36
11/13/78
Special Dist.
LB

MASTER

WAPD-TM-1314
DOE RESEARCH AND
DEVELOPMENT REPORT

**THE CALCULATIONAL MODEL USED IN
THE ANALYSIS OF NUCLEAR
PERFORMANCE OF THE LIGHT WATER
BREEDER REACTOR (LWBR)
(LWBR Development Program)**

AUGUST 1978

CONTRACT EY-76-C-11-0014

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

BETTIS ATOMIC POWER LABORATORY

WEST MIFFLIN, PENNSYLVANIA

Operated for the U. S. Department of Energy by

WESTINGHOUSE ELECTRIC CORPORATION

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

THE CALCULATIONAL MODEL USED IN THE ANALYSIS OF
NUCLEAR PERFORMANCE OF THE LIGHT WATER
BREEDER REACTOR (LWBR)
(LWBR Development Program)

Editor: L. B. Freeman

Contributors

B. R. Beaudoin	H. C. Hecker
R. J. Eckert	D. M. Kriek
L. B. Freeman	W. C. Schick
S. B. Gunst	E. Schmidt
G. L. Hartfield	N. M. Steen

Contract No. EY-76-C-11-0014

August 1978

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

Printed in the United States of America
Available from the
National Technical Information Service
U. S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22151

NOTE

This document is an interim memorandum prepared primarily for internal reference and does not represent a final expression of the opinion of Westinghouse. When this memorandum is distributed externally, it is with the express understanding that Westinghouse makes no representation as to completeness, accuracy, or usability of information contained therein.

BETTIS ATOMIC POWER LABORATORY
WEST MIFFLIN, PENNSYLVANIA

Operated for the U. S. Department of Energy by
WESTINGHOUSE ELECTRIC CORPORATION

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

for i

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States, nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights.

FOREWORD

The Shippingport Atomic Power Station located in Shippingport, Pennsylvania was the first large-scale, central-station nuclear power plant in the United States and the first plant of such size in the world operated solely to produce electric power. This project was started in 1953 to confirm the practical application of nuclear power for large-scale electric power generation. It has provided much of the technology being used for design and operation of the commercial, central-station nuclear power plants now in use.

Subsequent to development and successful operation of the Pressurized Water Reactor in the DOE-owned reactor plant at the Shippingport Atomic Power Station, the Atomic Energy Commission in 1965 undertook a research and development program to design and build a Light Water Breeder Reactor core for operation in the Shippingport Station. In 1976, with fabrication of the Light Water Breeder Reactor (LWBR) nearing completion the Energy Research and Development Administration established the Advanced Water Breeder Applications program (AWBA) to develop and disseminate technical information which would assist U.S. industry in evaluating the LWBR-concept. All three of these reactor development projects have been administered by the Division of Naval Reactors with the goal of developing practical improvements in the utilization of nuclear fuel resources for generation of electrical energy using water-cooled nuclear reactors.

The objective of the Light Water Breeder Reactor project has been to develop a technology that would significantly improve the utilization of the nation's nuclear fuel resources employing the well-established water reactor technology. To achieve this objective, work has been directed toward analysis, design, component tests, and fabrication of a water-cooled, thorium oxide fuel cycle breeder reactor to install and operate at the Shippingport Station. Operation of the LWBR core in the Shippingport Station started in the Fall of 1977 and is expected to be completed in about 3 to 4 years. Then the fissionable fuel inventory of the core will be measured. This effort, when completed in about 2 to 3 years after completion of LWBR core operation, is expected to confirm that breeding actually took place.

The Advanced Water Breeder Applications (AWBA) project was initiated to develop and disseminate technical information that will assist U.S. industry in evaluating the LWBR concept for commercial-scale applications. The project will explore some of the problems that would be faced by industry in adapting technology confirmed in the LWBR program. Information to be developed includes concepts for commercial-scale prebreeder cores which will produce uranium-233 for light water breeder cores while producing electric power, improvements for breeder cores based on the technology developed to fabricate and operate the Shippingport LWBR core, and other information and technology to aid in evaluating commercial-scale application of the LWBR concept.

Technical information developed under the Shippingport, LWBR, and AWBA projects has been and will continue to be published in technical memoranda, one of which is this present report.

TABLE OF CONTENTS

	<u>Page</u>
AUTHORSHIP AND ACKNOWLEDGMENTS	xi
I. INTRODUCTION	1
II. DESCRIPTION OF THE LWBR CORE AND IMPLICATIONS FOR THE CALCULATIONAL MODEL	4
A. Core Description	4
B. Implications of the Reactor Design for Neutron Calculations	6
III. GENERAL DESCRIPTION OF THE NUCLEAR CALCULATIONAL MODEL AND THE QUALIFICATION PROCEDURE	14
A. Nuclear Calculational Model	14
1. Input	14
2. PAX	15
3. CINDER	17
4. PDQ	17
B. Qualification Procedure	19
1. Reactivity	20
2. Power Distributions	21
3. Breeding	22
4. Other Qualification Procedures	23
REFERENCES	24
IV. DETAILED DESCRIPTION OF THE PRE-PDQ MODEL	27
A. Material Inventories and Homogenization	27
1. As-Built Material Inventories	27
2. Homogenization of Material Concentrations	30
B. Nuclear Data	32
1. Thorium	32
2. Uranium-233	34
3. Protactinium-233	35
4. Zirconium (Elemental) and Zircaloy-4	36
5. Hydrogen	38
6. Oxygen	39
7. Other Isotopes Except Fission Products	39
8. Xenon-135	39
9. Other Fission Product Cross Sections	40
10. Fission Product Yields and Decay Constants	40
11. Delayed Neutron Data	41
12. Energy per Fission	42
13. Processing Nuclear Data into XAP	42

TABLE OF CONTENTS (Cont)

	<u>Page</u>
C. Space-Energy Representations Within the Unit Cell	43
1. Energy Structure	43
2. Fast Advantage Factors	44
3. Resonance Treatment	46
4. Thermal Disadvantage Factors	47
5. Tests of the Model in an Infinite Lattice of Unit Cells	48
D. The Resonance Model	50
E. Determination of Few-Group Cross Sections for Use in Diffusion Theory Calculations	55
1. Infinite Medium Calculations	55
2. Time Varying Cross Sections	58
3. Temperature Dependence	59
4. Construction of Table Sets	59
F. Regional Space-Energy Correction Factors	61
1. Background	61
2. One-Dimensional Multigroup Computer Programs	63
3. Regional Few-Group Cross Sections from Multigroup Spectra	64
4. The Diffusion Coefficient	66
5. Assignment of Space-Energy Correction Factors to Regions Within the Core	70
6. Tests of Space-Energy Correction Factors	72
7. Automation of Space-Energy Correction Factors	76
REFERENCES	77
V. DETERMINATION OF THE NEUTRON FLUX DISTRIBUTION IN THE CORE AND THE REACTIVITY: THE USE OF PDQ	121
A. Depletion Chains	121
1. Fuel Chains	121
2. Fission Product Chains	122
B. Fission Product Treatment: CINDER	122
C. Transport Approximation for Fast Neutrons	125
D. The Multi-Region Core: Mesh and Depletion Block Size	125
E. Temperature Feedback	127
F. Xenon Feedback	129
G. Clad Shrinkage, Fuel Swelling, and Gap Conductance in PDQ	130
H. Depletion Timesteps	133
REFERENCES	133
VI. DETERMINATION OF NUCLEAR PERFORMANCE AND PREPARATION OF DATA FOR ENGINEERING ANALYSIS: POST-PDQ DATA MANIPULATION	144
A. Physics Analysis	144

TABLE OF CONTENTS (Cont)

	<u>Page</u>
B. Thermal-Hydraulic Analysis	145
C. Fuel Element Analysis	147
D. Structural Analysis	147
REFERENCES	148
VII. CORE KINETICS CALCULATIONS	150
A. Calculation of Kinetics Parameters	150
1. Temperature and Density Coefficients of Reactivity	150
2. Effective Delayed Neutron Fraction	151
3. Prompt Neutron Lifetime	152
B. Kinetics Calculations for LWBR	152
C. Stability and Xenon Transient	153
REFERENCES	153
VIII. QUALIFICATION OF THE MODEL	155
A. Fission-Product Treatment	155
1. Fission-Product Programs	155
2. Post-Irradiation Isotopic and Elemental Comparisons	156
3. Reactivity-Measurement Results Compared with Corresponding Calculations	156
4. Measured and Calculated Decay Heat	157
5. Conclusion	157
B. Core Reactivity	157
1. Experimental Core Program	157
2. Monte Carlo Calculation of Experiments	158
3. Development of Reactivity Bias for the Computational Model	159
C. Power Distributions	160
1. Experimental Core Power Distributions	160
2. PDQ Calculations of Experiments	160
3. Development of Experiment/Calculation Factors for Power Distributions	162
D. Core Breeding	162
1. η of U ²³³	162
2. Competition Between Thorium and Parasitic Materials - Cross Sections	163
3. Competition Between Thorium and Parasitic Materials - Flux Distribution	164
REFERENCES	166
IX. CONCLUSION	172

LIST OF TABLES

<u>Table</u>	<u>Title</u>	<u>Page</u>
II-1	LWBR Core Nominal Characteristics	8
II-2	LWBR As-Built Core Fuel Characteristics	9
IV-1	Typical LWBR Core Absorption Fractions After 8,000 Hours of Depletion at Full Power, Ordered by Magnitude	83
IV-2	Fission Product Nuclides in Order of Importance in LWBR High Zone Seed Spectrum After 10,500 Hours of Full Power Operation	84
IV-3	Thermal Cross Sections and Resonance Integrals for Fission Products	85
IV-4	Fission Product Yields from U^{233} Fission and Half-Lives	86
IV-5	Delayed Neutron Half-Lives and Yields	87
IV-6	Typical LWBR Fast Advantage Factors	88
IV-7	Thermal Disadvantage Factors for LWBR by the Multiple-Sauer Method	88
IV-8	Comparison of PAX and RCP Reaction Rates in Unit Cell Lattices	89
IV-9	Comparison of PAX and RCP Reaction Rates in Unit Cell Lattices	91
IV-10	Comparison of PAX and RCP Reaction Rates in Unit Cell Lattices	93
IV-11	Comparison of PAX and RCP Reaction Rates in Unit Cell Lattices	95
IV-12	Comparison of PAX and RCP Reaction Rates in Unit Cell Lattices	97
IV-13	Comparison of PAX and RCP Reaction Rates in Unit Cell Lattices	98
IV-14	Thermal-Hydraulic Feedback Variables	99
IV-15	LWBR Use of PAX Tables	100
IV-16	Time- and Temperature-Dependent Fitted Cross Sections for Fuel Regions in the LWBR Model	101
IV-17	Representative PAX Input Parameters for an LWBR Fuel Rod Cell	102

LIST OF TABLES (Cont)

<u>Table</u>	<u>Title</u>	<u>Page</u>
IV-18	Ranges of Typical Regional Space-Energy Correction Factors, with Movable Fuel Assemblies 14 Inches Below the Aligned Position	102
IV-19	Test of Space-Energy Constants for One-Dimensional Traverse T_1	103
IV-20	Test of Space-Energy Constants for One-Dimensional Traverse T_1	104
IV-21	Test of Space-Energy Constants for One-Dimensional Traverse T_2	105
IV-22	Test of Space-Energy Constants for One-Dimensional Traverse T_3	106
IV-23	Test of Space-Energy Constants for One-Dimensional Traverse T_4	107
IV-24	Test of Space-Energy Constants at Middle of Life	108
IV-25	Comparison of Fast G-Factors Between BOL and MOL	109
VIII-1	Eigenvalues from Critical Assemblies	167
VIII-2	Binary Fuel Power Distribution in Detailed Cells Experiment Versus RCP and PDQ	168
VIII-3	Isotopic Absorptions in Three-Dimensional LWBR Core Calculations at Beginning of Life	169

LIST OF FIGURES

<u>Figure</u>	<u>Title</u>	<u>Page</u>
II-1	LWBR Cross Section and Module Identification	10
II-2	LWBR Movable Fuel Control	11
II-3	Type I Module Cross Section	12
II-4	R-Z Schematic of Type I Module	13
III-1	LWBR Nuclear Calculational Model	26
IV-1	Generalized Fuel Pellet	110
IV-2	Fuel Rod Unit Cell	111

LIST OF FIGURES (Cont)

Figure	Title	Page
IV-3	Four Module Breeder Mockup BMU-2-4 (Power Flattened), per Atom Fission Distribution in 9 w/o Seed Slice (Mid-Plane)	112
IV-4	RZ Diagram of LWBR Type I Module	113
IV-5	Typical One-Dimensional Traverses for the Computation of Regional Few-Group Constants	114
IV-6	Relative U^{233} Fission Activation along Traverse through 9 w/o Seed of BMU-1B	115
IV-7	Test of Space-Energy Correction Factors for a Single Module	116
IV-8	Two-Dimensional Calculation of a Horizontal Slice through a Symmetric 1/6 Section of the Core	117
IV-9	Two-Dimensional Calculation of a Horizontal Slice through a Symmetric 1/6 Section of the Core	118
IV-10	Two-Dimensional Calculation of a Horizontal Slice through a Symmetric 1/6 Section of the Core	119
IV-11	Three-Dimensional Calculation of a Symmetric 1/6 Section of the As-Built LWBR Core	120
V-1	Natural U^{233} , Th^{232} Chain	135
V-2	Linear Fuel Chains	136
V-3	Explicit Fission Product Chains	137
V-4	Thermal Fission Product Cross-Section	139
V-5	Epithermal (Group 3) Fission Product Cross Section	140
V-6	Mesh Lines and Depletion Block Sizes in PDQ for 1/6 of Type I Module	141
V-7	Comparison of Seed Rod Temperature Calculation by PDQ and CYGRO-4, for 3 Depletion Blocks	142
V-8	Comparison of Regular Blanket Rod Clad Radius Calculation by PDQ and CYGRO-4 for 3 Depletion Blocks	143
VI-1	Cross Section of a Typical Depletion Block in PDQ Geometry	149
VIII-1	Results for Sample Irradiated to 89 Percent U^{233} Depletion	170
VIII-2	Hot Detailed Cell Power Fractions	171

AUTHORSHIP AND ACKNOWLEDGMENT

The authors of this report are shown in the following table:

<u>Report Section</u>	<u>Authors</u>
I, II, and III	L. B. Freeman
IV.A	B. R. Beaudoin
IV.B	N. M. Steen, L. B. Freeman, and G. L. Hartfield
IV.C	D. M. Kriek and L. B. Freeman
IV.D	E. Schmidt
IV.E	R. J. Eckert and L. B. Freeman
IV.F	L. B. Freeman
V.A and B	H. C. Hecker
V.C	L. B. Freeman
V.D, E, and F	H. C. Hecker
V.G	W. C. Schick
V.H	H. C. Hecker
VI	B. R. Beaudoin
VII	G. L. Hartfield
VIII.A	S. B. Gunst
VIII.B and C	G. L. Hartfield
VIII.D and IX	L. B. Freeman

The work performed in developing and testing the calculational model was done by a large group of engineers and scientists over a period of several years. The authors were part of this group, but were by no means all of it. The management and technical guidance for these developments were provided by G. H. Conley, H. F. Raab, D. H. Jones, S. Milani, M. Natelson, N. M. Steen, and E. M. Celbard.

The editor is grateful for the large typing effort of L. J. Clipper.

The purpose of the Light Water Breeder Reactor (LWBR) Program is to develop the technology to breed in a light water reactor. To achieve breeding in a water moderated and cooled thermal reactor required use of the U^{233} -thorium fuel cycle and neutron economic movable fuel reactivity control. The relatively small breeding margin in a light water reactor puts a premium on a precise prediction of the neutron economy. These considerations required the development of a novel and accurate calculational model of core physics behavior.

This report describes the calculational model used in the analysis of LWBR nuclear performance. The model was used to analyze the as-built core and predict core nuclear performance prior to core operation. The qualification of the nuclear model using experiments and calculational standards is described.

Features of the model include: an automated system of processing manufacturing data; an extensively analyzed nuclear data library; an accurate resonance integral calculation; space-energy corrections to infinite medium cross sections; an explicit three-dimensional diffusion-depletion calculation; a transport calculation for high energy neutrons; explicit accounting for fuel and moderator temperature feedback, clad diameter shrinkage, and fuel pellet growth; and an extensive testing program against experiments and a highly developed analytical standard.

The LWBR core is installed and operating in the Shippingport Atomic Power Station. After 3 to 4 years of operation, the spent core will be removed and shipped to the Idaho National Engineering Laboratory for a detailed examination and confirmation of breeding performance. The calculational model described in this report will be used to predict the results of core operation throughout core life and of spent core examination results which will serve to further validate the accuracy of the model.

THE CALCULATIONAL MODEL USED IN THE ANALYSIS OF NUCLEAR PERFORMANCE OF THE LIGHT WATER BREEDER REACTOR (LWBR) (LWBR Development Program)

Editor: L. B. Freeman

I. INTRODUCTION

The purpose of the Light Water Breeder Reactor (LWBR) Program is to develop the technology to breed in a light water reactor in order to provide a significant improvement in the fuel utilization compared to present types of light water thermal reactors. To breed in a water moderated and cooled thermal reactor it is necessary to use the U^{233} -thorium fuel cycle and neutron economic movable fuel reactivity control in the core design. The relatively small breeding margin in a light water reactor puts a premium on a precise treatment of the neutron economy. These considerations required the development of a novel and accurate calculational model of core physics behavior.

This report describes the calculational model used in the analysis of LWBR nuclear performance. The model was used to analyze the as-built core and predict core nuclear performance prior to core operation. (The performance predictions themselves will be the subject of a separate report.) The qualification of the

nuclear model against both experiments and calculational standards is also described in this report. These comparisons will indicate the degree of uncertainty in the model, and the amount of correction or allowance which is needed to assure that the actual core performance does not exceed any specified limit.

The calculational procedure starts with input core manufacturing data and nuclear data. The voluminous core manufacturing data are processed by an automated system for direct input to the analysis programs. The nuclear data are available from an extensively evaluated library for a U^{233} -Th system, for which critical experiments and evaluated nuclear data were previously lacking. From this input, nuclide concentrations and cross sections averaged over broad energy bands are generated for use in depletion calculations. The cross section generation includes an accurate resonance integral calculation which accounts for resonance self- and mutual-shielding without the use of correction factors. Space-energy corrections to the infinite media cross sections are applied to account for the finite size of each fuel zone.

The time and temperature-dependent cross sections are stored in computer files for input to the three-dimensional diffusion-depletion calculation. The depletion calculation treats fuel and fission product isotopes, handles movable fuel, and includes a transport calculation for high energy neutrons. Coolant and fuel temperature feedback to the neutron distribution are provided also, taking account of clad diameter shrinkage and fuel pellet growth. The output from this model is processed in a number of ways for use in engineering analysis of the core. Included are predictions of the lifetime variation of critical movable fuel position, power distributions, and breeding performance.

An extensive program tested both the individual and total aspects of the model against experiments and a highly developed analytical standard. The critical experiments included a mockup of part of the core but not a full scale mockup of the core. An explicit, accurate analytical standard provided the bridge from the experiments to the full core.

The LWBR core is installed and operating in the Shippingport Atomic Power Station. After 3 to 4 years of operation, the spent core will be removed and shipped to the Idaho National Engineering Laboratory for detailed examination and confirmation of breeding performance. The calculational model described in this report will be used to predict the results of core operation throughout core life and of spent core examination results which will serve to further validate the accuracy of the model.

The calculational methods developments and basic nuclear data analyses are themselves important to reactor technology apart from the LWBR core. The nuclear data have application to other thorium-based reactor systems, and the methods developments have general application where greater accuracy is needed in describing large cores with highly automated computational tools. The present report will provide an overall summary of these developments.

Section II of this report provides a brief description of the LWBR core and identifies those specific design features which differ from other pressurized water reactors. The effect of these features on the nuclear design model is also briefly discussed. Section III provides a summary description of the calculational model and its qualification. A detailed description of the model and how it is used to calculate the nuclear performance is presented in Sections IV, V, and VI. Section VII describes the calculational techniques employed to determine the core kinetics parameters which are required for transient performance analysis. A detailed discussion of the model qualification is presented in Section VIII.

II. DESCRIPTION OF THE LWBR CORE AND IMPLICATIONS FOR THE CALCULATIONAL MODEL

A. Core Description

The LWBR core is installed and operating in the Shippingport Atomic Power Station. To achieve breeding, the core has been designed to minimize parasitic neutron absorption in all core and structural materials.

Figure II-1 presents a cross-sectional view of the LWBR core showing the orientation of the basic types of modules which comprise the core configuration. As shown, the core contains the following principal types of fuel modules and fuel assemblies:

1. 12 movable seed fuel assemblies
2. 12 stationary blanket fuel assemblies composed of 2 blanket regions denoted as regular blanket and power-flattening blanket regions
3. 15 reflector blanket fuel modules.

The seed and blanket assemblies contain both fissile uranium-233 and fertile thorium-232, while the reflector blanket fuel modules contain only thorium. A hexagonal seed assembly and its surrounding annular blanket assembly form a seed/blanket module.

The 3 central fuel modules of the LWBR core are identical and symmetrical. They are designed as modules which could be used in a large central station reactor plant. The 9 modules surrounding these central modules have a slightly larger outer blanket region that is fueled with a somewhat higher uranium-233 content than the blanket regions of the inner modules. Use of this more highly loaded blanket region produces a relatively uniform power distribution within the interior of the core, thereby better simulating the environment of a typical large core. This power flattening increases the uranium-233 loading required for the small core used in Shippingport. In a large breeder core, power flattening could be accomplished with a smaller fractional increase in loading than used in the small core.

Surrounding the 12 hexagonal fuel modules is an annular region, about 9 inches thick, made up of 15 reflector blanket modules. These serve to reduce neutron leakage from the relatively small Shippingport Core to a value representative of a larger LWBR Core in the 300 to 400 MW(e) range. Surrounding the reflector blanket fuel modules are 15 stainless steel, nonfuel filler units whose purpose is to limit flow leakage by filling the space between the reflector modules and the lower barrel.

To eliminate the parasitic loss of neutrons in conventional control rod poison materials, core reactivity control is achieved by varying the geometric relationship between the movable seed fuel assemblies and the associated stationary annular blanket assemblies which surround each seed assembly. For LWBR operation, this reactivity control is achieved by uniformly positioning the 12 movable seed fuel assemblies in a bank via individual control drive mechanisms.

Changing the axial position of the seed assembly relative to the blanket assembly changes the relative amounts of neutron absorptions in the fissile (uranium-233) and fertile (thorium) fuel materials. The LWBR nuclear design is such that the more highly loaded seed has a k_{∞} greater than 1 and the lower loaded blanket has a k_{∞} less than 1. Reactivity is controlled by varying the leakage of neutrons from the high k_{∞} seed regions into the low k_{∞} blanket regions. The reactivity worth of the movable seed is increased by using different lengths of natural thorium in some of the seed and blanket rods; this concept is shown in Figure II-2. When the reactor is shut down, the seed assemblies are below the rest of fuel in the core as shown in Figure II-2. To start up the reactor, the operator raises the seed assemblies in a uniform bank. By moving the seed fuel up, more nearly into alignment with the rest of the core, the operator brings the uranium-233 bearing parts of the fuel closer together.

The height of the fuel is shown in Figure II-4, which shows a Type I module with the seed aligned with the blanket. It is seen that in this configuration there are 6 axial fuel zones between the thorium reflectors; each such zone is 14 inches high. At the beginning of core life, critical operation occurs with the tops of the seeds about 2 feet lower than the top of the stationary blanket. As the core operates, the seed assemblies are moved gradually upward toward a position about 2 feet higher than the blanket at the end of core life. From an operator's point of view, the movable fuel control system is similar in many respects to that of the movable poison rod control used in many light water reactors.

A typical fuel module cross section is shown in Figure II-3. Cylindrical fuel pellets were stacked inside hollow Zircaloy-4 cladding tubes. These tubes were then welded to solid end plugs at both ends to form the fuel rods. The fuel pellets are thorium (ThO_2) or binary ($\text{ThO}_2\text{-U}^{233}\text{O}_2$) ceramic, nominally 97 percent of their theoretical density. A plenum region is provided in all rods to accept fission gases and volatiles released from the pellets during

operation which limits internal gas pressure buildup. A helical coil spring is installed at the top of the fuel stack to maintain the position of the pellet stack. The fuel zoning for a Type I module is shown in Figure II-4. The 3 central modules are Type I. All twelve seeds are of identical design. The 9 outer modules are Type II if there are 2 sides that are the power flattening blanket and Type III if there are 3 such sides (Figure II-1). In the power flattening blanket region the fuel zoning is such that there are ten rows of fuel rods, of which seven rows are high zone fuel. Details of the lattice geometry and fuel loading are given in Tables II-1 and II-2.

The fuel rods are supported by a system of grids, axially positioned in each fuel assembly. Table II-1 indicates the distribution of the grids, which are made of AM-350 stainless steel. Each assembly contains a Zircaloy shell which acts as both a structural member and a defining boundary. The seed and reflector shells surround the outer perimeter of these assemblies. The blanket shell (guide tube) is located on the inside of the annular blanket assembly and provides a guide path for movement of the seed fuel assembly. Support posts for grids in each assembly are located along the outer boundary of the fuel rod lattice, cf., Figure II-3. For seeds and reflectors, these posts are located just inside the shells and are connected to the shells.

There are structural metal pieces above and below the fuel assemblies which provide support and form regions of different metal/water ratio. These regions must be accounted for in the calculational model.

B. Implications of the Reactor Design for Neutron Calculations

There are a number of design features which are different in LWBR than in other PWR's and which can either complicate or simplify the calculational problem. These features are briefly discussed here from the point of view of the nuclear analyst.

The most significant design aspect is the U^{233} -Th fuel system. The use of this fuel system led to the need for an extensive analysis of available cross section data and other basic nuclear data for U^{233} and thorium which had previously been given less attention than U^{235} and U^{238} . The U^{233} cross section dependence on energy is particularly complex with broad resonances and strong multilevel effects. In addition, the U^{233} cross section interferes with thorium resonances and with the resonances of its own precursor Pa^{233} .

A highly accurate Monte Carlo analytical standard was developed as a substitute for a full core mockup critical. Partial core mockup experiments were used to qualify this calculational standard.

The use of thorium results in a strong Doppler coefficient of reactivity which is important in both steady state and transient analysis. The relatively dry fuel lattices (Table II-1) lead to a strong sensitivity of lattice properties to water content. Both of these temperature effects necessitated the incorporation of thermal feedback into the neutron calculations, so that the neutron distribution would be consistent with the temperature distribution in the core. Similarly, changes in the fuel pellet and cladding geometry under irradiation alter the water content and fuel temperature in the lattices and had to be accounted for in calculating the neutron distribution.

The movable fuel control system used for LWBR tends to produce power peaks at interfaces between binary and thoria regions. In Figure II-4, the thoria regions in the rod rows with shorter binary fuel stacks are called thoria step or wedge regions. Power peaks along this thoria-binary interface and the rapid fuel temperature changes across the interface had to be accounted for in the nuclear model.

The movable fuel control system also gives added importance to accurately describing transport of neutrons from one region to another. This includes neutron leakage from seed to blanket, from binary region to thoria step region, cross core leakage from one module to another, and from fuel regions to metal-water regions above or below the fuel. Besides the direct transport of neutrons between regions, the effect of the transport on the neutron energy spectrum within a region must be considered. Except for the thoria steps the fuel zoning is radial, and the module dimensions are such that material changes occur more rapidly in the radial direction than in the axial direction. This aspect of the design provides a simplification for calculating neutron leakage.

TABLE II-1. LWBR CORE NOMINAL CHARACTERISTICS

	<u>Seed</u>	<u>Regular Blanket</u>	<u>Power Flattening Blanket</u>	<u>Reflector Blanket</u>
Rod OD (in.)	0.306	0.5715	0.5275	0.832
Clad thickness (in.)	0.0220	0.02775	0.02625	0.042
Grid thickness (in.)	0.0135	0.014	0.014	0.018
Grid volume/rod (in. ³)	0.1576	0.2592	0.2592	0.4300
Number of grid levels	9	8	8	6
Rod center-center spacing (in.)	0.369	0.630	0.630	0.900
Metal/water volume ratio*	1.726	2.981	1.752	3.506
Total number of rods	7428	3234	3581	3047
Total fissile loading (kg)**	198.6	116.3	186.1	None
Total Th-232 loading (kg)**	5206.5	9487.1	8788.3	18574.2

*Under nominal hot full-power conditions and assuming grid material homogenized throughout the fuel region.

**As built loadings indicated.

TABLE II-2. LWBR AS-BUILT CORE FUEL CHARACTERISTICS**

	Fellet OD (in.)	Pellet Length (in.)	U-Fissile (w/o)*	U-Fissile (grams/in.)	Fissile Loading (kg)	Loading Th-232 (kg)
<u>Seed</u>						
Thoria	0.2555	0.530	None	None	None	1846.6
Low zoned	0.2520	0.445	4.337	0.3416	61.28	1179.5
High zoned	0.2520	0.615	5.202	0.4114	137.31	2180.4
<u>Regular Blanket</u>						
Thoria	0.5105	0.615	None	None	None	3670.0
Low zoned	0.5105	0.530	1.214	0.3920	15.99	1141.6
Medium zoned	0.5105	0.870	1.668	0.5421	42.68	2205.9
High zoned	0.5105	0.785	2.005	0.6498	57.67	2469.6
<u>Power Flattening Blanket</u>						
Thoria	0.4695	0.445	None	None	None	2632.4
Low zoned	0.4695	0.870	1.654	0.4537	10.24	533.5
Medium zoned	0.4695	0.785	2.009	0.5509	13.58	580.1
High zoned	0.4695	0.700	2.739	0.7492	162.29	5042.3
<u>Racial Reflector Blanket</u>	0.7415	0.740	None	None	None	18574.2
TOTAL					501.04	42056.1

U Isotopic Composition

U-232	<0.001 w/o
U-233	98.23
U-234	1.29
U-235	0.09
U-236	0.02
U-238	0.37

$$*U\text{-Fissile (w/o)} = \frac{U\text{-233} + U\text{-235}}{UO_2 + ThO_2} \times 100$$

**Dimensions are nominal design values.
Loadings are as-built values.

Figure II-1. LWBR Cross Section and Module Identification

Figure II-2. LWBR Movable Fuel Control

Figure II-4. R-Z Schematic of Type I Module

III. GENERAL DESCRIPTION OF THE NUCLEAR CALCULATIONAL MODEL AND THE QUALIFICATION PROCEDURE

The expended LWBR is expected to contain about 1.2 percent more fissile fuel than it started with. The need to accurately describe the core performance, especially the small margin of breeding, imposed a need to develop a sophisticated calculational model and to test the degree of accuracy of the model. This section provides a summary description of the nuclear calculational model and the qualification procedure. A detailed description is provided in Chapters IV through VIII.

A. Nuclear Calculational Model

1. Input

A block diagram of the LWBR nuclear calculational model is presented in Figure III-1. The basic data input to the model are of 2 kinds - as-built core data and nuclear data. The as-built core data represent averages for each fuel zone, such as high zone seed, medium zone regular blanket, etc (Figure II-4). Data for each fuel rod and rod support grid were measured during core manufacture and input to a computer program for processing. The data include the weights of fissile and fertile fuel in each rod, isotopic distributions, pellet and fuel stack geometry, cladding diameter and wall thickness, and grid cell pitch and grid weight. As-built measurements were also used for the Zircaloy shells which bound the fuel rod assemblies. Nominal design data were used for the structural content above and below the fuel rods.

Averages of data from manufacturing are input to a computer program, PREP1, which converts the data into atom densities and geometry for fuel rod unit cells. The fuel rod unit cell is the basic repetitive unit in the assemblies and consists of a pellet stack, cladding tube, and an apportioned amount of water and structure. PREP uses the fuel rod cells and module-to-module pitch to construct seed and blanket assemblies. From these, PREP determines the dimensions of the channel regions that separate a seed from the surrounding blanket or one blanket from another. The unit cell information passes by computer file from PREP to the energy spectrum computer program PAX. The channel dimensions are used to set up input for the diffusion-depletion program PDQ. PREP also supplies fast advantage factors, which account for fuel rod cell heterogeneities, to PAX and fuel pellet conductivities for PDQ.

The cross section data came from the national Evaluated Nuclear Data File (ENDF), a Bettis evaluation, or another external evaluation. The data, in the form of resonance parameters or multigroup data, are processed and stored in a central repository for nuclear data called the XAP library (Reference III-1). From the main XAP library, the cross section generation code RCPL1 (Reference III-2) constructs a job library which includes detailed energy dependent cross section profiles constructed from resonance parameters. Such a job library is used as input to an RCP analytical standard calculation. A somewhat smaller job library together with the main XAP library is accessed by the energy spectrum program PAX (References III-3 and III-4).

2. PAX

The PAX program is one of two main parts of the LWBR calculational process (the other part being PDQ) and, as such, performs several major functions. The energy range from 0 to 10 Mev is divided into a thermal range from 0 to 0.625 ev and a fast range from 0.625 ev to 10 Mev. The fast range is further divided into 54 multigroups. For each fuel zone and each metal-water region, PAX computes infinite media (or simply buckled) flux spectra by multigroup and averages microscopic and macroscopic cross sections over the spectra. These spectral calculations were formerly performed by the MUFT and KATE codes, which have been subsumed within PAX. A special heterogeneous resonance calculation precedes the fast spectrum calculation. This resonance calculation is based on collision probabilities in a fuel rod unit cell infinite lattice and requires the RCPL1 resonance profiles as input. The resonance calculation uses ideas similar to the ZUT program (Reference III-5) and is sufficiently accurate that no self-shielding or mutual-shielding correction factors are needed. A "resonance escape probability" which includes both resonance and smooth cross sections is fed to the spectrum calculation for each multigroup and each isotope. With the unit cell heterogeneities accounted for by the fast advantage factor and resonance escape probabilities, the materials are homogenized and the fast flux spectrum is computed for the homogenized cell.

The output of the infinite medium calculations consists of cross sections for a "few-group" model. For the LWBR model there are 3 "few-groups" covering the fast energy range: 10 Mev to 0.8 Mev, 0.8 Mev to 5.5 Kev, and 5.5 Kev to 0.625 ev. The fourth few-group is the thermal group, and PAX includes a thermal disadvantage factor in the thermal cross sections of fuel rod cells which is

based on the Multiple Sauer approximation (Reference III-6). The thermal flux spectrum is then also computed for the homogenized cell. It has been observed by comparison to experiment that the LWBR model best matches power peaks near metal-water channels when the thermal few-group cross sections are a variant of the mixed number density scheme (Reference III-7). The variation is to use a diffusion coefficient midway between the softer Maxwellian and harder Wigner-Wilkins coefficients.

For each unit cell representing a fuel zone, a point depletion calculation is performed by PAX with enough depletion to at least cover the most depleted point in that fuel zone in the core. Microscopic cross sections for each few-group and isotope may be stored as functions of depletion in the form of accumulated fission density. Each such function is a table, and a computer file is automatically created containing a set of such tables. When the tables are used later in PDQ, an interpolation scheme is provided to obtain fission densities between the tabulated points. At selected time steps in the PAX depletion the moderator temperature or fuel temperature is varied and the infinite medium cross sections are recalculated. Tables are also stored containing these temperature effects for use in the thermal-hydraulic calculations in PDQ. Sensitivity studies were done to assess the magnitude of the cross section variations and their effect on core performance. Based on these studies certain cross sections are stored as functions of fission density (F/CC), hydrogen atom density (N_H), and fuel temperature ($\sqrt{T_F}$); certain cross sections are stored as constants, independent of F/CC , N_H , and $\sqrt{T_F}$; and other cross sections have intermediate complexity.

Comparisons to more accurate calculations indicated that the fast few-group cross sections produced from infinite media spectra led to significant errors in reactivity and reaction rate distributions. To improve the spectrum calculations, multigroup one-dimensional traverses or slices were run horizontally through the core. Originally these calculations used the P7MG option in PAX (Reference III-8) in a low order of transport; however a Discrete Ordinate Solver (DOS) has been added to PAX and is also being used. The one-dimensional traverses were run at sufficient axial positions to describe the varying fuel zoning. They start at the center of a module and run either to the edge of the module or to the edge of the core. The one-dimensional approximation works in LWBR because the material changes occur more rapidly radially than axially in the core. Few-group cross sections for prescribed spatial regions are stored in computer files. A program called PECOS accesses the files of DOS cross sections and infinite medium cross

sections and computes ratios using beginning of life uranium and thorium inventories. These ratios are collected with the other PAX output in table sets and are applied as constant correction factors to the time and temperature dependent infinite medium cross sections.

