U. S. DOE Nuclear Energy Research Initiative

**A Proliferation Resistant Hexagonal Tight Lattice BWR
Fueled Core for Increased Burnup and
Reduced Fuel Storage Requirements**

**Annual Progress Report:
August, 1999 to July, 2000**

Principal Investigators:

Hiroshi Takahashi Upendra Rohatgi

*Brookhaven National Laboratory
Building 475B
Upton, New York 11973*

T. J. Downar
*Purdue University
School of Nuclear Engineering
West Lafayette, IN 47906-1290*

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CONTENTS

EXECUTIVE SUMMARY	3
1.0 Introduction	4
1.1 <i>Project Overview</i>	4
1.2 <i>Background</i>	4
1.3 <i>Project Milestones: Year One</i>	6
2.0 Code Acquisition and Benchmarking	6
2.1 <i>Monte Carlo Burnup Code: MCBURN</i>	7
2.2 <i>Collision Probability Lattice Physics Code: HELIOS</i>	7
2.3 <i>Comparison of Monte Carlo and CP Methods for Tight Pitch Lattice</i>	9
3.0 Neutronics Design and Analysis	
3.1 <i>Basic Neutronics Studies of Uranium and Thorium Fuel</i>	13
3.1.1 <i>Nuclear Properties of Uranium and Thorium</i>	13
3.1.2 <i>Comparison of Uranium and Thorium Burnup Performance</i>	16
3.1.3 <i>Comparison of the Nuclear Properties Using the Equivalence Concept</i>	22
3.1.4 <i>Comparison of the Proliferation Resistance of Uranium and Thorium</i>	24
3.2 <i>Preliminary HCBWR Core Design Specifications</i>	25
3.3 <i>Monte Carlo Burnup Benchmark Model of the HCR</i>	33
4.0 Thermal-Hydraulics Design and Analysis	
4.1 <i>Preliminary Thermal-Hydraulics Design Calculations</i>	39
4.2 <i>Constitutive Relations for Tight Lattice Core</i>	43
4.3 <i>Coupled Neutronics / TH Subchannel Method</i>	45
5.0 Progress on Future Scheduled Milestones	
5.1 <i>Hexagonal Nodal Capability in the PARCS Code</i>	47
5.2 <i>Continuing Work</i>	48
6.0 References	49
 APPENDICES	
A <i>Paper Presented at PHYSOR-2000 Reactor Physics Meeting</i>	52
B <i>Paper Accepted for Presentation at the 2000 ANS Winter Meeting</i>	59
C <i>Paper Accepted for Presentation at the 2000 ANS Winter Meeting</i>	64
D <i>Paper Accepted for Presentation at the 2000 ANS Winter Meeting</i>	69

EXECUTIVE SUMMARY

The objective of this research is to design and analyze a proliferation resistant, economically competitive, high conversion, boiling water reactor (HCBWR) fueled with fissile plutonium and fertile thorium oxide fuel elements. The extensive previous research on high conversion LWRs in the U.S., Europe, and Japan over the last several years provided a useful starting point for the design developed here. The HCBWR developed here is characterized by a very tight lattice with a relatively small water volume fraction and operates with a fast reactor neutron spectrum. A design objective has been to achieve a high conversion of thorium to ^{233}U and to reduce the national accumulated inventory of plutonium, as well as to take advantage of the enhanced proliferation resistance of the thorium fuel cycle. The high burnups achievable with thorium fuel in a high conversion core will increase the plant operating factor and lower the cost of electricity. One of the concerns with a tight lattice core with a hard neutron spectrum is the potential for a positive void coefficient. Design features are being used in the HCBWR core design to insure inherent negative reactivity feedbacks to enhance core safety performance. All of these advantages are consistent with the Department of Energy's objectives for the development of Generation IV nuclear power systems and proliferation resistant fuel cycles.

Our 3-year R&D program is structured around specific task areas designed as a proof-of-principle demonstration of this reactor design. This report documents research performed during the first year of this program from August, 1999 to July, 2000 and focuses on the eight specific milestones which were reported to DOE for the first year activity. The code acquisition and benchmarking work has been completed. Both stochastic and deterministic analysis codes are being used in the work. The BNL Monte Carlo burnup code MCBURN has been benchmarked for high conversion lattices. The collision probability lattice code HELIOS was purchased from Studsvik/Scandpower and also was benchmarked for thorium depletion with hexagonal lattices. A basic neutronics study was performed comparing the performance of thorium and uranium fuels in both standard LWR and high conversion lattices. The preliminary design of the HCBWR fuel pin and fuel lattice was then completed using HELIOS and MCNP. Initial results show very favorable fuel burnup performance as well as good safety characteristics. The void coefficient was negative for all cases examined with thorium/plutonium fuel. Preliminary thermal-hydraulics analysis was also performed for the tight pitch channel using the RELAP5 code. Preliminary results are encouraging but there are concerns about the adequacy of constitutive relationships for the tight lattice cores. Work has progressed on schedule and some of the tasks on the second year have been initiated during the first year in order to facilitate the analysis. Specifically, the development of a hexagonal lattice capability in the nodal code PARCS was begun in the fourth quarter so that core burnup studies and core safety analysis could be started at the beginning of the second year. At this time there are no changes anticipated to the work scope and there are no foreseeable obstacles to meeting the scheduled milestones for this project.

1.0 Introduction

1.1 Project Overview

The overarching objective of this project is to advance the well-developed water-cooled reactor technology in order to make efficient use of the abundant thorium resources and enhance the proliferation resistance of the nuclear fuel cycle. Considerable effort has been invested in development of the sodium cooled fast reactor to breed fissionable ^{239}Pu from natural uranium. Much less effort has been expended into development of technologies that take advantage of the considerable experience with light water reactors as an alternative to the fast reactor for providing a hard neutron spectrum to convert thorium into the fissile U^{233} isotope.

This project investigates the feasibility of a plutonium-thorium (Pu-Th) fuel cycle for a new type of high conversion reactor cooled by boiling water (HCBWR). The technology will be developed to burn existing stocks of plutonium, while converting the fertile thorium to fissile ^{233}U . The high conversion will take place in a fast neutron spectrum produced by minimizing the volume of water in very tight fuel assembly lattices. High fuel burnup will be possible as a result of the continuous generation and fission of ^{233}U as the plutonium is consumed. Inherent safety will be designed into the reactor because of the favorable feedback neutronics characteristics of thorium and by the use of innovative core heterogeneities. This will insure a negative void coefficient for those accident sequences which result in off-normal coolant boiling.

The major technical objective of the proposed project is to develop a reactor design which will:

- (1) minimize the potential for proliferation of weapons grade materials,
- (2) maximize the inherent safety features of the reactor,
- (3) maximize the achievable fuel burn up and plant capacity factor,
- (4) minimize the cost of electricity generation.

1.2 Background

The Light Water Reactor with a hard neutron energy spectrum has been studied in the past, both in the US (EPRI) and in Europe (PSI). More recently, there has been considerable interest in the Japanese nuclear industry and research organizations. As background for the research here we evaluated several of the reactor designs proposed by the Japanese industry (Hitachi, Toshiba, Mitsubishi) and research institutes (JAERI, JAP). These designs included:

1. *High conversion BWR (HCBWR),*
2. *Long burn up cycle BWR (LBBWR)*
3. *BWR without blanket (BWRNB)*
4. *High conversion PWR (HCPWR),*
5. *PWR with Pu multi-cycle (PWRPM);*

The detailed analysis of high conversion cores have been carried out in Japan over the last two years under the auspices of a Japanese consortium and the results were published in the JAERI report 99-058. The general conclusions were that in order to achieve high burn up, a reactor with a hard neutron energy spectrum is required. A tight lattice BWR core can provide the hard neutron energy spectrum, however, the coolant void coefficient tended to be positive. The analysis showed that a negative void coefficient could be achieved by enhancing neutron leakage during coolant heat up.

The HCBWR proposed by the Hitachi company is a reactor with a pan-cake type flat core similar to the Na cooled fast reactor. The long burn up cycle BWR (LBBWR) proposed by Toshiba company utilized a core with neutron streaming channels to enhance the neutron leakage. The HCBWR core height is relatively small and the linear power density is high, so that heat removal becomes more severe than the LBBWR type reactor. By using a neutron streaming void tube, the core height can be higher than the HCBWR core height, thereby reducing the linear power density. The pressure water reactor proposed by Mitsubishi Company uses heavy water as coolant which hardens the neutron spectrum even though it uses a wider coolant channel than the H₂O cooled LWR. This mitigates the difficulty of heat removal encountered in the H₂O cooled RMWR.

From the preliminary analysis of the above reactors, we selected the LBBWR (RMWR) type reactor for our initial design study in the NERI program. Because nonproliferation is one of the key factors in the NERI program, we will use thorium as fertile material instead of the U-238 which is used in the Japanese study. The use of thorium as the fertile material can also eliminate fissile Plutonium more efficiently. Furthermore, the thorium fuel cycle does not accumulate a significant inventory of minor actinides which have very long half lives and does not exacerbate the high level waste disposal problem. A paper summarizing some of these findings as well as introducing some of the neutronics methods used for analyzing high conversion reactors was presented at the International Reactor Physics Meeting, PHYSOR-2000, in the Spring of last year and is included as Appendix A of this report.

1.3 Project Milestones: Year 1

The milestones presented to DOE for year one were as follows:

- 1) *Conceptual Design of the Reactor and Specifications of Parameters (BNL/Purdue)*
- 2) *Acquisition of CPM-03 Lattice Physics Code (Purdue)*
- 3) *Scoping study for core design with Monte Carlo burnup analysis (BNL)*
- 4) *Scoping fuel assembly lattice neutronics design (Purdue)*
- 5) *Comparison of Monte Carlo and analytic methods (BNL/Purdue)*
- 6) *Scoping thermal-hydraulics analysis (BNL)*
- 7) *Assessment of applicability of constitutive relationships of RELAP5 and RAMONA-4B code for tight lattice core (BNL)*
- 8) *Preparation of the annual report*

Progress on each of these milestones will be addressed in the following sections. In order to enhance the presentation of the report, the milestones will be presented in the following sequence:

2. **Code Acquisition and Benchmarking** (Milestones 2 and 5)
3. **Neutronics Design and Analysis** (Milestones 1, 3, and 4)
4. **Thermal-Hydraulics Design and Analysis** (Milestones 6 and 7)
5. **Preliminary Work on Future Milestones** (Milestone 4 from Year 2)

Progress on Individual Milestones for the First Year

2.0 Code Acquisition and Benchmarking

The neutronics analysis of complex reactor cores such as the high conversion BWR required both stochastic Monte Carlo methods and deterministic methods for solving the Boltzmann Transport equation. The intercomparison of results from the two methods will provide confidence in the predicted core neutronics behavior. This

section will describe activities during the first year in the acquisition and benchmarking of the codes used in this research.

2.1 Monte Carlo Burnup Code: *MCBURN*

The strongly anisotropic characteristics of highly voided regions such as those encountered in the HCBWR motivate the use of Monte Carlo methods. This is particularly important for the calculation of the void coefficients which is one of the most important safety parameters in the core. The Monte Carlo burn-up code (*MCBURN*) was developed at BNL for analysis of the accelerator driven reactor, but it has also been used successfully for analyzing reactors with hard neutron energy spectra. The nuclide depletion characteristics in *MCBURN* are calculated with the *ORIGEN-II* burnup code.

