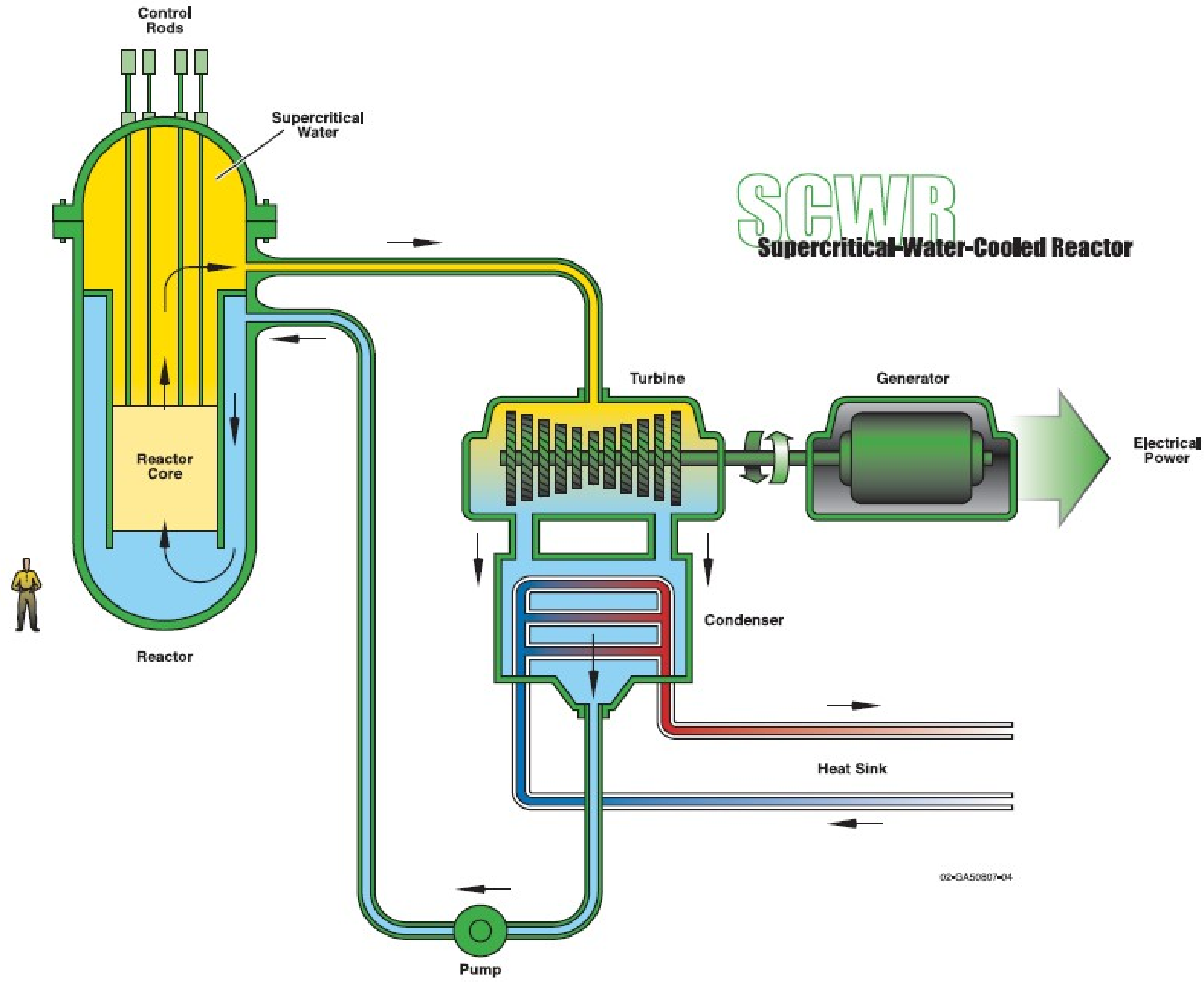

Figure 3: Diagram of an SCWR Power Generation System[5]

Sodium-Cooled Fast Reactors

The SFR design consists of a reactor core submerged in a pool of liquid sodium. Within the liquid sodium is a heat exchanger that converts the fission energy into steam in a secondary coolant cycle.[5] The generated steam then passes through another heat exchanger to transfer the heat energy to a third cycle, which then drives a steam turbine and generator.[5] This arrangement can be seen in Figure 4 below. The purpose of the third steam cycle is limiting plant exposure to radioactive material. The fuel in the reactor core is either a mixed uranium-plutonium oxide fuel

(MOX) or a uranium-plutonium-minor-actinide-zirconium metal mixture. It operates on the basis of a fast neutron spectrum.[5]

The advantages of the MSR design are primarily in safety and fuel utilization. The reactor can be designed with passive safety measures that require little intervention from a reactor operator, and the fuel design allows for a full actinide recycle fuel cycle.[5,13,14] This results in the opportunity for the implementation of a closed nuclear fuel cycle.

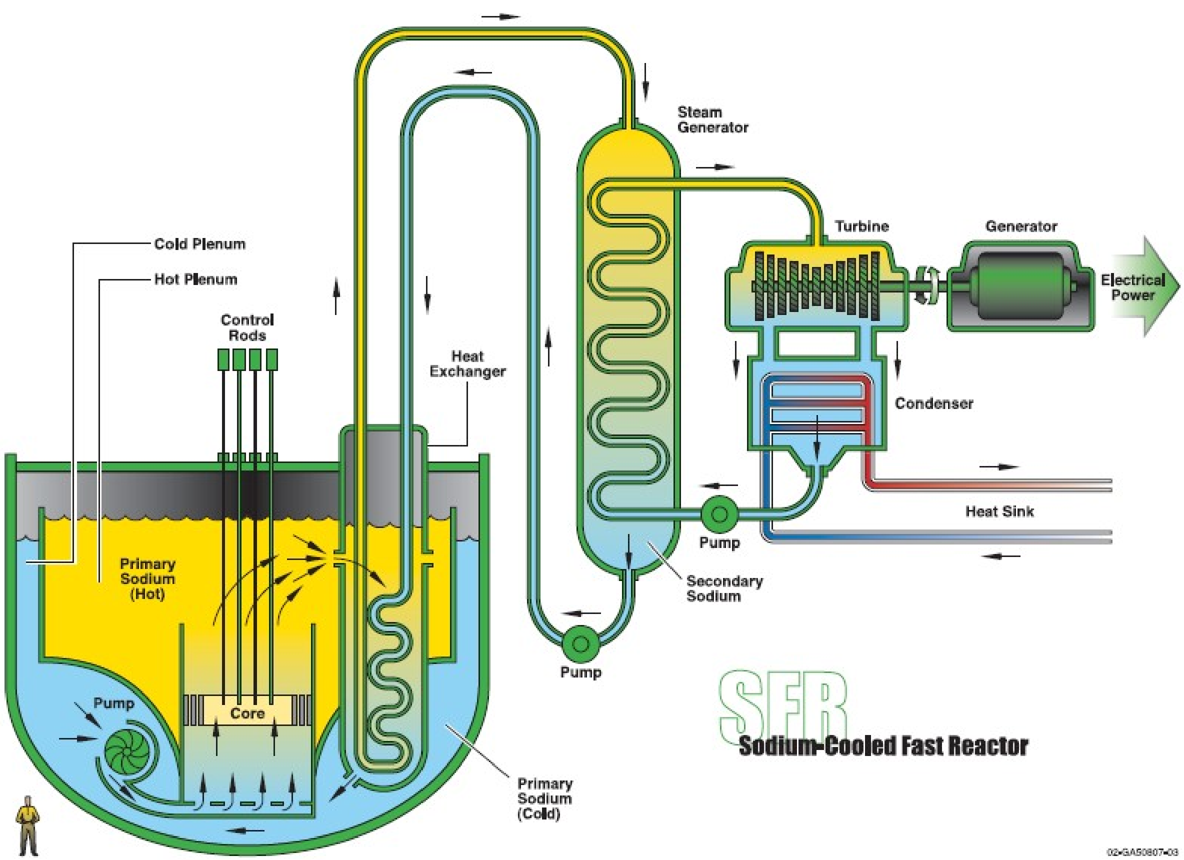

Figure 4: Diagram of an SFR Power Generation System[5]