3. CINDER

The three most important fission product chains, or series of reactions, are treated explicitly in the PAX depletion and in PDQ. The rest are described by a fission product "residual" which is computed using the CINDER program (Reference III-9). Few-group cross sections for isotopes in the fuel chains and fission product chains are input to a CINDER library. Few-group flux values as a function of time are obtained from a previous PDQ depletion for each fuel composition and are input to CINDER. Then two CINDER's are run for each fuel composition, one with the chains as used in PAX and PDQ, and one with 69 chains that describe essentially all the fission product absorption. The difference in total fission product absorption between the two CINDER's, expressed as barns per accumulated fissions, characterizes a fission product residual and is input to PAX and PDQ by few-group.

4. PDQ

All of the output data from PAX, PECOS, and CINDER, which are fed through PAX, are merged into one computer file called a HARMONY file. The HARMONY system (Reference III-10) is the part of PDQ which does the depletion calculation using the table sets of nuclear data. For LWBR, the PDQ program (Reference III-11) solves the diffusion-depletion equations in 3 spatial dimensions in hex,z geometry; that is, the horizontal planar geometry has fuel rods on a triangular pitch so hexagonal fuel assemblies may be described. The detailed structure of the fuel rod unit cell no longer appears in the PDQ nuclear calculations, the cells having been homogenized in PAX; but the fuel zones are described and no spatial synthesis is involved. One exception to the use of PAX data is the calculation of special removal cross sections for support post regions using Monte Carlo. Some of these regions are near power peaks and cannot be described even with one-dimensional PECOS correction factors.

Four energy groups (few-groups) are used, with the lower 3 groups using P_1 diffusion theory. Comparisons to experiment and to more accurate calculations indicated that diffusion theory would not adequately describe high energy neutron

leakage for all the configurations encountered. The simplified-P3 transport approximation is used in the highest energy few-group, resulting in a total of 5 diffusion-like equations for the 4 groups.

The program includes the capability of moving the fuel regions prior to a spatial flux calculation. The flux in each few-group is computed at over 200,000 spatial mesh points, describing a symmetric 1/6 of the LWBR core. One-sixth core symmetry is an assumption which neglects the 8 flux wire wells in the core, each of which replaces a single fuel rod. Both radially and axially, homogenized metal-water regions beyond the thorium reflector blankets are included. The depletion is done over a coarser grid than the spatial flux solution, there being about 64,000 "depletion blocks" (covering both fuel and metal-water regions) over which the material inventories are homogeneous.

The power distribution from the neutron calculation forms the heat generation rate in the thermal-hydraulic calculations in PDQ. One-dimensional axial flow is described up coolant channels or "tracks" between fuel rods; no mixing between tracks is described in the LWBR nuclear calculations. (The thermal-hydraulic performance analysis of LWBR is not done with PDQ. Thermal-hydraulic calculations within PDQ are used only to determine temperature distributions to improve the nuclear analysis.) A one-dimensional axial calculation of moderator temperature and density is done for each track; and at each axial height in the thermal-hydraulic grid, a one-dimensional radial calculation of the fuel pellet temperature in a fuel rod is performed. The thermal-hydraulic grid for LWBR is the same as the depletion block grid. Given the fuel and moderator temperature distributions, new cross sections are computed from the table sets which include the effects of revised Doppler broadening and moderator densities. Then the neutron flux distribution is recomputed. Generally, one such temperature feedback iteration is done in LWBR at each spatial calculation, though more than one has been used when appropriate. The result is that the neutron and temperature distributions are consistent with each other.

A calculation of the time-dependent clad diameter is incorporated in the thermal-hydraulic equations in PDQ. The clad diameter decreases with fast neutron irradiation until it is constrained by the fuel pellet. The swelling of the fuel pellet due to pellet temperature and accumulated fissions is also computed. After the swelling of the pellet is such that sufficient pressure is exerted on the clad, the clad diameter begins to increase. The clad diameter variation affects

the water content in the fuel lattice. The clad and pellet diameter variations, as well as the accumulated fissions, also affect the heat conduction in the pellet-to-clad gap; and together with the depletion-dependent pellet conductivity, a revised fuel temperature is obtained. Thus the inclusion of depletion-dependent pellet and clad properties was required to provide for the correct interaction of nuclear and thermal-hydraulic calculations.

Another feedback loop in PDQ, in addition to temperature feedback, is equilibrium xenon feedback. After each depletion timestep, when new nuclide concentrations are available, a new spatial flux solution is obtained. The equilibrium xenon and iodine distributions are then modified to be consistent with the new flux and the flux is recalculated.

The output from PDQ at each time in life is processed for several purposes. Nuclear analysis requires nuclide inventories and power and flux distributions. Thermal-hydraulic and fuel element analyses require power (heat flux) distribution data in different formats. Structural analysis requires heat flux and fast neutron flux distributions. Each need has been met by accessing the files of data stored by the computer for PDQ and computing the individual functions for each discipline using a special purpose program. Then the individual disciplines are provided either with edits of the functions or with computer files which can be read by their own analysis programs.

B. Qualification Procedure

A series of critical experiments including partial mockup experiments was performed to determine the degree of accuracy of the calculational model. Calculations of these experiments were done throughout the evaluation of the core design and the nuclear model. The partial core mockup consisted of a single Type II module surrounded by a uranium-fueled driver region and a thorium reflector. The seed assembly was movable in the mockup, as in the core, permitting the study of mockup properties as a function of fuel position.

A variety of neutron activation results from the experiments were examined. These contributed to the development of particular aspects of the model as discussed in Chapter IV. The most important comparisons between calculation and experiment were reactivity (multiplication factors) and power distributions which test the overall model. The problem arose as to how the bias between calculation and experiment for the critical experiments, in either power distribution or reactivity, should be related to the full core.

1. Reactivity

For reactivity, the connection between the critical experiments and the full core was made by developing a highly accurate analytical standard which could calculate both the experiments and the full core. The analytical standard is a Monte Carlo solution to the neutron transport equation with a particular set of neutron cross section libraries and is embodied in a computer program called RCP, written for the CDC-7600 computer (Reference III-12). The computer program was developed along with the core design and the nuclear model, and produces an "essentially exact" solution of the steady state transport equation in a core. This means that the core is represented in great geometric detail, energy and angular dependencies of the neutron cross sections are shown in substantial detail, and minimal calculational approximations are used. The limitations of RCP are that there is no depletion and no solution of thermal-hydraulic equations. In addition, the user imposes a practical limit on grinding down statistics and source convergence of the eigenfunction. For the calculation of a critical experiment, the main error expected is that due to the cross section data themselves.

RCP calculations were done for a variety of U^{233} and Th fueled critical experiments, including several seed positions in the partial mockup. The seed positions in the partial mockup spanned the range to be encountered throughout most of core operation. Temperatures in the experiments ranged from ambient to 477°F, compared to an average moderator temperature of about 530°F in the core.

The experiments also covered a wide range of geometric configurations, a wider range of material inventories than the design core, and they all included ThO_2 , $U^{233}O_2$, water, and Zircaloy. From the set of calculated multiplication factors an average bias between the analytical standard and experiment was obtained, and the associated variance in the bias was also obtained. This bias, RCP-Exp, is used for all conditions of core operation. Some basic cross section data which are used in the full core calculations were not tested in the critical experiments. These include data for fission products and other isotopes which build up during depletion, and Doppler effects at high power where the fuel temperature is considerably above the water temperature. The uncertainty in the predicted multiplication factor must therefore be increased from the variance in the RCP-Exp bias.

The analytical standard, with a consistent set of nuclear data libraries, was also used to calculate the full core at beginning of life. Although thermal-hydraulic feedback is not part of the RCP program, fuel temperatures characteristic of high power operation were used in the RCP calculations of the full core. Thus the Doppler broadening of thorium (and other) resonances at high power was described. In this way, the analytical standard together with the critical experiments provide a standard of truth for reactivity which extends the conditions covered beyond those that a mockup alone could provide. This extension is important for LWBR since about 2 percent in core multiplication factor is tied up in the "power defect," i.e., in the fuel temperature rise from essentially zero power with the moderator at operating temperature to full power.

The culmination of the reactivity predictions in the nuclear calculational model is the set of diffusion-depletion calculations done with the PDQ computer program (Reference III-11). A special PDQ calculation, done consistent with the RCP full core calculation at beginning of life, provides a bias between the nuclear analysis model and the analytical standard. The net reactivity bias is then taken as

$$\text{PDQ-Exp} = (\text{PDQ-RCP}) + (\text{RCP-Exp})$$

For later times in life, material inventories from the PDQ depletion calculations are averaged over specified core regions and consistent pairs of RCP and PDQ problems are run to generate a time-dependent reactivity bias, PDQ-RCP. These PDQ versus RCP comparisons constitute another extension of the truth standard provided by the analytical standard by showing considerably more depletion detail than a mockup could attain, including region-dependent concentrations of Xe^{135} , U^{234} , and Pa^{233} , as well as U^{233} and Th^{232} .

In summary, the nuclear calculational model is qualified by first qualifying the analytical standard against experiment. Then, with the degree of accuracy of the analytical standard known, the nuclear model is tested against the analytical standard using full core calculations.

2. Power Distributions

Regional power fractions are also examined using the analytical standard to demonstrate the adequacy of the nuclear model for describing the core. When discrepancies occur between calculation and experiment, the analytical standard

makes it possible to separate discrepancies due to cross section data or uncertainty in the constitution of the critical experiment from discrepancies due to approximate methods used in the nuclear model.

Since the analytical standard makes use of a Monte Carlo program, it is not possible to examine the power at points throughout a core or in fuel pellet-sized volumes throughout a core. The computer expense is such that these "local" or pointwise power distributions must be obtained from deterministic computer codes. Three-dimensional power distributions were measured for the partial core mockup, called the Detailed Cell, in sufficient detail to construct radial and axial power maps for various seed positions (Reference III-13). Direct PDQ calculations of these experimental power distributions yielded experiment-to-calculation (E/C) correction factors, or allowances, for the different configurations of the partial mockup. Since the partial core mockup was much smaller than the full core, it was not appropriate to take a local E/C factor from a particular location and seed position and apply it directly to a "corresponding" location in the full core. The environment of any point in the partial mockup is not the same as the environment in the full core. Rather, the totality of E/C data from all seed positions was examined together. Factors for each rod type were then chosen to correct the PDQ power distributions of the full core and account for the whole variety of experimental data for that rod type. For example, an E/C factor was chosen for the seed rods with 42 inches of low zone binary fuel (Figure II-4). This factor accounts for the worst possible underprediction of local power that would be expected in this type of seed rod in the full core, based on all the seed data from the experiments. This factor was then applied to PDQ power predictions at all points in the 42-inch binary seed rods in the full core to assure that a conservatively high local power estimate would be used for establishing the core power capability. Similar E/C factors were chosen for the other rod types in the seed, regular blanket, power flattening blanket, and the reflector blanket.

3. Breeding

The quantities which describe breeding performance are the conversion ratio (CR) and the fissile inventory ratio (FIR). The CR is the ratio of the instantaneous fissile production rate to the instantaneous fissile destruction rate. The FIR is the ratio of the fissile content at any time in life to the fissile content at beginning of life, and is a time integral which depends on the CR.

There are two basic quantities that determine the CR. One is the value of η of U^{233} and the other is the neutron capture competition between thorium and parasitic materials. Since the reactor is critical at some power level, for every neutron absorbed by U^{233} , there are $\eta-1$ neutrons remaining which are shared among thorium, water, cladding, structure, and the products of burnup. The fraction of the remaining neutrons which thorium absorbs determines the fissile production rate.

The η of U^{233} is qualified as follows. First, the basic nuclear data are tested against direct measurements of η . Accurate predictions of η require both accurate nuclear data and accurate predictions of the neutron energy spectrum because η is a complex function of energy. Since the multiplication factor is proportional to η , the wide variety of critical experiments which have been analyzed test the average η in those cores. The experiments include simple geometric configurations without thorium as well as the LWBR criticals discussed previously.

The qualification of the calculation of neutron competition between thorium and parasitic materials is really the qualification of the whole model. This competition is affected by the cross sections of the isotopes and by the relative absorptions in one region versus another. The neutron cross sections and other nuclear data are individually tested as part of the preparation of the nuclear data library. The different parts of the model which enter the calculation of the neutron distribution in space and energy are also individually tested. The overall model is tested by measuring three-dimensional power distributions and critical configurations as discussed previously.

The Monte Carlo analytical standard is used to obtain a bias in CR for the nuclear analysis model. Similar to the reactivity comparisons, the bias is obtained at beginning of life using fuel temperatures characteristic of high power operation. Then the bias is obtained for later times in life using consistent pairs of PDQ and RCP problems with material inventories from the PDQ depletion calculation.

4. Other Qualification Procedures

In addition to the overall qualification procedure of the nuclear model described above, individual parts of the model were tested against more exact calculations or against experiments during model development. These tests will be described in later sections dealing with the individual parts of the model or in Chapter VIII.

REFERENCES

- III-1. A. F. Henry, "54 Group Library for P-1 Programs," WAPD-TM-224, April 1960. The XAP library is an updated and extended system which includes the functions of this reference and the thermal library of Reference III-4.
- III-2. A. V. Dralle, N. R. Candelore, and R. C. Gast, "RCPL1 - A Program to Prepare Neutron and Photon Cross Section Libraries for RCP01," WAPD-TM-1268, August 1978.
- III-3. H. Bohl, Jr. and A. P. Hemphill, "MUFT-5, A Fast Neutron Spectrum Program for the Philco-2000," WAPD-TM-218, February 1961. Updated versions of MUFT and KATE (Reference III-4) are contained in the PAX program for the CDC-6600 and 7600 computers.
- III-4. H. J. Amctor and J. B. Callaghan, "KATE-1 - A Program for Calculating Wigner-Wilkins and Maxwellian Averaged Thermal Constants on the Philco-2000," WAPD-TM-232, October 1960.
- III-5. L. W. Nordheim, "A Program of Research and Calculations of Resonance Absorption," GA-2527, August 28, 1961.
- III-6. A. J. Buslik, "Calculational Method for Thermal Disadvantage Factor," Nuclear Science and Engineering 38 (1969) 71.
- III-7. R. J. Breen, "A One-Group Model for Thermal Activation Calculations," Nuclear Science and Engineering 9 (1961) 91.
- III-8. H. Bohl, Jr., et al, "P3MG1, A One-Dimensional Multigroup P-3 Program for the Philco-2000 Computer," WAPD-TM-272, September 1963. The P7MG option in PAX is an extended version of this reference.
- III-9. T. R. England, "CINDER - A One-Point Depletion and Fission Product Program," WAPD-TM-334 (Revised), June 1964. Also, T. R. England, R. Wilczynski, and N. L. Whitmore, "CINDER-7: An Interim Report for Users," LA-5885-MS, April 1975.
- III-10. R. J. Breen, O. J. Marlowe, and C. J. Pfeifer, "HARMONY: System for Nuclear Reactor Depletion Computation," WAPD-TM-478, January 1965.
- III-11. C. J. Pfeifer and C. J. Spitz, "PDQ-8 Reference Manual," WAPD-TM-1266, May 1978.

- III-12. N. R. Candelore, R. C. Gast, and L. Ondis, "RCP01 - A Monte Carlo Program for Solving the Neutron and Photon Transport Problems in Three Dimensional Geometry with Detailed Energy Descriptions," WAPD-TM-1267, August 1978.
- III-13. G. G. Smith, J. P. Semans, J. A. Mitchell, et al, "²³³U Oxide-Thorium Oxide Detailed Cell Critical Experiments," WAPD-TM-1101, October 1974.

Figure III-1. LWBR Nuclear Calculational Model

IV. DETAILED DESCRIPTION OF THE PRE-PDQ MODEL

A. Material Inventories and Homogenization

The accurate prediction of LWBR core lifetime, breeding, and power capability using the PDQ program and the post-PDQ engineering analysis programs required an accurate description of the core geometry and material inventories. Throughout the manufacturing stage of LWBR, sufficient as-built data were taken, recorded, and filed to ensure that the core met all design requirements. A subset of the data on file was stored on the CDC-6600 using the ASBLT as-built data collection and evaluation system. One important use for the computerized data and one important function of ASBLT is to provide an accurate description of the as-built fuel regions of the LWBR core in terms of input for the pre-PDQ program PREP.

The PREP program was developed during the design stages of LWBR and accepts dimensions from design drawings and computes input for the PAX and PDQ programs. In the as-built analysis, of course, the PREP input describes the as-built core rather than the nominal core. PREP performs the homogenization of material inventories and computes fast advantage factors which are part of the fuel lattice heterogeneity model described in IV.C. Input data generated by PREP for PAX and PDQ are written into computer files and linked automatically to those programs.

1. As-Built Material Inventories

The LWBR core contains approximately three million fuel pellets in 17,290 fuel rods assembled into 12 seed and blanket modules and 15 outer reflector blanket modules. The structure in each module consists of shells or cans which bound the rod assemblies, grids which support the rods, and grid support posts which hold the grids in the module. Approximately 1.6 million of the fuel pellets are binary (uranium oxide-thorium oxide) and the other 1.3 million are thorium (thorium oxide). Figure IV-1 shows the cross section of a generalized fuel pellet with end dishes, tapers, and chamfers.

Each powder blend, either binary or thorium, received a unique blend designation which was also used to identify the pellets made from that blend. A representative sample of pellets from a blend was taken and used to determine the characteristics of the blend. The pellet properties which were measured and needed for the as-built PDQ were length, diameter, and weight for all pellets in the sample, and weight percent of total uranium and uranium isotopic weight percents for binary pellets. Length, diameter, and weight were used to compute

pellet density assuming nominal design corrections for tapers, chamfers, and end dishes. The above properties for binary pellets were stored in a computer file for each binary blend manufactured and used to compute uranium and thorium loadings of binary fuel rods. The properties for thorium pellets were averaged for each of the four regions - seed, standard blanket, power flattening blanket, and reflector blanket - but not stored on the computer.

During fuel rod fabrication, pellets were stacked in a vee trough. The binary and thorium stacks were weighed and their lengths were measured. These data, along with the identities of the blends used in the rod, were entered into the computer and stored. The fuel rod data files and the binary blend data files were then used by one of the ASBLT options to compute the uranium and thorium loadings of each fabricated fuel rod. The clad thickness and rod outer diameter of each rod were also measured and these data were added to the ASBLT files.

During module assembly, the rod serial number, the installation sequence number, and the grid cell identity in the module were entered into the computer. These rod location data were then added to the rod fabrication data contained in the ASBLT files. With this information, ASBLT computed the fuel loadings of each module and the characteristics of each fuel composition to be described in PDQ.

Homogenized nuclide concentrations for fuel compositions in PDQ are computed by the PREP program. For fuel compositions, PREP requires input which describes the fuel pellets, the clad and the hexagonal arrangement of fuel rods. During the design stage this information had been taken from design drawings. For as-built calculations, the ASBLT system was programmed to collect data by composition (high zone seed, low zone standard blanket, etc.) and to compute the following input required by PREP for binary compositions:

- a. Root mean square rod outer diameter.
- b. Clad thickness (from root mean square rod inner diameter and item a).
- c. Pellet-clad gap thickness (from mean pellet area and item b).
- d. Mean void fraction (missing pellet volume due to end dishes, tapers, chamfers, and chips).
- e. Mean fraction of theoretical density.
- f. Mean weight percent of uranium oxide.
- g. Relative abundance of each uranium isotope (isotopic mix) by weight in the uranium.

For the thoria compositions in the PDQ, ASBLT computes items a through d only and requires that the mean pellet outer diameter and density fraction be furnished from the inspection results on the thoria samples.

The as-built fuel stack lengths (averaged for each composition) do not exactly equal the nominal values. It is impractical, however, to set up the PDQ axial mesh to exactly match the as-built lengths. Therefore, nominal stack lengths are used in PDQ for cold calculations and an axial expansion factor is applied to the lengths for hot calculations with the inverse of the factor applied to fuel and clad density to preserve inventories. Since nominal fuel stack lengths are used in PDQ, the total fissile loading and the grams of fissile fuel per inch of stack height cannot be simultaneously matched to as-built data. In the LWBR model the total fissile loading of each of the eight binary fuel zones is exactly matched to as-built data to assure an exact initial inventory for breeding calculations, and the weight percent of uranium oxide computed for PREP is made consistent with that choice.

Since all clad thickness and outer diameter measurements were taken during manufacturing at room temperature, ASBLT computes mean values for cold calculations directly from the data. Radial thermal expansion and beginning of life clad shrinkage effects are accounted for by supplying ASBLT with a perturbation on clad diameter. The program then computes hot rod diameters and clad thicknesses given the diameter change, preserving clad volume.

As discussed above, the ASBLT system was designed to automate the collecting and processing of the large quantity of as-built binary pellet data and fuel rod data. Other computer programs processed and evaluated grid inspection data and furnished root mean square grid cell pitch (cell center to center spacing) values for each fabricated grid. Completed grids were weighed and the weights and grid material density were used to determine the grid volume and the as-built grid area per rod required by PREP. The thermal expansion of the grid cell pitch and the grid volume were accounted for in PREP for hot calculations to obtain the correct water content in the fuel lattice. As-built dimensions for module cans and shells and grid support posts were obtained from inspection records, averaged, and input to PREP as required. For structure and water regions above and below the fuel bearing regions, nominal dimensions were used to compute material volume fractions for input to PREP.

This section has described the method whereby as-built fuel pellet, fuel rod, grid, and structure data were collected and transformed into input for the PREP program, a pre-processor for PAX and PDQ, with the goal of describing in PDQ as accurately as possible the as-built condition of the core. The next section will describe the model used by PREP to homogenize the material concentrations for use in PDQ.

2. Homogenization of Material Concentrations

The PREP program computes, among other parameters, homogenized nuclide concentrations for fuel regions and for nonfuel regions. In the case of fuel regions the input parameters required by PREP are pellet and clad dimensions, rod lattice pitch, fuel density fraction, uranium oxide weight percent, uranium isotopic mix, grid area per rod, and fuel stack heights. With this input PREP constructs a unit cell - i.e., a hexagonal area whose across-flats distance equals the rod pitch - containing fuel, void, clad, grid, and water (Figure IV-2). In general, a fuel pellet is cylindrical and has end dishes, tapers, and chamfers. It can have some surface volume missing due to chipping. In as-built analyses, ASBLT computes an overall pellet void fraction which accounts for the as-built end dishes, tapers, chamfers, and chips. The pellet input, therefore, for as-built analyses consists of pellet diameter, $\bar{d}$, and void fraction, $\bar{f}_v$. The equivalent diameter, d_c , of the fuel pellet within the unit cell is computed by PREP as follows:

$$d_c = \bar{d} \sqrt{1 - \bar{f}_v} .$$

A fuel region in PREP contains as many unit cells as there are rods in that fuel region. For example, the seed region of one LWBR module contains 619 fuel rods. The seed is described in the PREP input by identifying that the first seed rod row contains 1 rod (center of module), that the seed contains 15 rod rows, and that the last row is missing 12 rods to allow room for grid supports. Such a pattern of rods on a triangular pitch produces 619 rods. Therefore, the area of the seed region, A_s , having an average rod pitch P_o is computed as follows:

$$A_s = 619 \frac{\sqrt{3}}{2} P_s^2 = \frac{\sqrt{3}}{2} D_s^2 ,$$

where the seed across-flats distance is D_s .

A type I blanket region is described in PREP by identifying 60 cells in the first blanket row, 6 rows, and 6 rods missing from row 6 to allow room for the

grid supports. Since the blanket is an annular region, PREP must compute the across-flats distances for both the inner and outer boundaries. This is done by determining the number of cells present in an imaginary region within the blanket annulus. Since there are 60 cells in the first blanket row, the next inner row would have contained 54 cells, and each successive row toward the center would have contained 6 fewer cells than its outer neighbor all the way to the center row which would have contained one cell. Therefore, the number of cells in the imaginary region is 271. Given the blanket rod pitch, P_b , PREP computes the inner across-flats distance for the region as follows:

$$D_i = \sqrt{271} P_b .$$

The total number of unit cells in the blanket region (type I) is 444. PREP computes the area and the outer across-flats of the blanket region, A_b and D_o , as follows:

$$A_b = 444 \frac{\sqrt{3}}{2} P_b^2 ,$$

$$D_o = \sqrt{271 + 444} P_b .$$

The inner and outer boundaries of adjacent regions are used by PREP to determine the boundaries of metal-water regions between fuel regions.

A PREP composition, which in turn becomes a PDQ composition, is described by assigning fuel stack heights to each row of a fuel region. After computing the volume fractions of fuel, void, clad, grid, and water for a fuel composition based on the unit cell, PREP computes homogenized nuclide concentrations based on the fuel properties (density fraction, UO_2 weight percent and uranium isotopic mix), the clad material concentration, the grid material concentrations, and the water temperature and pressure. A mesh is generated for PDQ whereby at least one mesh interval spans a rod row. The mesh is generated such that the area of each rod row in PDQ equals the area of 1 unit cell times the actual number of cells in each row. Much of the temperature feedback input required by PDQ is generated by PREP - including reference moderator densities and temperatures, reference fuel temperatures, flow areas, heat transfer areas, pellet dimensions, and fuel thermal conductivity tables. All input for PDQ is written into a computer file which is then read by PDQ. PREP also writes a file for the PAX program containing the material, region, cell, and temperature feedback input.

PREP treats nonfuel regions in either of two ways: Channels between fuel regions can be described by specifying structure dimensions; regions above

and below the core can be described by specifying the material identifications and volume fractions. In the case of channels, the PREP input must identify the fuel regions on either side of the channel, the dimensions of hexagonal cans and/or shells, and the area of any other structure to be included. The outer boundary of the inner fuel region becomes the inner boundary of the nonfuel region, and the inner boundary of the outer fuel region becomes the outer boundary of the nonfuel region. The structure dimensions and channel dimensions are then used to compute material volume fractions which, in turn, are used to compute homogenized concentrations of hydrogen, oxygen, and structure nuclides. When metal volume fractions and material identifiers are input, PREP simply computes homogenized concentrations. The homogenized concentrations for nonfuel regions are written into a computer file for PDQ, and material, region, and cell descriptions are written into a file for PAX.

B. Nuclear Data

The accurate description of basic nuclear data is paramount to LWBR because of the small margin in core breeding. Uncertainties in the nuclear data are the largest contributors to uncertainties in breeding predictions. The use of the U^{233} -Th fuel system, however, involved isotopes which had been given less attention than those in the U^{235} - U^{238} fuel system. For these reasons, an extensive analysis of all nuclear data of importance to LWBR was conducted. Most of the resulting data base resides in a central repository called the XAP library.

The relative importance of various nuclides to LWBR is indicated by the ordered absorption fractions in Table IV-1. The fission product isotopes explicitly named in this table include those which are explicitly calculated in the 3 fission product chains in PDQ, and which lead to Xe^{135} and Sm^{149} . There are other fission product isotopes which are important and appear in Table IV-1 as part of the last item. This will be discussed further in later sections. The present section will briefly describe the data and how it is processed.

1. Thorium

Throughout core life thorium-232 is the largest single absorber in LWBR, accounting for 46 percent of all neutron absorptions. Thorium absorptions occur predominantly through the radiative capture reaction and, at high energy ($E > 1.5$ Mev), through fission. The fast fission reaction in Th^{232} constitutes almost 3 percent of all fission events. Other neutron interactions with Th^{232} of importance to LWBR analysis include the (n,2n) reaction, which leads to formation of U^{232} , and elastic and inelastic scattering.

The radiative neutron capture cross sections are taken directly from the evaluation by Steen (Reference IV-1). The data are fully parameterized using the single-level Breit-Wigner formalism. The 0.0253 ev cross section is 7.345 barns. The energy dependence of the thermal cross section is $\propto 1/v$ and is defined by use of a collection of negative energy resonances.

The infinitely dilute $1/E$ weighted resonance integral above 0.5 ev is 85.2 barns which is consistent with the measured value of 85.9 ± 3 barns by Hardy (Reference IV-2). Between 1.4 and 25 Kev the resonance distribution is represented by the unresolved resonance model for s, p, and higher order distributions.

The adequacy of the data set has been tested by comparison of calculated and experimental shielded resonance integrals for thorium metal and oxide rods at room temperature and elevated temperatures (Reference IV-1). The rod sizes included in these tests cover a much broader range of conditions than those encountered in the LWBR core. The calculated results were found to be consistent with the experiments. Other evidence that the LWBR Doppler broadening treatment is valid has been obtained by calculating the power defect for the initial core installed in the Indian Point #1 power station (Reference IV-3). The calculated power defect, defined as the reactivity difference between hot zero-power and full-power conditions at beginning of life, agreed with the experimental value of 1.29 ± 0.15 percent Δk within the experimental error. In addition, the Th^{232} fast-to-thermal absorption ratio and the ratio of Th^{232} fission to U^{233} fission in D_2O moderated lattice experiments has been calculated with these data. The results were found to be in agreement with experiment (Reference IV-4). Similar calculations, based on the ENDF/B-III data for Th^{232} , produced errors substantially larger than those obtained with the Steen evaluation.

The shape of the energy dependent fission cross section is primarily based on the measurements of Pankratov (Reference IV-5) and Kalinin and Pankratov (Reference IV-6) which cover the energy range 3.0 to 16 Mev. The shape indicated by these measurements was renormalized to the measurement by Sergachev (Reference IV-7). Near the fission threshold energy the energy dependence of the cross section was based on Reference IV-8, normalized to Reference IV-6. The energy dependent neutron yield per fission is in agreement with the data of Condé and Holmberg (Reference IV-9).

The (n,2n) reaction cross section data are consistent with the measurements by Butler and Santry (Reference IV-10).

The inelastic cross section is based on the summation of individual level contributions below 2 Mev (Reference IV-11) and optical model fits to the integral data of Batchelor et al (Reference IV-12) above 2 Mev. The optical model calculation used a complex potential, with spin-orbit coupling and energy dependent magnitudes of the real and imaginary components of the potential energy and the effective radii. The exit energies were obtained using individual level data below 1.35 Mev and an evaporation model at higher incident energies. For use in design programs, the (n,2n) emission is incorporated into the inelastic transfer matrix. The resulting emission spectrum is softened by the lower energy (n,2n) neutrons.

The total elastic scattering cross section was obtained as the difference between total cross sections and all nonelastic cross sections and was adjusted to the total cross section integral measurements of Green and Mitchell (Reference IV-13). Tests of the scattering properties of thorium are described in Reference IV-14. The calculated age in a thorium-water lattice is within 8 percent of experiment but some deficiency in the high energy scattering is indicated, possibly requiring an increase in the inelastic scattering.

The Th²³² fission neutron spectrum is assumed to be the same as the U²³³ spectrum ($\bar{E} = 2.012$ Mev) in LWBR core calculations.

2. Uranium-233

The data of most importance to LWBR are those of U²³³. The absorptive reactions in U²³³ that are important are those leading to fission and radiative neutron capture. In addition, the number of neutrons produced per fission $\bar{\nu}$ and per absorption η are of primary importance to accurate prediction of breeding performance. The data files for these quantities and all other quantities describing neutron interactions with U²³³, as well as the fission neutron energy distribution, are consistent with ENDF/B-IV. These data are based on the evaluation reported in Reference IV-15. The thermal parameters have been revised slightly to be consistent with Reference IV-16. Revision was also made to the resonance parameters of Reference IV-15 to correct a mechanical problem associated with the original data set.

The 0.0253 ev parameters are: $\eta = 2.2972$, $\bar{\nu}_t = 2.4980$, $\sigma_f = 525.1$ barns, $\sigma_c = 45.9$ barns, $\alpha = 0.0874$ and $\sigma_a = 571.0$ barns. The thermal cross sections

for fission and capture are significantly non- $1/v$, and the energy dependence of the capture and fission cross sections are primarily based on the measurement by L. Weston, et al, (Reference IV-20). Comparisons of the resulting shapes of $\sigma_f(E)$ and $\eta(E)$ to experimental data show good agreement (Reference IV-16).

Other measurements of Weston, et al, (Reference IV-21) were used in the epithermal range. Above 0.5 ev the $1/E$ weighted infinitely dilute resonance integrals of the capture and fission cross sections are respectively 134 barns and 761 barns. The data are fully parametrized using the multilevel formalism of Adler and Adler above thermal, up to 60 ev. Smooth data are used above 60 ev.

The mean energy of the equilibrium fission neutron spectrum is $\bar{E} = 2.012$ Mev; the shape accounts for emissions from two fragments and a stationary source associated with the scission event.

The qualification of all the above data by direct parameter measurements is described in References IV-15 through IV-19, which show good agreement with experiment. The above U^{233} data and the scattering cross sections discussed below have been further qualified, together with the hydrogen and oxygen cross sections, by comparison of calculated and experimental criticality. Comparisons were done for the homogeneous aqueous spheres and cylinders of Gwin and Magnuson, Reference IV-22. The results obtained with these data sets are summarized in Reference IV-16. The average error between calculated and experimental determination of the critical eigenvalue was less than 1×10^{-4} . The individual errors for the 10 experiments ranged from $+16 \times 10^{-4}$ to -31×10^{-4} , which is consistent with the anticipated variability of $\pm 25 \times 10^{-4}$ for the calculated values, due to uncertainty in the fuel inventory in the experiments.

The U^{233} scattering cross sections were taken from a previous ENDF/B evaluation performed by M. Drake (Reference IV-23).

The $U^{233}_{O_2}$ natural source was measured to be 6.3 ± 1.5 neutron/gm-sec (Reference IV-24). This source is higher than in a U^{235} based fuel and aids in core startup procedures.

3. Protactinium-233

Pa^{233} is the daughter product of neutron capture in Th^{232} and leads to formation of either U^{233} , through beta decay, or U^{234} , through neutron capture in Pa^{233} . Because Pa^{233} has a relatively long half-life of 27.0 days and comparatively large capture cross section, losses of U^{233} result from Pa^{233} neutron

capture in the LWBR core. Although neutron capture in Pa^{233} is only 1.4 percent of the Pa^{233} decay rate, these losses are significant to breeding. The value of 27.0 days for the Pa^{233} half-life is based on References IV-25 through IV-27.

For the as-built analysis the ENDF/B-III data, material 1119, for Pa^{233} has been adopted. Below 38.5 ev the cross section data are parameterized using the single-level Briet-Wigner formalism and are consistent with the total cross section measurements of Simpson and Coddington (Reference IV-28). The capture cross section in the thermal range is substantially non-1/v. The value of the 0.0253 ev capture cross section is 39.8 barns, consistent with the experimental value 39.5 ± 1.2 barns inferred by Connor (Reference IV-29). From 38.5 ev to 10 Kev the capture cross section is based on unresolved resonance distributions using averages of the resolved parameters, adjusted to yield a 1/E weighted dilute capture integral above 0.5 ev of 860 barns, which is in excellent agreement with the experimental value of 857 ± 35 barns reported by Connor (Reference IV-29).

The effect of self-shielding on Pa^{233} is small because of its low concentration throughout the LWBR core. However, over 50 percent of the total dilute resonance integral of Pa^{233} is due to two resonances located at 1.34 ev and 1.64 ev. The neutron flux in the vicinity of these resonances may be substantially depressed from the 1/E values by the presence of U^{233} . Specifically there are two U^{233} resonances at 1.42 ev and 1.78 ev which are large in magnitude and extensive in width and can alter the flux near the two Pa^{233} resonances. Consequently, there can be a strong internuclide shielding effect by U^{233} on Pa^{233} which reduces the effective Pa^{233} resonance integral to as little as 60 percent of the infinitely dilute value in certain regions of the LWBR core during core life.

4. Zirconium (Elemental) and Zircaloy-4

The neutron interactions with elemental zirconium that are important to LWBR are those leading to radiative neutron capture, scattering and, to a lesser extent, the high energy (n,p) and (n, α) reactions. The radiative capture data were evaluated using the nuclear data optimization procedure described in Reference IV-30 and are consistent with the data identified as "RUN-1" in that reference. These data reflect the results of pile oscillator measurements of the resonance integral as a function of sample size, low resolution radiative capture measurements, and several high resolution total and capture cross

section measurements. The resonance integral measurements encompass a broad range of sample sizes, including samples in which the self-shielding effects are comparable to those in LWBR geometries. These and the other experiments used in the analysis were carefully reviewed and the results adjusted to be consistent with current standards when necessary.