The computing time for Monte Carlo calculations can be substantial. As an example, the computer time required for whole core analysis using 20000 particles sampling is about 1-2 hours for each burn up time step. The *k* values can be obtained with a statistical variance of about 0.3 % which is adequate for many design studies. The *ORIGEN-II* depletion module requires one group cross sections for the decay chain calculation. The reaction cross sections for most isotopes involved in the thorium decay chain are obtained with reasonable accuracy from the tally data created with this sampling size. For performing design parametrics, a single cell calculation is usually adequate and requires a computing time about 5 times shorter than the whole core calculation. Monte Carlo results for pin cells will be compared to the collision probability method in the next two sections. Results for application of *MCBURN* to the HCBWR were presented at the *PHYSOR-2000* Reactor Physics conference this past spring and is included as Appendix A of this report.

2.2 Collision Probability Lattice Physics Code: *HELIOS*

The initial phase of the code acquisition and benchmarking was devoted to assessing the various lattice physics codes that were available for analyzing thorium fuel in general geometries. For puposes of assessing the performance of LWR lattice codes for thorium fuel applications a benchmark problem was proposed by MIT and is shown in Fig. 1.

Dimensions:

pin radius = 0.4114 cm
clad radius = 0.4712 cm
coolant radius = 0.6350 cm

Fuel Composition (w/o):

Th232=65.909
U-235=4.291; U-238=17.740
O-16=12.026

Pressure = 2250 psi

Fuel Average Temperature = 868°C

Linear Heat Rate = 167.6 W/cm

Figure 1. MIT Thorium Pin Cell Benchmark Problem

A comparison of the k -inf versus burnup results of CASMO-IV [Edenius, 1996], HELIOS [Stammeler, 1995], and two versions of MCNP [MCNP, 1998] are shown in Figure 2 for the pin cell benchmark. Very good agreement was achieved between the deterministic and stochastic predictions of the pin cell burnup performance.

Figure 2. K -inf versus Burnup for MIT Thorium Benchmark Problem

Because CASMO-IV and HELIOS are commercial codes and would require a formal purchase agreement with Studsvik/Scandpower, it was decided to investigate the use of a third lattice physics code, CPM-03 [Jones, 1996], which was available for free because of a pre-existing educational license agreement with EPRI [Agee, 1998]. It was discovered that although the thorium chain cross sections were available in CPM-03, the depletion chain for thorium was not included in CPM-03 and was added to the code. The pin cell problem shown in Fig. 1 was then performed with CPM-03 and large discrepancies compared to CASMO-IV and MCNP were observed (1000 pcm) for the first burnup point. A detailed investigation revealed that CPM-03 did not account for the resonance interference effects between Thorium and Uranium isotopes in the Thorium cross section library. An initial effort was made to reprocess the Thorium ENDF-VI cross section data with the NJOY code in order to add the resonance interference effects to CPM-03. It was then determined that the coding effort necessary to add the resonance interference parameters to the CPM-03 was going to be extensive.

It was then decided to purchase the commercial lattice physics code HELIOS [Stammler, 1995] from Studsvik/Scandpower because of its ability to treat generalized geometry. The results for HELIOS shown in Fig. 2 were included in a thorium neutronics benchmark paper co-authored with MIT and INEEL that was accepted for presentation at the winter ANS meeting. The paper is included as Appendix B of this report.

2.3 Comparison of Monte Carlo and CP Methods for Tight Lattice Cores

The HELIOS code was then benchmarked for the hard spectrum of a very tight lattice by comparing results to the MCNP depletion code. A tight lattice pin cell benchmark problem was developed for this purpose as shown below.

Thorium Pin Cell in Tight Lattice Core of BWR

(a) Geometry

Fuel Radius=0.5555 cm
 Clad Radius=0.5955 cm
 Moderator Pitch=1.35872 cm

(b) Material Composition

Material	Case	Temperature (K)	density (g/cc)	Isotope	Number Density($10^{24}/\text{cm}^3$)
Fuel	Weapon grade Pu	900	~10	Th-232	1.9259E-02
				Pu-239	1.9595E-03
				Pu-240	1.2455E-04
				O-16	4.2686683E-02
	U235			Th-232	2.0000E-02
				U-235	2.4000E-03
				O-16	4.4800E-02
Clad		620	6.505	Zr-2	4.29421E-02
Moderator		560	0.46432	H-1	3.10460E-02
				O-16	1.55253E-02

The benchmark problem was then analyzed with both the HELIOS and the MCNP depletion code MCNAP. The results are shown below for both the isotopics and for the k-inf.

HELIOS [Stammeler, 1995] is a multigroup two-dimensional collision probability method transport code for fuel or fuel assembly depletion analysis of thermal reactors. Because the neutron spectrum in the thorium fuel pin cell of tight lattice core is very different from a thermal reactor spectrum and almost like a fast reactor spectrum, the HELIOS prediction on the k-inf of thorium fuel cell was verified against the more reliable Monte Carlo depletion analysis codes.

MCNAP [Kim, 1999] is a continuous energy Monte Carlo code developed exclusively for neutronics analysis of multiplying systems such as a fuel pin, a fuel assembly, or a power reactor, etc. The program is capable of depletion analysis in which all the fuel and fission product isotopes are explicitly modeled like the ORIGEN code. The qualification of the MCNAP has been established through verification computations against fast and thermal integral experiments, k-effective, and pin power measurements of uranium and plutonium bearing VENUS cores. Additionally, the design analysis of fuel assemblies and the cores of the ABB-CE PWR plant built in Korea was performed using MCNAP.

Two types of thorium fuel pin cells were analyzed in this benchmark; one utilizing weapons grade plutonium fissile and the other using U-235 fissile. The MCNAP results are obtained by sampling a total of 300,000 particle histories on 100 cycles with 3,000 particle histories per cycle. The standard deviation of the k -inf is within 100 pcm. The continuous energy cross sections and their temperature dependence were obtained from ENDF/B IV version 3 using the NJOY code. The HELIOS results are obtained using 190 groups and resonance default option for thorium. It is shown that MCNAP generally overpredicts the k -inf in comparison with HELIOS. Nonetheless, two predictions on the k -inf versus burnup agree very well with each other. Figure 3 depicts discrepancies between two calculations and Figure 4 shows a comparison of HELIOS and MCNAP calculations for k -infinity versus burnup. Discrepancies are within 500 pcm for the thorium/plutonium pin cell and within 200 pcm for the thorium/U-235 pin cell over most of the burnup range beyond 100 MwD/KgHM. Considering that discrepancies such as shown in Figure 3 are often observed in the k -inf predictions with deterministic codes, the HELIOS code can be considered adequate for the thorium in tight pitch lattices. It is also worthwhile to note that the thorium fuel pin cell studies for PWR applications by deterministic codes such as CASMO-4 and the Monte Carlo depletion codes such as MOCUP show discrepancies of a similar order of the magnitude.

Figure 3. Difference of K_{inf} predictions by HELIOS and MCNAP.

Figure 4. Comparison of HELIOS and MCNAP predictions on k_{inf} versus burnup

(a) Thorium/Plutonium pin cell

(b) Thorium/U-235 pin cell

3.0 Neutronics Design and Analysis

As noted in the first section, the Japanese RMWR (Reduced Moderator Water Reactor) design was chosen for preliminary design analysis in the work here. It is important to note this core was used for preliminary design only. The RMWR core was fueled with U-238 fertile material, whereas the core designed here utilizes Th-232 fertile material which results in enhanced neutronics and safety performance of the core, as will be shown in subsequent sections.

3.1 Basic Neutronics Studies of Uranium and Thorium Fuel

Prior to initiating the HCBWR design, a basic neutronics study was performed to provide a consistent comparison of the neutronics characteristics of thorium and uranium fuels. This was determined to be important for affirming the fundamental advantages for the thorium fuel cycle. A paper reporting the results of this study were accepted for presentation at the ANS 2000 Winter Meeting and is included as Appendix C of this report.

3.1.1 Nuclear Properties of Thorium and Uranium

There are major differences in the nuclear properties of Th-232 and U-238. As shown in Table 1 and Figure 5, the thermal absorption cross section of Th-232 is about 3 times larger than that of U-238, whereas the resonance absorption of Th-232 is much less than

that of U-238. Both isotopes are fissionable above their respective fission threshold energy, however the fission threshold of Th-232 is higher than that of U-238, e.g., 1.4 Mev for Th-232 and roughly 1 Mev for U-238. At high energies, the fission cross section of Th-232 (200mb) is roughly one order less than that of U-238 (2 barns). Thus the fast fission effect of Th-232 will be much smaller than that of U-238.

These differences in nuclear properties of the two fertile isotopes impacts the neutronics performance of reactor cores employing these isotopes. For example, the k-infinity of the thorium fuel at the beginning of life is much less than that of U-238 fuel because of the larger thermal absorption of Th-232 compared to U-238. Because of the negligible fast fission contribution of Th-232 compared to U-238, the multiplication factor of Th-232 based fuel tends to be smaller than that of comparable U-238 fuels in fast reactor applications.

One of the most important impacts of the differences in the nuclear properties of Th-232 and U-238 is seen in the void reactivity feedback of a tight pitch lattice. As the coolant voids and the neutron spectrum becomes extremely hard (cf. Figure 12), the resonance absorption of U-238 decreases while its fast fission contribution increases. These combined effects lead to an increase in the multiplication factor, which is in turn responsible for the positive void coefficient in the tight lattice BWR core fueled with U-238. In contrast, the smaller fast fission effect and smaller resonance absorption of Th-232 leads to a decrease in the multiplication factor after voiding. This is very important from a safety standpoint since it is desirable that the core exhibit a negative void coefficient under all operating conditions.

The fissile isotopes bred from Th-232 and U-238, U-233 and Pu-239, respectively, also possess different nuclear properties. The U-233 has a larger ratio of σ_f/σ_a than any other fissile isotopes (cf. Table 2). Also, U-233 has a larger η value at thermal and epithermal energies than any other isotope. Because of this, U-233 is regarded as the best candidate fuel for a thermal breeder reactor. Conversely, Pu-239 has the lowest ratio of σ_f/σ_a and because it has a larger thermal absorption cross section, the Pu-239 fueled thermal reactor has a harder spectrum and also requires a greater fissile content in order to achieve the same initial core multiplication factor. The η value of Pu-239 increases at energies above 30 kev. Therefore, a Pu-239 fueled core has a tendency to have a more positive void reactivity coefficient in both thermal and fast reactors when compared to any other fissile isotopes.