Lead-Cooled Fast Reactors

The LFR design set forth by the Generation IV International Forum also features a fast neutron spectrum, however, it utilizes a lead or lead/bismuth eutectic coolant solution.[5] The coolant is in the form of a liquid metal surrounding the reactor core, as seen in Figure 5. The LFR design also features the versatility of being deployed in two primary forms. The first is a standard implementation of a relatively large core with a greater nominal power output (approximately 1200 MWe).[5] The second form is as a smaller, “battery” design that operates as a long-term heat source that can be used for either energy production or process heat.[5] The “battery” design has a nominal output ranging from 50 MWe to 150 MWe.[5]

Due to the fuel utilized in the LFR design, a full actinide recycle fuel cycle is possible.[5,13,14] This permits a closed fuel cycle and thus, greatly improved nuclear fuel utilization. The LFR concept also benefits from its long-life core design, which can last between 10 and 30 years.[5]

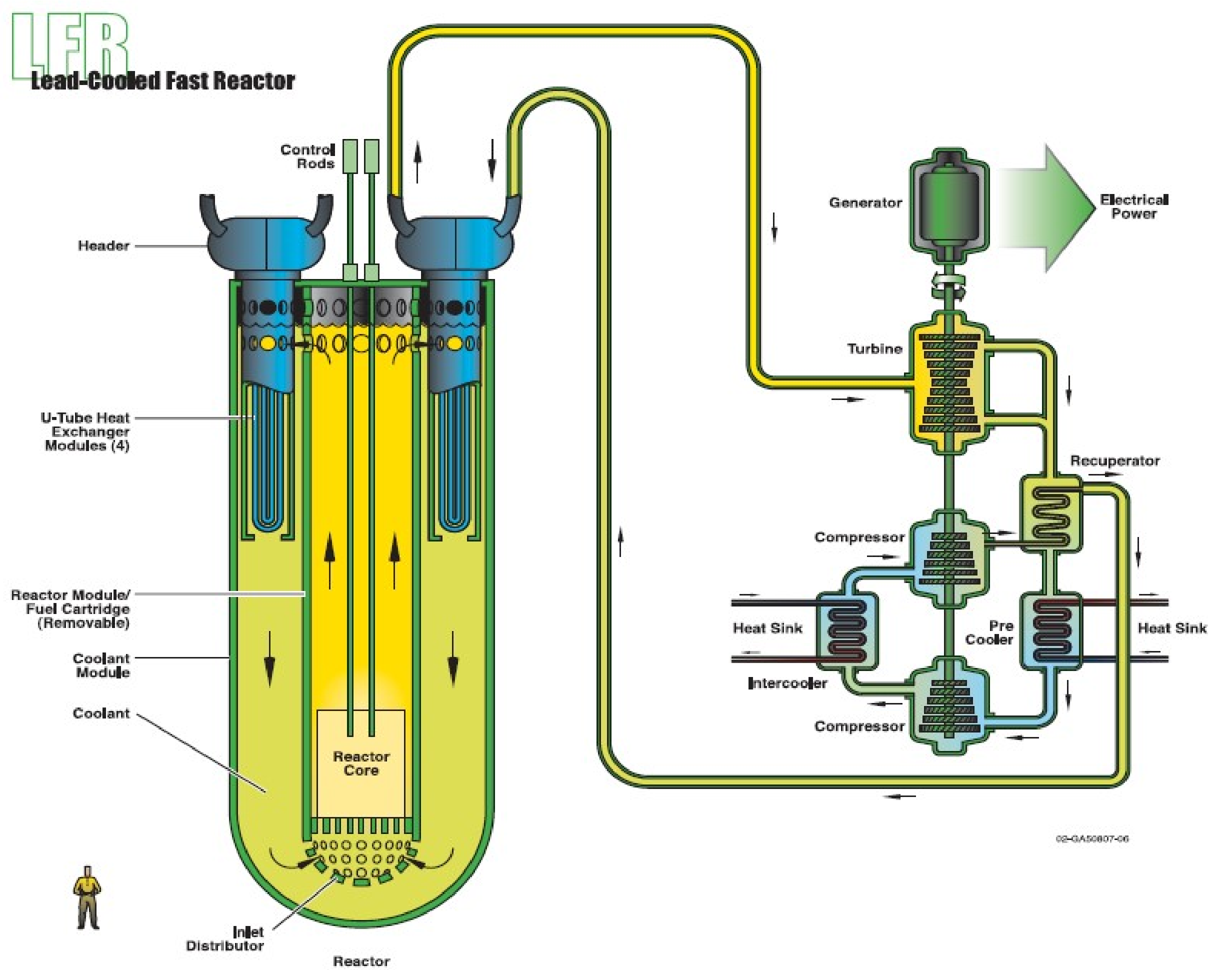

Figure 5: Diagram of an LFR Power Generation System[5]

Gas-Cooled Fast Reactors

The final advanced reactor design supported by the Generation IV International Forum is the GFR design.[5,8,15,16] The fuel types in a specific GFR can vary widely depending on the design of the reactor. GFR fuel can be in the form of pins, plates, or even prismatic blocks.[4,5,8,12,15-20] Regardless of the fuel type selected, the generation IV GFR design incorporates a pressurized helium coolant and operates with a fast neutron spectrum.[5,12,15-18,20] This design can be seen in Figure 6, where the reactor is used to power an electrical generator and turbine. However, the GFR design can also be used to produce process heat for the production of hydrogen.[5,16,17]

The inherent advantages of the GFR design are primarily in fuel optimization and thermal efficiency. It improves upon the fuel utilization of current reactors by allowing for a full actinide recycle, effectively closing the fuel cycle.[5,8,12-14,16-18,20] The advantage of improved thermal efficiency is due to the increased outlet temperature (up to 850°C) of the helium coolant.[5,12,16,18,20]