The data set is parametrized, using the single-level Breit-Wigner formalism with supplemental smooth cross sections added to account for unresolved resonances. The effect of possible self-shielding of the unresolved resonances was examined and found to be negligible. The $1/E$ weighted infinitely dilute total absorption integral above 0.5 eV is 0.970 barns. The evaluated data of Reference IV-30 use a radiative capture width, $\Gamma_\gamma = 81$ meV, for the important 293 eV Zr^{91} resonance. This value is smaller than the values (100 meV - 180 meV) inferred from experiments available at the time of the evaluation. The smaller value has now been confirmed experimentally by Macklin, et al, (Reference IV-31). These data were automatically qualified against the measurements which were part of the optimization procedure discussed above. The most important test is the comparison of the effective shielded resonance integral against experiment as a function of thickness of the sample. The evaluated data agreed with the experimental integral measurement within the experimental statistics (Reference IV-30). The comparison, which included the range of Zr thicknesses encountered in LWBR, was judged to be reliable within 3 percent in this range.

The 0.0253 eV radiative capture cross section is 183 millibarns. The energy dependence of the thermal capture data is $1/v$.

The (n,p) reaction cross section for elemental Zr is based on the reaction cross section of the individual zirconium isotopes. The most abundant of the isotopes is Zr^{90} . This isotope has the lowest energy threshold for the (n,p) reaction and its cross section is well established experimentally (References IV-32 and IV-33). The energy dependences of the (n,p) cross sections for the other isotopes were obtained from the Zr^{90} data by shifting the cross section curve to account for differences in Q values and a renormalization to isotopic measurements at 14 MeV.

The inelastic scattering cross sections are also based on isotopic data. The cross sections were calculated using evaluated optical model parameters with Hauser-Feshbach theory and fluctuation corrections. The calculations are supported by extensive measurements of γ -decay branching ratios from the excited

states and cross sections for excitation of individual levels up to about 3 Mev. Additional transmission measurements of the nonelastic cross section between 1 and 14 Mev were used to supplement the direct measurements of inelastic scattering data at higher energy. The uncertainty in the inelastic cross section is approximately 10 percent.

The integrated elastic scattering cross sections were taken to be the difference between the evaluated total minus the evaluated cross sections for all other reactions. The differential elastic cross sections are based on Hauser-Feshbach theory using evaluated optical model parameters. The theoretical model was used in place of reliance on individual experimental determination of the differential cross section since there is a significant spread in the experimental values.

In the nuclear analysis programs, a single "isotope" is used to represent the clad and structural material Zircaloy-4. For this purpose a Zircaloy residual data set was first constructed by combining, in the right proportions, cross sections for the alloying and impurity materials in Zircaloy-4. Then the residual data set was combined with zirconium to obtain the final data set. The most important elements in the residual data set are tin, iron, oxygen, chromium, and hafnium. A special low-hafnium material, containing not more than 35 ppm of hafnium, was used to reduce parasitic neutron absorption in Zircaloy-4 in a breeder.

5. Hydrogen

The hydrogen scattering cross sections above 80 ev are from ENDF/B material 1001 and are based on Gammel's data (Reference IV-34). Below 80 ev they are based on Melkonian's measurements (Reference IV-35).

In nuclear analysis calculations the chemical binding of hydrogen in water can be significant at epithermal energies. From 80 ev to the thermal cutoff (0.625 ev for LWR) the molecular binding is accounted for by adjusting the average lethargy change per collision ξ in each multigroup. The adjustment results in a flux shape as a function of energy, for an infinite medium of water at room temperature, which matches the Corngold expansion with Nelkin kernel parameters (Reference IV-36). At reactor operating temperatures the expansion differs little from that at room temperature. The adjusted lethargy change ξ also gives a good flux spectrum for an infinite medium of water poisoned to 6 barns/hydrogen atom, a range used in scattering law experimental work.

The thermal scattering kernel is based on ENDF/B material 1002 scattering law data for hydrogen bound in water. The hydrogen absorption cross section is $1/v$ with a value of 0.332 barns at 0.0253 ev.

6. Oxygen

The nuclear data for O^{16} , which comprises 99.8 percent of the natural element, are taken from ENDF/B-III, material 1134. In comparison to most other nuclides of significance to LWBR, a large number of measurements are available on oxygen cross sections.

The radiative capture (n,γ) cross section, which is $1/v$, is very small compared to those of other materials in the core, being only 0.178×10^{-3} barns at 0.0253 ev. For LWBR application the most significant absorptive reaction is that leading to emission of an alpha particle. This reaction has a threshold near 3.6 Mev and accounts for over 90 percent of the neutrons absorbed by oxygen.

Because of its relatively low mass and high abundance throughout the core, the moderating properties of oxygen and, hence, its scattering cross section are important. The elastic scattering cross section was primarily obtained as the difference between the evaluated total cross section and cross sections for nonelastic interactions. The evaluated total cross section is based on 9 separate experiments. The elastic scattering cross section at 0.0253 ev is 3.704 barns. The inelastic scattering cross section is also based on a collection of measurements.

7. Other Isotopes Except Fission Products

These isotopes include those which are part of the structural steels in the core, such as the AM-350 steel used in the fuel rod support grids, and other isotopes of uranium. The main steel constituents are Fe, Ni, and Cr and the fast cross section libraries are based on ENDF/B-I materials 1020, 1021, and 1018 respectively. The thermal cross section data were prepared from Bettis evaluations. U^{234} data were obtained from ENDF/B-III material 1043. Data for U^{232} , U^{235} , U^{236} , and U^{238} are based partly on ENDF evaluations and partly on internal evaluations at Bettis and at the Knolls Atomic Power Laboratory.

8. Xenon-135

As seen in Table IV-1, Xe^{135} absorption accounts for about 1/3 of all fission product absorption near the middle of core life. The absorption cross section of Xe^{135} used by LWBR is similar to the ENDF/B evaluation (Reference IV-37),

having about the same shape but values which are uniformly about 5 percent higher than ENDF/B. At 2200 m/s the cross section used is 2.77×10^6 barns. This higher level is in agreement with certain of the experiments used in Reference IV-37 and provides some conservatism in breeding predictions. The cross section above 0.625 ev is accounted for, but contributes very little.

9. Other Fission Product Cross Sections

The relative importance of various fission products in LWBR is indicated in Table IV-2. This table gives the absorption percentages for the high zone seed composition after 10,500 hours of full power operation, which is near the middle of core life. The relative importance depends on which core region is discussed and the time in life. For example, in Table IV-2 Xe^{135} is indicated as having 1/4 of the fission product absorption, whereas in Table IV 1 Xe^{135} has 1/3 of the fission product absorption. The reduction in Table IV-2 is about half due to the later time in life and half due to the hard high zone seed spectrum.

The Sm^{149} cross sections are taken from ENDF/B material 1027 used in versions I through IV (Reference IV-38). The 2200 m/s cross section is 41,200 barns. Numerous other cross section evaluations were used to construct either multi-group fission product libraries for use in PAX or few-group cross sections for direct use in CINDER or PDQ. The 2200 m/s cross section and the infinitely dilute resonance integral for the next eight most important fission products are given in Table IV-3.

The use of these cross sections, including spectral corrections, are discussed in Section V.B. Tests of the fission product data, both cross section data and the yields to be described in the next section, are given in Section VIII.A.

10. Fission Product Yields and Decay Constants

The isotope chains used by LWBR to describe fission product poisoning are given in Reference IV-39. These chains are used in the CINDER fission product program and are accounted for in the PDQ depletion calculation. In addition to the cross section data discussed previously, fission product yields and decay constants are also required in the calculations.

The cumulative yield of the Xe^{135} chain from U^{233} fission is 6.0 percent. This was originally based on the measurements of Reference IV-40. The value is

slightly conservative but within the range of a recent measurement, due to F. C. Schoenig and W. E. Moore at the Knolls Atomic Power Laboratory, which gives 5.87 ± 0.10 percent. For a two element fission product chain, as used in fission product absorption calculations, the independent yields are 4.8 percent for I^{135} and 1.2 percent for Xe^{135} . This breakdown was originally based on Reference IV-41, but is confirmed by the recent results of Schoenig and Moore. The half-lives of I^{135} and Xe^{135} are 6.70 hours and 9.16 hours, respectively.

The yields from U^{233} fission and half-lives of the most important isotopes after the mass 135 chain are given in Table IV-4. The isotopes in Table IV-4 dominate the production of the second through the seventh most important isotopes in Table IV-2. In those cases where data were not available for the independent yields, which make up the cumulative yield of a particular mass, a Gaussian distribution about a most probable charge was used to distribute the cumulative yield.

11. Delayed Neutron Data

The delayed neutron fractions for LWBR are based upon experimental data tabulated in References IV-43 through IV-46. The delayed neutron data of interest are for U^{233} and Th^{232} .

The total yield of U^{233} fission neutrons that are delayed was determined from an inverse variance weighting of 5 experimental values from the references. Three of the 5 values were adjusted slightly from the reported values to account for recalibration of a normalizing neutron source, and slight adjustments to neutron energies. The total delayed yield for Th^{232} is based on an inverse variance weighting of values reported in References IV-43 and IV-45. The resulting total yields were 0.0069 ± 0.0003 and 0.053 ± 0.003 neutrons per fission for U^{233} and Th^{232} , respectively.

The energy spectrum for emission of delayed neutrons is based on U^{235} fission. The effective delayed neutron fraction is influenced by the energies at which the delayed neutrons are emitted. Changes in the effective fraction due to the use of different spectra were determined to be small relative to one standard deviation in the total delayed neutron yield. In particular, spectra contained in Reference IV-47 for fast fission of U^{233} and thermal fission of U^{235} led to about a 1 percent difference in the effective delayed neutron fraction.

The LWBR delayed neutron model is based on the conventional 6 group scheme. The group fractional yields and precursor decay constants were taken from Reference IV-43. These data are listed in Table IV-5 for U^{233} and Th^{232} . The

isotopic data were combined into a single 6-delayed-group set. The U^{233} values for precursor half-lives and decay constants were adopted since more than 96 percent of the core power is produced by this isotope throughout core life. The differences between the U^{233} and the Th^{232} data are within 1 standard deviation for 5 groups and 2 standard deviations for the sixth group. The latter isotope produces approximately 3 percent of core power throughout core life. The fractional yields for the single 6-group set were based on weighting the data listed in Table IV-5 by the isotopic fission fractions. These 2 isotopes produce more than 99 percent of the core power throughout core life. The effect of neglecting the other fissionable isotopes is to underestimate the weighted core delayed neutron fraction by a maximum of 1 percent at the end of core life.

12. Energy per Fission

A constant value of 3.1×10^{10} fissions/joule or 201.3 Mev/fission is used for LWBR for all isotopes and few-groups at all times in life. The value chosen includes the energy from capture- γ rays and from β -decay in the Th^{232} - U^{233} chain.

The total energy per fission is treated in PDQ as if it were deposited at the fission site. Special external calculations are used for corrections to this approximation. However, these are primarily photon calculations and they will not be discussed in this report.

13. Processing Nuclear Data into XAP

The nuclear data used for LWBR analyses are stored in the XAP library and accessed by the analysis programs such as RCP and PAX. For each nuclide the XAP library contains spectrum-averaged multigroup cross sections, angular scattering patterns, and group transfer matrices. In addition the XAP file may contain resonance parameters, neutron yield data, fission neutron spectra, and other quantities as necessary. Most of the XAP data files used by LWBR are based on data from the national Evaluated Nuclear Data Files ENDF/B (Reference IV-48), maintained at the National Nuclear Data Center, Brookhaven National Laboratory (BNL). The ENDF/B files contain highly detailed descriptions of the nuclear properties of each nuclide. These detailed data files must be converted to the XAP format for use in LWBR analysis.

The ENDF/B files to be converted to XAP format are first checked by a computer program to ensure that the files are properly structured and can be accessed by subsequent data processing programs. This first program also

provides capability to correct or alter the files. The actual conversion of the ENDF/B files to XAP format is accomplished by 3 computer programs: ETOMX, ETOTX, and FLAN2. These programs are versions of ETOM-1 (Reference IV-49), ETOG-1 (Reference IV-50), ETOT (Reference IV-51), and FLANGE II (Reference IV-52) which were modified by Bettis. ETOMX produces the nonthermal data files for XAP. The conversion of the ENDF/B nonthermal data to XAP format includes construction of spectrum averaged multigroup cross sections from the detailed energy dependent ENDF/B files. The weighting spectrum used in the averaging process is a standard spectrum based on the energy distribution of fission neutrons in an infinite water medium. ETOTX constructs pointwise values of the thermal cross sections at a standard set of thermal energy points. The thermal neutron scattering kernel is calculated by FLAN2 from the ENDF/B description. This latter operation is only applied to hydrogen which is the principle moderator in the LWBR core.

Nuclear data for certain nuclides, such as Th^{232} , are not obtained from ENDF/B but are based instead on Bettis evaluations. These data are processed with different programs specifically tailored for the particular application. However, the basic processes are similar to those used in ETOMX and ETOTX.

XAP has the capability to store fission product yields and decay constants. However, these quantities are not retained in the XAP library at this time. Instead they are stored as part of the CINDER input library for use in calculating fission product poison cross sections and related quantities.

C. Space-Energy Representations Within the Unit Cell

The basic repetitive unit in the calculational model is the fuel rod unit cell, Figure IV-2. An infinite lattice of these cells, i.e., a unit cell with zero current boundary conditions, is assumed in order to calculate energy dependent reaction rates within the cell. This approximation is described in Sections IV.C, D, and E, and the output consists of few-group cross sections for homogenized cells. Section IV.F presents correction factors which modify the few-group cross sections to account for the core environment surrounding a unit cell. The homogenized representation is then used in PDQ, except that the internal cell structure is required to describe temperature feedback.

1. Energy Structure

The fast energy range is divided into 54 multigroups and 3 few-groups. The first few-group consists of multigroups 1 through 10 and covers the energy range

from 10 Mev to 0.821 Mev. Inelastic scattering occurs in this group as does the thorium (n,2n) reaction, in multigroups 1 and 2 above 6 Mev, and fission by thorium and the even-even uranium isotopes. The importance of inelastic scattering in LWBR is illustrated by the fact that in fuel regions the combined slowing down out of the first few-group due to thorium, oxygen, and zirconium is as important as that of hydrogen. In relatively dry fuel regions like the regular blanket, the thorium alone is as important as hydrogen for removal (slowing down) from few-group one. Seventy-five percent (75%) of the fission neutrons are emitted in this group, and there results a flux peak in a fuel pellet relative to the surrounding water in a fuel rod cell. This pellet flux peak is accounted for by a fast advantage factor.

The second few-group consists of multigroups 11 through 25 and covers the energy range from 821 Kev to 5.531 Kev. Inelastic scattering occurs in this group also, but it is less important, and no inelastic transfer is permitted out of few-group 2. Similarly, PDQ does not permit any transfer from few-group 1 to 3, so all transfer out of few-group 1 is put in few-group 2. Since 25 percent of the fission neutrons are emitted in this group, with hydrogen slowing down now dominating, a fast advantage factor is used to account for the cell heterogeneity. Resonances for Th and Zr are significant in few-group 2, but are not permitted currently in PAX so a special treatment is used (Section IV.C.3).

The third few-group consists of multigroups 26 through 54 and covers the energy range from 5531 to 0.625 ev. Doppler broadening and shielding of resonances in this "resonance group" and cell spatial heterogeneity are included in a special resonance treatment. Chemical binding of hydrogen in water is accounted for even though a full hydrogen scattering kernel is not used in this group (Section IV.B.5).

The fourth few-group covers the thermal energy range below 0.625 ev. Cross sections and a hydrogen scattering kernel for 25 energy points are used to compute the flux spectrum and few-group cross sections. A thermal disadvantage factor is used to account for flux depression in the fuel pellet.

2. Fast Advantage Factors

The fast advantage factor (FAF) in few-group 1 is based on measurements by Glickstein, et al, of the pellet-to-water fission activation ratio in thorium

foils (Reference IV-53). It was also demonstrated that for a cell the pellet-to-water ratio could be fit to the moderator chord length according to Sauer's formula (Reference IV-54). In terms of pellet and water fluxes ϕ_p and ϕ_w , the fit has the form

$$A \equiv \frac{\phi_p}{\phi_w} = a + b l_w$$

where the moderator chord length (cm) is

$$l_w = \frac{4V_w}{S}$$

in terms of the water volume V_w in the cell and the clad outer surface area S . The constant $a > 1.0$ if clad is present in the cell; the value was slightly modified from the original fit, using RCP Monte Carlo calculations (Section III.A.1 and Reference IV-55) of infinite unit cell lattices, because of changes in the clad since that time. The constant b is primarily the moderator removal cross section. Therefore the original slope was modified to account for temperature changes between the ambient temperature experiments and reactor operating temperatures. The resulting fit is

$$A = 1.0098 + 1.952 N_w l_w$$

where N_w is the water number density (molecules/barn cm). If we temporarily neglect differences between the flux in the clad, or pellet-to-clad gap, and the average cell flux $\bar{\phi}_{\text{cell}}$ then

$$\text{FAF}_w \equiv \frac{\phi_w}{\bar{\phi}_{\text{cell}}} = \frac{1}{v_w + A v_p}$$

where V_p is the pellet volume, $v_p = \frac{V_p}{V_p + V_w}$, and $v_w = \frac{V_w}{V_p + V_w}$.

Also

$$\text{FAF}_p \equiv \frac{\phi_p}{\bar{\phi}_{\text{cell}}} = (A)(\text{FAF}_w)$$

The quantities A , FAF_w , and FAF_p in the first few-group vary with geometry. The clad factor is taken as $\text{FAF}_c = 1.007 \text{FAF}_w$ in all binary rod regions. All FAF 's are set to 1.0 in thoria regions. The group 1 FAF 's are automatically supplied to PAX by PREP.

The second few-group FAF's were taken directly from the unit cell RCP calculations and varied little from one fuel region to another. Typical values of FAF's for both groups are given in Table IV-6. These values are input to flux spectrum and few-group cross section calculations in PAX. The FAF's in each few-group are worth roughly 0.1 percent in reactivity.

3. Resonance Treatment

The PAX resonance treatment is used in the third few-group and is described in Section IV.D, but we shall make use of the results of that calculation in the present section. The results are resonance integrals or resonance escape probabilities for each isotope and each multigroup in the third few-group that are input to the flux spectrum calculation. For LWBR both the explicit resonance and smooth parts of the cross section are treated as part of the "resonance integral" and are shielded at the same time. No externally generated correction factor is used to modify the treatment of resonance absorption in the third few-group.

Resonance interference is significant in LWBR and, in particular, the U^{233} cross section suppresses the flux seen by Th^{232} and Pa^{233} resonances. In contrast to earlier programs (Reference IV-56) which required external correction factors, interference is automatically accounted for because the flux seen by any resonance has interacted with the total cross section of all isotopes.

Certain materials, thorium and zirconium, have resonances which extend up into the second few-group where PAX does not permit an explicit resonance treatment. The current thorium library has unresolved resonances up to 25 Kev (Section IV.B.1) which covers 3 multigroups in few-group 2. The absorption properties of these resonances were obtained from an external deterministic evaluation (Reference IV-57). A single set of effective smooth capture cross sections was generated which was a good approximation for the rod arrays that occur in LWBR. These data were added to the thorium library stored in XAP.

Additionally, the current zirconium library has resolved resonances up to 89 Kev. Tests have shown that the resonance scattering in the second few-group has a significant effect on the zirconium absorption in that range, mainly in multigroup 25 which goes from 5.5 to 9 Kev. In this case, RCP was used to generate a single set of smooth capture cross sections for use with LWBR rod arrays.

4. Thermal Disadvantage Factors

The thermal flux dipping in the fuel pellet is treated by the Multiple-Sauer method for calculating thermal disadvantage factors (TDF's). This method is described in Reference IV-58 and PAX uses a similar approach except for the spectrum calculation. One-energy disadvantage factors $d_r(E)$ for each region r of the unit cell are calculated at each of the 25 thermal energies by the Sauer procedure (Reference IV-54) with Buslik's modified treatment of the clad. For region r of the unit cell with average flux $\phi_r(E)$, the disadvantage factors are

$$d_r(E) = \frac{\phi_w(E)}{\phi_r(E)}$$

where w refers to the water region. The moderator spectrum $\phi_w(E)$ is shown to solve an integral equation similar to the thermal flux spectrum equation for an infinite homogeneous medium (Reference IV-58). This equation is solved iteratively in PAX and the other $\phi_r(E)$ are determined from $\phi_w(E)$ and the disadvantage factors.

The one-group disadvantage factor, or thermal G-factor, for use in PDQ is then defined for isotope i and reaction type t (absorption or fission) as

$$G_i^t = \frac{\sum_r N_r^i V_r \int_0^{E_c} \sigma_i^t(E) \phi_r(E) dE}{\sum_r N_r^i V_r \bar{\phi}_{\text{cell}} \sigma_i^{t,\text{hom}}} .$$

Here $E_c = 0.625$ ev, N_r^i = concentration of isotope i in region r (atoms/barn cm), and V_r is the volume of region r . The average cell flux is

$$\bar{\phi}_{\text{cell}} = \frac{1}{V_{\text{cell}}} \sum_r V_r \int_0^{E_c} \phi_r(E) dE ;$$

and $\sigma_i^{t,\text{hom}}$ is the cross section of isotope i for reaction t averaged over the flux spectrum of the homogenized unit cell material without disadvantage factors. Thus two "infinite medium spectrum" calculations are done, one for the homogenized cell and one for $\phi_w(E)$. Both G_i^t and $\sigma_i^{t,\text{hom}}$ are passed to PDQ (see Section IV.E) and used as a product. The numerator in the equation for G_i^t represents the total

reaction rate t for i in the cell and when divided by $\bar{\phi}_{\text{cell}}$ gives the reaction rate per unit flux. The denominator gives the same quantity in the homogenized cell without disadvantage factors. Except for oxygen, an isotope only appears in one cell region and G_i^t simplifies to

$$\frac{1}{\bar{\phi}_{\text{cell}}} \frac{\int_0^{E_c} \sigma_i^t(E) \phi_r(E) dE}{\sigma_i^{t, \text{hom}}}$$

It is seen that the ratio of activation rates of one isotope to another in the unit cell will be matched to the Multiple-Sauer calculation by using the prescribed G-factor. Tests of the Multiple-Sauer disadvantage factors show that they can accurately represent flux and activation ratios from Monte Carlo calculations (Reference IV-58).

Typical thermal G-factors for LWBR are given in Table IV-7 for isotopes in the pellet (U^{233}), clad (Zircaloy-4, ZR-4), and moderator (H). The thorium G-factor is almost the same as the U^{233} G-factor, and the G-factor for U^{233} fission is essentially the same as those in the table which are for U^{233} absorption.

5. Tests of the Model in an Infinite Lattice of Unit Cells

The heterogeneous features of the fuel rod lattice that must be accounted for have been described, and so have the methods of accounting, except for the detailed discussion of the resonance treatment which is given in the next section. Comparisons were done at this level of complexity to check the overall model in the idealized geometry of the infinite lattice of unit cells. The comparison standard is an explicit Monte Carlo calculation of each lattice type using RCP (see Section III.B.1 and Reference IV-55).

The nuclear analysis model calculations were done in the PAX program (References IV-56 and IV-59) using spectrum calculations for homogenized unit cells with heterogeneities incorporated as described above. Since the calculation of the Multiple-Sauer thermal G-factor occurs in PAX after the homogeneous spectrum calculation is complete, a ruse was used to obtain reaction rates for the homogenized unit cell which included the G-factor. This ruse made use of a P_1 multi-group "spatial" calculation using the P7MG option in PAX (Reference IV-60), with

a single region and three widely spaced mesh points. The resulting "space-energy" calculations followed the homogeneous spectrum calculations and produced reaction rates for the homogenized cells which included the thermal G-factors.

The results of the comparisons are shown in Tables IV-8 through IV-11 for 4 of the 12 fuel rod cell types. The other cell types give similar results, although comparisons in thoria cells with no U^{233} are harder to interpret since virtually all source neutrons should come from leakage. The temperatures of the comparisons in Tables IV-8 through 11 were 545°F for the water and 920°F for the fuel pellet. A trace amount of Pa^{233} was included in one comparison to test the resonance treatment for this case. The data labeled "Total Zircaloy" include Zr (labeled "Zirc Absorption") and the residual materials. The data labeled "Total Oxygen" include oxygen in the pellet and water. All the reaction rates are normalized to one source neutron starting each generation in the cell. The total problem absorption is greater than unity (≈ 1.002) because of additional neutrons available in a given "generation" from (n,2n) reactions. The comparisons generally show good agreement between the calculational model and Monte Carlo, especially in the strong absorbers. The Zircaloy and U^{234} comparisons might have been improved by investing more computer time to sharpen the Monte Carlo statistics. The oxygen discrepancy is thought to be the result of using the same FAF for all 10 multigroups in few-group 1 - the energy dependence of oxygen absorption in this energy range is to increase with increasing energy, rather than to fall off or be generally flat as with most of the other reactions.

Table IV-12 shows a similar lattice comparison for the high zone seed cell where the fuel temperature has been raised to 1500°F and the water temperature is unchanged. The good results which may be compared to Table IV-8, demonstrate the accuracy of the Doppler broadening treatment. Table IV-13 shows the same cell where both the fuel and water temperature have been reduced to 80°F. These results are not as good as at the hot temperatures. They probably reflect the fitting of the second few-group parameters to the operating temperature conditions.

The notion of a unit cell does not apply to the metal-water regions in LWBR. The FAF's and TDF's are unity. Resonance absorption in Zircaloy was calculated using the same model as in fuel rod cells, but the materials were homogenized prior to the calculation so a homogeneous resonance integral was obtained. A test of this particular aspect was done by looking at an RCP calculation of a horizontal plane through a Type I module. An average absorption cross section

of Zircaloy-4 (ZR-4) was computed for the channel between the seed and the blanket, for the third (resonance) few-group. This cross section was an average of two ZR-4 cans which are separated by water, and RCP gave $\sigma_{a3}^{ZR-4} = 0.0654$ barns. The PAX calculation of the homogenized channel was modified by a set of space-energy correction factors which account for the core environment at various axial positions in which the channel appears (Section IV.F). This effect is separate from the resonance treatment, but it is the net cross section for each axial position which is comparable to the RCP and affects the flux in PDQ. The net PAX cross section averaged over the channel is 0.068 barns, 4 percent higher than the Monte Carlo estimate. Further discussion of the representation and testing of metal-water regions will be given in Sections IV.E and IV.F.

D. The Resonance Model

Resonance shielding is determined in PAX from a solution to the space and energy dependent Boltzmann equation in an infinite lattice of unit cells. The energy range included is the MUFT resonance range from thermal to 5531 ev. The Boltzmann equation is solved in discrete form with an energy mesh and distinct spatial regions. Physical assumptions included in the solution are that all scattering is isotropic, in both the center of mass and laboratory systems, and is uniformly distributed in each distinct spatial region. Initial conditions are that above 5531 ev the flux is spatially flat with an energy dependence proportional to $1/E$ and that the 5531 ev scattering cross sections apply. This flux is normalized such that the total slowing down at 5531 ev is unity.

The PAX model is in effect an improved version of earlier methods coupling slowing down and escape probability calculations, the basic idea for which was used in the ZUT program (Reference IV-61). The PAX method is a distinct improvement over integral approximation methods typified by the MINX program (Reference IV-62). These integral methods make many physical approximations such as the narrow resonance approximation, no heavy element moderation, no interference or overlap, no resonance scattering, and simplified line shapes. The PAX method does not make these assumptions. Both the PAX method and the other integral methods require the assumption of isotropic scattering in the center of mass and laboratory systems. The only additional assumption in PAX, which the other integral methods also make, is that the use of distinct spatial regions implies the assumption of constant sources in each region.

The absorption and fission rates for each isotope are determined for each MUFT multigroup and converted to resonance integral form

$$RI_i = \frac{-A_i}{A} \ln \left(1 - \frac{A}{q} \right)$$

where A_i is the absorption rate for isotope i , A is the total absorption rate, and q is the slowing down density at the top of the multigroup in the lattice. These resonance integrals (RI_i) are then passed to the other PAX sections, MUFT, P7MG, and DOS which treat the lattice as homogenized with resonance escape probabilities determined from these resonance integrals. No further resonance correction, such as the traditional MUFT L-factor, is used.

The energy mesh structure and corresponding cross section libraries are prepared by an option in the RCPL1 program (Section III.B.1 and Reference IV-55). The starting point for this calculation is an existing RCPL1 library as prepared for RCP. This library has detailed Doppler broadened resonance cross section profiles for each isotope. Taking each isotope separately, a subset of the RCPL1 energy mesh is selected to follow the detailed cross section profile for that isotope.

The criteria for inclusion of mesh point E_n in the subset include whether E_n is a local extremum of the cross section profile and whether the error in the resonance integral due to omitting E_n is "small enough," a term which is made precise as follows: Let E_{last} be the last point included in the subset from any isotope; so

$$\frac{1}{\ln \left(\frac{E_{last}}{E_{n+1}} \right)} \int_{E_{n+1}}^{E_{last}} \sigma_i \frac{dE}{E} \equiv \sigma_i^L$$

is a local average across section, from the last point included to the next point which could be included if E_n is omitted. Let E_{min} and E_{max} be the boundaries of a broader energy band containing E_n , called an RCP group (Reference IV-55) and similar to a multigroup. If the beginning or end of the resolved resonance range for isotope i falls within the particular RCP group, then E_{min} or E_{max} becomes that limit. Then

$$\frac{1}{\ln\left(\frac{E_{\max}}{E_{\min}}\right)} \int_{E_{\min}}^{E_{\max}} \sigma_i \frac{dE}{E} \equiv \sigma_i^B$$

is a broad average cross section over the RCP group. The error in the resonance integral due to omitting E_n is small enough if it is smaller than

$$\epsilon \ln\left(\frac{E_{\text{last}}}{E_{n+1}}\right) \left[c \sigma_i^L + (1 - c) \sigma_i^B \right]$$

where $0 \leq \epsilon$, $c \leq 1$ are prescribed by the user. In the LWBR model, $\epsilon = 0.001$, $c = 0.25$.

The union over all isotopes of these subsets is included in the PAX energy mesh for the resonance calculation. Additional points are selected, if necessary, to provide for an adequate description of slowing down for the heaviest element present. In the unresolved resonance range the RCPL1 energy mesh is used directly, in LWBR. For LWBR, a total of about 20,000 energy points is used to represent the resonance cross sections between 0.625 ev and 5,531 ev. The cross sections are transferred directly to the PAX library.

Smooth cross section data from XAP, which are not in the RCPL1 profiles, are taken as needed from the XAP library. In the MUFT and DOS sections of PAX, the smooth data may be treated as part of the resonance calculation and thus shielded. This is done in LWBR. This option is not appropriate for P7MG because the resonance absorption in a multigroup is proportional only to the slowing down into the group; in the DOS the resonance absorption is proportional to the multigroup flux.

The slowing down kernel for isotope i in region j of the unit cell, with isotropic scattering in the center of mass system, is given in the laboratory system by

$$K_{ij}(E' \rightarrow E) dE = \begin{cases} \frac{\Sigma_{sij}(E')}{E'(1 - \alpha_i)} dE & \text{for } \alpha_i E' \leq E \leq E' \\ 0 & \text{for } \alpha_i E' > E \text{ or } E > E' \end{cases}$$

with $\alpha_i = \left(\frac{\mu_i - 1}{\mu_i + 1}\right)^2$ and μ_i the mass of the scattering nucleus in units of

neutron mass. This kernel is numerically applied to the finite mesh structure for each isotope for each space region in the unit cell. The numerical treatment follows the analytic kernel as closely as possible, maintaining strict neutron balance. At epithermal energies where up-scattering and molecular binding effects become significant, the kernel is modified to approximate these effects. The approximation applied is similar to that used in RCP.

Neutron transport is calculated by PAX based on the physical assumptions of isotropic scattering in the laboratory system that is uniform on space for each unit cell region. Under these conditions the transport solution can be written in terms of first collision integrals which give the probability that neutrons born in one region make their first collision in any other region. Let P_{jk} be that probability for the j^{th} source region, with volume V_j , and the k^{th} final region. Then the neutron collision rate in region k is

$$\sum_j P_{jk}(E) S_j(E) V_j$$

where $S_j(E)$ is the source density in region j .

Using the assumptions stated above, the equation for the average flux in region k , $\bar{\phi}_k(E)$, is

$$V_k \Sigma_{Tk}(E) \bar{\phi}_k(E) = \sum_j V_j P_{jk}(E) \left[s_j(E, E_T) + \sum_i \int_E^{E/\alpha_i} \frac{\Sigma_{sij}(E') \bar{\phi}_j(E')}{(1 - \alpha_i)} dE' \right]$$

where $\Sigma_{Tk}(E)$ is the total cross section in region k and $s_j(E, E_T)$ is the source density from neutrons scattered from above the initial energy $E_T = 5531$ ev.

This latter source is

$$s_j(E, E_T) = C_o \sum_i \Sigma_{sij}(E_T) Z_i(E > E_T)$$

where

$$Z_i(E > E_T) = \begin{cases} \frac{1}{1 - \alpha_i} \left(\frac{1}{E_T} - \frac{\alpha_i}{E} \right) & \text{for } \alpha_i E_T \leq E \leq E_T \\ 0 & \text{for } E < \alpha_i E_T \end{cases}$$

and C_0 is a normalization constant given by

$$\sum_j V_j \int_0^{E_T} s_j(E, E_T) dE = 1 \quad .$$

The integrations are done using the trapezoidal rule.

The first collision integrals are expressed in terms of first flight transport kernels for an isotropic point source, $K(\vec{r}' \rightarrow \vec{r}, E)$, as

$$P_{jk}(E) = \frac{1}{V_j} \int_{V_k} d\vec{r}' \int_{V_j} K(\vec{r}' \rightarrow \vec{r}, E) d\vec{r} \quad .$$

The kernel is

$$K(\vec{r}' \rightarrow \vec{r}, E) = \frac{C_1 e^{-l(\vec{r}' \rightarrow \vec{r})}}{4\pi |\vec{r} - \vec{r}'|^2}$$

where $l(\vec{r}' \rightarrow \vec{r})$ is the optical path from $\vec{r}'$ to $\vec{r}$ and C_1 is a normalization constant given by

$$\int_{\text{cell}} K(\vec{r}' \rightarrow \vec{r}, E) d\vec{r} = 1 \quad .$$

First collision integrals for a rod lattice as used in LWBR are too complex to be expressed in closed form for evaluation by standard numerical techniques. Therefore, PAX uses a ray tracing procedure which is similar to Monte Carlo methods (Reference IV-63). The Monte Carlo approach would be to start neutrons on the surface of the source region with initial weight equal to the known flux from an internal uniform isotropic source. Each neutron is tracked through the lattice and the weight deposited in the various lattice regions recorded. The P_{jk} can then be determined from these weights. PAX uses the same technique deterministically with a uniform set of surface points and directions, Ω_i , i.e., each direction represents an equal solid angle. The user specifies the number of surface points and directions. The LWBR model uses six surface points for each 1/12 of a unit cell, which is a symmetric portion. The model also has, for each surface point, 55 directions per octant.

The effort required to determine the P_{jk} by this method limits the number of regions permitted and prohibits the calculation of the P_{jk} at each energy mesh point. It is recalled that the LWBR unit cell is divided into three

material regions which represent the fuel rod, clad, and moderator, with a void gap between the rod and clad. A prescribed set of total cross section values for each material region is selected by the user and tables of P_{jk} are precomputed over these cross section sets for the specific lattice geometry. Thus, $P_{jk}(E)$ becomes $P_{jk}(\Sigma_T^{\text{rod}}, \Sigma_T^{\text{clad}}, \Sigma_T^{\text{moderator}})$. The P_{jk} required during the main calculation are interpolated from these tables. Typical LWBR calculations use 10 values of Σ_T in the rod and clad and 2 values in the moderator.

The successive application of the P_{jk} matrix to determine the scattering densities at the n^{th} energy point, and the slowing down kernels to obtain the sources of the $n + 1^{\text{th}}$ point will completely determine both the reaction rates and the slowing down density for all points throughout the lattice. Test calculations comparing the PAX resonance model with RCP in LWBR seed and blanket lattices resulted in errors of 1 percent or less in isotopic resonance absorption rates.

For metal-water regions, such as the seed-blanket channel, the PAX resonance calculation is also performed because of the Zircaloy. The materials are homogenized, however, so a homogeneous resonance integral is obtained. Test calculations have shown that this is satisfactory, as discussed in Section IV.C.5.

E. Determination of Few-Group Cross Sections for Use in Diffusion Theory Calculations

The few-group cross sections for each fuel rod unit cell and for metal-water regions are determined by the PAX program (References IV-56 and IV-59). The few-group structure and the representation of unit cell heterogeneity were described in Section IV.C. In PAX the unit cell is homogenized so that an infinite lattice of cells becomes an infinite, homogeneous medium. The heterogeneous effects appear either in the coefficients determining the energy-dependent flux, or as a correction factor to be applied later in PDQ. Thus we shall speak of "infinite medium" flux calculations with the understanding that lattice heterogeneities are handled as in Section IV.C. The present section describes the determination of such infinite medium constants, including their time and temperature dependence. Section IV.F covers an additional correction which, for fixed time and temperature, accounts for the finiteness of the medium (or lattice) in the core.