Table 1. Summary of Nuclear Data for Natural Thorium and Uranium

	Thorium		Uranium		
	Th232	Th230	U238	U235	U234
Abundance	100 %	0 %	99.27%	0.72%	0.0057%
σ_a at thermal	7.4	23.2	2.7	680.8	100.2
σ_f at thermal	-	0.0012	2.7	582.2	0.6
RI at thermal	84.35		278.1	133.0	

Half life (yr)	1.4E10		4.46E09	7.03E08	-
Amount of RE	~ 12 ppm		~ 4 ppm

Figure 5. Absorption and fission Cross Sections of Th232 and U238

Table 2. Comparison of Nuclear Properties of Fissile Isotopes

		U ²³³	U ²³⁵	Pu ²³⁹
Capture XS	Thermal	54	100	267
	Resonance	140	144	200
	Fast	0.3	0.5	0.6
Fission XS	Thermal	527	579	741
	Resonance	764	275	301
	Fast	2.8	2.0	1.9
ν	Thermal	2.5	2.4	2.9
	Fast	2.5	2.5	2.9
η	Thermal	2.27	2.04	2.12
	Resonance	2.11	1.56	1.74
	Fast	2.26	2.0	2.2
σ_f/σ_c	Thermal	9.75	5.79	2.78
	Fast	9.33	4.0	3.17

3.1.2 Comparison of Thorium and Uranium Burnup Performance

In order to provide a consistent comparison of the burnup performance of thorium and uranium fuels the fuel types and fuel compositions shown in Table 3 were analyzed in both standard BWR and a high conversion BWR lattice. The fuel assembly designs are shown in Figures 6, 7, and 8 for the 8x8, 9x9, 10x10 BWR design and in Figure 9 for the tight lattice HCBWR fuel design. All calculations were performed using the collision probability code HELIOS for which satisfactory benchmarking results were shown in the previous section. In order to provide a consistent comparison of thorium in the existing BWR lattices, the fuel composition in the current 8x8, 9x9, and 10x10 BWR fuels was modified with an equivalently enriched thorium fuel. For example, $(\text{Th}+\text{U}^{235})\text{O}_2$, $(\text{U}^{238}+\text{Pu}^{239})\text{O}_2$, $(\text{Th}+\text{Pu}^{239})\text{O}_2$ were simply substituted for the existing UO_2 fuel. The fuel pin pitch of the high conversion BWR (HCBWR) was reduced in order to achieve a small moderator to fuel volume ratio.

Table 3. Summary of the BWR Fuel Pins Used in the Analysis

Fuel Type	8x8 ¹⁾	9x9 ¹⁾	10x10 ²⁾	HCBWR ³⁾
Power Density (W/g HM)	25.9	25.9	25.0	22.8
Pin pitch (cm)	1.6256	1.4529	1.2950	1.321
Fuel pellet				
Radius (cm)	0.5137	0.45275	0.4420	0.5555
Fuel/Enrichment	UO ₂ /3.2	UO ₂ /3.37	UO ₂ /4.0	(Th-Pu)O ₂
Density(g/cm ³)	9.7146	9.7146	-	~10.0
Temperature (K)	→	→	900	900
Cladding				
Thickness (cm)	0.0889	0.0762	0.0605	0.0400
Material	Zr-2	Zr-2	Zr-4	Zr-2
Density	-	-	-	6.505
Temperature (K)	→	→	600	620
Moderator				
Material	H ₂ O	H ₂ O	H ₂ O	H ₂ O
Density	→	→	0.740	0.73617
Temperature (K)	→	→	559	560.89
V_m/V_f ⁴⁾	1.3164	1.40155	1.1141	0.5589
Fuel Composition	UO ₂ (Th+U ²³⁵)O ₂	UO ₂ (Th+U ²³⁵)O ₂ (U ²³⁸ +Pu ²³⁹)O ₂ (Th+Pu ²³⁹)O ₂	UO ₂ (Th+U ²³⁵)O ₂	(U ²³⁸ +Pu ²³⁹)O ₂ (Th+Pu ²³⁹)O ₂

- 1) "Improving BWR Operation with a 9x9 Design," Nuclear Engineering Int'l, p49 (Sept. 1985)
- 2) OECD/NEA WPPR BWR Benchmark Problem
- 3) Research on Reduced Moderation Water Reactor(RMWR), JAERI-99-058
- 4) Fuel volume has not claddings. Here the moderator to volume ratio does not consider the water gaps between fuel assemblies and water holes in the fuel assembly.

Figure 6. 8x8 BWR Fuel Assembly Modeling for HELIOS

Figure 7. 9x9 BWR Fuel Assembly Modeling for HELIOS

Figure 8. 10x0 BWR Fuel Assembly Modeling for HELIOS

Figure 9. Tight Lattice BWR Fuel Assembly Modeling for HELIOS

A comparison of the fuel depletion performance and overall neutronics performance is shown in Tables 4 and 5 for the fuel pin cell and for the fuel assembly, respectively. Figures 10, 11, 12, and 13 show the k_{∞} values and the spectrum behavior. As expected, the current BWR fuels have similar initial k_{∞} values and depletion behavior. However, the k_{∞} values of the pins and assemblies loaded with Th^{232} as the fertile material show are very different than the corresponding U^{238} fuels. The initial k_{∞} values and the rate of depletion of the Th^{232} fuels are smaller than those of U^{238} fertile fuels. This performance is a direct result of the properties of Th^{232} described in the previous section. Specifically, this is because of the large absorption cross section of Th^{232} at thermal energies and the breeding capability of U^{233} . This is advantageous from the reactivity control standpoint since Th^{232} displays inherent poison capabilities at the beginning of the depletion and acts as a fissile source at the end of depletion. These

properties of Th^{232} fuel provide benefits for extended cycle and high burnup core operation. However, since the initial k_{∞} value of Th^{232} fuel is very low, the fuel enrichment must be somewhat higher.

In the hard spectrum of the HCBWR, the initial k_{∞} values for both U and Th are smaller than those of the current BWR fuels. Both fuels deplete more slowly in the hard spectrum because the fission and capture cross sections are much smaller than those in the standard BWR lattice. Therefore, the HCBWR is very conducive to extended cycle operations. However, as shown in Table 4, $(\text{U}^{238} + \text{Pu}^{239})\text{O}_2$ has the potential for a positive void coefficient.

Table 4. Summary of the BWR Fuel Pin Calculations

Cell Calculation										
Assembly	Vrn/Vf	Fuel			K-inf			FIR	Void Coefficients	
		Fertile	Fissile	Enrichment	BOC	Critical Burnup	Slope	Critical State	BOC	Critical State
8x8-case1	1.32	U238	U235	3.2	1.32092	29.5	-976	48.7	-230.8	-232.8
8x8-case2		Th232	U235	3.2	1.15924	23.5	-560	67.6	-182.9	-122.6
9x9-case1	1.4	U238	U235	3.37	1.33295	30.5	-979	47.6	-224.5	-227.9
9x9-case2		Th232	U235	3.37	1.17932	25.5	-584	66.3	-180.6	-120.3
9x9-case3		U238	Pu239	4.72	1.31100	40.5	-688	49.1	-249.0	-246.3
9x9-case4		Th232	Pu239	4.72	1.27697	34.5	-686	57.6	-254.4	-215.2
10x10-case1	1.11	U238	U235	4	1.32249	35.5	-824	60.3	-279.4	-268.3
10x10-case2		Th232	U235	4	1.17932	33.5	-511	68.0	-201.7	-85.2
HC-case1	0.56	U238	Pu239	9.3	1.25602	66.5	-266	84.4	-58.4	16.3
HC-case2		Th232	Pu239	9.3	1.16854	60.5	-231	80.0	-162.5	-96.8
BOC = Xe/Sm Equilibrium State										
Burnup in [GWD/t]										
Slope = $100000 \cdot (k(30) - k(10)) / 20$										
FIR = Weight of Fissile at EOC / Weight of Fissile in BOC										

Table 5. Summary of the BWR Fuel Assembly Calculations

Assembly Calculation								
Assembly	Vrn/Vf	Fuel			K-inf			FIR
		Fertile	Fissile	Enrichment	BOC	Critical Burnup	Slope	Critical State
8x8-case1	~2.5	U238	U235	3.2	1.32773	21	-1349.455	53.1
8x8-case2		Th232	U235	3.2	1.137407	13	-641.355	81.3
9x9-case1	~2.5	U238	U235	3.37	1.358276	25	-1303.56	47.7
9x9-case2		Th232	U235	3.37	1.178653	17	-698.995	75.8
9x9-case3		U238	Pu239	4.2	1.40234	29	-1237.3	33.6
9x9-case4		Th232	Pu239	4.2	1.33537	21	-1189.6	57.8
10x10-case1	~2.5	U238	U235	4	1.383096	30	-1154.67	42.4
10x10-case2		Th232	U235	4	1.208627	23	-675.545	69.8
HC-case1	0.56	U238	Pu239	9.3				
HC-case2		Th232	Pu239	9.3				
BOC = Xe/Sm Equilibrium State								
Burnup in [GWD/t]								
Slope = $100000 \cdot (k(30) - k(10)) / 20$								
FIR = Weight of Fissile at EOC / Weight of Fissile in BOC

Figure 10. Comparison of k_{inf} Values of BWR Fuel Pins

Figure 11. Comparison of k_{inf} Values of BWR Fuel Assemblies

Figure 12. Comparison of the Neutron Spectra for the BWR fuel pins

Figure 13 Comparison of the Neutron spectra for the BWR fuel Assemblies

3.1.3 Comparison of the Nuclear Properties Using the Equivalence Concept

The equivalent equilibrium cycle length concept is useful to perform a consistent comparison of the burnup performance of the various fuel compositions. In the Linear Reactivity Model (LRM), the reactivity change is assumed to be linear with the fuel burnup. Therefore, the cycle length at equilibrium can be written,

$$B_{Eq} = \frac{2}{n+1} \frac{\rho_0}{A}, \quad (1)$$

where

ρ_0 = initial reactivity,

A = slope of the reactivity,

n = number of batch size.

According to Equation 1, the same cycle length can be achieved with different fuel compositions by selecting the same ratio of the initial reactivity to the slope of the reactivity for the reference pre-designed fuels,

$$\frac{\rho_0^{ref}}{A^{ref}} = \frac{\rho_0}{A}, \quad (2)$$

where

ρ_0^{ref} = initial reactivity of a reference fuel,

A^{ref} = slope of the reactivity of a reference fuel.

Here the current 9x9 UO₂ fuel can be used as the reference fuel and the equivalent ratio of initial reactivity to the slope of the reactivity can be found by trial and error. Figure 14 shows the k_{∞} values designed by the equivalent concept. All fuels were designed such that their critical cycle lengths were equal to the current 9x9 BWR fuel. Figure 15 and Table 6 shows the void coefficients and proliferation resistance properties, respectively. As shown in Figure 14, the HCBWR fuels exhibit a very good behavior for longer cycle operations. Since their initial k_{∞} value is so small, it is easy to control the initial excess reactivity without chemical shim. The longer cycle operation can be easily implemented because of the flat slope of the k_{∞} value. However, the void coefficient of the HCBWR fuels becomes worse as shown in Figure 15. However, for the reactor concepts proposed here it is important to note that the void coefficient of (Th+Pu²³⁹)O₂ fuel remains negative at all burnups.

Figure 18 RMWR High Conversion BWR Fuel Assembly

Figure 19 RMWR High Conversion BWR Void Tube Assembly

Figure 20 RMWR High Conversion BWR Fuel Pin Geometry

Figure 21 RMWR High Conversion BWR Pin Cell Caculational Model ($V_m/V_f=0.5$)

For purposes of comparison some of the key features of the RMWR are shown in Table 8 along with the corresponding values of the General Electric ABWR.

TABLE 8 Comparison of the HCBWR/RMWR with the ABWR

Item	unit	HCBWR	ABWR
Thermal Power	MW	3926	3926
Core diameter	m	5.8	5.4
Core hight	m	1.6	3.7
Blanket hight	m	0.3 (upper) 0.3 (bottom)	
No of fuel elements	No/ assembly	469	62 (8x8)
Geometry of fuel arrangement	-	Triangle (in hexagonal tube assembly)	Square lattice
Outer dimeter of fuel cladding	cm	11.9	12
Cladding thickness	mm	0.4 (SUS)	0.9 (Zr)
Fuel element pitch	mm	13.2	16
Volume ratio water to fuel	-	0.5	3
Mass weight ratio of fissile plutonium	wt%	16	

Some of the important core burnup characteristics of the HCBWR and ABWR are shown in Table 9. The calculations here were performed using the HELIOS code with the pin cells shown in Table 10. The k-inf versus burnup is shown in Figure 22.