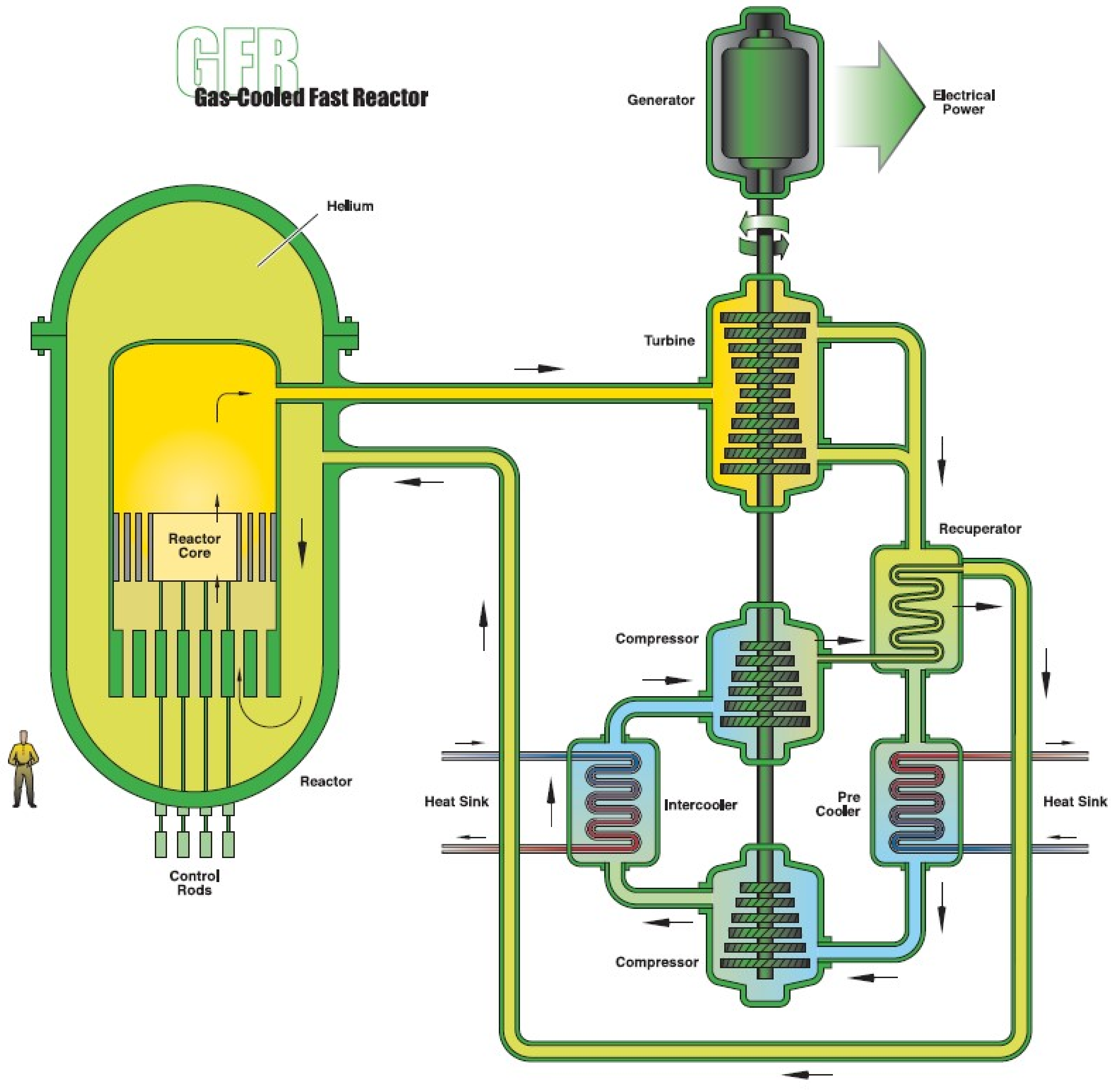

Figure 6: Diagram of a GFR Power Generation System[5]

ZPR-9 Critical Test Facility

The Zero Power Reactor No. 9 (ZPR-9) critical test facility was an experimental gas-cooled fast reactor model constructed and operated at the Argonne National Laboratory-West (ANL-West) site in Idaho.[21,22] It was part of the fast reactor critical experiments program that started in 1955 with the Zero Power Reactor No. 3 (ZPR-3) and ended when the Zero Power Physics Reactor (ZPPR) was shut down and decommissioned in 1990.[21]

The ZPR-9 facility itself operated between the years of 1963 and 1982.[21] Initially the ZPR-9 facility was used to support a nuclear rocket program.[21] This included the first 9 ZPR-9 assemblies.[21] The ZPR-9 facility was then used to study spectral dependent quantities and zone measurements for full-sized cores.[21] At the end of the ZPR-9 facility's lifetime it was used to model and evaluate several gas-cooled fast reactor designs.[21,22] The latter assemblies used for GFR analysis are of direct relevance to the research summarized in this paper. The ZPR-9 facility was officially shut down and decommissioned in 1981.[21]

The facility was used as a physics benchmark for a simple cylindrical reactor with an output of approximately 700 MWe and multiple zones with varying compositions.[21] It was constructed using a rack of rectangular stainless steel drawers measuring approximately 0.055 X 0.055 m, each with length 2.44 m.[21,22] The drawers were arranged to form a 2.44 X 2.44 X 2.44 m array that composed the ZPR-9 reactor.[21,22] Coolant in the form of pressurized helium was then circulated through the reactor core and a separate heat sink.[21] A radial cross section detailing the layout of the core regions is available in Figure 7.

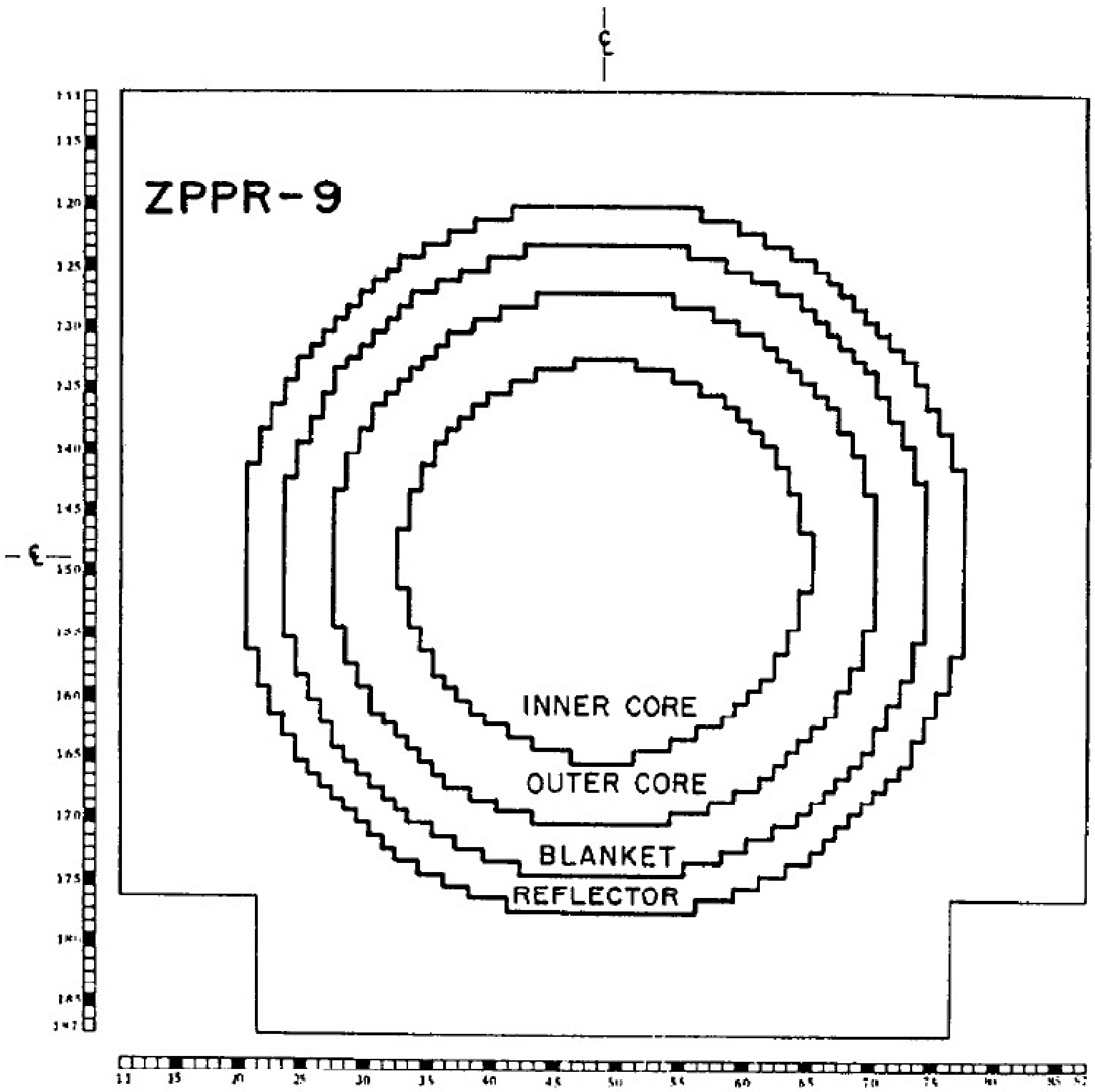

Figure 7: ZPR-9 Interface Diagram[21]

The standard drawer loading patterns can be seen in Figure 8 below.