1. Infinite Medium Calculations

There are 12 types of fuel rod unit cell in the core and there are 28 homogenized mixtures which represent the metal-water regions. For the latter, infinite

medium calculations are done at one time and one temperature per region. This temperature is chosen to represent the average temperature seen by that metal-water region in the core. For example, a region below the core is calculated at the inlet temperature and a region in the core is calculated at an average temperature depending on adjacent fuel regions. For the 12 fuel rod cells, infinite medium calculations are performed at several times in life and at two fuel temperatures and two moderator temperatures per cell, as described in Sections IV.E.2 and IV.E.3.

For all of the infinite medium calculations the input buckling is zero or essentially zero, so the designation "infinite" is appropriate. The fast multi-group spectrum calculation in PAX is done by solving the slowing down problem with multigroup transfer matrices. This differs from earlier versions which used a Greuling-Goertzel approximation (Reference IV-56). Other differences from earlier versions include the treatment of shielding and heterogeneous effects discussed in Sections IV.C and IV.D.

Constants for the thermal few-group are obtained by solving the thermalization problem using an iterative solution of the integral equation for the flux $\psi_0(E)$, rather than the Wigner-Wilkins differential equation as in earlier versions (Reference IV-59). From this hardened spectrum $\psi_0(E)$ and a Maxwellian spectrum $\psi_M(E)$, thermal few-group constants are defined according to a variant of the mixed number density scheme (References IV-64 and IV-65).

In the mixed number density scheme the thermal group equation to be solved by the spatial program PDQ is

$$-\nabla \cdot \left[\frac{D_M}{\left(\frac{1}{v}\right)_M} \nabla n \right] + \left[\frac{\Sigma_O^a}{\left(\frac{1}{v}\right)_O} \right] n = S,$$

where

n is the thermal neutron number density

S is the slowing down source to thermal

D_M is the thermal diffusion coefficient averaged over $\psi_M(E)$

$\left(\frac{1}{v}\right)_M$ is the cross section of a $\frac{1}{v}$ absorber averaged over $\psi_M(E)$

Σ_O^a is the thermal absorption cross section averaged over $\psi_O(E)$

$\left(\frac{1}{v}\right)_O$ is the $\frac{1}{v}$ absorption cross section averaged over $\psi_O(E)$.

Tests have shown that the mixed number density scheme will predict a higher value than experiment of local power peaking near a water channel, though the overall thermal flux shape is generally satisfactory. For example, power shape measurements were done across the BMU-2-4 critical experiment and compared to a three-dimensional PDQ calculation. With the mixed number density thermal constants, water channel peaks were overestimated by varying amounts up to 6 percent. The BMU-2-4 assembly had 4 modules in a line (Reference IV-66) and was one of a number of critical experiments which was used to study the properties of Th-U²³³ fueled systems and test calculational models.

In an effort to reduce the prediction of water channel peaks, while retaining continuity of the thermal neutron number density, consideration was given to using a hardened diffusion coefficient (Reference IV-64). The choice was made empirically by introducing a parameter β such that

$$D_{\beta} = \beta \frac{D_o}{\left(\frac{1}{v}\right)_o} + (1 - \beta) \frac{D_M}{\left(\frac{1}{v}\right)_M}, \quad 0 \leq \beta \leq 1.0,$$

and the resulting constants are called the " β number density" scheme. A value $\beta = 0.5$ is used for the LWBR as-built analysis. Figure IV-3 shows a calculation of a fission distribution across the BMU-2-4 experimental core using a three-dimensional PDQ and thermal diffusion coefficients with $\beta = 0.5$. It is seen that the predictions of water channel peaking, as well as the overall fission activation shape, are accurate for the BMU-2-4 when $\beta = 0.5$.

An additional modification to the usual few-group cross sections is needed to accommodate the thorium (n,2n) reaction in the PAX-PDQ scheme. The (n,2n) cross sections are incorporated into the inelastic scattering cross sections, which is a convenient place to incorporate the proper emission spectrum (Section IV.B.1). The inelastic scattering appears in the slowing down or removal cross section Σ^{R1} which removes neutrons from few-group 1 to few-group 2. Since the (n,2n) reaction results in more neutrons entering few-group 2 than leaving few-group 1, the single constant Σ^{R1} cannot describe both quantities. It does describe the source to few-group 2, but a negative correction to few-group 1 is then needed. Since Σ^{R1} appears in the group 1 diffusion equation only in the combination $(\Sigma^{a1} + \Sigma^{R1})$, an adjustment can be made to Σ^{a1} . This is done by replacing Σ^{a1} by $(\Sigma^{a1} - \Sigma^{n,2n})$, where $\Sigma^{n,2n}$ is the macroscopic (n,2n) cross section for few-group 1. With this modification, the reaction is correctly described in PDQ.

2. Time Varying Cross Sections

For the 12 fuel regions, the inventories change with depletion as neutron absorption, fission, and radioactive decay processes occur during the depletion. In PAX a point depletion calculation is performed for each fuel cell to generate time dependent inventories. A nuclide identification is assigned to the fission density accumulated since the beginning of the depletion (f/cc) to represent the depletion and to be used as a "clock" to represent the time dependence of all other nuclides. This clock is used in conjunction with the output and selected input for the PAX infinite media calculations.

The required input to PAX includes depletion chains, cross section libraries, and several sets of data. A depletion chain is a grouping of nuclides such that the precursors and daughters of a given nuclide are defined as well as the coupling mechanism which joins each nuclide to its precursor. If each nuclide in the chain can be formed from only one precursor, the system is known as a linear chain and the associated set of first order differential equations can be solved with the PAX program.

Some of the data do not change with time. For LWBR these data are the fast advantage factors and those fission product cross sections whose time dependence does not significantly affect the total fission product poison (Section IV.E.4). The PAX depletion represents 3 fission product chains explicitly and a fission product residual accounts for the remaining absorption. Discussion of the chains and residual, which are the same as in the LWBR PDQ model, is presented in Sections V.A and V.B. The fission product cross sections input to PAX are in the third and fourth few-groups only. The third group values are effective values which include small corrections to represent the top two few-groups.

Some of the input data to the PAX depletions are time-dependent quantities with values selected from previous PDQ depletion studies. These are the power density and few-group flux ratios, which are the ratios of the flux in each fast few-group to the thermal flux. All time-dependent quantities are input as tables of fitted data versus f/cc. Depletion intervals at which PAX calculations are to be performed are selected to represent the physical behavior of the system. For LWBR, calculations are performed at 7 times in life, viz., 0, 50, 1,000, 3,000, 8,000, 20,000, and 40,000 EFPH. The notation EFPH stands for "effective full power hours" and means the number of hours of depletion at a power density equivalent to full power operation in the core. These 7 times represent respectively the beginning of life, equilibrium xenon, equilibrium

samarium, equilibrium Pa^{233} , midlife, an approximate end of life, and an extended life depletion. This last point is used to prevent unwanted extrapolations beyond the data table, even for local fuel regions in PDQ which can deplete at greater than the average power density used in the PAX table generation.

3. Temperature Dependence

LWBR uses the thermal-hydraulic feedback option of PAX to correct the nuclear flux distribution for temperature variation encountered in the core. This requires the use of three pseudo-nuclides, N_{T_f} , N_ρ , N_{T_m} , which are defined in Table IV-14. N_{T_m} is not used in LWBR for cross section dependence because the small amount of boiling present does not significantly affect the nuclear characteristics. Thus, neutron calculations treat moderator density as a function of moderator temperature (at fixed pressure). Calculations are performed for nominal reference values of these parameters and for perturbed values in order to generate the temperature dependence of the cross sections. The reference value for the moderator temperature is 540°F and the perturbed value is 600°F. The reference value for the fuel is 920°F in the binary regions and 600°F in the thoria regions. In both cases the perturbed value is 500°F greater. PAX reference calculations are performed for each of the 7 values of f/cc. Pairs of perturbation calculations are performed at 3 times in life. These are at 0, 8,000, and 40,000 EFPH. In one perturbation calculation, only the moderator temperature is perturbed (i.e., thermal kernel and water density). In the other perturbation calculation, only the fuel temperature is changed.

4. Construction of Table Sets

The general cross section formulation in PDQ is given by:

$$\Sigma^{tg} = \Sigma_0^{tg} + \sum_i N_i \sigma_i^{tg} C_i^{tg}$$

where

t = type (transport, absorption, removal, fission),

g = group, and

i = nuclide.

Three types of tables are used in this formulation: a macro-table, a series of fixed micro-tables, and a series of fitted or interpolating tables. A macro-table contains time- and temperature-independent values of Σ_0^{tg} for all groups and, as with the other types of table, is assigned by material composition in

PDQ. A fixed micro-table contains time- and temperature-independent values of σ_i^{tg} . An interpolating table contains σ_i^{tg} and G_i^{tg} as functions of time (f/cc) and temperature. LWBR uses all of these types and the extent of the table usage in a typical region is given in Table IV-15. This lists all of the tables used by LWBR, including those which incorporate space-energy effects (Section IV.F) and those which describe time- and temperature-dependent cross sections.

The time- and temperature-dependent cross sections for fuel regions are presented in Table IV-16. In metal-water regions the cross sections are fixed. This table lists the nuclide, type, and group for the cross section being fitted, as well as the independent variables. Previous surveys have identified the nuclide cross sections for which explicit temperature or time dependence is required in order that an accurate description of both reactivity and breeding may be achieved. For example, the total reactivity error due to omitting all the other possible interpolations on time and temperature ≤ 0.15 percent. As part of these surveys, cross sections which are sensitive to moderator density alone and those which are sensitive to both moderator density and fuel temperature have been identified. All the cross sections in Table IV-16 are fit to f/cc. In addition, those which are sensitive to moderator density have also been fit to N_ρ and those which are sensitive to moderator density and fuel temperature have been fit to N_ρ and N_{Tf} . The temperature perturbations for the explicit cross sections in Table IV-16 have been incorporated into the fitted tables at one time in life, namely, at 8,000 EFPH.

The last three entries in this table describe the cross section formulation for the latent temperature-dependent cross sections. The purpose of these cross sections is to incorporate all thermally dependent cross section effects that have not been included by the explicit nuclides. The formulation is given by:

$$\sigma_x^{lg} \equiv \frac{1}{N_x} \left[\delta \Sigma^{tg} - \sum_i N_i \delta \left(\sigma_i^{tg} G_i^{tg} \right) \right]$$

where

$x = T_f$ or ρ ,

$t = \text{type}$,

$g = \text{group}$,

$i = \text{nuclide}$, and

δ represents the difference between the case with the perturbed temperature and the case with the reference temperature.

At this point in the calculation the only G-factor which is not unity is the thermal G-factor. (The space-energy corrections in the fast few-groups are independent of the temperature feedback calculation.) These latent cross sections are fitted against f/cc in a one-dimensional table with values at 0, 8,000, and 40,000 EFPH. These are the only times at which the perturbed temperature PAX calculations are performed.

A representative list of the important PAX input parameters for an LWBR fuel rod cell is given in Table IV-17.

All of the tables described in Table IV-15 and Table IV-16 are gathered into a "tableset" which is used to describe the time and temperature dependence of one fuel region type in the PDQ depletion. Tablesets for each fuel region type are generated in a similar manner. Tablesets containing only macro-tables and fixed micro-tables are generated to represent each metal-water region. All of these are combined with the tablesets containing regional space-energy correction factors (Section IV.F) to form a collection of tablesets called a HARMONY file (Reference IV-67) which is input to the PDQ program.

F. Regional Space-Energy Correction Factors

1. Background

The calculational model described previously has dealt with the energy dependence of the neutron flux in infinite lattices, or in infinite media with corrections based on lattices. The three-dimensional spatial calculations using PDQ will have 3 fast few-groups and 1 thermal few-group with each of the fast few-groups covering a broad energy range. Comparisons to more accurate calculations have shown that significant errors in reactivity and reaction rate distributions can result from having only 3 few-groups to cover the fast range. For example, reactivity errors of 1 percent were commonly observed.

Consideration was given to adding more few-groups or adjusting the boundaries between the present few-groups, and tests were done which included the addition of one fast few-group. The tests did not show improvement that could be depended upon - some calculations showed improvement and others did not. The addition of several fast few-groups, which perhaps could have solved the problem, was not practical in the large PDQ calculations required in LWBR (Section V).

Consideration was also given to adjusting the buckling in the infinite medium calculations (the "MUFT buckling," Reference IV-56) to provide a bare

core leakage which represented the actual core environment. The first tests of this approach were in 1 dimension using a P_1 multigroup calculation as a standard (Reference IV-60). Although the tests were not favorable to the buckling approach, they led to the use of few-group constants computed from the P_1 multigroup output itself. We will call these constants "PlMG constants" to indicate a P_1 angular approximation, though the computer programs had higher order angular capability (Reference IV-60).

There are two heuristic arguments which lead one to think that PlMG constants might work. The first argument is that material changes in LWBR occur more rapidly in a horizontal (radial) direction than in a vertical (axial) direction. This is illustrated in Figure IV-4 which shows an r, z sketch of a Type I module approximately to scale, made by passing a plane vertically through the module and showing the portion from the module centerline to the outside boundary. This figure should be compared to Figure II-4 which shows the same region of core, but not to scale. Figure IV-4 indicates that a one-dimensional (radial) space-energy correction to the infinite medium results might account for the most important part of this effect, since it will show the metal-water regions and the radial fuel zoning.

The other heuristic argument lies in the P_1 multigroup equations (Reference IV-60). If you run a one-dimensional multigroup problem and compute few-group constants for each spatial mesh interval, these constants could be input to a one-dimensional, few-group diffusion theory program. The few-group fluxes from the few-group diffusion theory program will then be the same as the few-group fluxes from the multigroup problem at each spatial mesh point. This assumes that the spatial difference equations in both programs are the same. Instead of editing few-group constants for each spatial mesh interval, they will be edited over larger, physically significant regions so the few-group fluxes will not reproduce the results from a multigroup calculation. One is led to guess that a large portion of the space-energy effect can nevertheless be accounted for.

A similar statement could be made connecting other multigroup calculations, such as discrete ordinate approximations, to few-group diffusion theory. All that is needed is that both programs have an implied neutron conservation equation, the same spatial difference equations, and that the few-group diffusion coefficients preserve the relation of current to flux in the multigroup program.

In most cases, however, if the geometry in the few-group problem differs from that in the multigroup problem, the few-group results will not closely represent the space-energy effect. The constants from a P_1 multigroup solution do represent the space-energy effect. Tests on LWBR systems have shown that PLMG constants will improve the few-group diffusion theory results not only in one-dimensional problems but also in large three-dimensional PDQ problems. Other multigroup calculations may be used if the few-group constants produced are like PLMG constants.

2. One-Dimensional Multigroup Computer Programs

Two multigroup solutions are available in PAX. One produces a P_1 solution (PLMG, Reference IV-60), including P_1 slowing down, and appropriate computations of few-group constants. This is an earlier option in PAX and retains a Grueling-Goertzel slowing down treatment. In addition, resonance absorption in a multigroup is proportional to the slowing down into the multigroup. This is a disadvantage in relatively dry regions because of the omission of resonance absorption in a multigroup, due to leakage of neutrons into the region in that same multigroup. The PLMG option has been used in LWBR to generate spatially dependent few-group cross sections and has proven generally satisfactory. The calculations are run in one-dimensional, cylindrical geometry with 54 fast multigroups and 1 thermal group. The thermal group uses the β -number density approximation (Section IV.E.1). In a typical radial traverse from the center of a Type I module to the module outer boundary, there are 36 mesh intervals whose size varies from 0.2 cm to 0.8 cm.

The other multigroup solution in PAX is a discrete ordinate solver (DOS). In the LWBR model, the polar angle is described by 3 single Gaussian cones per hemisphere. There are 10 equally spaced azimuthal directions headed away from the problem center per cone, so there are 30 angles per quadrant which describe the flux. A generalized diamond differencing scheme is used for the spatial variable and the methods of solution are based on Reference IV-68. P_1 scattering is used. The geometry and group structure are the same for generating DOS few-group constants as for PLMG constants. The β -number density approximation is not available in the DOS so a standard hardened thermal flux calculation was used. However, tests have shown that this change has a negligible effect on the resulting fast few-group constants in eigenvalue problems.

The DOS has the advantage of being more recent than the P_1 solution, with the result that the slowing down problem is expressed solely in terms of transfer

matrices. In addition, an effective smooth absorption cross section is calculated from the infinite lattice resonance escape probability and used in the DOS flux solution. Thus, the resonance absorption in a multigroup is proportional to the multigroup flux and includes resonance absorption of leakage neutrons in that same multigroup. It is this latter property which resulted in choosing the DOS computations of few-group σ_a , $v\sigma_f$, and the removal (slowing down) cross section σ_r . The few-group diffusion constant from the DOS differs from the P_1 diffusion constant, and a special treatment is required (Section IV.F.4).

3. Regional Few-Group Cross Sections from Multigroup Spectra

A set of one-dimensional radial traverses with zero axial buckling is prescribed to represent the different configurations of materials occurring in the core (Section IV.F.5). These traverses are from cylindricized versions of the hexagonal modules and divide the fuel compositions into smaller regions for purposes of computing few-group constants. Typical traverses are shown in Figure IV-5 where changes in material composition are indicated by solid vertical lines. Additional regions, indicated by dashed lines, are introduced adjacent to these composition boundaries because flux spectra will change most rapidly near boundaries. The boundary conditions are also shown. For each of the resulting set of regions, except for the metal-water filler region on the outside of the core, a set of few-group cross sections is computed from the DOS. This breakdown occurs for each one of the prescribed slices. Thus a given material composition which has one set of infinite medium cross sections has many sets of regional space-energy cross sections in the fast few-groups. For example, the high zone seed composition at beginning of life has 12 sets of spatially dependent few-group cross sections (Section IV.F.5). All regions in the core are assigned such a set of cross sections, except those which are of lesser importance or those for which the model of a one-dimensional traverse does not apply (Section IV.F.5).

The macroscopic few-group constants are computed as follows for isotope i , fast few-group g , and reaction type t in region s :

$$\Sigma_{is}^{tg} = \frac{\int_s \int_g \Sigma_i^t(u) \phi(u, r) r du dr}{\int_s \int_g \phi(u, r) r du dr}$$

where u = lethargy, Σ is a macroscopic cross section, ϕ is the scalar flux, and t = absorption, fission, and v -fission. Also,

$$\Sigma_s^{Rg} = \frac{\int_s [q_{el}(\hat{u}, r) + q_{in}(\hat{u}, r)] r dr}{\int_s \int_g \phi(u, r) r du dr}$$

where R = removal (slowing down), q_{el} and q_{in} are the elastic and inelastic slowing down densities at the maximum lethargy $\hat{u}_{eg}$. And

$$v_{is}^g = \frac{(\nu \Sigma^f)_{is}^g}{\Sigma_{is}^{fg}}$$

The diffusion constant will be discussed in the next section. Regional space-energy correction factors, or "fast G-factors," are defined by

$$G_{is}^{tg} \equiv \frac{\Sigma_{is}^{tg}}{\Sigma_{ic}^{tg}},$$

t = absorption and fission ,

where Σ_{ic}^{tg} is the infinite medium cross section ("MUFT cross section") for material composition c which spatial region s contains. Similarly

$$G_s^{Rg} \equiv \frac{\Sigma_s^{Rg}}{\Sigma_c^{Rg}}.$$

In the LWBR model, fast G-factors for absorption are computed for H, O, ZR-4, AM-350, Th²³², U²³³, U²³⁴, U²³⁵, U²³⁶, and Pa²³³, but not for fission products or other structural nuclides of lesser importance. Fission G-factors are computed for Th²³², Pa²³³, and the uranium isotopes. ν values from the DOS are used directly to replace infinite medium values for Th²³² and U²³³ in few-group 1 and U²³³ in few-group 2. No G-factor per se is created for ν . Isotopic removal cross sections are used in PDQ and the regional G_s^{Rg} is used for all isotopes in s . Fast G-factors G_s^{tg} for t = absorption, fission, and transport are computed in a similar way from the total macroscopic cross sections summed over all isotopes. As an approximation, these latter G-factors are applied to fictitious isotopes N_ρ and N_{Tf} which represent the latent temperature dependence (Section IV.E), a second order correction.

To give some idea of the size of the effects involved, Table IV-18 gives ranges of fast G-factors which occur in the LWBR core for a few of the nuclear reactions. It is seen that local effects for individual reactions can be substantial. The effect on gross core parameters involves an averaging of many local effects and will be less, but it is still significant (Section IV.F.6). Experience has shown that the regional space-energy cross sections are not strongly dependent on the order of the transport approximation. The detailed flux shape changes from a P_1 to a higher order angular approximation, but the few-group cross sections change very little. However, this is not true for the diffusion constant, as discussed below.

4. The Diffusion Coefficient

Contrary to the definitions of spatially dependent few-group cross sections given in the previous section, the choice of a diffusion coefficient is not as straightforward. If there were no P_1 slowing down, the averaging over lethargy could be accomplished by flux-weighting $(1/3\Sigma^{tr})$. But there is P_1 slowing down and this is what distinguishes a PLMG solution from a multigroup diffusion theory. The problem of averaging over a spatial region would remain even if there were no P_1 slowing down, because the few-group value of $(1/\Sigma^{tr})$ is a function of position.

Since few-group diffusion theory depends on using a Fick's Law approximation, the few-group diffusion coefficient has been defined as

$$D^g(r) = - \frac{\int_g J(r, u) du}{\int_g \frac{\partial \phi(r, u)}{\partial r} du} = - \frac{J_g(r)}{\frac{d}{dr} \phi_g(r)}$$

where J is the neutron current density (Reference IV-60). Using this $D^g(r)$ in a radial few-group calculation, it would be possible to reproduce the few-group current $J_g(r)$ from the multigroup calculation. Given that $J_g(r) = - D^g(r) \frac{d\phi_g(r)}{dr}$, there are several ways that one could think of to obtain a region average coefficient. Any average of the form

$$\bar{D} = \frac{\int_s D(r) w(r) r dr}{\int_s w(r) r dr}$$

with weight function $w(r)$ will approach the correct limit for small regions, i.e., as the region size approaches one mesh interval. One approach is to preserve the leakage term in the P_0 equation in an integral sense, i.e., the net leakage out of region s :

$$\int_s \frac{1}{r} \frac{d}{dr} (rJ) r dr \equiv - \bar{D}_I \int_s \frac{1}{r} \frac{d}{dr} \left(r \frac{d\phi}{dr} \right) r dr ,$$

or

$$\bar{D}_I \equiv - \frac{(rJ)_R - (rJ)_L}{(r\phi')_R - (r\phi')_L} = \frac{(rD\phi')_R - (rD\phi')_L}{(r\phi')_R - (r\phi')_L}$$

where $\phi' \equiv \frac{d\phi}{dr}$ and the subscripts R and L refer here to the right and left end points of region s . $\bar{D}_I$ has the disadvantage of not approaching the right value, $-J/\phi'$, for small regions. Also, the appearance of end point values of ϕ' would make $\bar{D}_I$ very sensitive to local fluctuations.

Another approach is to preserve Fick's Law in an integral sense:

$$\int_s Jr dr \equiv - \bar{D}_{FI} \int_s \frac{d\phi}{dr} r dr ,$$

or

$$\bar{D}_{FI} \equiv \frac{\int_s D\phi' r dr}{\int_s \phi' r dr} .$$

This expression does approach the correct limit for small regions.

The expression for a region average D , which we have chosen, is a modification of the above and also approaches the correct limit for small regions. This expression will preserve Fick's Law in a least squares sense. The approximate Fick's Law with a region average D is

$$J(r) \approx - \bar{D}_{FL} \phi'(r)$$

which results in an error

$$E(r) = J(r) + \bar{D}_{FL} \phi'(r) .$$

The mean square error is proportional to

$$\int_s E^2 r dr ,$$

and if this error is minimized with respect to $\bar{D}_{FL}$, there results

$$\bar{D}_{FL} = - \frac{\int_s J \phi' r dr}{\int_s (\phi')^2 r dr} = \frac{\int_s D (\phi')^2 r dr}{\int_s (\phi')^2 r dr} .$$

The squared gradient weighting function preserves Fick's Law in a least squares sense in any geometry, not just the one-dimensional cylindrical geometry used here.

Since D is an artifice from the viewpoint of a multigroup code with P_1 slowing down, it is not surprising that values may occur which look strange from the viewpoint of diffusion theory - regardless of how the region averages are defined. The point function $D^g(r)$ may be zero, negative, or infinite at some points because $J_g(r)$ and $\phi'_g(r)$ are not proportional to one another. The weight function $w(r) = (\phi')^2$ may be zero at some points, but in any practical problem the denominator in $\bar{D}_{FL}$ will be positive. Due to the point function $D^g(r)$, the region average $\bar{D}_{FL}$ may sometimes be very small or large or negative and these values may be a good set if one were ultimately interested in one-dimensional few-group calculations. Since we want to use the region average diffusion coefficients in three-dimensional PDQ calculations, and the only basis for this extension is empirical, values of D which are "far" from the traditional infinite medium values are excluded. In particular, negative values are excluded because they are not permitted in the PDQ numerical procedures. Calling the $\bar{D}_{FL}$ by D_s^g for region s , the allowed ranges are positive and surround the typical MUFT (infinite medium) values for LWBR systems. But they are considerably broader than the ranges of MUFT values:

$$0.5 \leq D_s^1 \leq 4.5 ,$$

$$0.2 \leq D_s^2 \leq 3.5 ,$$

$$0.1 \leq D_s^3 \leq 2.5 .$$

If some D_S^g falls outside of its allowed range, it is replaced by the MUFT value. In practice this does happen, but not very often.* For example, in the as-built core with the movable seed bank 14 inches above the aligned position, there are about 180 regions in the various one-dimensional traverses for which regional few-group constants are computed. Of the 180 values of D_S^1 , one negative value was rejected and $1.3 \leq D_S^1 \leq 2.5$ for the others. All of the 180 values of D_S^2 satisfy $0.6 \leq D_S^2 \leq 2.9$. There were two negative values of D_S^3 which were rejected and all the others satisfy $0.1 \leq D_S^3 \leq 1.9$.

When the regional diffusion coefficients are obtained from higher order transport calculations than P_1 (which are available in PAX, Section IV.F.2), their behavior is more erratic and less similar to infinite medium diffusion coefficients. This may be due to the presence of more rapid variations in flux gradients than are describable in P_1 , which are picked up in the higher order functions. Both the DOS and simplified $-P_L$ (Reference IV-60) approximations result in D's of this nature. More values fall outside the allowed ranges and PDQ calculations of experimental cores indicate poor reactivity results. This latter statement is not surprising since PDQ is, after all, basically a P_1 calculation. For these reasons, the regional D's for PDQ in the LWBR model are from PLMG, even though the other regional constants are from the DOS.

There is a modification in the definition of D which gives values very close to the PLMG values for a higher order calculation. If the P_L components of the flux are F_L , so $F_0 = \phi_g(r)$, the scalar flux, then the function $(F_0 + 2F_2)$ is a dependent variable in the simplified $-P_L$ equations (Reference IV-60 and Section V.C). Using $\frac{d}{dr} (F_0 + 2F_2)$ in the denominator for $D^g(r)$, instead of $\frac{d}{dr} F_0$, the region average D's are very close to PLMG values. This is probably because both $\frac{d}{dr} F_0$ in P_1 and $\frac{d}{dr} (F_0 + 2F_2)$ in simplified $-P_L$ are determined by the current. Application of this modified definition could provide a means of getting approximately PLMG D's from any multigroup calculation which is used to get the other few-group cross sections. In fact, this modified definition is used in Reference IV-60.

The use of PDQ by LWBR is such that Σ^{tr} rather than D is required input. The last stage of data preparation for PDQ takes $\frac{1}{3D_S^g}$ for input as $\Sigma_0^{tr,g}$. These macroscopic regional transport cross sections for the fast few-groups, $g = 1, 2$, and 3, are input directly to PDQ; no fast G-factors for Σ^{tr} are used. Once they are input to PDQ, the fast Σ^{tr} are only modified for temperature dependence using

the fictitious isotopes N_p and N_{Tf} (Section IV.E). It has been found that the fast Σ^{tr} is essentially constant in time and no time dependence is included in the LWBR model. For example, in a PAX depletion of the high zone seed material treated as an infinite medium (Section IV.E), the fast D_s^g values change by 0.6 percent or less through 20,000 hours of depletion at full power. The thermal transport cross sections are not assumed constant with time. They are described by depletable nuclide concentrations and microscopic cross sections.

5. Assignment of Space-Energy Correction Factors to Regions Within the Core

The one-dimensional traverses from which the fast G-factors will come must represent both regular and power flattening blanket regions around a seed and various seed positions which occur during the core lifetime. Referring to Figure II-1, one set of multigroup calculations starts at the center of the seed of an inner (Type I) module and runs to the boundary of that module. A typical one of these traverses is shown in Figure IV-5, part (a), and is from a cylindricized representation of a Type I module. The cylindrization maintains the same region areas as in the hexagonal module. This set of "inner traverses" is used to obtain space-energy constants for the 3 Type I modules and also for that portion of the Types II and III modules which have regular blanket around the seeds.

Again referring to Figure II-1, a second set of multigroup calculations starts at the center of the seed of an outer (Type II or III) module and runs through the power flattening blanket and reflector to the core boundary. A typical one of these traverses is shown in Figure IV-5, part (b), and is from a cylindricized representation where a seed is entirely surrounded by power flattening blanket and reflector. This set of "outer traverses" is used to obtain space-energy constants for that portion of the Types II and III modules which have power flattening blanket around the seeds and also for the thorium reflector modules.

The fuel zoning of a Type I module is shown in Figure II-4 where the seed is aligned with the surrounding blanket. Similar pictures apply for other portions of the core, with power flattening blanket and reflector replacing regular blanket in the outer regions. It can be seen in Figure II-4 that there are 6 unique axial fuel zones within the 84-inch high binary fuel region. An inner traverse multigroup calculation and an outer traverse multigroup calculation are run for each 14-inch high axial fuel zone, making 12 traverses in all.

If the movable seed assemblies are lowered 14 inches below the aligned position, there are 9 unique axial fuel zones which contain binary fuel. One of these zones is the lowermost 4 inches of seed which is opposite a metal-water region below the blanket lower thoria reflector. No unique multigroup traverses are run for this zone. Similarly, none are run for the zone with the uppermost 4 inches of blanket. Multigroup traverses are run for the 7 intermediate zones, so there are 14 traverses in all. These 14 traverses have about 180 regions for which space-energy corrections are obtained.

A third set of multigroup calculations is done for the movable seeds raised to 14 inches above the aligned position. With the 3 1/2 inch axial mesh in the PDQ core calculations (Section V.D), the extent of seed travel within the PDQ representation of the critical core is from 24 1/2 inches below the aligned position (the -24 1/2 inch position) to 24 1/2 inches above the aligned position (the +24 1/2 inch position). The sets of multigroup calculations are used as follows:

- 14 inch traverses are used from -24 1/2 inches to -7 inches;
- aligned traverses are used from -3 1/2 inches to +7 inches;
- +14 inch traverses are used from +10 1/2 inches to +24 1/2 inches.

Tests have indicated that this is an adequate representation. For example, a comparison showed little difference between a PDQ calculation with seeds at -21 inches and traverses from -14 inches and a similar PDQ with traverses at -21 inches.

All of the above multigroup calculations are performed at beginning of life. Tests have indicated that the change in the fast G-factors with time is small enough to neglect. In particular, the change with time is small in comparison with the change from infinite medium constants to the use of the space-energy corrections. Thus the fast G-factors generated at beginning of life, for movable seed positions encountered throughout life, are used for all times in PDQ.

Space-energy correction factors are used for all "important" regions of the PDQ problem which can be represented in a one-dimensional traverse. This includes all binary fuel regions and all thoria and metal-water regions which are in the same one-dimensional traverse as some binary regions. The fuel rod support grids do not appear as explicit regions, but are homogenized into the unit cell water. Therefore no separate G-factors are required. There are some thoria axial

reflectors above and below the binary fuel which, depending on the seed position, may not be opposite any binary fuel. No fast G-factors are generated for these regions. Nor are G-factors generated for the metal-water regions beyond the axial or radial thorium reflectors. There are also seed and blanket structural posts throughout the core, but they are not representable in one-dimensional traverses. In general, all of the PDQ regions for which fast G-factors are not generated make use of infinite medium constants. An exception to this is the set of seed and blanket structural post regions, for which special Monte Carlo calculations are performed using the analytical standard RCP (Sections III.B.1 and III.B.4). These calculations show a core region surrounding the posts. Effective removal cross sections are extracted from the RCP for use in PDQ.

6. Tests of Space-Energy Correction Factors

Some examples of test calculations will be presented in this section, emphasizing those which isolate the effect of space-energy correction factors from other model approximations. Tests of the overall model will be described in Chapter VIII.

The simplest tests use a one-dimensional multigroup calculation itself as the standard. Then 2 one-dimensional PDQ's are run, one with space-energy constants for regions similar to those in Figure IV-5 and one with infinite medium constants. Four such comparisons are shown in Tables IV-19 through IV-23 with all the reaction rate data being normalized to one starting fission neutron. The total absorption rate is slightly greater than unity due to the thorium (n,2n) reaction. Table IV-19 shows a comparison for traverse T_1 which is from a core design similar to the as-built core. Some physical data about the traverse are given along with a comparison of the regional absorptions in few-groups 3 and 4. Presented are results from the multigroup calculation, PLMG, and differences between PDQ and PLMG. One PDQ has infinite medium constants (MUFT) and the other has space-energy constants from a multigroup calculation (SpEn). The spatial distributions of A_3 and A_4 are sensitive indicators of model performance, since thorium and U^{233} absorptions occur predominantly in both of these groups. Table IV-20 gives results for the same traverse T_1 with all reaction types and few-groups, with the seed regions and blanket regions combined together.

Table IV-21 shows a comparison for traverse T_2 which is also from a core design similar to the as-built core, but with a different arrangement of the

seed and blanket regions. Table IV-22 shows traverse T_3 from an older core design with a central metal-water channel region. Table IV-23 shows a comparison for traverse T_4 which is from the experimental core BMU-1B (Reference IV-66). This core was one of a number of critical experiments which was used to study the properties of Th-U²³³ fueled systems and test calculational models. All 4 traverses show that the use of space-energy constants in one-dimensional few-group calculations does very well, much better than infinite medium constants.

The more interesting tests are in 2 and 3 dimensions, but they are also more difficult to interpret because of the lack of a "three-dimensional PLMG" to serve as a standard. Thus, the multidimensional comparison standard generally has more improvements than just the space-energy interaction and the isolation of the latter effect requires more judgment.

Three-dimensional PDQ calculations were done for the BMU-1B experimental core referred to above. A fission activation shape

$$A(r) = \int_0^{\infty} \sigma_f(E) \phi(E, r) dE$$

was measured using U²³³ foils placed in the BMU-1B fuel rods at a fixed height. Calculations of the same quantity across the BMU-1B core were obtained using the PDQ fluxes. One of the PDQ's was done with infinite medium constants and the other made use of space-energy corrections. The results for the fission activation traverse are shown in Figure IV-6. The use of space-energy corrections makes a significant improvement at nearly all points of the activation shape.

Calculations using PDQ in r,z cylindrical geometry were done for a single module of an earlier core design. The standard was a Monte Carlo calculation of the module showing each fuel rod explicitly in three-dimensional hex,z geometry using the RCP analytical standard (Section III.A.1). The outer boundary of the module was represented by a zero current condition radially and a vacuum condition on top and bottom. Figure IV-7 shows a sketch of this earlier design analogous to the sketch in Figure II-4, but with the seed lowered 21 inches to produce a near-critical condition for beginning of life. Power fractions are shown in Figure IV-7 for each fuel zone for RCP, PDQ with infinite medium constants, and PDQ with space-energy constants. Standard deviations on the RCP data range from

0.8 percent in high power regions to 2.6 percent in low power regions. The PDQ with space-energy constants shows improvement in the "gross" parameters (total seed and blanket power and reactivity) and in each fuel region. The degree of improvement varies from one region to another.

A two-dimensional horizontal slice, through a symmetric 1/6 section of a core design similar to the as-built core, is shown in Figure IV-8. The dashed lines mark fuel zone boundaries. Calculations using PDQ, with space-energy corrections, and RCP were done in hexagonal geometry with zero axial buckling. From the ratios of PDQ to RCP power, it is seen that the PDQ power shape is tilted toward the core center relative to the RCP values. PDQ overpredicts power in the central part of the core and underpredicts power in the outer core regions. Figure IV-9 shows a similar comparison except that the PDQ has infinite medium few-group cross sections without any fast G-factors. Here the PDQ power is tilted in the opposite way relative to the RCP. One possibility considered was that the RCP power shape might be tilted due to lack of source convergence; but enough histories and independent runs were done to make the judgment that convergence of the RCP was not a problem.