Table 9 Main Core Characteristics

Item	unit	RMWR	ABWR
Conversion ratio		1.015	0.6
Fuel shuffling pattern	-	4 batch / 2 years operation cycle	4 batch / 1 years operation cycle
Void reactivity coefficient	10**-4dk/k/% void	-2.6	-7
Linear heat density (Initial)	w/cm	200	195

Table 10 Comparison of Burnup Characteristics on BWR and HCBWR Core.

	BWR Pin	HCBWR

Pin Pitch	1.7 cm	1.5 cm
Initial Fissile	3.0 w/o	9.6 w/o
Maximum Discharge Burnup	37 GWd/tHM (4 batches)	73 GWd/tHM (3 batches)
Moderator to Fuel Ratio	1.5 (geometric)	0.6 (geometric)

Figure 22: HCBWR Burnup Comparison

The ABWR and HCBWR neutron spectrum are compared in Figure 23.. The HCBWR has a smaller neutron flux in the thermal neutron energy region and a larger neutron flux in the fast energy region. This reduces neutron moderation and thereby enhances the conversion ratio.

Figure 23 Comparison of Neutron Spectra for ABWR and HCBWR.

3.3 Monte Carlo Burnup Benchmark Model of the HCR

The design and fuel cycle analysis of the HCR will be performed with the advanced nodal neutronics code PARCS (Purdue Advanced Reactor Core Simulator) which is currently used by the U.S. NRC for best estimate analysis of U.S. LWRs. For purposes of benchmarking the PARCS calculation, a model of the HCR was developed and analyzed with the Monte Carlo burnup code MCBURN. This is particularly important because of the high voiding expected in the HCR and the uncertainty in multigroup diffusion theory predictions of neutron transport in highly voided core regions. Because the void coefficient of the HCR is expected to be close to zero and because it is an important safety parameter, a Monte Carlo calculation is important for providing confidence in the prediction of core behavior. This is particularly important in the HCR because of uncertainties in multigroup predictions of resonance capture in hard neutron spectrum cores. Continuous energy Monte Carlo calculations such as MCBURN do not incur the approximations of multigroup theory and can provide a reference to assess the error introduced by multigroup calculations.

The burnup of the HCR core was calculated with the Monte Carlo Burn Up (MCBURN) code which was developed at BNL by combining the MCNP code and the ORIGEN code. To calculate the burn up of the fuel assembly, the core is divided radially into 3 regions, and vertically into 5 regions as shown in the Figure 24. The burn up of the fuel elements and the generation of the fission products in each of the 15 (3x 5) segmented regions is calculated in six burn-up time steps of (0, 0.2, 0.5, 1.0, 2.0, 3.0x30 GWD/ton). The neutron flux at each time-steps was calculated by the Monte Carlo method using the newly obtained concentrations of the fertile materials and fission products. In this calculation, the upper and lower sections of the reflector which are each 30 cm in length are attached to the fuel assembly with a voided streaming channel. In the MCNP model, a hexagonal-lattice structure boundary is used instead of a circular boundary to simplify the calculation. Another simplification is to neglect the burnup induced change in the density of elements in the reflector regions. This is a reasonable simplification because of the very low flux levels in the reflector.

For a benchmark model, the core was designed with both a uniform and a non-uniform Pu density. The nonuniform density helps to reduce the power peaking factor. A reactor with these two types of fuel concentration was studied: one with a uniform distribution with 15 % Pu concentration, and the other had a non uniform Pu concentration. The core of the radius is divided into 3 regions of equal volume; the center 1/3 region had 10 % Pu enrichment, the middle had 12.5%, and the outer had 15 %.

This MCBURN calculation was performed using 100 particles with 100 batches for each burn up step, except for the case of the core with a uniform Pu concentration with U-238 fertile material, where 200 particle in 100 batches was used. Due to the small number of the sampling the statistical error is rather high of 0.4-0.6 % in the k values, but it provide adequate data for conceptual design for the HCWR. More exhaustive

calculations will be performed during the next quarter of the project. Recently, the MCBURN code was extended by Dr. Cetnar and their colleagues at BNL to the CBA code which use parallel computing with clustered PCs. Due to fast processor speeds and the low cost PC cluster architectures, the sampling number can be increased significantly with the MCBURN code. This will enable us to calculate more detailed analysis with a reasonable computing time.

Core Burnup Reactivity Behavior

The change in the core burnup reactivity is summarized in Table 11 and Figure 25. The core with a non-uniform distribution of Pu (case 2) gives the lowest initial reactivity, and the change in burn-up reactivity is very small (the k values at 30 MWD/ton burn up were almost unchanged or higher than the initial value). The other core with a uniform Pu concentration (case 1) gave a higher k value than the non uniform case, but it also shows a smaller reduction in k -values as burn-up progressed. Cores were also analyzed with U-238 fertile material. Similar to the analysis of k infinity for single cell calculation, the analysis of whole reactor which takes into account the neutron leakage from a finite sized reactor demonstrated that Th-232 fertile material has superior neutronic characteristics to U-238 fertile material. Due to the small initial reactivity and the small loss of reactivity with burnup, few control rods are required to regulate burn-up reactivity, thereby lessening the risk of a control rod drop accident.

Table 11 also shows the void coefficients which are calculated from the difference between k values of the reactor with full water density and zero water density. Although the uncertainty in the calculation is high due to the small sampling number, the void coefficient is predicted to be negative for Th-232 fertile material, but positive for U-238 fertile material. However, when the Pu concentration is distributed non uniformly, the void coefficient is negative in both cases. In all cases, the core with Th-232 fertile material has a larger negative void coefficient than U-238.

The Neutron Energy Spectrum and Fission Rate

The neutron energy spectrum in regions 410 and 210 (see Figure 24) are shown in Figures 26 and 27, respectively, for core burnups of 0., 1.5, 15, 30, 60, and 60 Gwd/kg. In the cases shown here, the Pu concentration is uniform. The change in the spectral shape during the increase in burn-up is rather small because the neutron spectrum is hard, unlike a typical thermal light water reactor.

The figure also shows that the energy spectrum in the 210 region is harder than that in the central core regions of 410. This difference is due to the fact that more neutrons leak out of the outer core regions than the inner core regions. The large fluctuation seen when the neutron flux is less than 100 eV reflects the small sampling number in the calculation. However, because of the small reactivity contribution of the neutrons at this low energy, the overall nuclear characteristics are not affected.

Table 1. Performance of the HCR Predicted by Monte Carlo Burnup

	1	2	3	4
Burn-up X30MWD/ ton	Uniform Pu-concent.		Non uniform Pu-concent.	
Fertile mat.	Th-232	U-238	Th-232	U-238
0.0	1.1782/.0059	1.2815/.0049	1.0768/.0063	1.1662/.0068
0.2	1.1697/.0066	1.2577/.044	1.0550/.0063	1.1407/.0060
0.5	1.1313/.0063	1.2184/.044	1.0635/.0054	1.1267/.0059
1.0	1.1605/.0064	1.1861/.0040	1.0752/.0055	1.1170/.0058
2.0	1.1171/.0057	1.1188/.0042	1.0618/.0067	1.0501/.0058
3.0	1.0770/.0056	1.0609/.0040		1.0132/.0054
Void H2O	1.1520/.0060	1.29105/.0072	0.9584/.0042	1.1118/.0053
Dk/k /% void	-2.62	+0.955	-11.84	-5.44
No of sampling	100*100	200*100	100*100	100*100

640 (upper reflector)	640	640
10	510	330
210	710	350
410	910	370
610	110	390
810	310	540
740(lower reflector)	740	740

Figure 24 Segmentation of the Reactor Core for the MCNP Model

Figure 25 Multiplication Factor Versus Burnup for Whole Core Reactor Model

Figure 26 Neutron Energy Spectrum in Region 410 of the Reactor

Figure 27 Neutron Energy Spectrum in Region 410 of the Reactor

4.0 Preliminary Thermal Hydraulics Design

The primary safety concern when reducing the moderator to fuel ratio and when using a tightly packed lattice arrangement is to maintain adequate cooling of the core during both normal operation and accident scenarios. A preliminary thermal-hydraulics design was performed by first utilizing an existing advanced BWR model with the RELAP5 code with an assumed power profile, and then by initiating the development of a coupled neutronic/thermal-hydraulic model to provide a robust method for analyzing a HCBWR fuel channel.

Comparison to SBWR Thermal Hydraulics Design

A tight lattice BWR core has a very narrow flow channel with a hydraulic diameter less than half of the regular BWR core. This type of configuration, while reducing moderation, leads to an increase in the frictional pressure drop and a reduced coolant inventory. Maintaining safety margins during the normal operation and during hypothetical accident scenario will be a challenge.

A scoping study was initiated to establish a reactor configuration, which would lead to safe operation with both simplicity and passive safety features. The Simplified Boiling Water Reactor (SBWR) provides these characteristics and was used to initiate the design study.

In the first preliminary configuration, the tight lattice core was placed in a vessel with a chimney in a similar geometry as an SBWR to investigate whether sufficient buoyancy head could be generated to provide a recirculation flow by natural circulation to maintain the core in a coolable condition without pumps. The heights of the vessel and other internal components such as the chimney were similar to those of the GE-SBWR (600MWe/ 2000MWt), however the areas of the flow paths of the internal components except core were sized to be approximately twice of GE-SBWR as the power of the proposed reactor (3926 MWt) was about twice of a SBWR. The geometry of this configuration is summarized in Table 12.

This design was analyzed with RELAP5 for steady state operation. Figure 28 shows the nodalization diagram of the vessel for the analysis. The configuration of the vessel is similar to that of a SBWR; the major components are the downcomer, core, chimney, separator and dryer. The core consists of four parallel channels, i.e., a bypass channel, a average fuel assembly channel, a water-tube assembly channel, and a hot channel. The core is divided into 10 axial nodes to reflect the axial power distribution. The main observation from the calculations was that the natural circulation with the current size chimney as the driver was not sufficient to cool the fuel in the core because of the relatively small flow areas and large friction losses in the tight lattice core. The flow

through the heated channels was not sufficient to maintain nucleate boiling and the heat transfer mode in the upper sections of the channels turned to film boiling. In addition the flow was not stable. The predicted peak clad temperature for this design was 1600K. It was apparent that a longer chimney would be needed to generate a sufficient driving force by natural circulation to overcome the large pressure drop in the core. A parametric study, where the height of the chimney was gradually increased, showed that about a twice-long chimney would be needed to generate sufficient natural circulation to cool the core; however, the recirculation ratio (ratio of core flow to feed water flow) was still much lower than that of the SBWR, i.e., about 2.6 compared to about 7.0 of the SBWR. To achieve the same recirculation ratio as an SBWR, the chimney had to be about 8 times longer than that of SBWR. Since the neutron kinetics will be affected by the recirculation ratio, the actual recirculation ratio will be calculated in conjunction with a neutron kinetics study.

Since a chimney height in the current analysis was 9m, it would require a chimney of at least 20 m long to generate sufficient flow to cool the core. Increasing the height of the core will increase the size of vessel and the containment, which will increase of the cost of this reactor system substantially. Therefore, it was concluded that it would be impractical to generate sufficient driving force using a chimney alone.