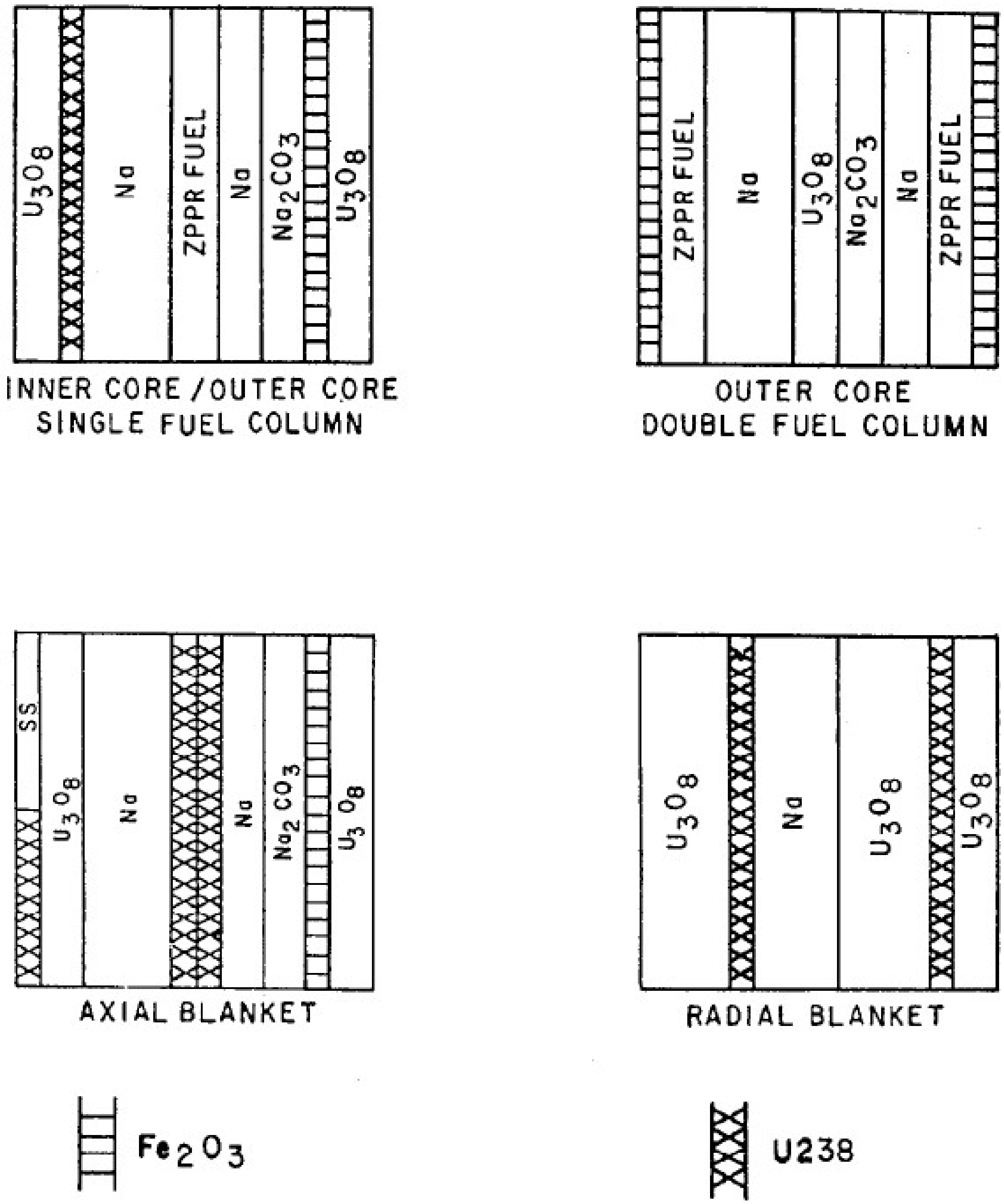

Figure 8: ZPR-9 Drawer Loading Patterns[21]

The research performed for this project recreates, through computer simulation, the experimental work published by E. M. Bohn et al. in 1977.[22] This experiment, coupled with reference calculations for the critical facility, was performed jointly with ANL and General Atomic (GA).[22] The purpose was to obtain the first official measurements of important physics parameters relevant to a General Atomic gas-cooled fast reactor design in a full-scale test.[22] They compared the experimental results to analytical calculations made by both ANL and GA personnel, as well as provide experimental data on safety coefficients necessary for safe reactor operation.[22] Three independent ZPR-9 assemblies were tested, but only data from the second will be referenced in this report.[22] The second assembly was the most extensively tested, and is featured prominently in the report published by E. M. Bohn et al.[22]

The experimental assembly tested by E. M. Bohn et al. varied slightly from the basic ZPR-9 facility design. The experiment involved only 3 radial core regions instead of 4.[22] These regions were labelled core, radial blanket, and radial reflector.[22] Additionally, the drawer compositions were varied axially in order to allow for multiple axial composition regions.[22] This allowed for the inclusion of an axial blanket to surround the core region and an axial reflector to surround the axial blanket regions.[22] The core blanket regions (radial and axial) incorporated U_3O_8 and depleted uranium in order to capture escaping neutrons and breed additional fissile material.[22] The purpose of this is to improve fuel utilization for the GFR design. The stainless steel reflector regions (radial and axial) served to improve neutron economy by scattering as many escaping neutrons as possible back into the nuclear core region. Figures 9 and 10 below summarize the alterations to the ZPR-9 facility's radial design and drawer loading patterns, respectively.