An attempt was made to empirically eliminate the power tilt of PDQ relative to RCP, which seems to be related to the space-energy treatment. We may recall that the fast G-factor G_{is}^{tg} for reaction type t , few-group g , isotope i , and spatial region s was defined as the ratio of a space-energy few-group cross section to the corresponding infinite medium few-group cross section and was calculated at beginning of life. Then the cross section used by PDQ at any time in life is σ_{is}^{tg} given by

$$\sigma_{is}^{tg} = G_{is}^{tg} \sigma_{ic}^{tg} ,$$

where σ_{ic}^{tg} is the infinite medium cross section for material composition c at any time in life, obtained from a PAX depletion (Section IV.E). Since the "cross-core" power tilt goes in opposite directions when σ_{is}^{tg} and σ_{ic}^{tg} are used in PDQ, the above computation was modified to

$$\sigma_{is}^{tg} = \left[\alpha_s^g G_{is}^{tg} + \left(1 - \alpha_s^g \right) \right] \sigma_{ic}^{tg} ,$$

where $0.0 \leq \alpha_s^g \leq 1.0$ is an empirical fitting parameter which produces the space-energy cross section ($\alpha_s^g = 1.0$), the infinite medium cross section ($\alpha_s^g = 0.0$), or anything in between. In the tables of G-factors used by PDQ, this modification is achieved by storing the G-factor $(G_{is}^{tg})'$ given by

$$(G_{is}^{tg})' = \alpha_s^g G_{is}^{tg} + (1 - \alpha_s^g) \quad .$$

In a similar way, the same value of the fitting parameter is used for the diffusion coefficient, so all macroscopic data will become averaged in the same way:

$$(D_s^g)' = \alpha_s^g D_s^g + (1 - \alpha_s^g) D_c^g \quad .$$

Testing has indicated that the space-energy constants should still be used in the first two few-groups, and the mixing should be done in the third few-group. Figure IV-10 gives a comparison for the same two-dimensional slice as in the previous two figures, but with

$$\alpha_s^1 = \alpha_s^2 = 1.0, \alpha_s^3 = 0.5 \text{ for all } s \quad .$$

There is a general improvement in the power comparison with $\alpha_s^3 = 0.5$ even though some regions are better with $\alpha_s^3 = 1.0$ or 0.0 . There is an additional change in Figure IV-10 from the previous two figures. The β -number density thermal model was used in the PDQ calculation for Figure IV-10 while the mixed number density model was used for Figures IV-8 and IV-9 (Section IV.E). This change, however, has been found to affect only local power peaks near water channels and not gross cross-core power shapes.

Additional testing, against RCP calculations of a two-dimensional horizontal slice from a single module, indicated that the full space-energy corrections are needed in the metal-water channel regions to properly describe the removal cross section Σ^{R3} . Thus, the final space-energy model adopted had

$$\alpha_s^1 = \alpha_s^2 = 1.0 \text{ for all } s \quad ,$$

$$\alpha_s^3 = 1.0 \text{ for channels} \quad ,$$

$$\alpha_s^3 = 0.5 \text{ for fuel regions} \quad .$$

The result of this final model is shown in Figure IV-11 where a full three-dimensional comparison of PDQ with the RCP power distribution is presented. The calculations represent the beginning of life, as-built core in "hex-z" geometry, i.e., hexagonal geometry in horizontal planes, with the movable seeds 21 inches below the aligned position. The final as-built nuclear analysis model is used insofar as it can be made compatible with RCP. That is, the model described in this chapter and the PDQ model described in Chapter V are used except there is no temperature feedback in the PDQ because it is not available in RCP. The fuel and moderator are each at representative fixed temperatures, 920°F and 550°F respectively. The results indicate that the PDQ nuclear analysis model is representing the core performance with considerable accuracy in reactivity and power distribution when compared to the Monte Carlo analytical standard. The overall qualification of the nuclear analysis model will be discussed further in Chapter VIII.

One final test will be described, namely, an example on the lifetime dependence of the fast G-factors. This example uses a one-dimensional radial traverse from an earlier core design with a central metal-water channel region. Table IV-24 gives the key physical data for the traverse. The "middle of life" inventories for the fuel regions were obtained from point depletions in PAX for 11,000 hours, at power densities characteristic of full power operation for each region. The middle of life (MOL) inventories were used to run a PLMG problem and thus generate fast G-factors for MOL. Some of these G-factors are compared to corresponding values at beginning of life (BOL) in Table IV-25. The major effects as represented by MOL G-factors are accounted for by BOL G-factors. One-dimensional PDQ calculations with MOL inventories and with and without BOL G-factors were also done. The reactivity and power distribution were compared as shown in Table IV-24. It is seen that the use of BOL G-factors is adequate to describe space-energy effects at other times in life and is much better than simply using the infinite medium constants.

7. Automation of Space-Energy Correction Factors

The output from each one-dimensional multigroup traverse is stored in a computer file, as is the output from the infinite medium spectrum calculations. A computer program called PECOS accesses the output files, computes the fast G-factors, and stores the values of G , Σ_{tr} , and v in a computer file. There is one resulting file for each traverse and these "traverse files" are then combined into a single file.

Since PDQ is attuned to quantities which vary by fitting them to nuclide concentrations, such a fit was created for the space-energy corrections. A fake nuclide was assigned an identification number, say 10, and its "atom density" N_{10} was given integral values. PECOS then forms a HARMONY file where the values of G , Σ_{tr} , and v are fitted to N_{10} in interpolating tables (Section IV.E), just like the other fitted quantities. Nuclide 10 is then used as a switch to define the spatial region in the three-dimensional PDQ problem to which a given set of G , Σ_{tr} , and v values are applied.

PECOS reads a PDQ concentration file, which contains the atom densities for real nuclides, and accepts input of the fake nuclide concentration N_{10} for each spatial region. Thus a revised concentration file is created. The spatial regions to which values of N_{10} are assigned are the depletion blocks (Section V.D) over which nuclide concentrations are constant. Since there are many more depletion blocks than regions with unique space-energy corrections, a single value of N_{10} is assigned to all depletion blocks with a unique space-energy correction. With N_{10} values assigned to spatial regions, and G , Σ_{tr} , and v fitted to N_{10} , then at any time in life in the PDQ calculation PDQ sees the fixed integer value of N_{10} for each depletion block. It then obtains the correct values of G , Σ_{tr} , and v from the "interpolating tables" and no actual interpolation is done on N_{10} .

REFERENCES

- IV-1. N. M. Steen, "An Evaluation of the Radiative Neutron Capture Cross Section of Thorium-232 for the Range 0.0 ev to 15 Mev (LWBR Development Program)," WAPD-TM-971, December 1970.
- IV-2. J. Hardy, Jr., "Influence of Molecular Binding Effects in Water on Measured Resonance Integrals," Nuc. Sci. Eng. 27 (1967) 135.
- IV-3. R. M. Ball, et al., "Operating Coefficients and Reactivity Behavior at Indian Point," Trans. A.N.S. 6 (1963) 343.
- IV-4. J. Hardy, Jr., J. J. Volpe, and D. Klein, "Measurement and Analysis of Parameters in Tight Th²³²-U²³⁵ and Th²³²-U²³³ Lattices Moderated with D₂O," WAPD-TM-1089, January 1974.
- IV-5. V. M. Pankratov, "Fission Cross Sections of Th²³², U²³³, U²³⁵, Np²³⁷ and U²³⁸ for 5-37 Mev Neutrons," Soviet At. Emer. 14 (1963) 167.

- IV-6. S. P. Kalinin and V. M. Pankratov, "Neutron Induced Fission Cross Sections of Th^{232} and U^{238} in the Energy Range of 3 to 11 Mev, and of U^{233} , U^{235} , Np^{237} , and Pu^{239} in the Energy Range of 3 to 8 Mev," Proc. 2nd U.N. Int. Conf. PUAE 16 (1958) 136.
- IV-7. A. I. Sergachev, et al, "Influence of Intermediate States of Fissioning Th^{233} Nucleus on the Mass and Kinetic Energy Distributions of the Fragments," Sov. J. Nuc. Phys. 7 (1968) 475.
- IV-8. M. Holmberg and L. Wallin, "Inelastic Neutron Scattering and Fission of Th^{232} Near the Fission Threshold," Nucl. Phys. A127 (1969) 149.
- IV-9. H. Condé and M. Holmberg, "The Physics and Chemistry of Fission," IAEA Conf. Vienna, 2 (1965) 61.
- IV-10. J. P. Butler and D. C. Santry, " Th^{232} (n,2n) Th^{231} Cross Section from Threshold to 20.4 Mev," Can. J. Chem. 39 (1961) 689.
- IV-11. A. B. Smith, "Elastic and Inelastic Scattering of Fast Neutrons from Th^{232} ," Phys. Rev. 126 (1962) 718. And, N. P. Glazkov, "Spectra and Inelastic Scattering Cross Sections of Neutrons in the 0.2-1.2 Mev Energy Range Scattered by Nuclei of V, Th, Hg, W, Sb, Cd, Mo, Nb, Fe," Soviet At. Ener. 14 (1963) 405.
- IV-12. R. Batchelor, W. B. Gilboy, and J. H. Towle, "Neutron Interactions with U^{238} and Th^{232} in the Energy Region 1.6 Mev to 7 Mev," Nuc. Phys. 65 (1965) 236.
- IV-13. L. Green and J. A. Mitchell, "Total Cross Section Measurements with a Cf^{252} Time-of-Flight Spectrometer," WAPD-TM-1073, April 1973.
- IV-14. R. E. Swaja, "Calculation of Neutron Slowing Down Properties in Thorium-Water Lattices," Trans. A.N.S. 13 (1970) 304.
- IV-15. N. M. Steen, "An Evaluation of the Neutron Reaction Cross Sections and Fission Spectrum of U^{233} for ENDF/B," WAPD-TM-691, December 1969.
- IV-16. N. M. Steen, "Revision of the Thermal Parameters of U^{233} ," WAPD-TM-1052, September 1972.
- IV-17. L. Green, J. A. Mitchell, and N. M. Steen, "The Uranium-233 Fission Neutron Spectrum from 0.8 to 10 Mev," Nuc. Sci. Eng. 52 (1973) 406.
- IV-18. J. J. Ullo and M. Goldsmith, "Monte Carlo Analyses of Direct Measurements of the Fission Neutron Yield per Absorption by Uranium-233 and Uranium-235 of Monochromatic Neutrons," Nuc. Sci. Eng. 60 (1976) 239.
- IV-19. M. Goldsmith and J. J. Ullo, "Monte Carlo Analysis of Thermal-Spectrum Averaged Measurements of η of Uranium-233 and Uranium-235," Nuc. Sci. Eng. 60 (1976) 251.

- IV-20. L. Weston, et al, "Neutron Fission and Capture Cross Section Measurements for U^{233} in the Energy Range 0.02 to 1 ev," ORNL-TM-2353, February 1, 1969.
- IV-21. L. W. Weston, R. Gwin, G. deSaussure, R. R. Fullwood, and R. W. Hochenbury, "Measurement of the Neutron Fission and Capture Cross Sections for U^{233} in the Energy Range 0.4 to 2000 ev," ORNL-TM-2140, 1968.
- IV-22. N. M. Steen, "Analysis of the Fission Neutron Spectrum of Uranium-233 and Criticality Computations for Homogeneous Uranium-233 - H_2O Spheres and Cylinders," WAPD-TM-997, June 1972.
- IV-23. M. Drake, "Neutron Cross Sections for Uranium-233," GA-7076, September 15, 1966.
- IV-24. C. J. Emert and S. Milani, "Measured Natural Neutron Source in $U^{233}O_2-ZrO_2$ and $U^{233}O_2-ThO_2$," WAPD-TM-601, April 1967.
- IV-25. F. L. Moore and S. A. Reynolds, "Determinations of Protactinium-233," An. Chem. 29 (1957) 1596.
- IV-26. H. W. Wright, et al, "Half-Lives of Radionuclides," Nuc. Sci. Eng. 2 (1957) 427.
- IV-27. L. D. McIsaac and E. C. Freiling, "Counting Efficiency Determinations of Pa^{233} ," Nucleonics 14 (1956) 65.
- IV-28. F. B. Simpson and J. W. Coddington, Jr., "Total Neutron Cross Section of Pa^{233} ," Nuc. Sci. Eng. 28 (1967) 133.
- IV-29. J. C. Connor, "Integral Measurements of the Protactinium-233 Neutron Capture Cross Section," WAPD-TM-837, June 1970.
- IV-30. N. M. Steen "Nonlinear Analysis Procedure for Evaluation of Resonance Range Capture Cross Sections," WAPD-TM-1246, January 1976.
- IV-31. R. L. Macklin, J. A. Harvey, J. Halperin, and N. W. Hill, "The 292.4 ev Neutron Resonance Parameters of Zirconium-91," Nuc. Sci. Eng. 62 (1977) 176.
- IV-32. E. E. Carroll and R. W. Stooksberry "Zirconium (n, p) Cross Section Measurements," Nuc. Sci. Eng. 25 (1966) 285.
- IV-33. B. P. Bayhurst and R. J. Prestwood, "(n, p) and (n, x) Excitation Functions of Several Nuclei From 7.0 to 19.8 Mev," J. Inorg. Nuc. Chem. 23 (1961) 1973.
- IV-34. J. L. Gammel, "The n-p Total and Differential Cross Sections in the Energy Range 0-40 Mev," in J. B. Marion and J. L. Fowler, eds., "Fast Neutron Physics, Part II, Experiments and Theory," Interscience, New York, 1963, Page 2185.

- IV-35. E. Melkonian, "A Precise Determination of the Slow Neutron Cross Section of the Free Proton," Phys. Rev. 76 (1949) 1744, and "Slow Neutron Velocity Spectrometer Studies of O₂, N₂, A, H₂, H₂O₂, and Seven Hydrocarbons," Phys. Rev. 76 (1949) 1750.
- IV-36. N. Corngold, "Thermalization of Neutrons in Infinite Homogeneous Systems," Annals of Phys. 6 (1959) 368.
- IV-37. H. M. Sumner, "The Neutron Cross Sections of Xe¹³⁵," AEEW-R 116, June 1962.
- IV-38. D. Garber, compiler, "ENDF/B Summary Documentation," BNL 17541 (ENDF-201) 2nd Edition, October 1975.
- IV-39. T. R. England, "Time-Dependent Fission-Product Thermal and Resonance Absorption Cross Sections (Data Revisions and Computational Extensions)," WAPD-TM-333, Addendum No. 1, January 1965.
- IV-40. D. R. Bidinosti, D. E. Irish, and R. H. Tomlinson, "The Thermal Neutron Fission Yields of U²³³," Can. J. Chem. 39 (1961) 628.
- IV-41. A. O. Okazaki, W. H. Walker, and G. B. Bigham, "The Ratio of the Direct to the Cumulative Fission Yield of Xe¹³⁵ in the Thermal Neutron Fission of U²³³, U²³⁵, Pu²³⁹, and Pu²⁴¹," Can. J. Phys. 44 (1966) 237. A correction is given in the following reference.
- IV-42. A. O. Okazaki, W. H. Walker, and G. B. Bigham, Erratum, Can. J. Phys. 49 (1971) 498.
- IV-43. G. Robert Keepin, Physics of Nuclear Kinetics, Ch. 4, Addison-Wesley Publishing Company, Inc., Palo Alto, 1965.
- IV-44. M. S. Krick and A. E. Evans, "The Measurement of Total Delayed-Neutron Yields as a Function of the Energy of the Neutron Inducing Fission," Nuc. Sci. Eng. 47 (1972) 311.
- IV-45. C. F. Masters, et al, "The Measurement of Absolute Delayed-Neutron Yields from 3.1- and 14.9-Mev Fission," Nuc. Sci. Eng. 36 (1969) 202.
- IV-46. F. J. Conant and P. F. Palmedo, "Measurement of the Delayed-Neutron Fractions for Thermal Fission of Uranium-235, Plutonium-239, and Uranium-233," Nuc. Sci. Eng. 44 (1971) 173.
- IV-47. G. W. Eccleston and G. L. Woodruff, "Delayed Neutron Spectra from Th²³², U²³³, U²³⁵, U²³⁸, and Pu²³⁹," Trans. A.N.S. 23 (1976) 492.
- IV-48. D. Garber, C. Dunford, and S. Pearlstein, editors, "ENDF-102, Data Formats, and Procedures for the Evaluated Nuclear Data File, ENDF," BNL-NCS-50496 (ENDF 102), October 1975.

- IV-49. R. A. Dannels and D. E. Kusner, "ETOM-1-A FORTRAN IV Program to Process Data from the ENDF/B File to the MUFT Format," WCAP-3688-1, May 1968.
- IV-50. D. E. Kusner, S. Kellman, and R. A. Dannels, "ETOG-1, A FORTRAN IV Program to Process Data from the ENDF/B File to the MUFT, GAM, and ANISN Formats," WCAP-3845-1 (ENDF 114), December 1969.
- IV-51. C. L. Beard and R. A. Dannels, "ETOT, A FORTRAN IV Program to Process Data from the ENDF/B File to Thermal Library Format," WCAP-7363 (ENDF 146), March 1971.
- IV-52. H. C. Honeck and D. R. Finch, "FLANGE II (Version 71-1), A Code to Process Thermal Neutron Data from An ENDF/B Tape," DP-1278, October 1971.
- IV-53. S. S. Glickstein, et al, "Thermal Disadvantage Factors and Fast Advantage Factors in Uranium-Thorium, Seed-Blanket Assemblies," Nuc. Sci. Eng. 30 (1967) 122.
- IV-54. A. Sauer, "Thermal Utilization in the Square Lattice Cell," J. Nuc. Ener. 18 (1964) 425.
- IV-55. A. V. Dralle, N. R. Candelore, and R. C. Gast, "RCPL1 - A Program to Prepare Neutron and Photon Cross Section Libraries for RCP01," WAPD-TM-1268, August 1978, and N. R. Candelore, R. C. Gast, and L. Ondis, "RCP01 - A Monte Carlo Program for Solving the Neutron and Photon Transport Problems in Three Dimensional Geometry with Detailed Energy Descriptions," WAPD-TM-1267, August 1978.
- IV-56. H. Bohl, Jr. and A. P. Hemphill, "MUFT-5, A Fast Neutron Spectrum Program for the Philco-2000," WAPD-TM-218, February 1961. An updated version of MUFT is contained in the PAX program for the CDC-6600 and 7600 computers.
- IV-57. N. M. Steen, "PUN-1-A FORTRAN-IV Program for the Evaluation of Unresolved Resonance Integrals and Related Multigroup Cross Sections," WAPD-TM-768, March 1969.
- IV-58. A. J. Buslik, "Calculational Method for Thermal Disadvantage Factor," Nuc. Sci. Eng. 38 (1969) 71.
- IV-59. H. J. Amster and J. B. Callaghan, "KATE-1, A Program for Calculating Wigner-Wilkins and Maxwellian Averaged Thermal Constants on the Philco-2000," WAPD-TM-232, October 1960. An updated version of KATE is contained in the PAX program for the CDC-6600 and 7600 computers.

- IV-60. H. Bohl, Jr., et al, "P3MG-1, A One-Dimensional Multigroup P-3 Program for the Philco-2000 Computer," WAPD-TM-272, September 1963. The P7MG option in PAX is an extended version of this reference.
- IV-61. G. F. Kuncir, "A Program for the Calculation of Resonance Integrals," GA-2525, March 14, 1962.
- IV-62. C. R. Weisbin, et al, "MINX: A Multigroup Interpretation of Nuclear X-Sections from ENDF/B," LA-6486-MS (ENDF-237), September 1976.
- IV-63. B. L. Anderson, E. M. Gelbard, and J. Spanier, "RESQ-2: A Combined Analytic-Monte Carlo Calculation of Resonance Absorption Based on Superposition," WAPD-TM-665, June 1967.
- IV-64. R. J. Breen, "A One-Group Model for Thermal Activation Calculations," Nuc. Sci. Eng. 9 (1961) 91.
- IV-65. A. J. Buslik, "The Description of the Thermal Neutron Spatially Dependent Spectrum By Means of Variational Principles," Bettis Technical Review, WAPD-BT-25, May 1962.
- IV-66. J. A. Mitchell, editor, "BMU Series of U²³³ Fueled Critical Experiments," WAPD-TM-1117, January 1975.
- IV-67. R. J. Breen, O. J. Marlowe, and C. J. Pfeifer, "HARMONY: System for Nuclear Reactor Depletion Computation," WAPD-TM-478, January 1965.
- IV-68. J. A. Davis and L. A. Hageman, "An Iterative Method for Solving the Neutron Transport Equation in x,y Geometry," SIAM J. Appl. Math. 17 (1969) 149.

TABLE IV-1. TYPICAL LWBR CORE ABSORPTION FRACTIONS AFTER 8,000 HOURS
OF DEPLETION AT FULL POWER, ORDERED BY MAGNITUDE

Heavy Elements	0.915
Clad, Water, and Structure	0.053
Fission Products	0.032
<hr/>	
Th-232	0.46253
U-233	0.43667
Zirc-4	0.02020
H	0.01855
Xe-135	0.01060
U-234	0.00802
Pa-233	0.00579
SS-304	0.00563
AM-350	0.00480
Sm-149	0.00380
O	0.00298
Pm-147	0.00192
Sm-151	0.00136
U-235	0.00133
Inc-718	0.00106
Pa-231	0.00083
Pm-148M	0.00048
Sm-150	0.00023
Pm-148	0.00018
U-232	0.00009
U-236	0.00002
Pm-149	0.00001
Other Fission Products	0.01292
	<hr/>
	1.00000

TABLE IV-2. FISSION PRODUCT NUCLIDES IN ORDER OF IMPORTANCE
IN LWBR HIGH ZONE SEED SPECTRUM AFTER 10,500 HOURS
OF FULL POWER OPERATION

<u>Fission Product Nuclide</u>	<u>Order of Importance in LWBR</u>	<u>Percent of Fission Product Absorption</u>	<u>Accumulated Absorption (Percent)</u>
Xe-135**	1	25.9	25.9
Sm-149**	2	11.3	37.2
Xe-131*	3	8.0	45.2
Cs-133*	4	7.2	52.4
Pm-147*	5	6.9	59.3
Nd-143*	6	6.2	65.5
Sm-151**	7	4.4	69.9
Tc-099*	8	4.3	74.2
Rh-103*	9	3.5	77.7
Nd-145*	10	3.3	81.0
Sm-152*	11	2.8	83.8
Mo-095*	12	1.8	85.6
Pm-148M	13	1.6	87.2
Eu-153*	14	1.3	88.5
Kr-083	15	0.96	89.5
Sm-150	16	0.89	90.4

*Spectrum dependent few-group 3 cross sections were calculated by the PAX program for these 10 nuclides.

**Spectrum dependent thermal cross sections were calculated by the PAX program for these 3 nuclides.

TABLE IV-3. THERMAL CROSS SECTIONS AND RESONANCE
INTEGRALS FOR FISSION PRODUCTS
(Units Are Barns)

Isotope	$\sigma_a (2200\text{m/s})$	$\int_{0.625 \text{ ev}}^{\infty} \sigma_a \frac{dE}{E}$
Xe ¹³¹	90	872
Cs ¹³³	29.9	454
Pm ¹⁴⁷	181	2092
Nd ¹⁴³	337	118
Sm ¹⁵¹	15000	3300
Tc ⁹⁹	22	306
Rh ¹⁰³	148	1174
Nd ¹⁴⁵	47	304

TABLE IV-4. FISSION PRODUCT YIELDS FROM U^{233}
FISSION AND HALF-LIVES

<u>Isotope</u>	<u>Fission Yield (%)</u>	<u>Half-Life (hours)</u>
Te ^{131M}	1.68	30.00
I ¹³¹	1.83	193.57
Xe ¹³¹	0.00	∞
Xe ¹³²	0.53	96.27×10^5
I ¹³³	5.96	20.80
Xe ¹³³	0.10	126.51
Cs ¹³³	0.00	∞
Cs ¹³⁴	0.00	18.06×10^3
Ce ¹⁴²	6.71	∞
Ce ¹⁴³	5.85	33.00
Pr ¹⁴³	0.00	325.92
Nd ¹⁴³	0.00	∞
Nd ¹⁴⁴	0.01	∞
Pr ¹⁴⁵	3.37	5.98
Nd ¹⁴⁵	0.00	∞
Nd ¹⁴⁶	2.53	∞
Nd ¹⁴⁷	1.78	265.44
Pm ¹⁴⁷	0.00	23.00×10^3
Pm ^{148M}	0.00	995.97
Pm ¹⁴⁸	0.00	129.66
Pm ¹⁴⁹	0.77	53.10
Sm ¹⁴⁹	0.00	∞
Sm ¹⁵⁰	0.01	∞
Sm ¹⁵¹	0.00	81.52×10^4
Sm ¹⁵²	0.19	∞

TABLE IV-5. DELAYED NEUTRON HALF-LIVES AND YIELDS

U^{233}	<u>Group</u>	<u>Half-Life*</u> <u>(Seconds)</u>	β_i
			<u>(Delayed Neutrons per Fission Neutron)</u>
U^{233}	1	55.11 ± 2.75	0.000237
	2	20.74 ± 1.27	0.000756
	3	5.30 ± 0.29	0.000627
	4	2.29 ± 0.27	0.000875
	5	0.546 ± 0.16	0.000201
	6	0.221 ± 0.063	0.000064
			$\beta_{TOT} = 0.002760$
Th^{232}	1	56.03 ± 1.40	0.000751
	2	20.75 ± 0.99	0.003312
	3	5.74 ± 0.36	0.003422
	4	2.16 ± 0.12	0.009848
	5	0.571 ± 0.063	0.003798
	6	0.211 ± 0.029	0.000949
			$\beta_{TOT} = 0.022080$

*The quoted uncertainties are one standard deviation.

TABLE IV-6. TYPICAL LWBR FAST ADVANTAGE FACTORS

Few-Group	Core	Fuel Region	A	FAF _w	FAF _p
1	hot, as-built core	seed	1.032	0.983	1.015
		regular blanket	1.033	0.977	1.010
		power flattening blanket	1.047	0.973	1.020
1	cold, Detailed Cell experiment	seed	1.037	0.980	1.017
		regular blanket	1.039	0.972	1.011
		power flattening blanket	1.055	0.968	1.023
2	hot	all binary	1.018	0.991	1.010
2	cold	all binary	1.027	0.984	1.012
1, 2	all	all thorium	1.0	1.0	1.0

TABLE IV-7. THERMAL DISADVANTAGE FACTORS FOR
LWBR BY THE MULTIPLE-SAUER METHOD

t = absorption

Cell	Time*	i = U ²³³ G _i ^l	Th G _i ^t	ZR-4 G _i ^t	H G _i ^t
High Zone Seed	0	0.981	0.983	1.100	1.163
	8,000	0.982	0.983	1.099	1.162
	40,000	0.989		1.089	1.143
Low Zone Seed	0	0.989		1.094	1.150
Seed Thorium	0	1.010	1.010	1.036	1.051
	20,000	1.000	1.000	1.046	1.071
High Zone Regular Blanket	0	0.981		1.104	1.166

*Hours of PAX depletion (see Section IV.E).

TABLE IV-8. COMPARISON OF PAX AND RCP REACTION RATES
IN UNIT CELL LATTICES

	HIGH ZONE SEED		OPERATING TEMP		
U-233 CAPTURE	GROUP 1	GROUP 2	GROUP 3	GROUP 4	TOTAL
PAX VALUE	0.256120E-03	0.275660E-02	0.539818E-01	0.204141E-01	0.774085E-01
RCP VALUE	0.254803E-03	0.274139E-02	0.543528E-01	0.202790E-01	0.776279E-01
1 PROB ERROR	0.747669E-06	0.518851E-05	0.133035E-03	0.487797E-04	0.141793E-03
% PE/RCP	0.293430E+00	0.189266E+00	0.244763E+00	0.240543E+00	0.182658E+00
%RCP-PAX/RCP	-0.516868E+00	-0.554897E+00	0.682581E+00	-0.666092E+00	0.282617E+00
RCP-PAX/PE	-0.176147E+01	-0.293184E+01	0.278875E+01	-0.276912E+01	0.154725E+01
TH-232 CAPTURE					
PAX VALUE	0.127342E-01	0.554306E-01	0.192553E+00	0.439143E-01	0.304633E+00
RCP VALUE	0.126634E-01	0.558313E-01	0.192364E+00	0.434780E-01	0.304337E+00
1 PROB ERROR	0.379200E-04	0.958483E-04	0.594467E-03	0.102378E-03	0.611962E-03
% PE/RCP	0.299446E+00	0.171675E+00	0.309032E+00	0.235472E+00	0.201080E+00
%RCP-PAX/RCP	-0.559122E+00	0.717702E+00	-0.983920E-01	-0.100361E+01	-0.971665E-01
RCP-PAX/PE	-0.186719E+01	0.418059E+01	-0.318387E+00	-0.426211E+01	-0.483222E+00
U-234 ABSORPTION					
PAX VALUE	0.153896E-03	0.126073E-03	0.487226E-02	0.495326E-03	0.564756E-02
RCP VALUE	0.153732E-03	0.125837E-03	0.493597E-02	0.489609E-03	0.570515E-02
1 PROB ERROR	0.448104E-06	0.267575E-06	0.675912E-04	0.117966E-05	0.676035E-04
% PE/RCP	0.291484E+00	0.212636E+00	0.136936E+01	0.240939E+00	0.118496E+01
%RCP-PAX/RCP	-0.106542E+00	-0.187927E+00	0.129068E+01	-0.116757E+01	0.100945E+01
RCP-PAX/PE	-0.365516E+00	-0.883795E+00	0.942542E+00	-0.484591E+01	0.851890E+00
PA-233 ABSORPTION					
PAX VALUE	0.377436E-09	0.705377E-09	0.284129E-07	0.127315E-08	0.307689E-07
RCP VALUE	0.378857E-09	0.697940E-09	0.282108E-07	0.127287E-08	0.305605E-07
1 PROB ERROR	0.122335E-11	0.161587E-11	0.108526E-09	0.306778E-11	0.108588E-09
% PE/RCP	0.322905E+00	0.231520E+00	0.384694E+00	0.241013E+00	0.355321E+00
%RCP-PAX/RCP	0.374986E+00	-0.106551E+01	-0.716359E+00	-0.222645E-01	-0.681897E+00
RCP-PAX/PE	0.116129E+01	-0.460224E+01	-0.186215E+01	-0.923790E-01	-0.191910E+01
O-PELLET ABSORPTION					
PAX VALUE	0.194496E-02	0.624794E-07	0.181341E-05	0.240736E-05	0.194924E-02
RCP VALUE	0.198773E-02	0.619349E-07	0.182233E-05	0.239246E-05	0.199201E-02
1 PROB ERROR	0.175609E-04	0.127666E-09	0.367971E-08	0.562398E-08	0.175609E-04
% PE/RCP	0.883465E+00	0.206129E+00	0.201923E+00	0.235071E+00	0.881568E+00
%RCP-PAX/RCP	0.215174E+01	-0.879158E+00	0.489522E+00	-0.622760E+00	0.214679E+01
RCP-PAX/PE	0.243557E+01	-0.426508E+01	0.242430E+01	-0.264924E+01	0.243520E+01
TOTAL OXYGEN					
PAX VALUE	0.286956E-02	0.926595E-07	0.276657E-05	0.379993E-05	0.287621E-02
RCP VALUE	0.291065E-02	0.920452E-07	0.278192E-05	0.377375E-05	0.291730E-02
1 PROB ERROR	0.198923E-04	0.152668E-09	0.399869E-08	0.830612E-08	0.198923E-04
% PE/RCP	0.683431E+00	0.165862E+00	0.143739E+00	0.220102E+00	0.681874E+00
%RCP-PAX/RCP	0.141188E+01	-0.667405E+00	0.551520E+00	-0.693641E+00	0.140827E+01
RCP-PAX/PE	0.206587E+01	-0.402385E+01	0.383697E+01	-0.315145E+01	0.206529E+01
ZIRC ABSORPTION					
PAX VALUE	0.407575E-03	0.267202E-02	0.681139E-02	0.102399E-02	0.109150E-01
RCP VALUE	0.405368E-03	0.265583E-02	0.695538E-02	0.102287E-02	0.110394E-01
1 PROB ERROR	0.183202E-05	0.148107E-04	0.751969E-04	0.607684E-05	0.769039E-04
% PE/RCP	0.451940E+00	0.557669E+00	0.108113E+01	0.594099E+00	0.696628E+00
%RCP-PAX/RCP	-0.544530E+00	-0.609547E+00	0.207029E+01	-0.109848E+00	0.112757E+01
RCP-PAX/PE	-0.120487E+01	-0.109303E+01	0.191492E+01	-0.184898E+00	0.161861E+01

TABLE IV-8 (Cont)

TOTAL
ZIRCALOY

PAX VALUE	0.439104E-03	0.287852E-02	0.839866E-02	0.119088E-02	0.129072E-01
RCP VALUE	0.436840E-03	0.286122E-02	0.852615E-02	0.118975E-02	0.130140E-01
1 PROB ERROR	0.183827E-05	0.148248E-04	0.754558E-04	0.622086E-05	0.771715E-04
% PE/RCP	0.420811E+00	0.518129E+00	0.834993E+00	0.522871E+00	0.592990E+00
%RCP-PAX/RCP	-0.518284E+00	-0.604864E+00	0.149525E+01	-0.951333E-01	0.820545E+00
RCP-PAX/PE	-0.123163E+01	-0.116740E+01	0.168956E+01	-0.181944E+00	0.138374E+01

HYDROGEN
ABSORPTION

PAX VALUE	0.777541E-05	0.549444E-04	0.232866E-02	0.511869E-02	0.751007E-02
RCP VALUE	0.770334E-05	0.548031E-04	0.234409E-02	0.507719E-02	0.748379E-02
1 PROB ERROR	0.226613E-07	0.676064E-07	0.382640E-05	0.224776E-04	0.228011E-04
% PE/RCP	0.294175E+00	0.123362E+00	0.163236E+00	0.442717E+00	0.304673E+00
%RCP-PAX/RCP	-0.935576E+00	-0.257838E+00	0.658362E+00	-0.817344E+00	-0.351144E+00
RCP-PAX/PE	-0.318034E+01	-0.209009E+01	0.403319E+01	-0.184620E+01	-0.115253E+01

AN-330
ABSORPTION

PAX VALUE	0.898592E-04	0.267278E-03	0.175048E-02	0.255443E-02	0.466204E-02
RCP VALUE	0.839310E-04	0.266299E-03	0.175795E-02	0.253371E-02	0.464694E-02
1 PROB ERROR	0.542610E-06	0.363767E-06	0.223319E-05	0.112172E-04	0.114560E-04
% PE/RCP	0.609804E+00	0.136601E+00	0.127034E+00	0.442718E+00	0.246527E+00
%RCP-PAX/RCP	-0.986953E+00	-0.367766E+00	0.425029E+00	-0.817584E+00	-0.324964E+00
RCP-PAX/PE	-0.161848E+01	-0.269227E+01	0.334580E+01	-0.184674E+01	-0.131817E+01

U-233
TOTFIS

PAX VALUE	0.123587E-01	0.287673E-01	0.325301E+00	0.208983E+00	0.575411E+00
RCP VALUE	0.123419E-01	0.286714E-01	0.326749E+00	0.208103E+00	0.575865E+00
1 PROB ERROR	0.359214E-04	0.522356E-04	0.583327E-03	0.488471E-03	0.763475E-03
% PE/RCP	0.291052E+00	0.182187E+00	0.178525E+00	0.234726E+00	0.132579E+00
%RCP-PAX/RCP	-0.136041E+00	-0.334532E+00	0.442980E+00	-0.423304E+00	0.788084E-01
RCP-PAX/PE	-0.467409E+00	-0.183620E+01	0.248134E+01	-0.180340E+01	0.594427E+00

U-235
TOTFIS

PAX VALUE	0.533310E-05	0.125047E-04	0.973409E-04	0.123785E-03	0.238964E-03
RCP VALUE	0.532744E-05	0.124484E-04	0.972529E-04	0.122567E-03	0.237596E-03
1 PROB ERROR	0.155971E-07	0.228392E-07	0.270712E-06	0.294301E-06	0.400828E-06
% PE/RCP	0.292769E+00	0.183471E+00	0.278359E+00	0.240115E+00	0.168702E+00
%RCP-PAX/RCP	-0.106273E+00	-0.452645E+00	-0.904988E-01	-0.994109E+00	-0.575965E+00
RCP-PAX/PE	-0.362991E+00	-0.246712E+01	-0.325116E+00	-0.414014E+01	-0.341410E+01