In the second configuration, the chimney (9m) was retained and a pump was added between the lower plenum and the downcomer similar to the Advanced BWR (ABWR). The pump was sized to achieve a recirculation ratio similar to that of the ABWR, which was about 7. The flow in this case was stable and the fuel was cooled. The predicted peak temperature was 561K. It is concluded that a pump would be needed to have adequate flow in the core without substantially increasing the vessel size. While the reactor operation will not be passive, the pump will provide easy startup and better control. Furthermore, this chimney/pump design will provide an important protection by providing sufficient flow in the core to maintain the core coolable in case of loss of power (thus, loss of forced flow by pump) such as a station blackout accident. A parametric study was performed by gradually decreasing the reactor power without pumps; it showed that the chimney/pump design would generate a sufficient flow to cool the core without pumps in case of a station blackout accident up to 50 % level of power.

The thermal-hydraulic study to determine the optimal vessel design will continue; the reactor design will be further refined based on transient and accident analysis with the system codes that have constitutive relationships applicable to the tight lattice geometry.

TABLE 12 Summary of Core Specifications for Core Thermal-Hydraulics Model

Number	Item	SBWR	Tight Lattice BWR*
1	Power, MWt	2000	3926
2	Core Height, m	3.2	2.2
3	Chimney Height, m	9.1	9.1
4	Hydraulic Diameter Average Channel, cm	1.56	0.43
5	Hydraulic Diameter, peripheral channel, cm	1.56	
6	Hydraulic Diameter, Void Channel, cm		0.62
7	Flow Area Average Channels, m ²	5.74	5.04
8	Flow Area Peripheral Channels, m ²	1.62	
9	Flow Area Void Channels, m ²		1.036
10	Flow Area Bypass, m ²	5.3	2.19
11	Flow Area Downcomer, m ²	6.5	13
12	Pressure Drop Across Core, bar	1.1	3.4
13	Recirculation Flow Ratio	7.0	7.4
14	Peak Clad Temperature, K	580.	578.

* With recirculation pump

Figure 28 RELAP5 Nodalization Diagram

4.2 A Coupled Thermal-Hydraulic / Neutronics Fuel Channel Model

The preliminary design calculations described in the previous section assumed a power profile as input, whereas there is obviously a tight coupling between the power and void distribution. Therefore, the development of a coupled thermal-hydraulics/neutronics method was initiated based on the RELAP5 TH code and the HELIOS neutronics code. The collision probability code HELIOS was used to model a two-dimensional fuel channel (r-z) and an iterative procedure was developed to achieve a converged power/void profile. A simplified drift flux TH model was built into HELIOS to accelerate the convergence, however the final converged power/void model will be consistent with the six equation solution in RELAP5.

The convergence procedure is shown in Figure 29 and proceeds as follows. Initially, typical BWR power profiles were input into the drift flux code in order to obtain revised void profile information. This information was then input to HELIOS to obtain corrected power profiles. Finally, the drift flux - HELIOS iterations were further checked and validated by running the information through various RELAP5 and parametric analyses. Based on the trends and information given by RELAP5 and parametrics, the drift flux - HELIOS inputs and design parameters were changed accordingly until desired end points were achieved. Areas of investigation in the RELAP5 and parametric analyses consisted of CHF, heat flux, mass flow rate, void profile, quality, fuel centerline and clad temperatures, hydraulic diameter, delta P across the core, and thermal power output. These variables were changed until the modified loop structure yielded agreeing results and then a final RELAP analysis was done to evaluate thermal - hydraulic feasibility.

Figure 29 RELAP5/HELIOS Convergence Method

The simplified ten-node RELAP5 model used here is shown in Figure 15. This model included an infinite source at constant inlet temperature and an infinite outlet sink. In addition, the model also included both lower and upper plenum assemblies. Assembly geometry was modeled as a heated pipe with the associated hydraulic and heated diameters, wetted perimeters, wall roughness, flow areas, power, and other required flow parameters characteristic of the assembly. The model was validated using RELAP5 assembly input values shown below.

Table 13 RELAP5 Assembly Input for Coupled Code Model

Flow Area	(m ²)		0.01534
Assy. Length	(m)		1.5
Wall Roughness	(m)		4.60E-05
Delta P	(kPa)		77

Ave. Pressure	(Mpa)		6.7015
T inlet	(K)		533.1
D – hydraulic	(m)		6.08E-03
D – heated	(m)		6.08E-03
Assy. Power	(MWth)		6.94

Testing and validation of the coupled code model is currently being completed. This model will provide a useful tool for performing preliminary subchannel design and analysis. Final TH design and analysis of the core will be performed with a full three dimensional neutronics model of the core using the coupled codes RELAP5/PARCS.

4.3 Constitutive Relationships for Tight Lattice Core

Most of the widely available system codes such as RELAP5 (, RAMONA-4B, and TRAC, etc. have been developed for the current generation of reactor systems such as PWR, AP-600, BWR, ABWR and SBWR. In these reactor systems, the typical channel hydraulic diameter in the core is in the order of 1 cm. However, in the proposed tight lattice core, the hydraulic diameter is less than 0.5 cm.

The size of the channel affects the distribution of phases in the channel as well as the wall heat transfer and friction pressure drop when boiling occurs. The critical heat flux and, thus, MCPR (Minimum Critical Power Ratio) are also highly dependent on the channel gap sizes. Therefore, the boiling phenomena in the channels of the proposed core design are expected to be substantially different from those in the conventional reactor cores.

The purpose of this task is to review the existing data base and the literature to find the best possible set of constitutive relationships applicable to the tight lattice core.

We are currently reviewing an option in RELAP5, which was incorporated in the code for Oak Ridge National Laboratory Advanced Nuclear Source (ANS) applications to account for flow and heat transfer in narrow channels between fuel plates (Miller and Shumway, 1992). The Oak Ridge option includes Griffith's drift flux correlation for bubbly and slug flow regimes for estimating interfacial momentum transfer, single phase wall heat transfer based Petukhov's correlation, and critical heat flux at higher flows ($> 7500 \text{ kg/m}^2\text{-s}$) by Gambill. The other source is literature related to Savannah River Site K-Reactor Restart. Both these applications have narrow channels.

The Japanese organizations such as Kyushu University (Kuncoro et. al. 1995, Fugita et. al. 1990, Ishibashi et. al. 1969), Japanese Atomic Energy Research Institute (Kumamaru et. al. 1993), University of Tokyo (Aoki et. al., 1982) and Kyoto University (Mishima et.

al.) have performed tests for narrow channels, and the literature from these organizations are also being reviewed for applicability to the tight lattice core. Other papers which are relevant for current need are by Bao et. al. (2000) and by Chang et. al. (1983). The first paper describes the experimental results for pressure drop and heat transfer for air-water flows in narrow channel (diameter 1.95 mm). Most of the data is for horizontal channel but there are some data for vertical channels also. The second paper describes the data for critical heat flux in narrow channels (gap 0.25mm) with closed bottom. The data from this paper will provide the lowest limit for critical heat flux.

5.0 Progress on Future Scheduled Milestones

5.1 Hexagonal Nodal Capability in PARCS Code (Task 4, Year 2)

A methods development effort during the past year was focused on the development of a hexagonal nodal capability for the PARCS core simulator. This task was initiated in the first year since it became evident that the calculation of core wide parameters was going to be crucial to the neutronics design.

The PARCS code has been chosen by the US NRC for its best estimate reactor analysis and has been coupled to the NRC system thermal-hydraulics codes RELAP5 and TRAC-M. This will enable the HCBWR to be analyzed with the coupled codes.

The hexagonal nodal method developed for PARCS as part of this work is based on a polynomial flux expansion for an arbitrary number of triangular nodes within each hexagon.

$$\phi(x, y) = c_0 + a_x x + a_y y + b_x x^2 + b_u u^2 + b_p p^2 + c_x x^3 + c_u u^3 + c_p p^3$$

The 9 unknown coefficients are determined using constraints on the node average flux, the fluxes at the three corners, the surface average fluxes at three surfaces, and the flux moments:

Where,

$$\bar{\phi}_x = \frac{1}{h} \int \phi(x, y) dy$$

$$\tilde{\phi}_y = \frac{2}{h} \frac{1}{V} \iint y \phi(x, y) dy dx$$

Constraint equations can be written for the surface average currents, for the corner point net leakage, and for the flux moments. These can be combined with the nodal balance equation for the triangle which can be written as;

$$\left(80\frac{D}{h^2} + \Sigma_r\right)\bar{\phi} = \frac{1}{k} \nu \Sigma_f \bar{\phi} + 32\frac{D}{h^2}(\bar{\phi}_x + \bar{\phi}_u + \bar{\phi}_p) - \frac{16D}{3h^2}(\phi_x + \phi_u + \phi_p)$$

The resulting system of equations for the triangle can be written in matrix form as:

$$\begin{bmatrix} C_{aa} & 0 & 0 & C_{as} & C_{aj} & C_{ap} \\ 0 & C_{xx} & 0 & C_{xs} & C_{xj} & C_{xp} \\ 0 & 0 & C_{yy} & C_{ys} & 0 & C_{yp} \\ C_{sa} & C_{sx} & C_{sy} & C_{ss} & 0 & C_{sp} \\ C_{ja} & C_{jx} & 0 & 0 & C_{jj} & C_{jp} \\ 0 & C_{px} & 0 & 0 & C_{pj} & C_{pp} \end{bmatrix} \begin{bmatrix} \bar{\phi} \\ \tilde{\phi}_x \\ \tilde{\phi}_y \\ \phi_s \\ j_o \\ \phi_p \end{bmatrix} = \begin{bmatrix} \bar{q} + S_{ji} \\ \tilde{q}_x + \tilde{S}_{xji} \\ \tilde{q}_y \\ 0 \\ S_{j_o j_i} \\ S_{pj_i} \end{bmatrix}$$

This method has been implemented in the PARCS code and is currently undergoing testing for a suite of hexagonal benchmark problems. The nodal code benchmarking will be described in the annual report. Work has also been initiated on the development of a depletion capability for the PARCS code.

5.2 Continuing Work

For the last three months of the first year of the project, work will be completed on some outstanding items on the remaining tasks listed in the milestones. There are currently no obstacles or changes foreseen for the project, other than the initiation of some second year tasks during the first year which have already been noted.

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APPENDIX A

Paper Presented at PHYSOR-2000 Reactor Physics Meeting

COOLANT OPTIONS FOR A WATER-COOLED REACTOR WITH A HARD NEUTRON SPECTRUM

H. Takahashi, J. Zhang, D. Cokinos, U. Rohatgi
Brookhaven National Laboratory
Upton, New York. 11973

takahash@bnl.gov ; zhang@bnl.gov, cokinos@bnl.gov ; rohatgi@bnl.gov

T. Downar
Purdue University
School of Nuclear Engineering
West Lafayette, IN 47907-1290

ABSTRACT

A thorium-plutonium-fueled, water-cooled reactor with hard neutron spectrum has been analyzed by using the Monte Carlo (MC) burn-up code MCBURN developed at BNL. Preliminary analyses have shown that thorium fertile fuel has better neutronics characteristics than U-238. Reasonable computer time is required to analyze, by the MC method, a whole reactor consisting of many lattice cells. It is demonstrated that the MCBURN code can be a useful tool for a reactor with a complicated geometry. The application of the MC method to RELAP and PARCS code systems to analyze the kinetic behavior in the case of an accident is discussed.