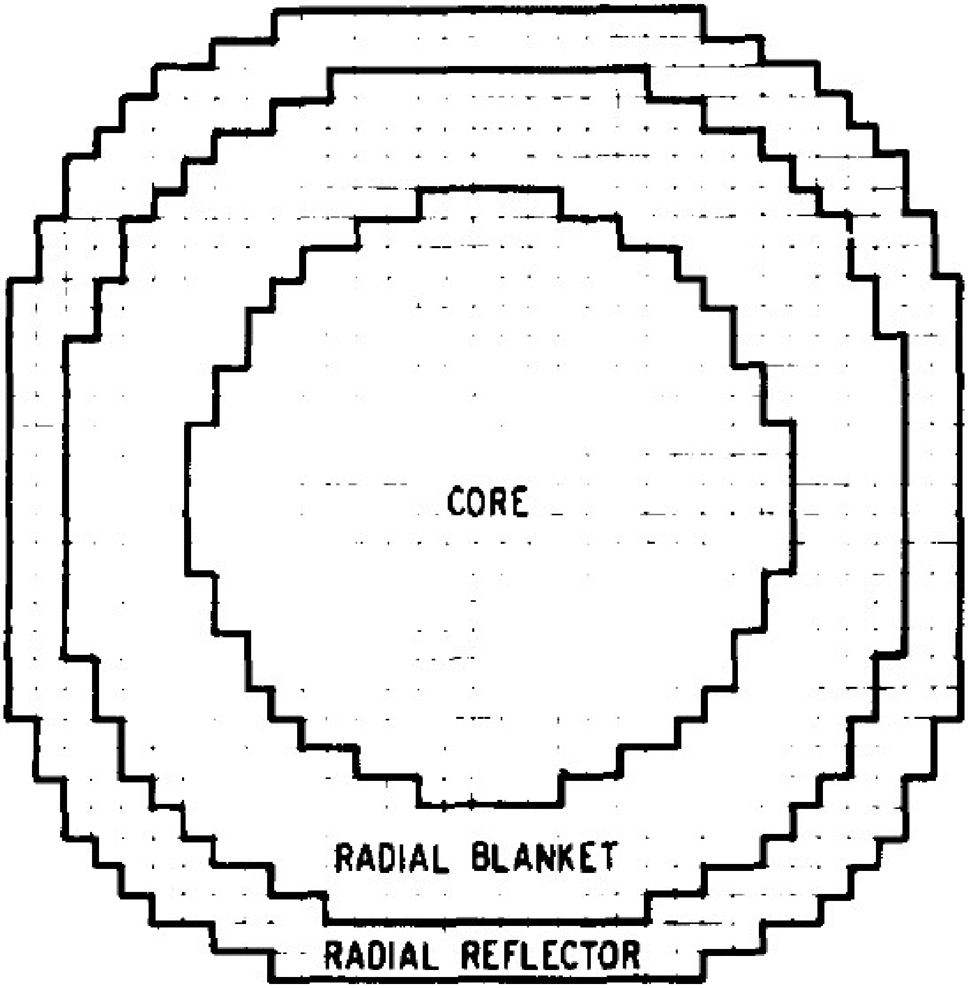

Figure 9: Midplane View of GFR Assembly for ZPR-9 Experiment[22]

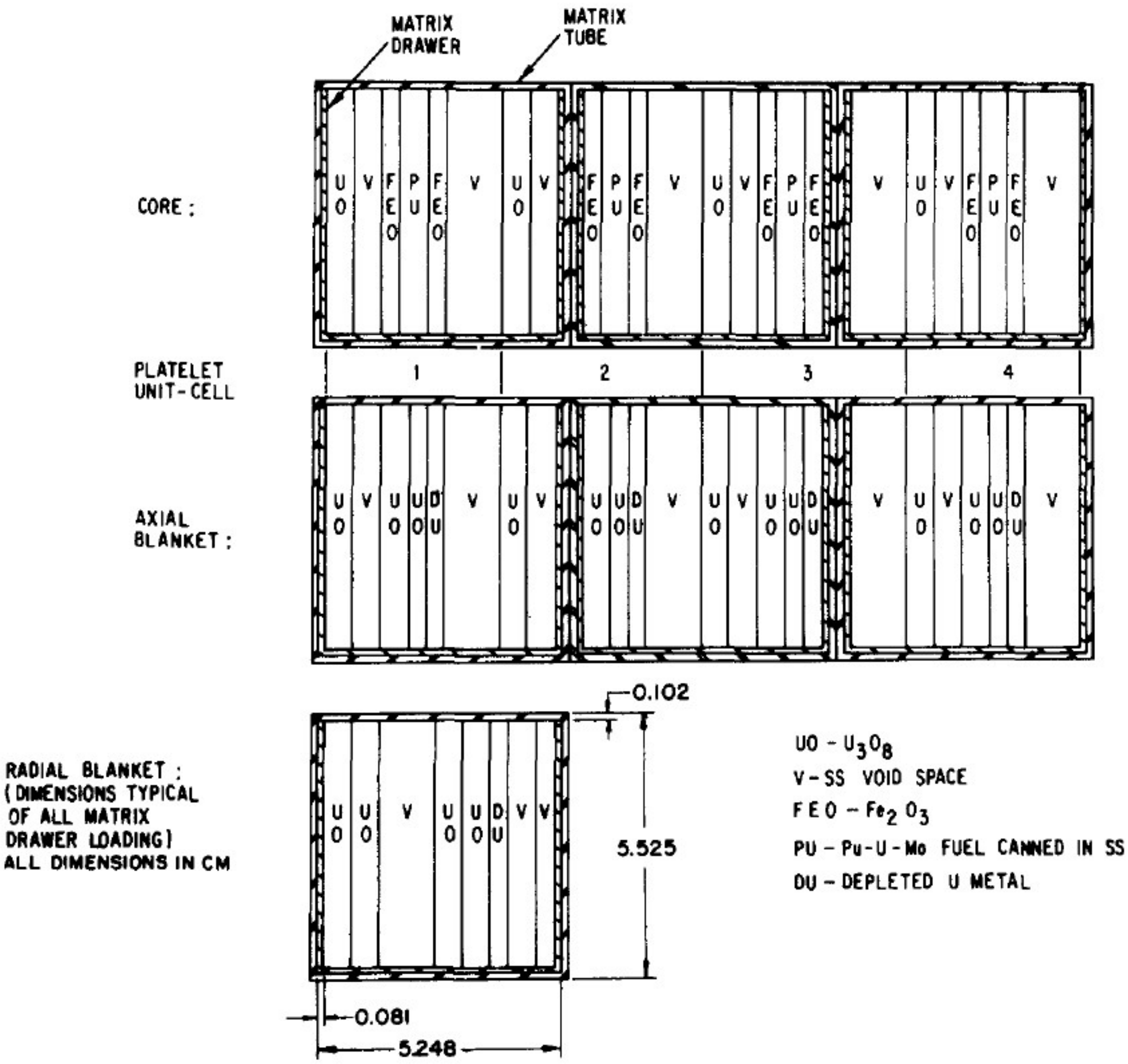

Figure 10: Drawer Loading Pattern for GFR Assembly Used for ZPR-9 Experiment[22]

The alterations included in this experiment also affected the atom densities of the reactor materials, fissile and otherwise, found in each region of the experimental design. These values are critical to any simulation used for calculating or analyzing important characteristics of this GFR design. The region-dependent average unit-cell atom densities used in the experimental ZPR-9 assembly and corresponding calculations are summarized in Table 1.

Table 1: Average Unit-Cell Atom Densities for ZPR-9 Experiment (10^{21} atoms/cm^3)[22]

Material	Core	Axial Blanket	Radial Blanket	Axial Reflector	Radial Reflector
^{239}Pu	1.1832	-	-	-	-
^{240}Pu	0.1569	-	-	-	-
^{241}Pu	0.0163	-	-	-	-
^{242}Pu	0.0023	-	-	-	-
^{241}Am	0.0093	-	-	-	-
^{235}U	0.0122	0.0186	0.0194	-	-
^{238}U	5.5421	8.6998	9.0911	-	-
O	13.4423	14.5819	17.7994	-	-
Fe	15.3210	8.8023	8.7909	52.8807	55.5448
Ni	1.3281	1.1426	1.1373	6.6746	6.7956
Cr	2.8828	2.5122	2.5087	15.0985	15.7448
Mn	0.2260	0.1944	0.1944	1.4434	1.3279
Mo	0.3121	0.0097	0.0099	0.0055	0.0730
C	0.0303	0.0278	0.0281	0.2370	0.2164
Si	0.1791	0.1591	0.1591	1.0056	0.9052

After the ZPR-9 experiment was performed, a number of reactor parameters and characteristics were calculated from the results obtained.[22] Both ANL and GA personnel independently computed the values shown in this report, using different methods developed by both laboratories.[22] These parameters and characteristics included, but were not limited to, core eigenvalues, reactivity parameters, region and isotope cross sections, neutron energy spectrum, fission rates, and reactivity worths.[22] While all of these values are pertinent to GFR operation, only the eigenvalues and neutron energy spectrum will be used for comparison to the computer simulations performed in the research summarized in this report. Table 2 and Figure 11 display the calculated eigenvalues for the test facility and the neutron spectrum, respectively.