TH-232
TOTFIS

PAX VALUE	0.104454E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.104454E-01
RCP VALUE	0.105504E-01	0.163167E-11	0.000000E+00	0.000000E+00	0.105504E-01
1 PROB ERROR	0.420803E-04	0.110056E-11	0.000000E+00	0.000000E+00	0.420803E-04
% PE/RCP	0.398850E+00	0.674499E+02	0.000000E+00	0.000000E+00	0.398850E+00
%RCP-PAX/RCP	0.994892E+00	0.100000E+03	0.000000E+00	0.000000E+00	0.994892E+00
RCP-PAX/PE	0.249440E+01	0.148258E+01	0.000000E+00	0.000000E+00	0.249440E+01

TOTAL
ABSORPTION

PAX VALUE	0.393606E-01	0.902979E-01	0.589355E+00	0.282821E+00	0.100183E+01
RCP VALUE	0.394144E-01	0.905687E-01	0.591199E+00	0.281298E+00	0.100248E+01
1 PROB ERROR	0.699940E-04	0.110283E-03	0.849495E-03	0.502131E-03	0.995409E-03
% PE/RCP	0.177585E+00	0.121767E+00	0.143690E+00	0.178505E+00	0.992947E-01
%RCP-PAX/RCP	0.136404E+00	0.299022E+00	0.311921E+00	-0.541377E+00	0.644234E-01
RCP-PAX/PE	0.768107E+00	0.245568E+01	0.217078E+01	-0.303284E+01	0.648810E+00

TABLE IV-9. COMPARISON OF PAX AND RCP REACTION RATES
IN UNIT CELL LATTICES

	LOW ZONE BLANKET		OPERATING TEMP			
U-233 CAPTURE	GROUP 1	GROUP 2	GROUP 3	GROUP 4	TOTAL	
PAX VALUE	0.359687E-04	0.122223E-02	0.295578E-01	0.148086E-01	0.456746E-01	
RCP VALUE	0.851271E-04	0.121259E-02	0.292688E-01	0.147649E-01	0.453315E-01	
1 PROB ERROR	0.307454E-06	0.259311E-05	0.114179E-02	0.383835E-04	0.114243E-02	
% PE/RCP	0.361171E+00	0.213849E+00	0.390103E+01	0.259964E+00	0.252017E+01	
%RCP-PAX/RCP	-0.983633E+00	-0.794909E+00	-0.987227E+00	-0.295462E+00	-0.756797E+00	
RCP-PAX/PE	-0.273732E+01	-0.371715E+01	-0.253069E+00	-0.113655E+01	-0.300295E+00	
TH-232 CAPTURE						
PAX VALUE	0.192807E-01	0.110049E+00	0.295036E+00	0.144386E+00	0.568752E+00	
RCP VALUE	0.190817E-01	0.109867E+00	0.293638E+00	0.143612E+00	0.571198E+00	
1 PROB ERROR	0.703974E-04	0.210544E-03	0.934771E-03	0.363073E-03	0.102708E-02	
% PE/RCP	0.368926E+00	0.191635E+00	0.313012E+00	0.252816E+00	0.179812E+00	
%RCP-PAX/RCP	-0.104305E+01	-0.165344E+00	0.120593E+01	-0.539299E+00	0.428249E+00	
RCP-PAX/PE	-0.282727E+01	-0.862810E+00	0.385266E+01	-0.213317E+01	0.238165E+01	
U-234 ABSORPTION						
PAX VALUE	0.508828E-04	0.546478E-04	0.249777E-02	0.364137E-03	0.296744E-02	
RCP VALUE	0.506996E-04	0.542496E-04	0.248983E-02	0.361775E-03	0.295655E-02	
1 PROB ERROR	0.180920E-06	0.128731E-06	0.426058E-04	0.935629E-06	0.426167E-04	
% PE/RCP	0.356047E+00	0.237294E+00	0.171120E+01	0.258622E+00	0.144143E+01	
%RCP-PAX/RCP	-0.361368E+00	-0.733993E+00	-0.319159E+00	-0.652075E+00	-0.368332E+00	
RCP-PAX/PE	-0.101267E+01	-0.309320E+01	-0.186512E+00	-0.252444E+01	-0.255532E+00	
U-236 TOTALS						
PAX VALUE	0.126693E-06	0.171697E-06	0.660548E-05	0.103688E-06	0.700696E-05	
RCP VALUE	0.125772E-06	0.170808E-06	0.673913E-05	0.103541E-06	0.713925E-05	
1 PROB ERROR	0.465054E-09	0.356535E-09	0.119676E-06	0.262036E-09	0.119678E-06	
% PE/RCP	0.369760E+00	0.208764E+00	0.177584E+01	0.253075E+00	0.167634E+01	
%RCP-PAX/RCP	-0.255303E+00	-0.520754E+00	0.198324E+01	-0.141828E+00	0.185308E+01	
RCP-PAX/PE	-0.690457E+00	-0.249447E+01	0.111679E+01	-0.560421E+00	0.110543E+01	
O-PELLET ABSORPTION						
PAX VALUE	0.257653E-02	0.119235E-06	0.392607E-05	0.751644E-05	0.258809E-02	
RCP VALUE	0.266520E-02	0.117701E-06	0.390547E-05	0.750579E-05	0.267673E-02	
1 PROB ERROR	0.289239E-04	0.273844E-09	0.106457E-07	0.189946E-07	0.289239E-04	
% PE/RCP	0.108524E+01	0.232661E+00	0.272584E+00	0.253066E+00	0.108057E+01	
%RCP-PAX/RCP	0.332707E+01	-0.130346E+01	-0.527465E+00	-0.141838E+00	0.331151E+01	
RCP-PAX/PE	0.306573E+01	-0.560243E+01	-0.193505E+01	-0.560480E+00	0.306460E+01	
TOTAL OXYGEN						
PAX VALUE	0.317199E-02	0.147268E-06	0.491129E-05	0.956224E-05	0.318661E-02	
RCP VALUE	0.328766E-02	0.145672E-06	0.489154E-05	0.954945E-05	0.330224E-02	
1 PROB ERROR	0.305689E-04	0.276908E-09	0.108556E-07	0.216356E-07	0.305689E-04	
% PE/RCP	0.929808E+00	0.190090E+00	0.221926E+00	0.226563E+00	0.925701E+00	
%RCP-PAX/RCP	0.351810E+01	-0.109573E+01	-0.403817E+00	-0.133917E+00	0.350153E+01	
RCP-PAX/PE	0.378369E+01	-0.576426E+01	-0.181961E+01	-0.591077E+00	0.378257E+01	
ZIRC ABSORPTION						
PAX VALUE	0.348999E-03	0.300710E-02	0.739786E-02	0.185933E-02	0.126133E-01	
RCP VALUE	0.347154E-03	0.301941E-02	0.723530E-02	0.185403E-02	0.124559E-01	
1 PROB ERROR	0.219707E-05	0.216828E-04	0.953676E-04	0.112136E-04	0.984668E-04	
% PE/RCP	0.632881E+00	0.718113E+00	0.131809E+01	0.604823E+00	0.790524E+00	
%RCP-PAX/RCP	-0.531462E+00	0.407759E+00	-0.224685E+01	-0.285994E+00	-0.126368E+01	
RCP-PAX/PE	-0.839750E+00	0.567820E+00	-0.170463E+01	-0.472855E+00	-0.159853E+01	

TABLE IV-9 (Cont)

TOTAL
ZIRCALOY

PAX VALUE	0.375490E-03	0.324125E-02	0.917148E-02	0.216190E-02	0.149501E-01
RCP VALUE	0.373682E-03	0.325223E-02	0.898121E-02	0.215629E-02	0.147634E-01
1 PROB ERROR	0.220433E-05	0.217018E-04	0.957474E-04	0.114795E-04	0.988694E-04
% PE/RCP	0.589893E+00	0.667288E+00	0.106609E+01	0.532373E+00	0.669692E+00
%RCP-PAX/RCP	-0.483798E+00	0.337562E+00	-0.211861E+01	-0.259967E+00	-0.126469E+01
RCP-PAX/PE	-0.820146E+00	0.505872E+00	-0.198728E+01	-0.488318E+00	-0.188847E+01

HYDROGEN
ABSORPTION

PAX VALUE	0.536407E-05	0.510899E-04	0.240710E-02	0.752059E-02	0.998415E-02
RCP VALUE	0.533007E-05	0.510102E-04	0.240904E-02	0.751271E-02	0.997809E-02
1 PROB ERROR	0.238436E-07	0.827052E-07	0.519437E-05	0.380964E-04	0.384490E-04
% PE/RCP	0.447341E+00	0.162135E+00	0.215620E+00	0.507093E+00	0.385334E+00
%RCP-PAX/RCP	-0.637897E+00	-0.156176E+00	0.805301E-01	-0.104941E+00	-0.607086E-01
RCP-PAX/PE	-0.142598E+01	-0.963250E+00	0.373482E+00	-0.206945E+00	-0.157548E+00

AM-350
ABSORPTION

PAX VALUE	0.493574E-04	0.203156E-03	0.142519E-02	0.308460E-02	0.476230E-02
RCP VALUE	0.498845E-04	0.202454E-03	0.142604E-02	0.308136E-02	0.475974E-02
1 PROB ERROR	0.473673E-06	0.365075E-06	0.243699E-05	0.156254E-04	0.158256E-04
% PE/RCP	0.949539E+00	0.180325E+00	0.170892E+00	0.507094E+00	0.332489E+00
%RCP-PAX/RCP	0.105661E+01	-0.346661E+00	0.596693E-01	-0.105032E+00	-0.537888E-01
RCP-PAX/PE	0.111276E+01	-0.192243E+01	0.349164E+00	-0.207125E+00	-0.161776E+00

U-233
FISSIONS>

PAX VALUE	0.408954E-02	0.126786E-01	0.168956E+00	0.151305E+00	0.337029E+00
RCP VALUE	0.407287E-02	0.126091E-01	0.168099E+00	0.151394E+00	0.336176E+00
1 PROB ERROR	0.145306E-04	0.259455E-04	0.451998E-03	0.383407E-03	0.593454E-03
% PE/RCP	0.356766E+00	0.205768E+00	0.268888E+00	0.253250E+00	0.176531E+00
%RCP-PAX/RCP	-0.409234E+00	-0.551459E+00	-0.509669E+00	0.590434E-01	-0.253903E+00
RCP-PAX/PE	-0.114707E+01	-0.268000E+01	-0.189547E+01	0.233142E+00	-0.143829E+01

U-235
TOTFIS

PAX VALUE	0.176121E-05	0.552010E-05	0.441767E-04	0.905298E-04	0.141988E-03
RCP VALUE	0.175515E-05	0.548320E-05	0.436828E-04	0.901017E-04	0.141023E-03
1 PROB ERROR	0.628802E-08	0.113706E-07	0.135760E-06	0.233333E-06	0.270266E-06
% PE/RCP	0.358261E+00	0.207372E+00	0.310785E+00	0.258966E+00	0.191647E+00
%RCP-PAX/RCP	-0.345361E+00	-0.672880E+00	-0.113065E+01	-0.475107E+00	-0.684241E+00
RCP-PAX/PE	-0.963994E+00	-0.324480E+01	-0.363805E+01	-0.183463E+01	-0.357032E+01

TH-232
TOTFIS

PAX VALUE	0.150773E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.150773E-01
RCP VALUE	0.152260E-01	0.596428E-11	0.000000E+00	0.000000E+00	0.152260E-01
1 PROB ERROR	0.737892E-04	0.284583E-11	0.000000E+00	0.000000E+00	0.737892E-04
% PE/RCP	0.484626E+00	0.477146E+02	0.000000E+00	0.000000E+00	0.484626E+00
%RCP-PAX/RCP	0.976678E+00	0.100000E+03	0.000000E+00	0.000000E+00	0.976678E+00
RCP-PAX/PE	0.201532E+01	0.209580E+01	0.000000E+00	0.000000E+00	0.201532E+01

TOTAL
ABSORPTION

PAX VALUE	0.421886E-01	0.127507E+00	0.509132E+00	0.323747E+00	0.100257E+01
RCP VALUE	0.422349E-01	0.127256E+00	0.511391E+00	0.322999E+00	0.100388E+01
1 PROB ERROR	0.107478E-03	0.213260E-03	0.154686E-02	0.531154E-03	0.165286E-02
% PE/RCP	0.254476E+00	0.167583E+00	0.302481E+00	0.164444E+00	0.164647E+00
%RCP-PAX/RCP	0.109685E+00	-0.197315E+00	0.441892E+00	-0.231695E+00	0.130157E+00
RCP-PAX/PE	0.431023E+00	-0.117742E+01	0.146089E+01	-0.140896E+01	0.790523E+00

TABLE IV-10. COMPARISON OF PAX AND RCP REACTION RATES
IN UNIT CELL LATTICES

	HIGH ZONE BLANKET OPERATING TEMP				
U-233 CAPTURE	GROUP 1	GROUP 2	GROUP 3	GROUP 4	TOTAL
PAX VALUE	0.142953E-03	0.201843E-02	0.393407E-01	0.147429E-01	0.562449E-01
RCP VALUE	0.141177E-03	0.200816E-02	0.393946E-01	0.147484E-01	0.562923E-01
1 PROB ERROR	0.496189E-06	0.419816E-05	0.130486E-03	0.439103E-04	0.137741E-03
% PE/RCP	0.351466E+00	0.209055E+00	0.331227E+00	0.297730E+00	0.244688E+00
%RCP-PAX/RCP	-0.125784E+01	-0.511520E+00	0.136875E+00	0.371979E-01	0.841531E-01
RCP-PAX/PE	-0.357083E+01	-0.244682E+01	0.413235E+00	0.124938E+00	0.343920E+00
TH-232 ABSORPTION					
PAX VALUE	0.190747E-01	0.108141E+00	0.278055E+00	0.848940E-01	0.490165E+00
RCP VALUE	0.188206E-01	0.108530E+00	0.277692E+00	0.846208E-01	0.489663E+00
1 PROB ERROR	0.675471E-04	0.203687E-03	0.859269E-03	0.245892E-03	0.919161E-03
% PE/RCP	0.358900E+00	0.187678E+00	0.309433E+00	0.290582E+00	0.187713E+00
%RCP-PAX/RCP	-0.134987E+01	0.358186E+00	-0.130641E+00	-0.322821E+00	-0.102371E+00
RCP-PAX/PE	-0.376114E+01	0.190852E+01	-0.422196E+00	-0.111095E+01	-0.545357E+00
U-234 ABSORPTION					
PAX VALUE	0.846362E-04	0.903499E-04	0.349125E-02	0.357069E-03	0.402330E-02
RCP VALUE	0.839929E-04	0.898827E-04	0.361766E-02	0.355605E-03	0.414714E-02
1 PROB ERROR	0.291733E-06	0.208497E-06	0.577009E-04	0.105582E-05	0.577116E-04
% PE/RCP	0.347331E+00	0.231966E+00	0.159498E+01	0.296908E+00	0.139160E+01
%RCP-PAX/RCP	-0.765920E+00	-0.519759E+00	0.349412E+01	-0.411670E+00	0.298594E+01
RCP-PAX/PE	-0.220516E+01	-0.224067E+01	0.219070E+01	-0.138652E+01	0.214568E+01
U-236 T0TABS					
PAX VALUE	0.209764E-06	0.283686E-06	0.962916E-05	0.102967E-06	0.102256E-04
RCP VALUE	0.208370E-06	0.282559E-06	0.979138E-05	0.103000E-06	0.103853E-04
1 PROB ERROR	0.752183E-09	0.578183E-09	0.166562E-06	0.299453E-09	0.166565E-06
% PE/RCP	0.360984E+00	0.204624E+00	0.170111E+01	0.290708E+00	0.160385E+01
%RCP-PAX/RCP	-0.669151E+00	-0.398802E+00	0.165674E+01	0.397545E-01	0.153811E+01
RCP-PAX/PE	-0.185369E+01	-0.194895E+01	0.973916E+00	0.136751E+00	0.959010E+00
O-PELLET ABSORPTION					
PAX VALUE	0.257706E-02	0.118188E-06	0.327067E-05	0.448333E-05	0.258493E-02
RCP VALUE	0.266953E-02	0.117113E-06	0.328758E-05	0.448512E-05	0.267742E-02
1 PROB ERROR	0.284197E-04	0.265835E-09	0.830035E-08	0.130382E-07	0.284197E-04
% PE/RCP	0.106460E+01	0.226990E+00	0.252476E+00	0.290699E+00	0.106146E+01
%RCP-PAX/RCP	0.346394E+01	-0.917920E+00	0.514293E+00	0.400162E-01	0.345439E+01
RCP-PAX/PE	0.325376E+01	-0.404243E+01	0.203700E+01	0.137655E+00	0.325438E+01
TOTAL OXYGEN					
PAX VALUE	0.317209E-02	0.145948E-06	0.410643E-05	0.574696E-05	0.318209E-02
RCP VALUE	0.328921E-02	0.144783E-06	0.412979E-05	0.575666E-05	0.329924E-02
1 PROB ERROR	0.299941E-04	0.268774E-09	0.849368E-08	0.147898E-07	0.299942E-04
% PE/RCP	0.911896E+00	0.185639E+00	0.205669E+00	0.256916E+00	0.909123E+00
%RCP-PAX/RCP	0.356066E+01	-0.804925E+00	0.565747E+00	0.168556E+00	0.355080E+01
RCP-PAX/PE	0.390468E+01	-0.433597E+01	0.275077E+01	0.656072E+00	0.390574E+01
ZIRC ABSORPTION					
PAX VALUE	0.348190E-03	0.297819E-02	0.713169E-02	0.113608E-02	0.115942E-01
RCP VALUE	0.340462E-03	0.298008E-02	0.750272E-02	0.114894E-02	0.119722E-01
1 PROB ERROR	0.211499E-05	0.204615E-04	0.947172E-04	0.803061E-05	0.972574E-04
% PE/RCP	0.621212E+00	0.686608E+00	0.126244E+01	0.698959E+00	0.812360E+00
%RCP-PAX/RCP	-0.226989E+01	0.632767E-01	0.494530E+01	0.111893E+01	0.315770E+01
RCP-PAX/PE	-0.365398E+01	0.921583E-01	0.391726E+01	0.160085E+01	0.388707E+01

TABLE IV-10 (Cont)

TOTAL
ZIRCALOY

PAX VALUE	0.374630E-03	0.321007E-02	0.879570E-02	0.132127E-02	0.137017E-01
RCP VALUE	0.366396E-03	0.320875E-02	0.915228E-02	0.133660E-02	0.140640E-01
1 PROB ERROR	0.212181E-05	0.204800E-04	0.950423E-04	0.822167E-05	0.975939E-04
% PE/RCP	0.579102E+00	0.638255E+00	0.103846E+01	0.615117E+00	0.693926E+00
%RCP-PAX/RCP	-0.224702E+01	-0.412601E-01	0.389612E+01	0.114703E+01	0.257649E+01
RCP-PAX/PE	-0.388018E+01	-0.646453E-01	0.375184E+01	0.186474E+01	0.371292E+01

HYDROGEN
ABSORPTION

PAX VALUE	0.535352E-05	0.505666E-04	0.204179E-02	0.464473E-02	0.674244E-02
RCP VALUE	0.529658E-05	0.503978E-04	0.205735E-02	0.467379E-02	0.678683E-02
1 PROB ERROR	0.232577E-07	0.795572E-07	0.440602E-05	0.256744E-04	0.260499E-04
% PE/RCP	0.439108E+00	0.157858E+00	0.214160E+00	0.549327E+00	0.383829E+00
%RCP-PAX/RCP	-0.107494E+01	-0.335017E+00	0.756376E+00	0.621824E+00	0.654181E+00
RCP-PAX/PE	-0.244801E+01	-0.212226E+01	0.353183E+01	0.113197E+01	0.170435E+01

AM-350
ABSORPTION

PAX VALUE	0.492881E-04	0.201084E-03	0.125700E-02	0.190505E-02	0.341243E-02
RCP VALUE	0.500072E-04	0.200439E-03	0.126444E-02	0.191697E-02	0.343186E-02
1 PROB ERROR	0.464857E-06	0.349999E-06	0.210848E-05	0.105304E-04	0.107552E-04
% PE/RCP	0.929580E+00	0.174616E+00	0.166752E+00	0.549325E+00	0.313392E+00
%RCP-PAX/RCP	0.143797E+01	-0.321643E+00	0.580015E+00	0.621804E+00	0.566146E+00
RCP-PAX/PE	0.154691E+01	-0.184200E+01	0.352628E+01	0.113194E+01	0.180651E+01

U-233
FISSION

PAX VALUE	0.680227E-02	0.209486E-01	0.231227E+00	0.150951E+00	0.409929E+00
RCP VALUE	0.674697E-02	0.208794E-01	0.231702E+00	0.151296E+00	0.410625E+00
1 PROB ERROR	0.234225E-04	0.420542E-04	0.544422E-03	0.439845E-03	0.701552E-03
% PE/RCP	0.347156E+00	0.201415E+00	0.234966E+00	0.290718E+00	0.170850E+00
%RCP-PAX/RCP	-0.819623E+00	-0.331609E+00	0.204983E+00	0.228079E+00	0.169372E+00
RCP-PAX/PE	-0.236097E+01	-0.164640E+01	0.872394E+00	0.784540E+00	0.991352E+00

U-235
FISSION

PAX VALUE	0.292959E-05	0.911913E-05	0.660088E-04	0.892999E-04	0.167357E-03
RCP VALUE	0.290771E-05	0.907881E-05	0.659958E-04	0.889898E-04	0.166972E-03
1 PROB ERROR	0.101419E-07	0.184201E-07	0.190917E-06	0.264350E-06	0.331498E-06
% PE/RCP	0.348793E+00	0.202891E+00	0.301409E+00	0.297057E+00	0.198535E+00
%RCP-PAX/RCP	-0.752533E+00	-0.444063E+00	-0.196229E-01	-0.348457E+00	-0.230721E+00
RCP-PAX/PE	-0.215753E+01	-0.213868E+01	-0.651039E-01	-0.117303E+01	-0.116212E+01

TH-232
FISSION

PAX VALUE	0.149305E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.149305E-01
RCP VALUE	0.150039E-01	0.557639E-11	0.000000E+00	0.000000E+00	0.150039E-01
1 PROB ERROR	0.714394E-04	0.266165E-11	0.000000E+00	0.000000E+00	0.714394E-04
% PE/RCP	0.476139E+00	0.477307E+02	0.000000E+00	0.000000E+00	0.476139E+00
%RCP-PAX/RCP	0.489060E+00	0.100000E+03	0.000000E+00	0.000000E+00	0.489060E+00
RCP-PAX/PE	0.102714E+01	0.209509E+01	0.000000E+00	0.000000E+00	0.102714E+01

TOTAL
ABSORPTION

PAX VALUE	0.446397E-01	0.134673E+00	0.564325E+00	0.258927E+00	0.100256E+01
RCP VALUE	0.445108E-01	0.134979E+00	0.564997E+00	0.259059E+00	0.100355E+01
1 PROB ERROR	0.105449E-03	0.209031E-03	0.103158E-02	0.506649E-03	0.117288E-02
% PE/RCP	0.236907E+00	0.154862E+00	0.182581E+00	0.195573E+00	0.116874E+00
%RCP-PAX/RCP	-0.289532E+00	0.227114E+00	0.119103E+00	0.508940E-01	0.978991E-01
RCP-PAX/PE	-0.122214E+01	0.146656E+01	0.652330E+00	0.260230E+00	0.837647E+00

TABLE IV-11. COMPARISON OF PAX AND RCP REACTION RATES
IN UNIT CELL LATTICES

	HI ZONE PFB		OPERATING TEMP		
U-233 CAPTURE	GROUP 1	GROUP 2	GROUP 3	GROUP 4	TOTAL
PAX VALUE	0.154430E-03	0.173469E-02	0.415343E-01	0.224920E-01	0.659155E-01
RCP VALUE	0.153317E-03	0.173149E-02	0.414093E-01	0.224962E-01	0.657903E-01
1 PROB ERROR	0.528670E-06	0.390069E-05	0.137459E-03	0.532560E-04	0.147468E-03
% PE/RCP	0.344822E+00	0.225279E+00	0.331953E+00	0.236734E+00	0.224148E+00
%RCP-PAX/RCP	-0.725940E+00	-0.184814E+00	-0.301959E+00	0.184206E-01	-0.190321E+00
RCP-PAX/PE	-0.210526E+01	-0.820378E+00	-0.909643E+00	0.778113E-01	-0.849084E+00
TH-232 CAPTURE					
PAX VALUE	0.149145E-01	0.677204E-01	0.214137E+00	0.947503E-01	0.391522E+00
RCP VALUE	0.147904E-01	0.683540E-01	0.213755E+00	0.945136E-01	0.391413E+00
1 PROB ERROR	0.520733E-04	0.138714E-03	0.759920E-03	0.217772E-03	0.804273E-03
% PE/RCP	0.352075E+00	0.202934E+00	0.355510E+00	0.230413E+00	0.205480E+00
%RCP-PAX/RCP	-0.838807E+00	0.926943E+00	-0.178803E+00	-0.250411E+00	-0.279340E-01
RCP-PAX/PE	-0.238247E+01	0.456771E+01	-0.502948E+00	-0.108679E+01	-0.135945E+00
U-234 ABSORPTION					
PAX VALUE	0.929238E-04	0.790089E-04	0.362930E-02	0.554624E-03	0.435586E-02
RCP VALUE	0.925068E-04	0.793892E-04	0.349182E-02	0.552950E-03	0.421667E-02
1 PROB ERROR	0.317028E-06	0.198907E-06	0.616788E-04	0.130368E-05	0.616938E-04
% PE/RCP	0.342708E+00	0.250547E+00	0.176638E+01	0.235768E+00	0.146309E+01
%RCP-PAX/RCP	-0.450764E+00	0.479078E+00	-0.393710E+01	-0.302794E+00	-0.330088E+01
RCP-PAX/PE	-0.131530E+01	0.191213E+01	-0.222891E+01	-0.128429E+01	-0.225610E+01
U-236 TOTABS					
PAX VALUE	0.231835E-06	0.243812E-06	0.100504E-04	0.157501E-06	0.106835E-04
RCP VALUE	0.230910E-06	0.244202E-06	0.991770E-05	0.157601E-06	0.105504E-04
1 PROB ERROR	0.825592E-09	0.535998E-09	0.189652E-06	0.362849E-09	0.189655E-06
% PE/RCP	0.357538E+00	0.219490E+00	0.191226E+01	0.230233E+00	0.179761E+01
%RCP-PAX/RCP	-0.400441E+00	0.159724E+00	-0.133792E+01	0.632992E-01	-0.126181E+01
RCP-PAX/PE	-0.112000E+01	0.727706E+00	-0.699653E+00	0.274936E+00	-0.701936E+00
O-PELLET ABSORPTION					
PAX VALUE	0.223383E-02	0.742688E-07	0.254757E-05	0.501678E-05	0.224147E-02
RCP VALUE	0.230351E-02	0.737504E-07	0.256313E-05	0.501996E-05	0.231117E-02
1 PROB ERROR	0.237455E-04	0.181111E-09	0.655425E-08	0.115572E-07	0.237455E-04
% PE/RCP	0.103084E+01	0.245573E+00	0.255713E+00	0.230225E+00	0.102742E+01
%RCP-PAX/RCP	0.302487E+01	-0.702877E+00	0.606942E+00	0.634307E-01	0.301564E+01
RCP-PAX/PE	0.293438E+01	-0.286219E+01	0.237353E+01	0.275516E+00	0.293514E+01
TOTAL OXYGEN					
PAX VALUE	0.311282E-02	0.104362E-06	0.368185E-05	0.752364E-05	0.312413E-02
RCP VALUE	0.321092E-02	0.103712E-06	0.370688E-05	0.754875E-05	0.322228E-02
1 PROB ERROR	0.263071E-04	0.185579E-09	0.690715E-08	0.163753E-07	0.263071E-04
% PE/RCP	0.819299E+00	0.178937E+00	0.186333E+00	0.216928E+00	0.816411E+00
%RCP-PAX/RCP	0.305530E+01	-0.626675E+00	0.675156E+00	0.332648E+00	0.304607E+01
RCP-PAX/PE	0.372917E+01	-0.350221E+01	0.362338E+01	0.153345E+01	0.373105E+01
ZIRC ABSORPTION					
PAX VALUE	0.273567E-03	0.190495E-02	0.517217E-02	0.131147E-02	0.866215E-02
RCP VALUE	0.276118E-03	0.191903E-02	0.526571E-02	0.128959E-02	0.875046E-02
1 PROB ERROR	0.171313E-05	0.149599E-04	0.773801E-04	0.852554E-05	0.792912E-04
% PE/RCP	0.620434E+00	0.779553E+00	0.146951E+01	0.661104E+00	0.906138E+00
%RCP-PAX/RCP	0.923751E+00	0.733807E+00	0.177649E+01	-0.169628E+01	0.100912E+01
RCP-PAX/PE	0.148888E+01	0.941317E+00	0.120890E+01	-0.256582E+01	0.111365E+01

TABLE IV-11 (Cont)

TOTAL
ZIRCALOY

PAX VALUE	0.294769E-03	0.205236E-02	0.636523E-02	0.152474E-02	0.102371E-01
RCP VALUE	0.297437E-03	0.206639E-02	0.643159E-02	0.149961E-02	0.102950E-01
1 PROB ERROR	0.171889E-05	0.149738E-04	0.776601E-04	0.872712E-05	0.795891E-04
% PE/RCP	0.577900E+00	0.724638E+00	0.120748E+01	0.581960E+00	0.773083E+00
%RCP-PAX/RCP	0.897122E+00	0.678656E+00	0.103181E+01	-0.167582E+01	0.562632E+00
RCP-PAX/PE	0.155238E+01	0.936545E+00	0.854519E+00	-0.287962E+01	0.727778E+00

HYDROGEN
ABSORPTION

PAX VALUE	0.733668E-05	0.548187E-04	0.277135E-02	0.921617E-02	0.120497E-01
RCP VALUE	0.732399E-05	0.545556E-04	0.279421E-02	0.929683E-02	0.121529E-01
1 PROB ERROR	0.270902E-07	0.812525E-07	0.532922E-05	0.426685E-04	0.430001E-04
% PE/RCP	0.369383E+00	0.148935E+00	0.190724E+00	0.458958E+00	0.353825E+00
%RCP-PAX/RCP	-0.173308E+00	-0.482237E+00	0.818207E+00	0.867600E+00	0.849554E+00
RCP-PAX/PE	-0.468549E+00	-0.323790E+01	0.429001E+01	0.189037E+01	0.240105E+01

AM-350
ABSORPTION

PAX VALUE	0.480217E-04	0.150212E-03	0.112170E-02	0.259271E-02	0.391265E-02
RCP VALUE	0.484231E-04	0.149414E-03	0.112860E-02	0.261539E-02	0.394183E-02
1 PROB ERROR	0.371146E-06	0.246663E-06	0.171560E-05	0.120035E-04	0.121337E-04
% PE/RCP	0.766465E+00	0.165087E+00	0.152011E+00	0.458956E+00	0.307818E+00
%RCP-PAX/RCP	0.828879E+00	-0.534046E+00	0.610951E+00	0.867013E+00	0.740126E+00
RCP-PAX/PE	0.108143E+01	-0.323494E+01	0.401911E+01	0.188910E+01	0.240443E+01

U-233
FISSIONS

PAX VALUE	0.746129E-02	0.180791E-01	0.243453E+00	0.229553E+00	0.498546E+00
RCP VALUE	0.742406E-02	0.181137E-01	0.244124E+00	0.229970E+00	0.499632E+00
1 PROB ERROR	0.254022E-04	0.391863E-04	0.580022E-03	0.529187E-03	0.786541E-03
% PE/RCP	0.342160E+00	0.216335E+00	0.237593E+00	0.230112E+00	0.157424E+00
%RCP-PAX/RCP	-0.501481E+00	0.190751E+00	0.274967E+00	0.181438E+00	0.217329E+00
RCP-PAX/PE	-0.146563E+01	0.881738E+00	0.115730E+01	0.788479E+00	0.138053E+01

U-235
FISSIONS

PAX VALUE	0.322078E-05	0.786185E-05	0.669980E-04	0.137626E-03	0.215707E-03
RCP VALUE	0.320655E-05	0.786532E-05	0.666194E-04	0.137368E-03	0.215060E-03
1 PROB ERROR	0.110417E-07	0.171526E-07	0.216151E-06	0.322956E-06	0.389151E-06
% PE/RCP	0.344348E+00	0.218079E+00	0.324457E+00	0.235102E+00	0.180950E+00
%RCP-PAX/RCP	-0.443711E+00	0.441763E-01	-0.568342E+00	-0.187553E+00	-0.300854E+00
RCP-PAX/PE	-0.128855E+01	0.202571E+00	-0.175167E+01	-0.797749E+00	-0.166264E+01

TH-232
FISSIONS

PAX VALUE	0.122953E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.122953E-01
RCP VALUE	0.123331E-01	0.000000E+00	0.000000E+00	0.000000E+00	0.123331E-01
1 PROB ERROR	0.579976E-04	0.000000E+00	0.000000E+00	0.000000E+00	0.579976E-04
% PE/RCP	0.470260E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.470260E+00
%RCP-PAX/RCP	0.306622E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.306622E+00
RCP-PAX/PE	0.652027E+00	0.000000E+00	0.000000E+00	0.000000E+00	0.652027E+00

TOTAL
ABSORPTION

PAX VALUE	0.383849E-01	0.898811E-01	0.513129E+00	0.360853E+00	0.100225E+01
RCP VALUE	0.383611E-01	0.905593E-01	0.513252E+00	0.361114E+00	0.100329E+01
1 PROB ERROR	0.861171E-04	0.144971E-03	0.970910E-03	0.576492E-03	0.114168E-02
% PE/RCP	0.224491E+00	0.160084E+00	0.189168E+00	0.159643E+00	0.113794E+00
%RCP-PAX/RCP	-0.622070E-01	0.748992E+00	0.238650E-01	0.722571E-01	0.103444E+00
RCP-PAX/PE	-0.277103E+00	0.467875E+01	0.126158E+00	0.452618E+00	0.909040E+00

TABLE IV-12. COMPARISON OF PAX AND RCP REACTION RATES
IN UNIT CELL LATTICES

	<u>High Zone Seed</u>		<u>1500°F Fuel</u>		
	<u>Group 1</u>	<u>Group 2</u>	<u>Group 3</u>	<u>Group 4</u>	<u>Total</u>
U^{233} Capture					
RCP Value	0.255E-3	0.274E-2	0.5352E-1	0.1999E-1	0.7650E-1
%(RCP-PAX)/RCP	-0.4 E+0	-0.7 E+0	0.3 E+0	-0.2 E+0	0.2 E+0
(RCP-PAX)/PE	-0.13 E+1	-0.38 E+1	0.14 E+1	-0.8 E+0	0.8 E+0
Th^{232} Capture					
RCP Value	0.1267E-1	0.5611E-1	0.2023E+0	0.4286E-1	0.3139E+0
%(RCP-PAX)/RCP	-0.5 E+0	0.12 E+1	-0.4 E+0	-0.5 E+0	-0.2 E+0
(RCP-PAX)/PE	0.16 E+1	0.72 E+1	-0.15 E+1	-0.21 E+1	-0.9 E+0
Pa^{233} Absorption					
RCP Value	0.377E-9	0.699E-9	0.2785E-7	0.1254E-8	0.3018E-7
%(RCP-PAX)/RCP	0.0 E+0	-0.9 E+0	-0.3 E+0	0.4 E+0	-0.3 E+0
(RCP-PAX)/PE	0.0 E+0	-0.37 E+1	-0.8 E+0	0.16 E+1	-0.8 E+0
Zirc Absorption					
RCP Value	0.402E-3	0.264E-2	0.682E-2	0.999E-3	0.1086E-1
%(RCP-PAX)/RCP	-0.15 E+1	-0.11 E+1	0.3 E+0	-0.6 E+0	-0.3 E+0
(RCP-PAX)/PE	-0.33 E+1	-0.21 E+1	0.2 E+0	0.10 E+1	-0.4 E+0
U^{233} Total Fission					
RCP Value	0.1232E-1	0.2871E-1	0.3219E+0	0.2050E+0	0.5680E+0
%(RCP-PAX)/RCP	-0.3 E+0	-0.2 E+0	0.4 E+0	0.0 E+0	0.2 E+0
(RCP-PAX)/PE	-0.11 E+1	-0.11 E+1	0.21 E+1	0.0 E+0	0.14 E+1

TABLE IV-13. COMPARISON OF PAX AND RCP REACTION RATES
IN UNIT CELL LATTICES

	<u>High Zone Seed</u>		<u>80°F</u>		<u>Total</u>
	<u>Group 1</u>	<u>Group 2</u>	<u>Group 3</u>	<u>Group 4</u>	
U^{233} Capture					
RCP Value	0.218E-3	0.213E-2	0.5121E-1	0.2643E-1	0.7999E-1
%(RCP-PAX)/RCP	-0.5 E+0	-0.14 E+1	-0.1 E+0	0.5 E+0	0.1 E+0
(RCP-PAX)/PE	-0.16 E+1	-0.75 E+1	-0.4 E+0	0.27 E+1	0.4 E+0
Th^{232} Capture					
RCP Value	0.1082E-1	0.4315E-1	0.1455E+0	0.5893E-1	0.2584E+0
%(RCP-PAX)/RCP	-0.7 E+0	-0.9 E+0	-0.12 E+1	0.1 E+0	-0.8 E+0
(RCP-PAX)/PE	-0.26 E+1	-0.49 E+1	-0.35 E+1	0.5 E+0	-0.41 E+1
Pa^{233} Absorption					
RCP Value	0.328E-9	0.542E-9	0.2713E-7	0.1669E-8	0.2970E-7
%(RCP-PAX)/RCP	-0.3 E+0	-0.22 E+1	0.2 E+0	0.8 E+0	0.3 E+0
(RCP-PAX)/PE	-0.10 E+1	-0.92 E+1	0.4 E+0	0.42 E+1	0.7 E+0
Zirc Absorption					
RCP Value	0.343E-3	0.203E-2	0.573E-2	0.137E-2	0.948E-2
%(RCP-PAX)/RCP	-0.12 E+1	-0.27 E+1	0.20 E+1	-0.8 E+0	0.5 E+0
(RCP-PAX)/PE	-0.27 E+1	-0.46 E+1	0.18 E+1	-0.15 E+1	0.7 E+0
U^{233} Total Fission					
RCP Value	0.1063E-1	0.2231E-1	0.3070E+0	0.2773E+0	0.6172E+0
%(RCP-PAX)/RCP	-0.5 E+0	-0.12 E+1	0.3 E+0	0.7 E+0	0.4 E+0
(RCP-PAX)/PE	-0.17 E+1	-0.63 E+1	0.15 E+1	0.40 E+1	0.34 E+1

TABLE IV-14. THERMAL-HYDRAULIC FEEDBACK VARIABLES

Let T_f = fuel temperature ($^{\circ}\text{F}$), T_m = moderator temperature ($^{\circ}\text{F}$),
and N_H = hydrogen atom density (atoms/barns cm).