1. INTRODUCTION

A proliferation-resistant, hexagonal, tight-lattice BWR fuel core is proposed as part of the Nuclear Energy Research Initiative (NERI) program [1]. Basic objectives of this program include non-proliferation, advancement of nuclear technology, and the maintenance of the computational tools and scientific and engineering talent required for the future of nuclear engineering. Our objective is to advance the well-established technology of the water-cooled reactor to develop a design for a proliferation resistant, economically competitive, high burnup boiling water reactor (HBBWR), fueled with fissile plutonium and fertile thorium-oxide fuel elements. The proposed HBBWR has a very tight lattice with a relatively small water-volume fraction, and a fast-reactor neutron spectrum. Design goals are to achieve a high conversion of thorium to U-233, and reduce the accumulated national inventory of plutonium while producing useful energy. Through a combination of high concentration of plutonium and a large rate of production of U-233, the tight-lattice core can achieve high fuel burn-up. The consequent reduction in the required fuel reshuffling will increase the plant's operating factor and lower the cost of electricity.

2. CORE CONFIGURATION

To safely operate a light water cooled reactor with a hard neutron energy spectrum [2,3,4], prone to positive void coefficient, the incorporation of a neutron-leaky core, similar to that in the Na-cooled fast reactor, was proposed. One such type of reactor, has a very flat core. Another type consists of fuel assemblies with and without void channels through which neutrons can stream out when there is extensive boiling of the coolant. Thus, the increase in reactivity due to hardening of the neutron-energy spectrum can be reduced by neutron leakage. To get a high powered LWR, the pancake-type flat core must have a large diameter relative to its height. This requirement results in the need for a thick pressure vessel with a large radius.

Neutronic characteristics for various fuel and coolant options for a hexagonal tight lattice using light water as coolant and their corresponding initial k-inf values and neutron energy spectra have been calculated by the Monte Carlo method. Tables 1A and 1B list the fuel rod assembly characteristics and neutronic characteristics, respectively. Table 1B shows that the nitride fuel has higher multiplication rates than the oxide fuel due to its higher density.

TABLE 1A
FUEL ROD ASSEMBLY GEOMETRY - HEXAGONAL LATTICE

Fissile and fertile fuel	PuN-ThN	PuO ₂ -ThO ₂
Fissile enrichment (cm)	10%	10% and 20%
Fuel rod diameter(cm)	0.7068	0.484
Gap (cm)	0.02	0.02
Clad (cm)	0.046	0.046
Pitch (cm)	0.572	1.1945
Hexagonal can width (cm)	0.3	0.3
Distance between rod and can(cm)	0.061	0.061
No. of fuel rods in assembly	61	231
Density of H ₂ O (gr/cc)	0., 0.3, 1.0, 3.0	0., 0.3,

TABLE 1B

NEUTRONICS CHARACTERISTICS OF PuN-ThN, PuN-UN, PuO₂-ThO₂ FUEL ASSEMBLIES

Case	Fuel Fissile, Fertile, fissile %	Coolant density (gr/cc)	k-inf	Number weighted energy	Flux weighted energy	Capture in Th or U	Fission in Th or U
1	PuN,ThN 10%	H ₂ O 1.0	1.4611	2.2720e-2	9.2262e-1	8.2369e-2	3.053e-3
2	PuN,ThN,10%	H ₂ O 0.3	1.6679	5.6494e-2	7.8791e-1	1.0322e-1	4.856e-3
3	PuN,UN,10%	H ₂ O 0.3	1.2583	3.0613e-2	7.245e-1	2.2430e-1	3.8939e-2
4	PuN, ThN,10%	H ₂ O 0.0	2.1489	2.6506e-1	6.1005e-1	9.7822e-2	6.7340e-3
5	PuN,ThN,10%	H ₂ O 3.0	1.3398	9.9413e-3	9.9788e-1	5.7222e-2	1.4736e-3
6	PuO ₂ ,ThO ₂ ,10%	H ₂ O 0.3	0.9310	1.7809e-2	6.7822e-1	3.0573e-1	1.1077e-2

7	PuO ₂ ,ThO ₂ ,20%	H ₂ O 0.3	1.2067	2.9658e-2	7.3128e-1	2.3174e-1	9.8173e-3
8	PuO ₂ ,ThO ₂ ,20%	D ₂ O .33	1.1451	6.1732e-2	4.6313e-1	3.4269e-1	9.9600e-3
9	PuO ₂ ,ThO ₂ ,20%	H ₂ O 0.0	1.3446	1.4584e-1	4.7803e-1	3.3497e-1	1.3365e-2

3. D₂O COOLED REACTOR

A tight lattice limits the ability to remove heat, thus jeopardizing operation. A hard neutron spectrum can also be achieved by using D₂O coolant that has a lower slowing-down power for neutrons than H₂O coolant. Thus, a higher amount of heavy water coolant than light water can be used for heat removal.

To remove heat from the tight lattice, a high pressure pump is needed and this arrangement might incur difficulties in removing heat during an accident. A D₂O-cooled pressurized water reactor might possibly offer a harder neutron-energy spectrum without using a tight lattice.

Figure 1 shows the neutron energy spectra for the fuel assemblies listed as cases 1 through 9 in Table 1B. We note that the neutron flux of the D₂O-cooled reactor is negligibly small in the low-energy region of 20 eV. By contrast, the neutron flux in the H₂O-cooled reactor in this energy range is still substantial.

Figure 1. Neutron Energy Spectra of Various Fuel Assemblies

4. CORE BURNUP WITHOUT VOID CHANNEL

Table 2 shows the change of the multiplication factor as a function of burnup for the reactor whose dimensions are tabulated in the second type core without void channel (Table 3). This

figure shows that the thorium fertile fuel needs a higher Pu-239 fissile content than the Pu-239 content in the U-238 fertile fuel due to the larger neutron capture cross-section. In the burnup region from 0 to ~50 MWD/ton, the reactivity increases with burnup. After this burn-up level, k_{inf} decreases rather rapidly. In the case of the U-238 fertile material, k_{inf} decreases monotonically as the burn-up increases. Neutron capture by control rods is required for criticality control. This requirement, however, worsens the burn up characteristics of the U-238 fertile fuel.

TABLE 2
K-INF AS FUNCTION OF THE BURN UP FOR THE REACTOR

Burn Up in Units of 30MWD/ton	qqq11 U238 O2 H2O 0.3 gr/cc (1000, 50)*	Qqq16 U-238 O2 H2O 0.3 gr/cc (200,35)*	qqq14 Th O2 H2O 0.3 gr/cc (200, 35)*
0	1.1495 0.0031	1.1777 0.0068	1.0096 0.0067
0.2	1.1183 0.0031	1.1357 0.0069	1.0533 0.0062
0.5	1.0756 0.0029	1.0810 0.0073	1.0607 0.0064
1.0	1.0048 0.0030	1.0177 0.0072	1.0022 0.0064
2.0	0.8654 0.0025	0.8751 0.0053	0.8583 0.0052
3.0	0.7221 0.0021	0.7210 0.0047	0.6856 0.0042
4.0	0.5233 0.0014	0.5221 0.0033	0.4795 0.0032

* No. of sampling for initial neutrons source (No. of particle , No of Batches)

The use of thorium does not create Np-237 or the other minor actinides created when U-238 fertile material is used. This feature offers a great advantage in the use of thorium over U-238 as fertile material.

The results of the calculations shown in the first column of Table 2 are based on sampling 1000 initial source neutrons and 50 batches. Results in the next column have been obtained by using a smaller number of particles: 200 neutrons and 33 batches. Due to the smaller sampling number in the latter case, the statistical errors of the results are relatively larger, but even this small number of sampling provides a useful trend. It thus shows that this Monte Carlo burn-up calculation can be used for parameter study of the conceptual design.

Due to the need for many cells in the core, the calculation time (125 min) for sampling numbers of 1000 particles * 50 batches is five times longer than the single cell calculation time (25 min) for using the same sampling numbers.

TABLE 3
SPECIFICATION OF THE WATER-COOLED REACTOR WITH A HARD
NEUTRON SPECTRUM

Design Parameters	Specification with Void Tube	Specification Without Void Tube
Rod Outer Diameter	11.91 mm	14.5 mm
Rod Inner Diameter	11.11 mm	14.mm
Pitch Of Rod	13.21 mm	15.8mm
Number Of Rods In Bundle	469	217(271)
Smeared Fuel Density	93 %	88%=10/11.3
Inner Distance Of Channel Box	298 mm	206.3 mm
Outer Distance Of Channel Box	299 mm	213.mm
Pitch Of Fuel Assemblies	304.2 mm	219.7 mm
No Of Fuel Assembly	252	974(924)
No Of Void Tube Assemblies	61	0
Core Diameter	5651 mm	7200 mm
Core Height	1600 mm	1000 mm
Upper Blanket	300 mm	No
Lower Blanket	300 mm	No

5. MONTE CARLO BURN-UP CODE DEVELOPED AT BNL

The neutronic characteristics of the reactor without void channel were calculated using the Monte Carlo burnup code (MCBURN) [5]. The MCBURN code was developed at BNL, first by Yang combining the MCNP [6] and ORIGEN [7] codes. This code was then revised by Cetnar using the Unix system and C-language to facilitate handling of the large number of files created during the calculations and their reuse. This code was further developed by Cetnar in collaboration with a Swedish university. Reference 8 describes recent developments with this code.

In the analysis of this reactor, void channels have been introduced to suppress the positive void-coefficient by neutron streaming when coolant boiling occurs. It is very crucial to properly analyze neutron transport, using the Monte Carlo method, although this requires a longer computer time than using analytical methods based on the first-flight collision probability method [9], which we developed in 1960, to analyze the heterogeneity of the fuel assembly configuration. The regular first-collision probability method assumes isotropic neutron scattering. To take anisotropic scattering into account, one of the authors developed a generalized collision probability method [10] for a cylindrical lattice system, which can be easily extended to other geometries such as square or hexagonal lattice. However, extension of this

method to three-dimensional problems becomes a rather complicated operation. The collision-probability methods are analytical deterministic methods, so that the uncertainty associated with the probabilistic Monte Carlo method, due to the statistically small number of samples, does not exist. Since an energy group approximation has to be used, the calculation is inexact for the analysis of a core system composed of material that has resonance cross sections, although the H₂O coolant can provide some relief for this approximation.

The Monte Carlo method can handle continuous-energy cross section representation and is also free from any approximation in geometry. Thus, we adopted the Monte Carlo method for our burn-up calculation. In carrying out this reactor calculation, the core has been segmented into many separate regions. In each region, the change of composition due to burnup is calculated by the ORIGEN code. Hence, while this approach is not completely approximation-free, the streaming of neutrons can be treated without any approximation.

6. DEVELOPMENT OF THE KINETICS CODE

To evaluate the safety of a tight lattice reactor, the neutronics and thermo-hydraulics codes RELAP [11] and PARCS [12] will be used. The PARCS code, developed for a square lattice by Downar, was recently extended to enable calculations of hexagonal lattice geometries, so that it can be used to analyze the Russian-designed PWRs. The PARCS code uses a diffusion approximation for neutron transport. To implement strong anisotropic neutron flux distributions, it can use the S_n type transport method, but this calculation takes a long time, and its deterministic methodology is not as powerful as the Monte Carlo method.