Table 2: Calculated Eigenvalues for the ZPR-9 Experiment[22]

	ANL	GA
K_{inf} (core average)	1.5808	1.5533
K_{eff} (isotropic diffusion)	1.0148	1.1048
K_{eff} (anisotropic diffusion)	0.9994	0.9977
Δk due to streaming	-0.0154	-0.0171

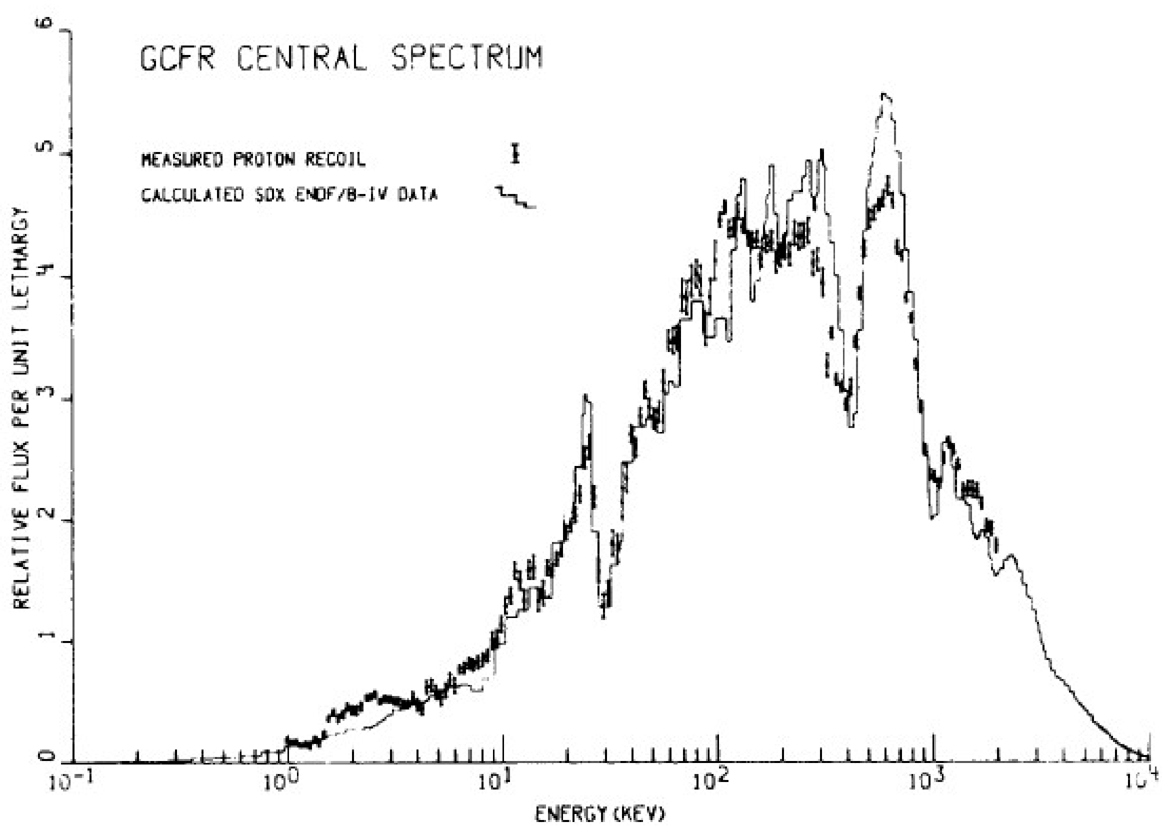

Figure 11: Measured and Calculated Neutron Spectra for the ZPR-9 Experiment[22]

Nuclear Reactor Computer Simulation

Crucial to the development of any nuclear reactor design is the ability to accurately model reactor core operation and performance through the use of computer programs. By modeling a reactor type or design in a software program, many different iterations and improvements can be made to the design without the costly process of experimentation. A reactor design must still be proven to function as intended through actual experimentation, but computer simulation can avoid much of the costly and time-consuming process of multiple reactor experiments for a single design. However, most nuclear simulation programs differ from one another through a number of factors, including calculation methods, inherent assumptions, and more. As a result, not every nuclear simulation code is suitable for modeling every type of reactor. Before a specific code is used to model a reactor design, it must first be verified as accurate for that reactor type. This is accomplished by modeling a benchmark nuclear system and comparing the results from the program in question to those of the benchmark experiment or a previously verified program. The specific nuclear programs and codes described in this chapter were selected for their ability to aid in the nuclear reactor design development process. Therefore, throughout the course of the research performed, each program's validity was investigated appropriately.

Serpent is a continuous-energy Monte Carlo reactor physics burnup calculation code developed in 2004 by VTT Technical Research Centre of Finland.[10,23] It was originally developed for the Linux operating system, though it has been compiled on some UNIX systems and MAC OS X as well.[10] It is run primarily from the command line interface, with user and code interaction taking place through the use of one or more input files that the user develops.[10] Serpent primarily utilizes data from ACE format cross section libraries, including JEF-2.2, JEFF-

3.1, ENDF/B-VI.8, and ENDF/B-VII data files.[10,23] Input file development requires the user to construct the desired reactor geometry in terms of single material cells, which are defined by geometric boundary surfaces, and universes, within which the defined cells are located.[10] The combination of multiple universes and cells within them allows for the construction of more complex reactor systems. Additionally, Serpent provides the option for premade special universes, called lattices, to be used.[10] These lattices are filled with a regular structure of other universes, which include infinite 3D structures and circular cluster arrays, among others.[10] Similarly, Serpent provides a shortcut for defining reactor pin geometries.[10] When the desired reactor geometry and materials contained within are defined, the input code can be compiled. After which, Serpent will produce a number of output files, dependent on what the user requests. These can include, but are not limited to, eigenvalue calculations, neutron energy spectra, and reactor burnup characteristics, all of which can be used for reactor design evaluation and further development.[10,23]

Serpent has been tested extensively against reactor experiments and other nuclear core calculation programs in order to verify its accuracy. Table 3 summarizes some of the research papers that have investigated the accuracy of the Serpent program.

Table 3: Prior Investigations of the Serpent Code

Research Paper Title	Brief Summary of Work	Conclusions
Solution of the OECD/NEA neutronic SFR benchmark with Serpent-DYN3D and Serpent-PARCS code systems[24]	Serpent was used to generate homogenized energy group constants for a large U-Pu MOX SFR system. Two other codes, DYN3D and PARCS, utilized these group constants to continue 3-D full core calculations. The results were then compared to a full core Serpent reference solution.	Serpent was able to accurately model the MOX SFR system, including the generation of homogenized energy group constants.

Comparison between Serpent and MONTEBURNS codes applied to burnup calculations of a GFR-like configuration[25]	Criticality and burnup calculations were performed on a configuration representing the Allegro MOX GFR design using both Serpent and MONTEBURNS nuclear calculation codes, then compared.	Serpent was able to accurately model and calculate criticality values for the GFR design.
Full Core modeling techniques for research reactors with irregular geometries using Serpent and PARCS applied to the CROCUS reactor[26]	Serpent was used to model the irregular LWR design of the zero-power teaching and research CROCUS reactor, which employs an irregular geometry.	Serpent successfully modelled the irregular CROCUS and provided accurate results.
Modeling of SFR cores with Serpent–DYN3D codes sequence[27]	Serpent was used in conjunction with DYN3D to perform calculations on a fast spectrum reactor and provide a reference for comparison to another nuclear code system, ERANOS.	Serpent was shown to be able to successfully model reactors operating with a fast neutron spectrum.