Then

$$N_{T_f} \equiv \sqrt{T_f} - \sqrt{T_f^*}$$

$$N_{\rho} \equiv N_H - N_H^*$$

$$N_{T_m} \equiv T_m - T_m^*$$

*Represents the reference value.

TABLE IV-15. LWBR USE OF PAX TABLES

1. Fixed macro-tables of cross sections: For the LWBR model, only Σ^{tr1} , Σ^{tr2} , and Σ^{tr3} contain nonzero entries for fuel regions and these data are taken from the 8000 EFPH time step. For metal-water regions, Σ_{tr}^4 is also nonzero and these are taken from the beginning of life calculation. In general, any entries that are not replaced by interpolated macroscopic data will be used in the PDQ calculation. For LWBR, interpolated values of Σ^{tr} from the space-energy corrections are used in most regions (Section IV.F).
2. Fixed micro-tables: The data types which are put into this kind of table are σ^{tr} , σ^a , σ^R , (σ^f , ν , κ).

A separate table by energy group is used to define time-independent data for each of the following nuclides:

- a. Fuels: Th²³², U²³², U²³³, U²³⁴, U²³⁵, U²³⁶, Pa²³¹, Pa²³³
- b. Fission products: f/cc, Xe¹³⁵, Nd¹⁴⁷, Pm¹⁴⁷, Pm¹⁴⁸, Pm^{149M}, Pm¹⁴⁹, Sm¹⁴⁹, Sm¹⁵⁰, Sm¹⁵¹
- c. Metal-water: H, O, ZR-4, AM-350
- d. Thermal-hydraulic feedback variables: N_ρ , N_{Tf}

For fuel regions, these data are taken from the 8,000 EFPH time step. For metal-water regions, these data are taken from the beginning of life. Any entries that are not replaced by fitted microscopic data will be used in the PDQ calculation. One source of such data is the temperature-dependent fitted cross sections shown in Table IV-16.

3. Interpolating thermal G-factor tables: For fuel regions only, a separate table is generated as a function of f/cc to be used as a multiplier on σ^{a4} and σ^{f4} for the same nuclides listed in item 2 and also for the pseudo-nuclides N_ρ and N_{Tf} . For U²³³ and Xe¹³⁵ the thermal G-factor is fit on the same basis as the temperature-dependent cross sections indicated in Table IV-16.
4. Interpolating cross-section tables: For fuel regions only, selected cross sections which have significant temperature and burnup dependence are shown in Table IV-16.
5. Space-energy corrections: Adjustments to infinite medium data in few-groups 1, 2, and 3 are made to account for the influence of neighboring regions with different neutron spectra. Tables include Σ^{tr} , $\nu(\text{Th}^{232})$, $\nu(\text{U}^{233})$, and G-factors on absorption, removal, and fission cross sections for the nuclides which represent the metal-water regions, the fuel regions, and the thermal-hydraulic feedback variables. The method is discussed in Section IV.F.

TABLE IV-16. TIME- AND TEMPERATURE-DEPENDENT FITTED CROSS SECTIONS FOR FUEL REGIONS IN THE LWBR MODEL

Nuclide	Type*	Group	Interpolating Parameters
Th ²³²	a	3	$f/cc, N_{\rho}, N_{T_f}$ ↓ $f/cc, N_{\rho}$ ↓ f/cc ↓
U ²³³	a, f	3	
H	a, r	3	
O	r	3	
ZR-4	a	3	
U ²³³	a, f	4**	
Pa ²³³	a	3	
U ²³⁴	a	3	
Xe ¹³⁵	a	4**	
ZR-4	r	3	
N _{T_f}	a, r, f	3	
N _ρ	a, r, f	3	
N _ρ	tr, a, f	4	

*a = absorption; r = removal; f = fission; tr = transport.

**The thermal G-factor is fit on the same interpolating basis as the corresponding group 4 cross-section.

TABLE IV-17. REPRESENTATIVE PAX INPUT PARAMETERS FOR AN
LWBR FUEL ROD CELL

Rod Geometry

Fast Few-Group Breakpoints at multigroups 10,
25, and 54

25 groups in the thermal
few-group

Input Fast Advantage Factors

Multiple-Sauer Thermal G-factor
calculated by PAX

Fast $B^2 = 0.00001$

Thermal $B^2 = 0.0$

Moderator Temperature

Fuel Temperature

Reference 540°F

Reference 920°F (binary)
600°F (thoria)

Perturbed 600°F

Perturbed 1420°F (binary)
1100°F (thoria)

For fuel rod cells, infinite medium calculations are performed at seven times in life: 0, 50, 1000, 3000, 8000, 20,000, and 40,000 EFPH. The source of the data for the time-independent macro-table and micro-tables is the 8000 EFPH calculation. This is also the time at which perturbed temperature values are placed in the fitted cross section tables for the explicit temperature dependent nuclides. Perturbed temperature calculations are also performed at 0 and 40,000 EFPH to supply values for the latent temperature cross sections.

TABLE IV-18. RANGES OF TYPICAL REGIONAL SPACE-ENERGY CORRECTION
FACTORS, WITH MOVABLE FUEL ASSEMBLIES 14 INCHES
BELOW THE ALIGNED POSITION

<u>Few-Group</u>	<u>Reaction</u>	<u>Isotope</u>	<u>Regions</u>	<u>Range of Fast G-Factor</u>
1	fission	^{232}Th	fuel	0.98 to 1.07
2	absorption	ZR-4	fuel	0.96 to 1.06
2	absorption	ZR-4	metal-water channels	1.00 to 1.07
3	absorption	^{232}Th	fuel	0.98 to 1.02
3	absorption	^{233}U	fuel	0.93 to 1.11
3	removal	total	fuel	0.90 to 1.20
3	removal	total	metal-water channels	0.65 to 1.04

TABLE IV-19. TEST OF SPACE-ENERGY CONSTANTS FOR ONE-DIMENSIONAL TRAVERSE T_1

Region	Hi Sd	Lo Sd	ThO ₂ Sd	Chan	Lo Bkt	Md Bkt	Hi Bkt	Md Bkt	Chan	Zero Current
r (cm)	0.0	9.0	9.8	12.3	13.9	16.8	18.3	21.2	22.6	23.0
meshpoint	0	21	23	29	33	41	45	53	57	59
N ^{U233} (atoms/barn cm)	0.00058	0.00039				0.00014	0.00022	0.00027	0.00022	
N Th	0.0086	0.0088	0.0094		0.013	0.012	0.012	0.012		
N ^H	0.019	0.019	0.019	0.025	0.013	0.013	0.013	0.013	0.038	
A ₃ : PLMG	0.1204	0.0209	0.0280	0.0030	0.0732	0.0469	0.1132	0.0559	0.0006	
PDQ (MUFT)-PLMG	0.0027	-0.0005	-0.0019	-0.0003	-0.0011	-0.0001	-0.0007	-0.0009	0.0000	
PDQ (SpEn)-PLMG	0.0001	0.0000	0.0000	0.0000	-0.0001	-0.0001	-0.0001	0.0000	0.0000	
A ₄ : PLMG	0.0796	0.0260	0.0361	0.0051	0.0875	0.0398	0.0886	0.0502	0.0012	
PDQ (MUFT)-PLMG	-0.0018	0.0012	0.0038	0.0006	0.0020	-0.0021	-0.0043	0.0030	0.0002	
PDQ (SpEn)-PLMG	-0.0001	0.0000	0.0003	0.0001	0.0000	-0.0001	-0.0002	0.0000	0.0000	

A_g = absorption fractions in few-group g

Traverse multiplication factor K: PLMG 1.0852
 PDQ (MUFT)-PLMG -0.0212
 PDQ (SpEn)-PLMG -0.0005

TABLE IV-20. TEST OF SPACE-ENERGY CONSTANTS FOR ONE-DIMENSIONAL TRAVERSE T_1

	PLMG				PDQ(MUFT)-PLMG				PDQ(S _E) _{p-n} -PLMG			
	Sd	Chan	Bkt	Chan	Sd	Chan	Bkt	Chan	Sd	Chan	Bkt	Chan
Few-group 1												
source	0.2977		0.4568		0.0049		-0.0050		-0.0001		0.0001	
leakage	0.0326	-0.0470	0.0437	-0.0293	-0.0018	0.0006	-0.0052	0.0028	-0.0005	-0.0001	0.0006	0.0000
absorption	0.0130	0.0002	0.0246	0.0001	-0.0002	0.0000	-0.0003	0.0000	0.0000	0.0000	-0.0001	0.0000
removal	0.2520	0.0468	0.3885	0.0292	0.0029	-0.0006	0.0004	-0.0028	0.0004	0.0001	-0.0006	0.0000
Few-group 2												
source	0.0980		0.1501		0.0016		-0.0017		0.0000		0.0000	
leakage	0.0202	-0.0540	0.0709	-0.0370	0.0000	0.0032	-0.0018	-0.0014	0.0000	0.0001	-0.0003	0.0001
absorption	0.0270	0.0009	0.0606	0.0002	0.0003	0.0000	-0.0002	0.0000	0.0000	0.0000	-0.0001	0.0000
removal	0.3028	0.1000	0.4072	0.0661	0.0042	-0.0038	0.0008	-0.0014	0.0003	0.0000	-0.0003	-0.0001
Few-group 3												
source	0.0001		0.0001		0.0000		0.0000		0.0000		0.0000	
leakage	-0.0001	0.0367	-0.0710	0.0344	0.0028	-0.0170	0.0298	-0.0156	0.0001	0.0000	0.0000	0.0000
absorption	0.1693	0.0030	0.2892	0.0006	0.0003	-0.0003	-0.0027	0.0000	0.0001	0.0000	-0.0002	0.0000
removal	0.1336	0.0603	0.1891	0.0311	0.0012	0.0135	-0.0263	0.0142	0.0001	0.0000	-0.0001	0.0000
Few-group 4												
leakage	-0.0081	0.0552	-0.0769	0.0299	-0.0020	0.0130	-0.0251	0.0141	-0.0001	0.0000	0.0002	0.0000
absorption	0.1417	0.0051	0.2661	0.0012	0.0032	0.0005	-0.0013	0.0002	0.0002	0.0000	-0.0003	0.0000

TABLE IV-21. TEST OF SPACE-ENERGY CONSTANTS FOR ONE-DIMENSIONAL TRAVERSE T_2

Region	<u>Hi Sd</u>		<u>Lo Sd</u>	<u>Chan</u>	<u>ThO₂ Bkt</u>	<u>Hi Bkt</u>	<u>Md Bkt</u>	<u>Chan</u>	Zero Current ↓
r (cm)	0.0	9.0	12.3	13.9	18.3	21.2	22.6	23.0	
A_3 : PLMG	0.1270	0.0932	0.0030	0.0755	0.1146	0.0548	0.0006		
PDQ (MUFT)-PLMG	0.0064	-0.0005	-0.0003	-0.0027	-0.0024	-0.0010	0.0000		
PDQ (SpEn)-PLMG	0.0016	0.0003	0.0000	-0.0004	-0.0007	-0.0003	0.0000		
A_4 : PLMG	0.0655	0.0943	0.0044	0.0872	0.1093	0.0534	0.0013		
PDQ (MUFT)-PLMG	0.0002	0.0021	0.0004	0.0041	-0.0064	0.0000	0.0001		
PDQ (SpEn)-PLMG	0.0005	0.0000	0.0000	0.0000	-0.0007	-0.0003	0.0000		

A_g = absorption fractions in few-group g

Traverse multiplication factor K:

PLMG	1.0636
PDQ (MUFT)-PLMG	-0.0160
PDQ (SpEn)-PLMG	0.0017

TABLE IV-22. TEST OF SPACE-ENERGY CONSTANTS FOR ONE-DIMENSIONAL TRAVERSE T_3

Region	Chan	Hi Sd	Lo Sd	ThO ₂ Sd	Chan	ThO ₂ Bkt	Hi Ekt	Chan	Zero Current ↓ 22.9
r(cm)	0.0	1.1	10.1	11.6	12.3	13.9	18.2	22.5	
N^{U233} (atoms/barn cm)		0.00052	0.00041				0.00024		
N^H	0.019	0.029	0.029	0.029	0.030	0.016	0.016	0.048	
A_{Fast} : PLMG	0.0002	0.1889	0.0526	0.0107	0.0041	0.1026	0.2018	0.0009	
PDQ(MUFT)-PLMG	0.0005	0.0090	-0.0003	-0.0005	-0.0003	-0.0021	-0.0075	0.0000	
PDQ(SpEn)-PLMG	0.0000	0.0031	0.0002	0.0000	0.0000	0.0004	-0.0034	0.0000	
A_4 : PLMG	0.0001	0.1170	0.0578	0.0092	0.0047	0.0933	0.1548	0.0012	
PDQ(MUFT)-PLMG	0.0000	0.0030	0.0019	0.0007	0.0004	0.0037	-0.0080	0.0001	
PDQ(SpEn)-PLMG	0.0000	0.0016	0.0002	0.0001	0.0000	0.0008	-0.0029	0.0000	
A = absorption fractions									
Traverse multiplication factor K:									
				PLMG		1.0323			
				PDQ(MUFT)-PLMG		-0.0115			
				PDQ(SpEn)-PLMG		-0.0010			

TABLE IV-23. TEST OF SPACE-ENERGY CONSTANTS FOR ONE-DIMENSIONAL TRAVERSE T_4

Region	Chan	Seed	Chan	ThO ₂	Blanket	ThO ₂	Water	vacuum
r (cm)	0.0	1.1	12.3	13.7	16.9	24.4	34.6	54.6
N^{U233} (atoms/barn cm)		0.00063			0.00023			
N^H	0.018	0.030	0.034	0.018	0.018	0.018	0.067	
N^{Th}		0.0066		0.012	0.012	0.012		
A_3 : P1MG	0.0001	0.2087	0.0017	0.0270	0.0987	0.0322	0.0004	
PDQ(MUFT)-P1MG	0.0000	0.0022	-0.0001	-0.0013	-0.0011	-0.0002	0.0000	
PDQ(SpEn)-P1MG	0.0000	0.0001	0.0000	0.0003	-0.0001	-0.0001	0.0000	
A_4 : P1MG	0.0001	0.2104	0.0046	0.0565	0.1281	0.0949	0.0442	
PDQ(MUFT)-P1MG	0.0000	0.0070	0.0005	0.0033	-0.0056	-0.0050	0.0007	
PDQ(SpEn)-P1MG	0.0000	0.0002	0.0000	-0.0003	0.0004	-0.0002	0.0002	

A_g = absorption fractions in few-group g

Traverse multiplication factor K:

P1MG	1.0978
PDQ(MUFT)-P1MG	0.0065
PDQ(SpEn)-P1MG	0.0010

TABLE IV-24. TEST OF SPACE-ENERGY CONSTANTS AT MIDDLE OF LIFE

Region	Chan	Hi Sd	Lo Sd	ThO ₂ Sd	Chan	ThO ₂ Bkt	Lo Bkt	Hi Bkt	Chan	Zero Current
r(cm)	0.0	1.1	9.4	10.9	12.3	13.8	15.2	18.1	22.4	22.8
BOL N ^{U233} (atoms/barn cm)		0.00054	0.00038				0.00017	0.00026		
BOL N Th		0.0068	0.0070	0.0082		0.013	0.013	0.013		
N ^H	0.014	0.022	0.022	0.022	0.023	0.012	0.012	0.012	0.037	
MOL N ^{U233}		0.00044	0.00030	0.000036		0.000017	0.00018	0.00026		
MOL N Th		0.0068	0.0069	0.0082		0.013	0.013	0.013		
Power: PLMG		0.3345	0.1110	0.0205		0.0287	0.1635	0.3417		
PDQ(MUFT)-PLMG		0.0088	0.0037	0.0019		0.0012	-0.0043	-0.0112		
PDQ(SpEn)-PLMG		-0.0018	0.0004	0.0005		0.0000	0.0000	0.0011		

BOL = Beginning of Life

MOL = Middle of Life

Traverse multiplication factor K: PLMG 1.0384
 PDQ(MUFT)-PLMG -0.0233
 PDQ(SpEn)-PLMG 0.0026

TABLE IV-25. COMPARISON OF FAST G-FACTORS BETWEEN BOL AND MOL

<u>Few-Group</u>	<u>Region</u>	$G^a_{U^{233}}$		$G^a_{Th^{232}}$		G^R	
		<u>BOL</u>	<u>MOL</u>	<u>BOL</u>	<u>MOL</u>	<u>BOL</u>	<u>MOL</u>
1	Chan					0.936	0.936
	Hi Sd	1.001	1.001	0.996	0.996	1.013	1.012
	ThO ₂ Sd	1.001	1.001	0.995	0.995	1.009	1.010
	Chan					1.006	1.008
	Hi Bkt	0.999	0.999	1.004	1.004	0.987	0.988
	Chan					1.108	1.108
2	Chan					0.939	0.951
	Hi Sd	0.994	0.995	0.993	0.995	0.972	0.984
	ThO ₂ Sd	1.006	1.006	1.006	1.007	1.029	1.029
	Chan					1.032	1.021
	Hi Bkt	0.999	0.998	0.997	0.996	0.992	0.992
	Chan					0.999	1.002
3	Chan					0.556	0.593
	Hi Sd	1.008	1.011	1.004	1.002	1.063	1.057
	ThO ₂ Sd	1.099	1.081	0.950	0.958	0.831	0.850
	Chan					0.808	0.762
	Hi Bkt	1.116	1.110	0.926	0.930	1.258	1.224
	Chan					0.678	0.652

(Not to scale. Not all pellets had chamfers, tapers, or end dishes.)

Figure IV-1. Generalized Fuel Pellet

NOTE: Unit cell dimensions are given in Tables II-1 and II-2

Figure IV-2. Fuel Rod Unit Cell

Figure IV-3. Four Module Breeder Mockup BMJ-2-4 (Power Flattened),
per Atom Fission Distribution in 9 w/o Seed Slice (Mid-Plane)

Figure IV-4. RZ Diagram of LWBR Type I Module

- (a) Traverse from Center of Module (Center of Seed) to Module Outer Boundary through Regular Blanket

- (b) Traverse from Center of Module (Center of Seed) to Core Outer Boundary through Power Flattening Blanket

Figure IV-5. Typical One-Dimensional Traverses for the Computation of Regional Few-Group Constants

Figure IV-6. Relative U^{233} Fission Activation Along Traverse through 9 w/o Seed of BMU-1B

Regional Power Fractions are tabulated in the order:

RCP
PDQ (MUFT)
PDQ (SpEn)

.0002		ThO ₂	
.244 .231 .241	.0018 .0019 .0018		
Hi Sd		ThO ₂ Sd	
.197 .206 .191	.046 .050 .047		
	Hi Sd		
	Lo Sd		
.028 .042 .031	.008 .014 .010		.0057 .0104 .0079
	Hi Sd		Hi Sd
	Lo Sd		Hi Sd
ThO ₂			

ThO2	
.051 .047 .051	.064 .056 .060
	HiBkt
Lo Bkt	.253 .237 .257
	Hi Bkt
.0042 .0048 .0047	.097 .101 .099
ThO2 Bkt	Hi Bkt
ThO2	.0002

	<u>Total Sd</u>	<u>Total Bkt</u>	<u>Module Multiplication Factor</u>
RCP	0.531	0.469	1.0081
PDQ (MUFT)	0.555	0.445	0.9941
PDQ (SpEn)	0.530	0.471	1.0061

Figure IV-7. Test of Space-Energy Correction Factors for a Single Module

Data shown are ratios of power from PDQ(SpEn)/power from RCP, for binary fuel zones.

Figure IV-8. Two-Dimensional Calculation of a Horizontal Slice through a Symmetric 1/6 Section of the Core

Data shown are ratios of power from PDQ(MUFT)/power from RCP, for binary fuel zones.

Figure IV-9. Two-Dimensional Calculation of a Horizontal Slice through a Symmetric 1/6 Section of the Core

Data shown are ratios of power from $PDQ(\alpha_s^3 = 0.5)$ /power from RCP, for binary fuel zones.

Figure IV-10. Two-Dimensional Calculation of a Horizontal Slice through a Symmetric 1/6 Section of the Core

Data shown are ratios of power from PDQ/power from RCP, for binary fuel zones, with power fractions from PDQ shown parenthetically.

Core Multiplication Factor

RCP 1.0091 $\pm$ 0.0010 (1 σ)

PDQ 1.0105

Figure IV-11. Three-Dimensional Calculation of a Symmetric 1/6 Section of the As-Built LWBR Core

V. DETERMINATION OF THE NEUTRON FLUX DISTRIBUTION IN THE CORE AND THE REACTIVITY: THE USE OF PDQ

The PDQ program (Reference V-1) as used for LWBR solves the diffusion-depletion equations in 3 spatial dimensions. An eigenvalue calculation at each fixed time gives the core reactivity. The depletion begins after an initial (time zero) spatial flux and power calculation is performed, which includes 2 recalculations of fuel and coolant temperature distributions (Section V.E.). Subsequent calculations, referred to as "timesteps," consist of:

1. Depletion from time T_1 to T_2 using the spatial flux distribution from the previous timestep at T_1 and holding it constant in time;
2. Upward motion of the movable fuel to a new estimated critical fuel position;
3. Spatial flux calculations including, for a constant power depletion, one recalculation of temperature and xenon distributions.

An explicit three-dimensional flux solution is used rather than a synthesized solution because the latter has been demonstrated to yield insufficient accuracy due to the axial fuel zoning in LWBR (Figure II-4). The PDQ model for LWBR is presented in the following sections.

A. Depletion Chains

Solution of the depletion equations in the PDQ program requires couplings in which nuclides are fed by a single parent. Thus, nuclides coupled to one another through neutron capture and decay processes must be resolved into two "linear" chains, one involving capture only and the other with decay only.

Two types of nuclide chains are permitted in PDQ. Nuclides with no direct yield from fission are specified in type one chains, which may include dummy chains ($dN/dt = 0$) for nondepleting nuclides. Chain type two is used for fission product nuclides.

LWBR depletion calculations are done with 3 fuel depletion chains and 4 chains to represent fission products.

1. Fuel Chains

The natural $\text{Th}^{232} \rightarrow \text{U}^{233}$ chain is shown in Figure V-1. For use in PDQ this is broken into 3 linear chains, as shown in Figure V-2, which neglect the short lived nuclides Th^{231} , Th^{233} , Th^{234} , Pa^{232} and Pa^{234} . The nonphysical (decay + capture) coupling from Th^{232} to Pa^{233} and the "counter" nuclide are used to

preserve atom balance for bookkeeping purposes. Half-lives given in Figure V-2 for Th^{232} and the "counter" are used to avoid roundoff difficulties with extremely small numbers in the computer.

The third fuel chain, shown in Figure V-2, is used primarily to measure the U^{232} buildup for health physics studies. Its significance is minor in normal design calculations. For convenience, the Pa^{231} concentration is treated as a direct fission yield from Th^{232} rather than as an n,2n product. This avoids carrying n,2n cross sections in PDQ. The fake yield is a ratio of thorium cross sections averaged over the first few-group: $\sigma^{n,2n}/\sigma_f$.

Uranium fuel produced for LWBR fuel elements contains a small amount (less than 1/2 percent core average) of U^{238} . The U^{238} is not treated explicitly in a depletion chain, but its effect on the atom balance (for breeding analysis) is accounted for by a post-PDQ correction.

2. Fission Product Chains

Four linear chains are used in PDQ to represent fission product nuclides. Three explicit linear chains, shown in Figure V-3, were specified to account for the bulk of the poisons which depend on power level and few-group flux level, as suggested in Section A-V of Reference V-2. The fourth fission product chain contains a single nuclide, which has a yield of unity from each isotope which fissions, and serves to accumulate the total fissions/cm³ (f/cc) as a function of position in the PDQ calculation. This nuclide is also used to represent the "residual" fission product poison not included in the 3 explicit chains of Figure V-3, as discussed in the next section.

B. Fission Product Treatment: CINDER

As discussed in Section III.A.3 and above, the fission product residual isotope accounts for the remaining fission product poison. The cross sections for this isotope come from the CINDER program and are fed into the PAX depletion calculation. Cross sections for the fission products treated explicitly in the PAX and PDQ chains are input directly to the PAX depletion. The Xe^{135} thermal cross section is time-dependent (Section IV.E.4) while the other cross sections are fixed. The energy averaging is handled in the same way as for input to CINDER (described below). The HARMONY file which gathers all the PAX output for PDQ (Section IV.E.4) contains all the fission product cross sections.

Residual fission product cross sections are calculated using the CINDER program, Reference V-3, which does a "point depletion" calculation for any specified number of linear fuel and fission product chains. For each of the 12 fuel compositions in the LWBR core a total fission product CINDER and a 3 chain CINDER calculation, with chains as used in PDQ, are done. The residual fission product cross sections are obtained for each composition by subtracting the 3 chain contribution from the total. Fuel composition dependent input to CINDER consists of initial fuel nuclide concentrations, time-independent few-group cross sections, decay constants, and few-group flux values, the latter as a function of time. Fuel nuclide few-group cross sections and a thermal disadvantage factor are taken from the middle of life tables in a previous PAX depletion calculation. Composition averaged few-group flux values as a function of time are obtained from a previous PDQ depletion calculation.

Nuclide chains used to describe fission product poisoning in CINDER contain 179 different nuclides in 69 linear chains, as given in Reference V-2. The data which appear in Reference V-2 have been updated for LWBR calculations, including the use of cross sections for 4 few-groups. These data have been discussed in Section IV.B for the most important fission product absorbers.

As recommended in Reference V-2, the thermal cross sections for Xe^{135} , Sm^{149} and Sm^{151} in the CINDER library are adjusted for each fuel composition by using spectrum dependent thermal cross sections calculated by the PAX program. Thermal cross sections for the other fission products are the 2200 m/s values. These are appropriate for the β number density thermal treatment (Section IV.E.1) since the thermal group cross section would be exact for any 1/v isotope.

The CINDER library cross sections in the epithermal range are 1/E - weighted values. These are adjusted by spectrum correction factors for all 179 fission product nuclides. The 10 most important epithermally absorbing nuclides, identified in Table IV-2, account for over 75 percent of the total epithermal fission product absorption. Spectrum-dependent few-group 3 cross sections for these 10 nuclides are obtained from special infinite medium multigroup PAX calculations with fixed inventories for each fuel composition. The PAX calculations contain middle of life concentrations for these nuclides, which are obtained from a previous CINDER calculation using estimated fission product spectrum correction factors. Correction factors for each of the 10 epithermal absorbers are given by

$$R_{ij} = (\sigma_{3ij}^{\text{PAX}} / \sigma_{3i}^{\text{CINDER Library}}) ,$$

for nuclide i in composition j , where the infinitely dilute resonance integral in the CINDER library is consistent with the data in PAX. The arithmetic average over all 10 epithermal absorbers, $\bar{R}_j$, is defined as the correction factor for the other 169 fission products, which contribute less than 25 percent of the total epithermal fission product absorption.

Because the most important power-dependent nuclides are represented in the 3 explicit chains, the cross sections per fission of the fission product residuals are approximately constant in time. These constant values σ_c^{ag} of absorption cross section (a) are obtained for each composition c from

$$\sigma_c^{ag} \text{ (barns/fission)} = \frac{\sum_c^{ag} (\text{cm}^{-1})}{(\text{fissions/barn cm})_c},$$

where g is the few-group index. In this expression $\sum_c^{ag}$ is the total macroscopic poison cross section of the residual nuclides. Figures V-4 and V-5 show the thermal and epithermal microscopic residual cross sections for 1 composition. The abscissa KEFPH in the figures stands for thousands of effective full power hours, Section IV.E.2. A time-independent value of each residual cross section is obtained by averaging the cross section from 3000 EFPH to end of life. The biggest error in the assumption of a constant value occurs in the epithermal cross section early in life, since the constant value is chosen to represent times after the transient has passed; but for these early times the error has a minimal effect since the accumulated fission concentration is small.

The PAX program permits fixed cross section input only for few-groups 3 and 4. Thus, the CINDER calculated residual cross sections for few-groups 1, 2, and 3 are combined by lethargy weighting into an effective few-group 3 cross section, i.e.,

$$\sigma_{\text{effective}}^3 = (2.5\sigma^1 + 5.0\sigma^2 + 9.0884\sigma^3)/9.0884.$$

This approximate weighting is used because fission product absorption in few-groups 1 and 2 is a minor part of the total fast absorption. The total fission product cross section in few-groups 1 or 2 is less than 1 percent of the few-group 3 value.

C. Transport Approximation for Fast Neutrons

The need for consideration of the transport effect in the high energy few-group (few-group 1) was brought to light in early critical experiments performed in support of LWBR (Reference V-4). Measurements and calculations of thorium (fast) fission activation shapes had 20 percent discrepancies which were shown to be due to the use of diffusion theory. Using the simplified- P_3 approximation in few-group 1, instead of diffusion theory, resulted in correcting the major portion of the discrepancy and this approximation was adopted for the analysis model.

The simplified- P_3 (SP_3) approximation, originally proposed by Gelbard for non-slab geometries (Reference V-5), involves 2 diffusion-like second order equations for few-group 1. The diffusion-like character of the equations is desirable to make use of the efficient numerical procedures in PDQ. To obtain the coefficients in the equations spherical harmonic components of the scattering cross section are required. The "transport approximation" is made, whereby scattering is assumed isotropic but of reduced magnitude, and is exact in a P_1 approximation. Then the coefficients are simple functions of the usual few-group constants D^1 , $\sum^{a1}$, and $\sum^{R1}$. PDQ solves the equations for the 2 unknowns in the first few-group and couples them to the single diffusion equation for the second few-group. The 2 unknowns in group 1 are coalesced into the usual group 1 flux after the spatial calculation, so the flux is available for computing reaction rates or depletion.

For isotropic sources, isotropic scattering, and constant total cross section the SP_3 equations yield the same scalar flux and current density as the P_3 equations. In LWBR, the group 1 total cross section is not constant but is slowly varying. Studies were done which indicate that SP_3 gives good results in describing the high energy transport for systems like LWBR and is a practical addition to diffusion theory programs (Reference V-6). It was also demonstrated that SP_3 is better behaved than certain other diffusion-like approximations. In the variety of cores studied during the development of LWBR, the reactivity effect of using SP_3 rather than P_1 in the high energy few-group varied from about 0.2 percent to over 2 percent in some small critical experiments.

D. The Multi-Region Core: Mesh and Depletion Block Size

The PDQ calculations for the LWBR core are done in three-dimensional hex, z geometry; that is, the horizontal planar geometry has fuel rods on a triangular

pitch so hexagonal fuel assemblies may be described. The detailed structure of the fuel rod cells (fuel pellet, clad, support grid and coolant) does not appear in PDQ neutron calculations. (The structure is used in the temperature calculations Sections V.E. and V.G.) Homogenized fuel regions are represented by discrete three-dimensional "depletion blocks" which cover the regions. A depletion block is a subregion such that nuclide concentrations are spatially constant over the block, but may vary from block to block as burnup occurs. Initially the blocks are assigned with piecewise constant materials such that the transverse and axial fuel zones (see Figure II-4) are described.

Most LWBR core calculations are done with a PDQ geometry, described below, which represents a symmetric 1/6 core sector. Calculations for a few nonsymmetric core configurations are also done, such as a single movable fuel assembly out of alignment with the others (stuck seed accident) or a simulation of a steam line rupture in one of the four coolant loops. These configurations are done with a 1/2-core geometry which contains less detail (larger mesh spacings and fewer material blocks) than the 1/6 core geometry described in this section.

In Figure V-6 is a sketch which shows both the transverse mesh, used in the PDQ spatial flux solution, and the coarser "depletion block" grid, in 1/6 of a type I module (see Figure II-3). The transverse mesh lines, shown on the periphery of the module in Figure V-6, extend through the module in both directions. Only those mesh lines which bound the depletion blocks (42 in the seed region and 43 in the blanket region) are drawn through the module in the figure.

Relatively small depletion blocks have been assigned in regions of the core where previous calculations have shown that power peaks exist and in certain other regions to provide additional data for thermal-hydraulic analyses. In the type I module these small blocks are along the core center-line diagonal, as shown in Figure V-6. Other larger depletion blocks generally contain between 2 and 4 fuel rod unit cells such that a reasonably detailed end of life fissile fuel distribution will be available for use in breeding performance analysis.

The mesh line spacing and depletion block sizes assigned to the type II and type III modules in the PDQ geometry are very similar to those shown in Figure V-6 for the type I module. Comparable spacings and block sizes are also used for the larger diameter rods in the radial reflector region (module types IV and V). In addition, radially and axially homogenized metal-water regions beyond the thorium reflector blankets are included in the 1/6 core PDQ geometry.

Forty-five planes, with a uniform mesh of 3.5 inches, are used to describe the core in the axial direction. Thirty-one of these planes contain fuel, with the upper and lower thoria reflectors represented by 10.5 inches rather than the actual 10 inches (see Figure II-4). The other 14 planes contain axial metal-water regions. Note that a nonuniform axial mesh would not work in PDQ with the LWBR movable fuel requirement. Each axial plane serves as a depletion block boundary such that depletion blocks, as shown in Figure V-6, each have a height of 3.5 inches.

Fuel movement for LWBR is accomplished in the PDQ program by specifying a list of transverse depletion blocks and the upper and lower planes which constitute the region to be moved. Several axial metal-water regions above and below the fuel are moved along with the fuel such that these regions remain in the correct position relative to the seed and blanket fuel.

The 1/6 core geometry, as described above, contains 1472 transverse blocks where the material may vary from one block to another. Of these, 1390 are depletion blocks in fuel regions representing 2883 fuel rod locations. With 31 axial fuel planes, there are 41,700 three dimensional fuel blocks. Transverse mesh points (84 columns by 82 rows) total 7055 but about 2000 of these are "void" points outside the 1/6 core region to fill-in the 120-degree chevron required by PDQ in hexagonal geometry. Thus, out of about 317,500 total points over 220,000 spatial points are contained in the 1/6 core solution.