Instead of calculating the dynamics of the whole reactor with the Monte Carlo method which requires a substantial amount of computer time, we can provide the diffusion coefficient which will be used for the PARCS assessment by calculating the segmented core regions with the Monte Carlo method, with suitable boundary conditions. We have successfully applied this approach to calculate the one-dimensional kinetics problem [13]. This approach shortens the kinetics calculation while properly treating the neutron streaming through the voided tubes by tabulating the diffusion coefficient or by formulating it in an analytical form.

CONCLUSIONS

Preliminary studies of a water-cooled reactor with a hard neutron spectrum indicates that thorium fertile material yields higher burn ups than U-238, without producing Pu and minor actinides. This approach meets the objective of a proliferation-resistant design, as required in the NERI program. The Monte Carlo method is a useful tool for the analysis of a reactor with complicated geometry, although the computer time is longer than that required for the analytical method. Even when analyzing the whole reactor with many lattice cells and small uncertainties, computing does not require prohibitively long times.

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APPENDIX B

Paper Accepted for 2000 ANS Winter Meeting

Comparison of CASMO-4, HELIOS, and MOCUP for ThO_2 Pincell Burnup

By

Xianfeng Zhao (MIT), Kevan D. Weaver (INEEL),
Yunlin Xu (Purdue), Thomas J. Downer (Purdue)

As part of an effort to evaluate the potential benefits of using thorium in LWR fuel, initially under a strategic nuclear research collaboration between MIT and INEEL and more recently as NERI projects at MIT/INEEL and Purdue/ANL, comparisons are being made between state-of-the-art codes for core burnup calculations with thorium fuel. The results reported here compare CASMO-4^[1], HELIOS^[2], and MOCUP^[3]. Both CASMO-4 and HELIOS are multigroup two-dimensional transport codes for burnup calculations based on collision probability method. MOCUP^[3] is the MCNP-ORIGEN2 Coupled Utility Program which employs the MCNP (version 4B) generalized-geometry Monte Carlo transport code to give the neutronics solution and the ORIGEN2 code to compute the time-dependent compositions of the individually selected MCNP cells.

The pin cell problem that was analyzed here is representative of a fuel pin in a standard 17x17 fuel assembly in a Westinghouse PWR. The usual all- UO_2 pellets are replaced by ThO_2 - UO_2 pellets having the characteristics documented in Table 1. Because of some modeling differences in the codes used here, a entirely consistent comparison was not possible. For example, MOCUP and HELIOS employ a square pin cell model whereas CASMO-4 uses an equivalent circular pin cell. Other minor differences were also encountered, such as the inability of HELIOS to treat temperature expansion effects and to model Zr-4. The impact of these differences on the results was quantified and in most cases were found to result in only minor discrepancies in the results. The prediction of the pin cell k -inf between MOCUP and HELIOS vs. CASMO as a function of burnup is shown in Figure 1. Selected nuclide concentrations are shown in Table 2 at a burnup of 60 MWd/kg.

In general there is good agreement in the k -inf versus burnup predicted by the three codes as shown in Figure 1. The differences that do exist in the k -inf are attributable in part to the fact that stochastic codes (like MOCUP) can have large statistical variations in the results. The

number of particle histories used here in the MOCUP calculations were 225,000, which results in a statistical uncertainty in k_{inf} of about 0.002. A second source of differences in the results is that different nuclear data libraries were used: CASMO-4's 70-group library is based on the evaluated data files JEF-2.2 and ENDF/B-6, MCNP4B's continuous library is based on the ENDF/B-5, ENDF/B-6, LLNL, or T2, and HELIOS's 190-group library is based on ENDF/B-6. A third source of differences is the fission product modeling used in the codes. CASMO and HELIOS employ slightly different lumped fission products but they do model all fission product absorption. However, MOCUP only includes the major fission products and misses about 3% of the fission product absorption effects. Finally, one other difference in the calculations is that MOCUP depletes the fuel with an infinite medium spectrum, whereas CASMO and HELIOS employ a more realistic critical spectrum. These spectral differences will result in small differences in the conversion ratio and slight differences in the slope of the k_{inf} versus burnup curve. The overall impact of these differences in the modeling and calculation methods do not appear to be large, possibly because of a fortuitous cancellation of effects.

As shown in Table 2, good agreement was observed in the prediction of most of the important nuclide concentrations. For example, all codes predict the U-233 nuclide concentration within 4% of each other. Discrepancies were observed in the prediction of the PU-239 concentration but these are not inconsistent with the results of recent NEA MOX and all-U unit cell benchmarks^{[4],[5]}. Some points of particular interest are:

- (1) The percentage differences at 60MWd/kg are consistent with those noted at 20 and 40 MWd/kg.
- (2) U-234 displays by far the largest difference: ~18%
- (3) Th-232 chain nuclide concentrations are consistently higher in MOCUP.

The work reported here helps establish the framework for confidence in the credibility of predictions of thorium core performance. Because of the recent interest in Thorium fuel for the next generation of light water reactors, it will be important to resolve any differences that may exist in code predictions. This is particularly important because of previous shortcomings in predicting the performance of thorium fueled cores (e.g. Indian Point I). In the future, additional code benchmark comparisons are planned, as well as the re-analysis of thorium fueled criticals by FRAMATOME under the auspices of a NERI project^[6].

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Table 1: Pin-cell Model Parameters

Parameter	Cold Zero Power	Hot Full Power
Fuel Temperature (°K)	300	900
Power Density (KW/KgHM)	0.0	38.1347
Power Density (KW/liter cell)	0.0	107.284
Fuel Pellet Density (g/cm3)	9.614	9.424
Cladding Temperature (°K)	300.0	621.1
Cladding Density (g/cm3)	6.550	6.505
Coolant Pressure (bars)	155.13	155.13
Coolant Temperature (°K)	300.0	583.1
Coolant Density (g/cm3)	1.003	0.705
Fuel Pellet Radius (mm)	4.096	4.1274
Cladding Inner Radius (mm)	4.178	4.1896
Cladding Outer Radius (mm)	4.750	4.7609
Pin Pitch (mm)	12.6	12.626
Fuel Composition		
Th-232 (weight percent %)	65.909	
U-234 (weight percent %)	0.034	
U-235 (weight percent %)	4.291	
U-238 (weight percent %)	17.740	
O-16 (weight percent %)	12.026	

Table 2 Fractional Difference⁽¹⁾ in Isotope Concentration @ 60 MWd/Kg

Isotopes	CASMO-4	MIT MOCUP	INEEL MOCUP	HELIOS
Th-232	1.53769e+22	-0.003	-0.003	-0.001
Pa-231	1.70440e+18	0.048	0.018	-0.071
Pa-233	1.95229e+19	0.035	0.045	0.028
U-232	1.56006e+18	0.034	-0.003	-0.057
U-233	2.74202e+20	0.040	0.044	0.022
U-234	5.15172e+19	0.176	0.174	-0.001
U-235	1.78104e+20	-0.021	-0.033	-0.013
U-236	1.39420e+20	0.054	0.057	0.058
U-238	3.88419e+21	0.004	0.003	0.007
Np-237	1.82660e+19	-0.058	-0.035	-0.105
Np-238	5.46097e+16	-0.037	-0.096	-0.096
Np-239	7.61806e+17	-0.043	-0.019	-0.070
Pu-238	8.90932e+18	-0.026	-0.099	-0.102
Pu-239	5.37090e+19	-0.071	-0.050	-0.101
Pu-240	1.82233e+19	-0.032	0.021	-0.081
Pu-241	1.90707e+19	-0.024	-0.041	-0.075
Pu-242	9.96772e+18	-0.036	0.027	-0.090

(1) Fractional Diff. = $(N - N_{\text{Casmo4}})/N_{\text{Casmo4}}$, where N is nuclide concentration

Pincell model for westinghouse PWR Assembly
(25%UO₂+75%ThO₂;hot full power)

Fig. 1 Eigenvalues as a Function of Burnup

Appendix C

Paper Accepted for Presentation at the 2000 Winter ANS Meeting, Washington, D.C.

Thorium Fuel Depletion Analysis for Boiling Water Reactors

T.J. Downar, T.K. Kim, Y. Xu, C.H. Kim
Purdue University

1. Introduction

Thorium-based fuel (simply thorium fuel hereafter) has attracted renewed interest because of its potential advantages such as its desirable non-proliferation characteristics, its suitability as a fertile host for burning weapons grade plutonium, its lower production of long-lived radiotoxic wastes, its potential for higher burnup than uranium based fuel, and its beneficial reactivity characteristics leading to more acceptable safety characteristics than Conventional uranium-based fuels.^{1,2} Many previous studies have been performed on thorium fuels with the primary objective of demonstrating these advantages within the existing reactor technology.³⁻⁷ These studies were performed primarily for the pressurized water reactor (PWR). The purpose of the work reported here is to analyze the burnup performance of thorium and UO_2 fuel in current boiling water reactor (BWR) designs and to assess the potential advantages of thorium fuel over UO_2 fuel with respect to proliferation resistance, possibility of longer cycle operation, and void reactivity characteristics.

2. Comparison of Thorium and Uranium Burnup Performance

In order to provide a consistent comparison of the burnup performance of thorium and UO_2 fuels, the fuel pin designs used for 8x8, 9x9, 10x10 BWR fuel assemblies^{8,9} are analyzed using the collision probability code HELIOS¹⁰. For thorium fuels, two different fuel compositions are considered; $(\text{Th}+\text{U}^{235})\text{O}_2$ in which Th^{232} replaces U^{238} and $(\text{Th}+\text{Pu}^{239})\text{O}_2$ in which both U^{238} and U^{235} are replaced by Th^{232} and fissile Pu^{239} , respectively. For comparison an additional fuel is considered, $(\text{U}^{238}+\text{WGPu}^{239})\text{O}_2$ where the weapon grade (WG) Pu^{239} replaces the U^{235} fissile. For the initial analysis, the UO_2 fuel pin composition is simply modified with an equivalently enriched thorium fuel. Table 1 and Figures 1(a) show the comparison of the depletion performance of different fuel pin compositions. The current UO_2 fuel pins have similar initial k_{inf} values and depletion behavior. However, the thorium fuel pins show a very different behavior. The initial k_{inf} values and the rate of depletion of the thorium fuel pins are smaller than the corresponding UO_2 fuel pins. This performance is a direct result of the larger thermal absorption cross section of Th^{232} than U^{238} and of the breeding capability of U^{233} . This is advantageous from the reactivity control standpoint because Th^{232} displays inherent poison capabilities at the beginning of the depletion cycle and acts as a fissile source at the end of the depletion cycle. These properties of Th^{232} have potential benefits for extended cycle and high burnup core operation. Since the initial k_{inf} value of Th^{232} fuel is very low, however, the fuel enrichment must be somewhat increased in order to meet the required cycle burnup.