MC^2-3 is a multigroup cross section generation code designed by Argonne National Laboratory researchers for fast spectrum nuclear reactor analysis.[11] It was developed as part of the Advanced Fuel Cycle Initiative (AFCI), which strived to develop simulation tools for fast reactors.[11] MC^2-3 utilizes ENDF/B-VII.0 data files to generate multigroup neutron cross sections for the reactor geometry selected.[11] Reactor geometries and material compositions are defined through the use of an input file generated by the user.[11] This input file, which can be one of several, is constructed through the use of input blocks.[11] These input blocks divide the input file into various command groups that control code calculations.[11] Examples of these blocks include the control block, which determines the method by which MC^2-3 solves for reactor characteristics, the geometry block, where the core geometry is modelled into basic geometric configurations, and the material block, where the chemical compositions of the various materials in the model are defined.[11] After the input is defined and the code is executed, MC^2-3 produces several output files, depending on the user's needs. These outputs can include a summary of neutronics calculations, neutron energy spectra, homogenized group constants, and more.[11] Depending on the needs of the user, some of these outputs can then be passed on to other programs for further reactor analysis.

The NEAMS Workbench is a program contained within the NEAMS Integration Product Line (IPL) developed by the Argonne National Laboratory.[28] It is currently in pre-release status, as additional features and functionality are being incorporated. The purpose of the 2017 Workbench initiative is to aid in the transition from conventional tools to high fidelity tools for fast spectrum nuclear reactor analysis.[28] The Workbench operates as a common user interface that allows the user a more convenient method to create reactor models, execute nuclear calculation codes, and perform output processing for the suite of deterministic neutronics codes provided.[28] These codes included within this suite are MC^2-3, DIF3D, REBUS-3, and PERSENT.[28] MC^2-3 generates multigroup cross sections, DIF3D performs flux calculations, REBUS-3 calculates depletion and equilibrium values, and PERSENT executes perturbation theory calculations.[11] The NEAMS Workbench improves the ease of use for these codes by providing a single, intuitive interface that incorporates multiple codes into a single model analysis operation.[28] This allows for easier definitions for material compositions, reactor geometries, calculation restrictions and assumptions, and more.

Chapter 3

Project Summary

Introduction

Since 1957, commercial nuclear power has been safely and efficiently providing reliable baseload electricity to the United States public.[2] In 2015, nuclear power produced approximately one-fifth of all US energy.[1] Unfortunately, recent years have started to see a decline in the percentage of US power production from the nuclear sector, with the possibility for further, more rapid decline. Slow growth in the construction of new nuclear plants over past decades has resulted in an aging US commercial nuclear fleet with a relatively few number new plants. A large portion of the commercial nuclear reactors operating in the country today were built in the 1960s, 1970s, and 1980s, which means that many reactors are approaching the end of their operating licenses.[2] While many reactors are seeking license extensions for 20 more years, this process cannot continue indefinitely. Either the aging US fleet will continue to shrink in the near future, or new nuclear reactors will need to be built. In the case of the former, the US will lose one of its most reliable sources of energy and will have to find a way to replace the role that nuclear has played in the power industry for the past 60 years. This is further complicated by the fact that under this scenario, the US will lose its primary source of carbon-free energy. In 2015, nuclear reactors produced 58% of American carbon-free energy.[2] For a society with an increasing interest in the reduction of carbon emissions, this is potentially a major problem. However, the loss of American commercial nuclear power is not guaranteed. In addition to the push for reactor operation license extensions, the nuclear industry is also pursuing newer, safer, and more efficient nuclear reactor designs.[5,6,812]

The most prominent organization supporting new nuclear reactor designs is the Generation IV International Forum.[3,5,6] It supports reactor designs that feature improvements over current reactors in matters of safety and reliability, economic viability, sustainability, and resistance to nuclear proliferation.[5,6,8,12] The GIF supports the research and development of 6 reactor types, but the Gas-cooled Fast Reactor is of the most relevance to the research summarized in this report. GFR designs have been investigated and used for years, including some of the very first operational nuclear reactors.[3,5,12,18,20] However, when all of the currently operating commercial US reactors were built, the more popular LWR design was chosen.[2] Fortunately, GFR research and development has continued in the years since, allowing for significant technological advances and vast improvements in GFR design.

One crucial component of research into GFR systems is the development and use of reactor simulation and modelling software. Accurate simulation software provides researchers and designers with the ability to theoretically test designs and concepts, without having to invest the time and expense associated with the performance of an experiment. However, as with any tool, nuclear codes and programs must be used appropriately. Using a given nuclear simulation software for the wrong situation or without proper verification of its accuracy can lead to inaccurate and invalid results. Given the nuclear industry's desire to avoid unnecessary risk, this explains the importance of validating nuclear software calculations against experiments and similar programs.

Accordingly, the main purpose of this research was to investigate the ability of the multigroup cross section generation code MC^2-3 to accurately model an existing gas-cooled fast reactor system. The system in question was the ZPR-9 critical test facility located at the Argonne National Laboratory. The specific ZPR-9 assembly was the same assembly that was used in an experiment performed by E. M. Bohn et al. This assembly consists of an approximated cylindrical U-Pu mixed oxide core contained within a uranium oxide blanket and stainless steel reflector, respectively. The accuracy of the MC^2-3 code was determined by comparing the MC^2-3 outputs to those of the experiment, as well as Serpent.

A secondary purpose of this research was to demonstrate the ability of the NEAMS Workbench program to model the ZPR-9 style of reactor system. For simplicity purposes, the NEAMS Workbench was used to model the same assembly as the MC^2-3 and Serpent codes. The goal was to show that the NEAMS Workbench, which was developed to combine the utility of several ARC codes into one program with a simplified user interface, was capable of providing the same functionality of the MC^2-3 program.

Methods

Serpent was used as the reference program for this research, and as such, it was the first program within which the experimental ZPR-9 assembly was modelled. Due to the geometric and material complexities associated with the experimental assembly and limitations contained within the other nuclear codes used, the Serpent model was simplified to an infinite reactor system with zero neutron leakage. The purpose of this was to maintain a higher degree of consistency with the compared models.

Because only the core region was modelled for all programs, the blanket and reflector regions, both axial and radial, were neglected. The material within the simplified Serpent assembly core was homogenized. The material for the Serpent and all other computer models was an identical match to the core region material composition expressed in Table 1. This was completely consistent between the ZPR-9 experiment and the programs used in this research.

The Serpent simulation program outputs selected for analysis and later comparison were the homogenized region eigenvalue calculation and the neutron energy spectrum at the center of the simulated reactor system. The eigenvalue calculation would be compared to those of both other computer simulations, and the actual ZPR-9 experiment. The neutron energy spectrum was compared directly to that of the MC^2-3 model.

The MC^2-3 input file for the ZPR-9 simulation was identical in geometry and material to the Serpent model. The MC^2-3 model consisted of a homogenized infinite core of identical material composition matching that of the core region of Table 1. Similar to the Serpent outputs, the MC^2-3 code outputs include eigenvalue calculations for the homogenized core region and the neutron energy spectrum.

For the ZPR-9 assembly model created in the NEAMS Workbench, the infinite geometry was the same as the models for Serpent and MC^2-3. The remainder of the Workbench input was also identical to the previous computer models, including material composition. Currently, the pre-release version of the NEAMS Workbench does not include the functionality to produce a neutron energy spectrum from the MC^2-3 executable alone, so there is no Workbench neutron spectrum to compare to the others. However, there are full intentions to include this in later versions. Nevertheless, reactor eigenvalue calculations are included within the MC^2-3 optional calculations in the NEAMS Workbench, so the Workbench eigenvalue was used to compare results.