The equivalent equilibrium cycle length concept is useful to perform a consistent comparison of the burnup performance of the various fuel compositions. According to the linear reactivity model (LRM)¹¹, the equilibrium cycle length of an n -batch core is given by:

$$B_{Eq} = \frac{2}{n+1} \frac{\rho_0}{A}, \quad (1)$$

where ρ_0 =initial reactivity and A =slope of the reactivity. By using Eq. (1), the burnup potential of fuel having different compositions can be compared by selecting the same ratio of the initial reactivity to the slope of the reactivity for the reference pre-designed fuel:

$$\frac{\rho_0^{ref}}{A^{ref}} = \frac{\rho_0}{A}, \quad (2)$$

where ρ_0^{ref} and A^{ref} are the initial reactivity and slope of the reactivity versus burnup, respectively, for a reference fuel. The current 9x9 UO₂ BWR fuel design was chosen as the reference and the equivalent ratio of initial reactivity to the slope of the reactivity was determined by trial and error so that the critical cycle length of each fuel composition became equivalent to that of the current 9x9 UO₂ fuel. Four different fuel compositions were analyzed and the results in Table 1 and Figure 1(b) summarize the burnup behavior of the kinf, as well as the void coefficients and proliferation resistance characteristics of the fuel. The case D fuel composition shown here is a mixture of 75 % ThO₂ and 25 % UO₂ enriched to 18 % U²³⁵. Similar to results reported in earlier studies on thorium fuel performance in the PWR, the above results show that thorium fuel has the potential for higher conversion and for more desirable proliferation resistance characteristics.

3. Conclusion

The improved conversion performance of thorium fuel provides the potential benefit of a high burnup fuel design and longer cycle operation of the BWR without the adverse effects of a positive void coefficient. It is possible to further enhance the proliferation resistance by long cycle operation of thorium fuel because of the accumulation of gamma-emitting U²³². The study here indicates that thorium fuel has considerable advantages as a BWR fuel and merits further investigation.

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Table 1. Current BWR fuel pin design data and depletion characteristics

Fuel Type	8x8		9x9				10x10	
Power density(W/g)	25.9		25.9				25.0	
Pin pitch (cm)	1.6256		1.4529				1.2950	
Fuel pellet								
Radius(cm)	0.5137		0.45275				0.4420	
Density(g/cc)	94% TD		94% TD				94% TD	
Temperature(K)	900		900				900	
Cladding								
Thickness(cm)	0.0889		0.0889				0.0889	
Material	Zr-2		Zr-2				Zr-4	
Density(g/cc)	6.505		6.505				6.505	
Temperature(K)	600		600				600	
Coolant								
Material	H2O		H2O				H2O	
Density(g/cc)	0.740		0.740				0.740	
Temperature(K)	559		559				559	
Fuel composition								
Fissile	U^{235}	U^{235}	U^{235}	U^{235}	U^{238}	Th^{232}	U^{235}	U^{235}
Fertile	U^{238}	Th^{232}	U^{238}	Th^{232}	WG-Pu ^{a)}	WG-Pu	U^{238}	Th^{232}
Enrichment	3.20	3.20	3.37	3.37	4.72	4.72	4.00	4.00
K-inf								
BOC	1.27118	1.11702	1.28420	1.14000	1.28779	1.25273	1.25030	1.13027
Slope(pcm)	-729	-347	-751	-380	-606	-512	-661	-318
Critical burnup	23.5	17.5	24.5	21.5	31.5	28.5	22.5	24.5
Void coefficient								
BOC(pcm/K)	-529	-497	-523	-488	-477	-566	-518	-547
Critical(pcm/K)	-534	-453	-536	-446	-431	-455	-454	-501
FIR at critical(%)	49	68	48	66	49	58	60	68
Equivalent equilibrium cycle length concept								
Fuel Composition			U^{235}	U^{235}	WG-Pu	WG-Pu		
Fissile			U^{238}	Th^{232} (75)	U^{238}	Th^{232}		
Fertile (weight percent)				U^{238} (25)				
Enrichment, (%)			3.37	18.0	3.65	4.50		
Void coefficient, (pcm/void)								
BOC			-562	-567	-545	-582		
EOC			-530	-531	-482	-470		
Proliferation resistance								
Fraction of long-lived isotopes ^{b)} , (%)			0.15	0.08	0.36	0.34		
Relative spontaneous fission rate ^{c)}			11.18	10.64	11.08	13.19		
Relative specific decay heat ^{d)}			4.45	6.7	2.4	2.5		
U^{232} contamination ^{e)} , (%)			-	0.21	-	0.22		
Fraction of plutonium at EOC, (%)			1.03	0.39	3.25	2.5		
Dirtiness of Plutonium ^{f)} , (%)			24.6	21.4	26.7	33.5		

a) WG-Pu = weapon grade plutonium (98% Pu^{239} and 2% Pu^{240})

b) Fraction of long-lived isotope = $100 \times (\text{amount of } Np^{237} + \text{its precursors}) / (\text{total amount of HM isotopes})$

c) Relative spontaneous fission rate = relative spontaneous fission rate to the weapon grade plutonium

d) Relative specific decay heat = relative specific decay heat to the weapon grade plutonium

e) U^{232} contamination = $100 \times (\text{amount of } U^{232}) / (\text{total amount of heavy metal isotopes})$

f) Dirtiness of plutonium = $100 \times (Pu^{238} + Pu^{240} + Pu^{242}) / (Pu^{239} + Pu^{241})$

(a) Current BWR pins depletion behavior with different fuel compositions

(b) Comparison of the depletion behavior having the same equilibrium cycle length.

Figure 1. k_{inf} Depletion Behavior of BWR Fuel Pin with Different Fuel Compositions.

Appendix D

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Feasibility Study of a Plutonium-Thorium Fuel Cycle for a High Conversion Boiling Water Reactor

T. Downar, , H. Takahashi, K. Rohatgi, C.H. Kim, T.K. Kim, Y. Xu

1. Introduction

During the past several years there has been considerable interest in high conversion (HC) light water reactors (LWRs) which can achieve high fuel burnup, long fuel cycle operation, and fissile plutonium recycle.¹ Recently, Japanese industry and research organizations have presented a reduced moderation water reactor (RMWR) based on a tight lattice BWR design concept. The purpose of the work here was to investigate the feasibility of fissile plutonium and fertile thorium fuel cycle for a HCBWR similar to the RMWR concept. Unlike previous studies on HCLWRs, the objective of the work here is to achieve the most efficient use of the abundant thorium resources, while enhancing the proliferation resistance of the nuclear fuel cycle and burning the weapon grades plutonium effectively.

The HCBWR operates with a fast neutron energy spectrum which results from minimizing the water to fuel volume ratio through the tight fuel pin spacing of a hexagonal lattice. The fast neutron spectrum enhances the conversion of U^{238} to Pu in uranium fueled HCBWR through increased resonance absorption. When the spectrum shifts to ultra fast region with the voiding of the core, the resonance absorption by U^{238} decreases and fast fission of U^{238} increases. As a result, the uranium-fueled HCBWR exhibits the drawback of a positive void coefficient. Conversely, thorium fuel with fissile plutonium has a negative void coefficient in a tight lattice spectrum because both resonance absorption and fast fission are considerably less in Th^{232} than in U^{238} . Additionally, Th^{232} is highly proliferation resistant because the fissile Plutonium simply burns out in the absence of fertile U^{238} . The purpose of the research here is to examine these qualities of thorium with fissile plutonium through the analysis of fuel pins using the lattice physics code HELIOS.

2. Burnup analysis of Thorium fuel pin cell in Tight Lattice BWR core

The HCBWR core of the RMWR concept is characterized by tight fuel pin spacing in a hexagonal fuel lattice. The ratio of the rod diameter to lattice pitch is 0.9 which is much larger than that of a standard BWR/6 core (0.623). The water to fuel volume ratio of the HCBWR is 0.5 while that of standard BWR/6 is 2.7. This results in a neutron energy spectrum for the HCBWR which resembles that of the fast reactor. Figure 1(a) shows the fuel assembly configuration and the fuel pin cell geometry of the 3926 MW(th) Japanese RMWR design which is used here for the HCBWR. Figure 1(b) illustrates the neutron energy spectrum in the HCBWR lattice in comparison with that of the standard BWR lattice. For purposes of comparison, four different

fuel compositions are considered; 10 % enriched UO_2 , a mixture of 50 % ThO_2 and 50 % UO_2 with 20 % U^{235} enrichment, weapons grade (WG) PUO_2 with U^{238}O_2 and WGPuO_2 with ThO_2 . To present a consistent comparison, the fissile enrichment is set to be the same as 10 %. The pin cell analysis was performed with the collision probability code HELIOS.³ The validation of HELIOS for the fast spectrum lattice was performed with a Monte Carlo depletion code.⁴ Figures 1(c) and 1(d) show the variation of the k_{inf} and coolant void coefficient of four fuel compositions as a function of burnup.

There are several important differences in the nuclear properties of Th^{232} and U^{238} . The resonance absorption of Th^{232} is about 3.5 times less than that of U^{238} . Both Th^{232} and U^{238} are fissionable above 1.4 and 1 Mev, respectively. But the fission cross section of Th^{232} (200mb) is roughly one order less than that of U^{238} . Because of these differences in the nuclear properties, thorium fuels burn more slowly than corresponding U^{238} fuels (cf. Fig. 1 (c)). Thorium fuel can maintain a negative void coefficient in a tight lattice while U^{238} fuel exhibits the positive void coefficient when voiding in a tight lattice (cf. Fig. 1(d)). The smaller fast fission contribution of Th^{232} is responsible for the lower initial k_{inf} of thorium fuel than U^{238} fertile fuel as shown in Fig. 1(c). It is worth noting that the initial k_{inf} of thorium fuel with WG plutonium fissile (1.11033) is considerably lower than that of the corresponding U^{238} fuel (1.25560) but the critical burnups, e.g., the burnup when $k_{\text{inf}}=1$, are almost comparable to each other. This indicates the possibility of designing very long thorium cycle of the HCBWR using WG plutonium fissile.

For further comparison, Table 1 presents plutonium burning and proliferation resistance characteristics of thorium and uranium fuels with WG plutonium. A comparison of the Pu isotopic composition of the two fuels at BOC and EOC indicates that thorium fuel burns the Pu isotopes more effectively than uranium fuel because the fertile U^{238} for breeding Pu isotopes are absent in the thorium fuel. Table 1 also indicates that the thorium fuel discharged at the EOC is more proliferation resistant than the corresponding uranium fuel, as measured by the spontaneous fission rate and the decay heat rate.

3. Conclusion

Based on the pin cell analysis performed here, we can conclude that the thorium fertile and WG plutonium fissile fuel provide substantial advantages for realizing the objectives of increased proliferation resistance and increased fuel burnup which will result in reduced fuel storage requirements.

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Table 1. Pu Burning and Proliferation Resistance Characteristics of Th and U Fuel

		Uranium fuel		Thorium fuel	
		BOC	EOC	BOC	EOC
Isotopic composition (Kg/assembly)	Pu ²³⁸	-	0.3589	-	0.1759
	Pu ²³⁹	65.1909	47.5179	65.1909	19.9850
	Pu ²⁴⁰	4.1610	15.5928	4.1610	11.3451
	Pu ²⁴¹	-	3.8249	-	2.88180
	Pu ²⁴²	-	0.5705	-	0.45466
	Th ²³²	-	-	582.5528	529.5476
	U ²³²	-	-	-	0.1004
	U ²³³	-	-	-	26.1400
	U ²³⁸	582.5528	523.3431	-	-
Burnup(GWD/t)		0	90	0	85
k _{inf}		1.25560	1.00106	1.11033	1.00063
Spontaneous neutron for 1 Kg Pu (n/s)		54620.7	237143.0	54620.7	331630.0
Decay heat for 1Kg Pu (watts)		2.19400	6.09212	2.19400	6.47909

(a) Fuel assembly configuration and the fuel pin cell geometry

(b) Spectrum comparison

(c). Depletion behavior of k_{inf}

(d) Coolant void reactivity coefficient with burnup

Figure 1. Tight Lattice BWR Fuel and Their Depletion Characteristics