Additionally, it should be noted that since the modelled reactor systems are for an infinite geometry the computer eigenvalue calculations are for k_∞ rather than for k_{eff}. The motivation for this decision was based in the fact that modelling constraints prevented the inclusion of either the reactor blanket or reflector. This was expected to have a noticeable effect on the output comparison. Therefore, the comparison between the code outputs and the experimental results will be restricted to the ANL and GA calculations for the k_{inf} eigenvalue of the ZPR-9 critical assembly.

Results

A goal of this project was to investigate the ability for MC^2-3 to accurately model a realistic gas-cooled fast reactor system. The GFR system chosen for this analysis was the ZPR-9 critical fast reactor assembly at the Argonne National Laboratory. It was an approximated cylindrical reactor core of U-Pu mixed oxide fuel surrounded by a uranium blanket with a stainless steel reflector. The original experiment was performed by E. M. Bohn et al. and involved the calculation of important reactor characteristics. Of these reactor characteristics, the core averaged k_{inf} eigenvalues, as independently calculated by Argonne National Laboratory and General Atomic personnel, were used to compare to the same values obtained by modern neutronics codes. One of these modern codes was the Monte Carlo code Serpent, and the other was the deterministic code MC^2-3. Additionally, the NEAMS Workbench, a program designed by ANL with the expressed purpose of providing a method of integrating multiple ARC codes into one efficient interface, also modelled the ZPR-9 experimental reactor. Though the NEAMS Workbench uses the MC^2-3 code to evaluate the system, the Workbench was included in order to demonstrate its ability to model the ZPR-9 system. Table 4 below displays the k_{inf} eigenvalues that each program generated.

Table 4: ZPR-9 Calculated k_{inf} Eigenvalues

	K_{inf}	Δk_∞ from Serpent (pcm)
ANL	1.5808	13374
GA	1.5533	10624
Serpent	1.44706	-
MC^2-3	1.44972	266
NEAMS Workbench	1.44972	266

As Table 4 shows, the ANL and GA eigenvalue calculations disagree with the modern Serpent eigenvalue by several orders of magnitude of pcm. This is a significant difference that could indicate that the modern simulation techniques of Serpent and MC^2-3 are invalid for this type of GFR system. Alternatively, this difference could be the result of significant assumptions and simplifications that were involved with the simulation process. By neglecting both the reactor blanket and reflector regions, as well as simplifying the geometry to that of an infinite system, it is reasonable to assume that significant errors were introduced into the eigenvalue calculations. This would make the comparison of the simulation eigenvalues to the experimental eigenvalues invalid. Table 4 also shows the agreement between the Serpent and MC^2-3 models, which was notably better. Because Serpent has been shown in previous experiments to be capable of modelling GFR systems with a reasonable degree of accuracy, the agreement between Serpent and MC^2-3 indicates that, for a GFR system approximated by the assumptions and simplifications performed within this project, MC^2-3 can also provide a reasonably accurate analysis. This conclusion is also supported by the excellent agreement shown between the neutron spectra for both Serpent and MC^2-3. Figure 13 shows the normalized neutron flux distribution as a function of energy for the ANL 2082 group structure.

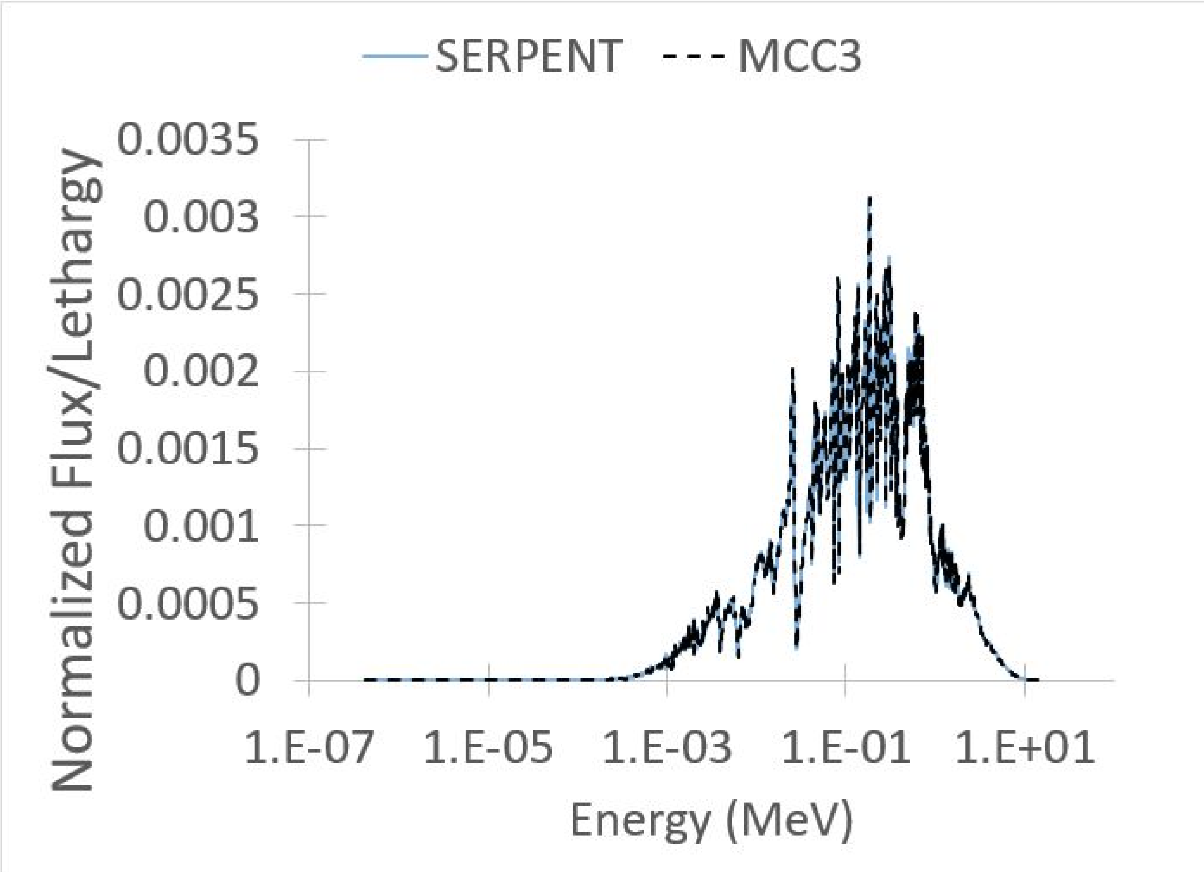

Figure 12: Neutron Flux Spectra for Serpent and MC2-3 Simulations

From Figure 12 it can be seen that the neutron flux spectra are in very close agreement. The Serpent and MC^2-3 normalized flux spectra are virtually indistinguishable from one another.

The second goal set for this project was to demonstrate the NEAMS Workbench as a viable alternative for performing GFR analysis. Because the Workbench relies upon MC^2-3 for cross section generation, just through an alternative user interface, it can only be a viable alternative in a situation where MC^2-3 is valid. In order for the Workbench to be used, both it and MC^2-3 must produce similar outputs for a similar reactor system. As can be seen from Table 4, for the ZPR-9 reactor, the difference in eigenvalue calculation was 0 pcm. This allows for the conclusion that the Workbench is a viable alternative to using MC^2-3 alone for multigroup cross section generation in a reactor of size and configuration similar to the ZPR-9 assembly. The additional ARC codes packaged with the NEAMS Workbench may have to be verified independently before the full suite of codes can be integrated together, but this research supports verification of the NEAMS Workbench as an alternative source for MC^2-3 cross section generation.

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