E. Temperature Feedback

The procedure called thermal feedback provides the capability to compute a spatial flux distribution which is consistent with the spatial distribution of fuel temperature, moderator temperature, and moderator density. This feedback procedure consists of first calculating the power (flux) distribution, assuming some temperature and moderator density distribution, and then calculating temperature and density distributions based on this power distribution. A new power distribution is then calculated using the latest temperature and density distributions. The initial spatial flux calculation for LWBR (zero depletion time) contained uniform temperatures and moderator density and was followed by two iterations of temperature feedback. In all subsequent timesteps, the temperatures and water density distributions were input from the previous timestep and a single iteration through temperature feedback was performed.

Reference V-7 contains the general specifications for the thermal calculations. Changes to the specifications, as implemented in the PDQ program, include the following. The fuel element temperature calculation has been modified to allow the fuel conductivity to be input in table form as a function of fuel temperature and depletion. Turbulent mixing (cross flow) is not included in three-dimensional solutions; i.e., all flow is assumed to be in the axial direction. The equations to determine the fuel temperature have been modified slightly to allow a non-zero gap between the fuel and the clad. Calculations of clad shrinkage and pellet expansion effects have been included. These calculations affect the gap conductance and water content and are described in Section V.G.

Reference V-7 specifies a method of obtaining the fuel temperature, moderator temperature, and moderator density when the power distribution is known. The basic method is still used except for the modifications described in Section V.G. The power distribution results from solving the spatial flux problem and combining this flux with a spatial distribution of the cross sections. The fundamental assumption in the thermal solution is that the moderator flow in the core is known and is independent of the power distribution. The thermal calculations are coupled to the reactor diffusion-depletion calculation through the power distribution and the depletion of the fuel, which influences the thermal conductivity of the fuel material. The thermal-hydraulic grid for LWBR is the same as the depletion block grid - each transverse depletion block constitutes a thermal track for which a one-dimensional axial calculation of moderator temperature and density is done. At each axial height in the thermal-hydraulic grid, which for LWBR corresponds to the PDQ axial planes, a one-dimensional radial calculation of the fuel pellet temperature in a fuel rod is performed. Note that temperature feedback equations apply only in regions where power is generated. In non-fueled structural regions a time-independent moderator density is assigned which corresponds to the estimated region average temperature.

The temperatures and density are represented as nuclide concentrations and have the following form:

$$\text{fuel temperature: } N_{T_F} = \sqrt{T_F + 459.72} - \sqrt{T_F^{\text{ref}} + 459.72}$$

$$\text{moderator density: } N_\rho = N_H - N_H^{\text{ref}}$$

In these forms, T_F represents the calculated fuel temperature (in °F) and N_H is the calculated density of hydrogen. The same quantities with the superscript "ref" are specified reference values of the parameters. The moderator temperature is treated as a function of moderator density in LWBR because boiling effects on nuclear calculations are not significant. These particular "nuclides" possess a spatial distribution, not as the result of a depletion calculation but as the result of a thermal calculation. Since the cross section calculations do not treat these pseudonuclides in any special way, the "concentrations" may have the same kind of effect on macroscopic and/or microscopic cross sections as any other nuclide concentration. That is, these pseudo-concentrations are assigned microscopic cross sections and self-shielding factors and serve as independent variables in cross section interpolation tables, as discussed in Section IV.E.

F. Xenon Feedback

The xenon feedback calculation provides the capability to compute the spatial flux distribution associated with equilibrium nuclide concentrations of iodine and xenon. This iterative procedure consists of (1) calculate the spatially-dependent cross sections for some spatial distribution of iodine and xenon concentrations; (2) solve the diffusion equations to determine the spatial flux distribution; (3) normalize the flux to the core power level and use this flux to solve the asymptotic iodine and xenon equations; (4) repeat from step (1) again, using the latest iodine and xenon concentrations. In LWBR core depletion calculations a single iteration through xenon feedback was performed in each depletion timestep.

The equations solved for iodine (I) and xenon (Xe) are:

$$N_I^{i+1} = \frac{Y_I^i}{\lambda_I + A_I^i}$$

$$N_{Xe}^{i+1} = \theta N^{i+1} + (1 - \theta) N_{Xe}^i$$

where i is an iterate number and

$$Y_{j,k}^i = \sum_j \gamma_{j,k} N_j \sum_g \sigma_{j,g}^f C_{j,g}^f \phi_g^i$$

$$A_k^i = \sum_g \sigma_{k,g}^a G_{k,g}^a \phi_g^i$$

$$N^{i+1} = \frac{Y_{Xe}^i + \lambda_I N_I^{i+1}}{\lambda_{Xe} + A_{Xe}^i}$$

θ = An input extrapolation factor used to improve convergence. The physical interpretations for the basic symbols are:

- N_j = the concentration of nuclide j
- λ_j = the decay constant for nuclide j
- $Y_{j,k}$ = the fractional yield of nuclide k from fissile nuclide j
- $\sigma_{j,g}^a \text{ or } f$ = the microscopic absorption (a) or fission (f) cross section for nuclide j in group g
- $G_{j,g}^a \text{ or } f$ = the self-shielding factor for absorption (a) or fission (f) for nuclide j in group g
- ϕ_g = The power normalized flux for group g averaged over the appropriate depletion block mesh. This flux is the flux associated with the previous iterate iodine and xenon concentrations.

In general, $0.0 < \theta \leq 1.0$. For LWBR, $\theta = 0.9$.

G. Clad Shrinkage, Fuel Swelling, and Gap Conductance in PDQ

The thermal feedback procedure in PDQ includes the explicit calculation of the thermal conductance of the fuel-clad gap for each depletion block. The procedure takes into account the following factors:

1. Clad shrinkage due to fast-neutron-induced creep;
2. Fuel contraction due to pellet densification;
3. Fuel expansion due to fission product swelling and thermal expansion;
4. Changes in the conductivity of the gas in the gap due to release of noble gas fission products.

The purpose of the inclusion of these factors is to provide accurate calculations of fuel temperature (and hence of Doppler-broadened cross sections) and accurate determinations of the hydrogen number density. The hydrogen concentration changes because of the change in coolant channel area caused by clad shrinkage (or clad swelling due to outward pressure of the expanding fuel after the gap disappears).

The time-dependent geometry procedure described above was devised for analysis of LWBR, but it could be applied to any light water moderated reactor with rod-type fuel. The approach taken is a compromise between the objectives of, on one hand, a thorough, comprehensive treatment of the factors outlined above and, on the other hand, a sufficiently simple treatment that the PDQ computation time is not significantly increased.

The clad shrinkage is taken to be proportional to the fast neutron flux. After the gap disappears the clad diameter is assumed to be determined solely by the fuel diameter. Provision has been made to account in an elementary fashion for fuel-clad interaction, such as might be caused by clad ovality, where the gap is small but has not yet disappeared. Fuel densification is treated by an empirical model depending on grain size. Fuel swelling is assumed to be proportional to depletion. The fuel thermal expansion is calculated as a quadratic function of temperature.

The treatment of thermal conductance of the gap is a simplification of the method used in FIGRO (Reference V-8). The thermal conduction coefficient h (BTU/hrft² °F) is given by

$$h = k / (C_o + t)$$

where

k = the conductivity of the gas in the gap (BTU/hrft °F)

C_o = an input parameter

t = the gap thickness.

A modified expression is used as t approaches zero. The calculation of k assumes that the gap and plenum have an initial charge of He which is subsequently diluted with fission product Kr and Xe (as well as a small amount of He from ternary fission). The release of the fission product gases into the gap is calculated under the assumption that the fraction of gas released, R , is given by

$$R = C_1 + C_2 f + C_3 V_F$$

where

C_1 , C_2 , and C_3 = input parameters

f = depletion (f/cc)

V_F = the volume fraction of fuel above the gas release temperature.

This temperature is an input quantity. V_F is calculated for each depletion block during the initial pass through the core in the thermal feedback loop of PDQ. The amount of released gas is summed over the axial length of the core for each track (i.e., each axial stack of depletion blocks). This sum is combined with the known amount of fill gas in the fuel-clad gap and residual plenum to determine the composition of the gas in the rods in each track.

On successive passes through the core in the thermal feedback loop, an iterative procedure is employed for each depletion block to obtain consistent values for the gap conductance, the fuel temperature, the fuel radius (corrected for thermal expansion), and the resulting gap thickness (which affects the gap conductance). Convergence of this iterative procedure is defined by a change of less than 2°F in the fuel surface temperature on successive iterations. In nearly all test cases examined convergence was achieved within 5 iterations.

The net output of the above procedure are the changes in moderator density and fuel temperature for each depletion block due to the irradiation history. These changes are combined with the changes in moderator density and fuel temperature caused by the spatial power distribution and become part of the temperature feedback process described in Section V.E.

The method has been tested by comparison with the much more sophisticated mechanical and thermal calculations of CYGRO-4 (Reference V-9). A number of individual LWBR fuel rods from various regions of the core and with varying power histories have been analyzed over core life. Agreement of the PDQ calculations with CYGRO-4 for fuel temperature averaged over a depletion block was within 40°F in nearly all cases, and usually well within this figure. For comparison, the temperature rise of a fuel depletion block above the moderator ranged up to 1450°F in these tests. Agreement in the calculation of clad radius was within 0.3 mil in nearly all cases where the change in clad radius ranged up to 3 mils in these tests.

Figure V-7 shows a comparison of PDQ and CYGRO-4 calculations of fuel temperature for three depletion blocks from one seed rod. Block A is high in the rod and gets cooler with time as the seed moves up and the axial seed power shape shifts downward. Conversely, block C is low in the rod and becomes hotter with time. Figure V-8 shows a comparison of clad radius for 3 depletion blocks from 1 blanket rod. The time at which pellet-clad contact causes the clad to

stop shrinking and start expanding is seen to be early where the flux is high at the center of the rod (block E). It is late where the flux is low near the ends of the rod.

H. Depletion Timesteps

The notion of a timestep as the unit in a depletion calculation was defined at the beginning of Chapter V. Since the axial mesh spacing is 3.5 inches (Section V.D.), each spatial flux calculation is done with the movable fuel position no more than 1.75 inches from the nominal critical position. In some cases the timestep lengths ΔT during the PDQ depletion calculations are adjusted to further improve the proximity of the fuel position to the estimated critical position. Additional depletion calculations are done with movable fuel positions adjusted to simulate a core for which the reactivity is ± 1 percent off-nominal.

The main-line depletion calculations described above, performed prior to core operation, are done assuming continuous operation at 100 percent of full power, with equilibrium levels of xenon and protactinium. Additional calculations are done at various times in life, with xenon and/or protactinium removed and the movable fuel position adjusted to the critical seed position, to calculate off-equilibrium power distributions.

Timestep lengths (ΔT) of 100, 900, and 2000 effective full power hours (EFPH, Section IV.E.2.) are used for the initial 3000 EFPH during which time xenon, protactinium, and samarium are building up to near equilibrium levels. During the middle portion of lifetime a ΔT of 2500 EFPH is used, since the movable seed bank is close to being axially aligned with the blanket (see Figure II-2), and the fuel motion is relatively slow. A reduction in ΔT to 1500 or 1000 EFPH is made for the period of more rapid fuel motion late in core lifetime, so that the change in movable seed critical position between PDQ timesteps does not exceed 7 inches.

REFERENCES

- V-1. C. J. Pfeifer and C. J. Spitz, "PDQ-8 Reference Manual," WAPD-TM-1266, May 1978.
- V-2. T. R. England, "Time-Dependent Fission-Product Thermal and Resonance Absorption Cross Sections (Data Revisions and Computational Extensions)," WAPD-TM-333, Addendum No. 1, January 1965.

- V-3. T. R. England, "CINDER - A One-Point Depletion and Fission Product Program," WAPD-TM-334 (Revised), June 1964. Also, T. R. England, R. Wilczynski, and N. L. Whitmore, "CINDER-7: An Interim Report for Users," LA-5885-MS, April 1975.
- V-4. S. Milani and S. H. Weiss, "Small Uranium-233 Fueled Seed-and-Blanket Critical Experiments," WAPD-TM-614, November 1967.
- V-5. E. M. Gelbard, "Application of Spherical Harmonics Method to Reactor Problems," Bettis Technical Review, WAPD-BT-20, September 1960, page 73 and "A Simplified Form of the Spherical Harmonics Equations and Its Use in Shielding Problems," Trans. A.N.S. 3 (1960) 349.
- V-6. L. B. Freeman and H. W. Ryals, "Numerical Comparison of Diffusion-Like Transport Approximations for Very Fast Neutrons," Nuc. Sci. Eng. 34 (1968) 67 and "Numerical Comparison of Neutron Transport Approximations for Application at Energies Above 0.8 Mev," WAPD-TM-690, April 1968.
- V-7. J. N. Sorenson, "Thermal Feedback Calculations in the PDQ-5 Few Group Neutron Diffusion-Depletion Computer Program," WAPD-TM-639, January 1967.
- V-8. L. A. Waldman, L. L. Lynn, and I. Goldberg, "FIGRO (Addendum) - CDC-6600 Computer Program for the Analysis of Fuel Swelling and Calculation of Temperature in Bulk-Oxide Cylindrical Fuel Elements," WAPD-TM-618, Addendum I, October 1967.
- V-9. J. B. Newman, J. F. Giovengo, and L. P. Comden, "The CYGRO-4 Fuel Rod Analysis Computer Program," WAPD-TM-1300, July 1977.

Figure V-1. Natural U^{233} , Th^{232} Chain

Th²³² Yielding Pa²³¹ + U²³²

Figure V-2. Linear Fuel Chains

Figure V-3. Explicit Fission Product Chains

Second Samarium Chain

Accounts for production and daughters of ground state Pm^{148} . 0.526 of the captures in Pm^{147} give ground state Pm^{148} nuclei. For accounting purposes, the Pm^{147} is said to come from direct fission yield, but this Pm^{147} is not counted in the total when concentrations are summed over all chains.

Figure V-3. (Cont)

Figure V-4.- Thermal Fission Product Cross-Section

Figure V-5. Epithermal (Group 3) Fission Product Cross Section

Figure V-6. Mesh Lines and Depletion Block Sizes in PDQ for 1/6 of Type I Module

Figure V-7. Comparison of Seed Rod Temperature Calculation by PDQ and CYGRO-4, for 3 Depletion Blocks

Figure V-8. Comparison of Regular Blanket Rod Clad Radius Calculation by PDQ and CYGRO-4 for 3 Depletion Blocks

VI. DETERMINATION OF NUCLEAR PERFORMANCE AND PREPARATION OF DATA FOR ENGINEERING ANALYSIS: POST-PDQ DATA MANIPULATION

Computer files generated by the PDQ depletion are used by a series of post-PDQ programs to prepare data summaries and data files for engineering analyses. These programs assist in the evaluation of core performance with respect to reactivity lifetime, breeding capability, power distributions, thermal capability, fuel element performance, and other aspects. The extensive computer automation designed into the post-PDQ data processing system for LWBR results in timely and accurate transmittal of data to the engineering groups.

A. Physics Analysis

The physics analysis of LWBR core performance utilizes the results of the PDQ depletion to assess reactivity, power performance, and breeding. The core reactivity behavior is characterized by predictions of the movable fuel position versus time. Power performance is described by gross power sharing between seed and blanket or among the modules, and by distributions of average power in each rod and pointwise power, fast fluence, and depletion. The breeding parameters of interest are the conversion ratio (CR) which is an instantaneous quantity and the fissile inventory ratio (FIR) which is a time integral quantity. The CR is the ratio of the instantaneous fissile production rate to instantaneous fissile destruction rate. The FIR is the ratio of the fissile content at any time in life to the fissile content at beginning of life.

Because of the 3.5 inch axial mesh used in the PDQ calculation, the movable fuel is not necessarily at the exact critical position for each PDQ timestep. Given the PDQ axial fuel position (Z_o), the PDQ eigenvalue (λ_o), the desired critical eigenvalue (λ_c) which accounts for PDQ-to-experiment bias, and the movable fuel worth (W in $\Delta\lambda/\text{cm}$) at the particular time in life, a corrected axial fuel position (Z_c) is computed at each timestep as follows:

$$Z_c = Z_o + \frac{\lambda_c - \lambda_o}{W} .$$

The best estimate reactivity lifetime is then the time in life at which the corrected fuel position reaches the maximum position allowed (Section II.A).

Having computed the corrected fuel position at each PDQ timestep, corrections are next made to the PDQ neutron balance (nuclide absorption and fission fractions). These corrections are made to account for the changes in neutron losses to the structure regions above and below the core, caused by the fuel position adjustments, and to account for the redistribution of these neutron losses among

the nuclides. The correction to the neutron balance is made in two steps: First, the change in neutron loss is obtained from a previously generated sensitivity of neutron loss to fuel position. Then, the change in loss is distributed among the nonfissile isotopes in proportion to their capture fractions. The corrected neutron balances are used to compute the corrected conversion ratio at each time-step. A final correction is made to the conversion ratio to account for effects not included in the PDQ depletion - for example, U^{238} , fuel impurities and in-core instrumentation.

At beginning of life the conversion ratio is at its maximum value and is greater than 1. As the core depletes and fission products build up, the conversion ratio decreases with lifetime. When the conversion ratio reaches unity late in core life, the fissile content of the core is at its maximum. The fissile inventory ratio is computed by integrating the conversion ratio over time; that is, the change in FIR between times t_1 and t_2 is

$$\Delta \text{FIR} (t_1 \rightarrow t_2) = \left[\frac{A_f(t_1) + A_f(t_2)}{2 N_0} \right] \left[\frac{\text{CR}(t_1) + \text{CR}(t_2)}{2} - 1 \right] (t_2 - t_1) ,$$

where A_f is the absorption rate in fissile material and N_0 is the initial number of fissile atoms in the core. Then, the FIR at any time t_n is

$$\text{FIR}(t_n) = 1 + \sum_{i=1}^n \Delta \text{FIR}(t_{i-1} \rightarrow t_i) .$$

The curve of FIR versus time will peak at the time in life when CR drops to a value of 1. The computations of neutron absorption fractions, CR and FIR are performed by a computer program which reads files of integral data. These files are part of the PDQ output computer files generated for each timestep during the depletion calculations (Reference VI-1).

The physics analysis of power, fast fluence, and depletion distributions involves the evaluation of regionwise power fractions (power sharing), the examination of local power peaks (ratios of pointwise power to average power), and computation of local fast fluence and depletion values. Computer programs have been written which access the PDQ output files and generate computer files and/or tabular data for use in thermal-hydraulic, fuel element and structural analyses.

B. Thermal-Hydraulic Analysis

The preparation of computer files for thermal-hydraulic analyses requires operating on the PDQ partition power files for each timestep. The partition

power is defined by the neutron fluxes at a mesh point and the macroscopic fission cross sections in a mesh block adjacent to the point (Reference VI-1). It is used to construct heat flux values for axial segments of fuel rods. The PDQ mesh and depletion block model discussed in Section V.D was designed with the post-PDQ analyses in mind. Depletion blocks in the PDQ calculation are assigned to rod segments which are important in thermal-hydraulic performance.

In general, the cross sectional representation of a depletion block in PDQ is a parallelogram, as shown in Figure VI-1. The block is bounded by PDQ mesh columns C_l and C_r and mesh rows R_f and R_r . The as-built model uses 31 PDQ mesh planes to divide the fuel height axially. Therefore, each axial stack of fuel depletion blocks consist of 30 depletion blocks or plane intervals which become rod segments in the thermal-hydraulic data files. A rod segment is bounded by an upper plane, z_u , and a lower plane, z_l . As shown in Figure VI-1, each PDQ mesh point has 6 sectors in a horizontal plane. The PDQ partition power file contains 12 relative power values for each PDQ mesh point, 6 for the sectors above the plane and 6 for the sectors below the plane. The pointwise power values for a 3-1/2 inch high axial segment are taken from the top of the lower plane and the bottom of the upper plane, for the sectors which lie within the parallelogram that defines the depletion block.

The power values at the top of the segment are compared to obtain the maximum at the top, $\hat{P}_{top}$, and averaged to obtain the average at the top, $\bar{P}_{top}$. Similar operations are done for the bottom values to obtain $\hat{P}_{bot}$ and $\bar{P}_{bot}$. Data files transmitted to the thermal-hydraulic analysis group contain, for each segment h (each depletion block) at each PDQ timestep, the segment averaged heat flux (BTU/hr-ft²) computed as follows:

$$\bar{\phi}_h = \frac{1}{2} C_h \bar{f}_h (\bar{P}_{top} + \bar{P}_{bot})$$

and the peak sector heat flux in the segment computed as follows:

$$\tilde{\phi}_h = \frac{1}{2} C_h \hat{f}_h (\hat{P}_{top} + \bar{P}_{top}) \text{ if } \hat{P}_{top} \geq \hat{P}_{bot}$$

or

$$\tilde{\phi}_h = \frac{1}{2} C_h \hat{f}_h (\hat{P}_{bot} + \bar{P}_{bot}) \text{ if } \hat{P}_{bot} > \hat{P}_{top} .$$

Here, C_h converts relative power density to heat flux, $\bar{f}_h$ is a physics factor on segment average power for correcting PDQ data, and $\hat{f}_h$ is a physics

factor on "local" power. Local power refers to power in any small region, such as a sector. These data files are used with various thermal-hydraulic analysis tools - for example, the HOTROD program (Reference VI-2) and the XITE program (Reference VI-3).

C. Fuel Element Analysis

Fuel element analyses require estimates of local and axial segment average heat fluxes, depletion (f/cc), and fast neutron fluxes (above 1 Mev) and fuel rod average depletion. In a fashion similar to that for thermal-hydraulic analyses, post-PDQ computer programs read the PDQ partition power and pointwise flux files and prepare files for use in fuel element analyses. For fuel element analysis, local power refers to averages at a PDQ plane, $\bar{P}_{top}$ or $\bar{P}_{bot}$, rather than to sector powers. The procedure for obtaining local power includes the power values on both the thoria and binary sides of the binary-thoria interface in stepped rods (rods with less than 84 inches of binary fuel). As for the thermal-hydraulic data, the local and segment average power values are converted to heat flux values and multiplied by the appropriate physics correction factors which account for uncertainties and off-equilibrium conditions.

To obtain depletion levels which are consistent with the heat flux values, the local and average heat fluxes are integrated over time to produce local and average depletions in fissions per cc. Upper envelope plots of local heat flux versus depletion are constructed and the segments which make up the upper envelopes over lifetime are identified.

The PDQ pointwise flux file is used to obtain fast flux (few-group 1) values which are maximum at each segment boundary and average in the axial segment. The PDQ group 1 fluxes are multiplied by 0.88 to account for the fact that the few-group 1 lower energy boundary is 0.821 Mev, whereas fuel element evaluations require the fast flux above 1 Mev.

These data for limiting locations are collected in computer files and transmitted to the Fuel Element group for evaluation, for example, with the CYGRO-4 computer program (Reference VI-4).

D. Structural Analysis

Structural analyses require heat fluxes, heat flux gradients across fuel rods, and fast fluence (fast flux integrated over time). Relative power values are obtained for selected rods (depletion blocks) from the PDQ partition power files. These data are used to compute heat flux values on either side of the

rods along PDQ mesh columns or mesh rows, depending on the direction of the steepest gradient. The pointwise flux files are used to obtain fast flux at each timestep for the locations of importance for structural analyses and the fast fluence is computed by integrating these fluxes over time.

Other requests for power or fast neutron flux data are generally less frequent and involve smaller amounts of data. These are usually handled by editing PDQ data rather than by transmission of computer files.

REFERENCES

- VI-1. C. J. Pfeifer and C. J. Spitz, "PDQ-8 Reference Manual," WAPD-TM-1266, May 1978.
- VI-2. S. G. Bens, J. H. Anderson, and R. J. DeCristofano, "HOTROD - A Computer Program for Subchannel Analysis of Coolant Flow in Rod Bundles," WAPD-TM-1070, November 1973.
- VI-3. Safety Analysis Report for the Light Water Breeder Reactor, Section 15.1.0.6.4.
- VI-4. J. B. Newman, J. F. Giovengo, and L. P. Comden, "The CYGRO-4 Fuel Rod Analysis' Computer Program," WAPD-TM-1300, July 1977.

Figure VI-1. Cross Section of a Typical Depletion Block in PDQ Geometry

VII. CORE KINETICS CALCULATIONS

A. Calculation of Kinetics Parameters

The nuclear parameters important to determining the kinetic behavior of the LWBR and associated power plant were evaluated using the nuclear calculational model described in the preceding chapters. The important core parameters include temperature and density coefficients of reactivity, effective delayed neutron fraction, and prompt neutron lifetime. The parameters may be used to study typical transients or hypothetical accidents. In the latter case the best estimate of the parameter is varied to allow for possible uncertainties.

1. Temperature and Density Coefficients of Reactivity

Two temperature coefficients of reactivity are determined using the LWBR nuclear calculational model, namely, the fuel and moderator temperature coefficients. Three-dimensional PDQ calculations, as described in Chapter V, are utilized for determining both zero-power and at-power coefficients.

Each zero-power coefficient is determined by performing 2 complete sets of PREP-PAX-PDQ calculations with uniform temperatures and no temperature feedback, which is equivalent to zero power conditions. The 2 sets of calculations are identical except for the perturbation of a single core parameter such as moderator temperature or fuel temperature.

The at-power coefficients are determined simultaneously from a set of 3 temperature feedback PDQ calculations, all at the movable seed bank position and core lifetime of interest. The 3 cases involve the following conditions: 100 percent power - 100 percent flow; 75 percent power - 75 percent flow; and 75 percent power - 100 percent flow - inlet temperature perturbed (21°F increase). From the first pair of cases the fuel temperature coefficient is determined directly as the resulting reactivity change per unit square root of fuel temperature. The moderator temperature distribution remains constant in these 2 cases due to the constant power-to-flow ratio. The moderator temperature coefficient is determined from cases 1 and 3 and use of the previously determined fuel temperature coefficient. In case 3, relative to case 1, the reactivity effects of reduced fuel temperatures and increased moderator temperatures approximately cancel. However, the moderator temperature coefficient can be inferred from the observed temperature changes of fuel and the moderator and the fuel coefficient predetermined as discussed above.

For some applications the moderator temperature coefficient, which is primarily a density effect, is obtained in the form of a density coefficient of

reactivity rather than a temperature coefficient. This density coefficient is determined in the same manner as the moderator temperature coefficient, except that the reactivity change due to moderator effects is related to the corresponding density changes rather than to the temperature changes.

2. Effective Delayed Neutron Fraction

The fraction of total fission neutrons that are delayed is determined by weighting the isotopic delayed neutron fractions, from the basic data presented in Section IV.B.11, by the corresponding fission fractions within LWBR. An effective fraction is then determined by multiplying this weighted fraction by an importance factor ($\bar{\beta}/\beta$) resulting from delayed neutrons being emitted at lower energies than prompt neutrons and thus having an increased importance. The calculation of $\bar{\beta}/\beta$ involves determining the ratio of the total fissions resulting from a delayed neutron, relative to the total fissions resulting from a core average neutron, based on methods described in Reference VII-1. The procedure involves following a delayed neutron population through several generations until an asymptotic fission rate equal to that of an average core neutron is reached. The increased importance is due primarily to the first generation. However, succeeding generations contribute to the total effectiveness. Both the PDQ calculational model, discussed in Chapters IV and V, and the analytical standard, discussed in Chapter III, are utilized for this calculation.

The PDQ method for determining $\bar{\beta}/\beta$ is based on a converged three-dimensional eigenvalue calculation with multiplication factor λ_1 , followed by several one-iteration calculations giving multiplication factors λ_2 to λ_n . The first one-iteration calculation uses as input the converged source distribution from the eigenvalue calculation, while each of the succeeding one-iteration calculations uses as input the output source distribution from the preceding calculation. In addition, the first one-iteration calculation uses few-group cross sections based on a delayed neutron spectrum, while the other iterations are based on the total neutron spectrum. $\bar{\beta}/\beta$ is then calculated as

$$\bar{\beta}/\beta = \frac{\lambda_2}{\lambda_1} \frac{\lambda_3}{\lambda_1} \frac{\lambda_4}{\lambda_1} \dots \frac{\lambda_n}{\lambda_1} .$$

The one-iteration calculations are continued until $\lambda_n \approx \lambda_1$.

The RCP model for determining the importance factor is similar to the PDQ model, discussed above, in that a converged eigenvalue calculation, λ_1 , provides the starting point and the delayed neutron population is calculated through several generations. The RCP method differs from the PDQ method in that, prior

to the series of generation-by-generation calculations, the converged fission site locations are separated into 2 subsets - one for U^{233} and one for Th^{232} - by a pair of fixed source calculations. Each one of this pair of calculations is then followed by a series of fixed source calculations, in the same way as with the one-iteration PDQ calculations. A multiplication factor for each step in each one of the pair of calculational chains is determined as the output source relative to the input source. The total delayed neutron importance factor is then determined by combining the 2 sets of calculations as follows:

$$\bar{\beta}/\beta = \frac{\beta^{Th232} \left(\frac{\lambda_2 \lambda_3 \dots \lambda_n}{\lambda_1 \lambda_1 \dots \lambda_1} \right)^{Th^{232} \text{ fissions}} + \beta^{U233} \left(\frac{\lambda_2 \lambda_3 \dots \lambda_n}{\lambda_1 \lambda_1 \dots \lambda_1} \right)^{U233 \text{ fissions}}}{\beta^{Th232} + \beta^{U233}}$$

3. Prompt Neutron Lifetime

The prompt neutron lifetime is determined using the method described in Reference VII-1. In this technique the value of the neutron generation time, Λ , is shown to be identical to the reactivity change resulting from a uniform perturbation of the absorption cross sections throughout the entire core by an amount

$$\Delta \Sigma_a(E) = \frac{1}{v(E)}$$

where $v(E)$ is the neutron speed.

The perturbation is implemented into PDQ calculations by adding equal traces of Boron-10 throughout all regions of the calculation. Because of the small reactivities resulting from the boron additions, the amount of boron is increased by a factor of 100 to provide a reactivity perturbation that is easier to calculate.

B. Kinetics Calculations for LWBR

A summary of the methods used for kinetics calculations of LWBR is contained in Reference VII-2. Transient behavior of the core is determined primarily using 3 computer programs PARK-1, PARK-2 and FLASH. PARK-1 and FLASH are based on point-kinetics and make use of the total core kinetics parameters discussed above, while PARK-2 is based on three-dimensional, space-time techniques and requires different kinetics-related parameters.

In PARK-2 the reactor is described three-dimensionally using axially discontinuous synthesis techniques as described in Reference VII-3. To permit

analysis of a core accident or transient, a core model is developed using PDQ and fed into PARK-2 to permit the three-dimensional power distribution to be calculated throughout the transient. Each model contains a three-dimensional geometry description and temperature-feedback cross section library consistent with those used in static PDQ analysis of the core, as discussed in Chapter V. In addition, a synthesis package is necessary which consists of sets of two-dimensional trial functions that apply to all core configurations that may be encountered during the transient calculation in PARK-2.

The PARK-2 calculations require the effective delayed neutron fractions as input. The values used are those calculated by methods discussed above. The prompt neutron lifetime is not used, but 4 parameters equal to the inverse of the neutron velocity in each of the 4 neutron few-groups are used, and these characterize neutron lifetime. The inverse neutron velocity parameters are determined from the PAX calculations discussed in Chapter IV. Temperature coefficients are not required by PARK-2. The reactivity effects due to temperature changes in the core are calculated directly in the PARK-2, utilizing the temperature dependent cross sections in the HARMONY file (Section IV.E.4) and the three-dimensional nuclear synthesis model.

C. Stability and Xenon Transient

The methods for investigating the xenon stability characteristics of the LWBR are based on the techniques contained in Reference VII-4. These techniques are applied in analyzing the LWBR characteristics and require determination of overtone mode eigenvalues, effective thermal flux levels, and xenon and iodine yield characteristics for U^{233} . These core parameters are also important for determining maximum-to-equilibrium xenon poisoning following core power transients. The high direct yield to Xe^{135} and the low thermal flux levels result in a very small maximum-xenon transient and are also important in producing a core which is stable with respect to power oscillations.

REFERENCES

- VII-1. A. F. Henry, "The Application of Reactor Kinetics to the Analysis of Experiments," Nuc. Sci. Eng., 3 (1958) 52.
- VII-2. Safety Analysis Report for the Light Water Breeder Reactor, Section 15.1.0.6.

- VII-3. J. B. Yasinsky, "Combined Space-Time Synthesis with Axially Discontinuous Trial Functions," WAPD-TM-736, October 1967.
- VII-4. T. R. England, G. L. Hartfield, and R. K. Deremer, "Xenon Spatial Stability in Large Seed - Blanket Reactors," WAPD-TM-606, April 1967.

VIII. QUALIFICATION OF THE MODEL

Testing of individual parts of the nuclear analysis model has been discussed in the preceding sections where those parts are described. This chapter discusses testing of the model as a whole with critical experiments and the analytical standard. Because critical experiments do not provide any test of fission product poisoning predictions, fuel irradiation experiments were performed to test the fission product data. Those comparisons are also described in this chapter.

A. Fission-Product Treatment

1. Fission-Product Programs

The CINDER program (Reference VIII-1), a point depletion and fission-product program, has been used for the LWBR calculational model. This program was developed for nuclear design purposes. It has had widespread application and has been very useful to nuclear designers on a wide variety of nuclear cores in addition to LWBR.

The COMBO program (Reference VIII-2), like CINDER in many respects, was developed expressly for use with experimental data rather than for nuclear design. As such, it efficiently handles detailed exposure histories comprising hundreds or thousands of neutron flux timesteps. It takes account of thermal and epithermal neutron self-shielding that vary with nuclide concentrations as functions of irradiation. In addition, it has been used to process reactivity measurement data obtained on irradiation experiments.

Although the COMBO program is used with experimental data, its nuclear data library is taken primarily from the CINDER library. The basic nuclear data which were used to generate few-group cross sections were essentially the same for both the COMBO and CINDER libraries. The COMBO and CINDER programs have been shown to give essentially the same results for a number of conceptual problems selected for the express purpose of comparing the two programs under a variety of conditions. Because of the demonstrated agreement between the two programs, the comparison of explicit COMBO calculations with the detailed experimental measurements is tantamount to comparing CINDER calculations with experiment.

The calculations have had extensive experimental verification. The calculations have been compared with results of physics irradiation experiments carried out on samples representing all fissile and fertile reactor fuels. The experiments included irradiations in both soft and hard neutron spectra and covered both short and long exposures.

2. Post-Irradiation Isotopic and Elemental Comparisons

Post-irradiation mass analyses have been compared with calculations of corresponding quantities. Results of the comparisons are presented in References VIII-2 and VIII-3. Isotopic and elemental uranium have been compared for 5 irradiated samples of Th^{232} , 5 irradiated samples of U^{233} , 6 irradiated samples of natural uranium, and 1 irradiated sample of U^{238} . For the most part, the agreement is within 1 wt percent for the isotopic results and within 2 percent for the total uranium.

Measured and calculated Cs^{137} have been compared for 5 irradiated samples of Th^{232} , 5 irradiated samples of U^{233} , 6 irradiated samples of natural uranium, and 1 irradiated sample of U^{238} . The agreement is about 5 percent on the average.

Measured and calculated results of 6 neodymium isotopes have been compared for 3 irradiated samples of Th^{232} and 4 irradiated samples of U^{233} . The agreement is within about 1 wt percent for the isotopic neodymium results.

3. Reactivity-Measurement Results Compared with Corresponding Calculations

Experimental results obtained from reactivity measurements on irradiated fuel samples provide the content of fissile material and the two-group fission-product poisoning. The two-group poisoning is expressed in terms of the thermal and the epithermal neutron absorption cross sections. From the two-group poisoning, an effective one-group fission-product cross section is derived for the irradiation spectrum. These experimental results of the fissile content, the two-group poisoning, and the effective one-group poisoning are obtained as functions of irradiation and cooling time and are compared with corresponding COMBO calculations for the irradiation spectrum. Such results have been presented in References VIII-2 and VIII-3 for 5 irradiated samples of U^{233} .

Typical calculated and measured results for 1 sample of irradiated U^{233} are shown graphically in Figure VIII-1. The abscissa is the number of three-week cycles irradiated. On Part a of the figure the fuel fraction (of the initial fuel) is plotted. Part c of the figure shows σ_{2200} , the total thermal poisoning in barns per fission. Part d of the figure shows the epithermal resonance integral I above 0.105 ev (appropriate for the irradiation spectrum) in barns per fission. Included on parts c and d are triangles showing the barns per fission calculated for transient Xe^{135} , Sm^{149} , and their isobaric precursors. The results presented in Figure VIII-1 are typical of results obtained from reactivity measurements and corresponding calculations on a variety of irradiated samples exposed in different spectra and for different irradiation and cooling times.

The typical results shown in Figure VIII-1 illustrate the fact that measured and calculated results agree to about 1 percent for the fissile content and to about 3 percent for the one-group effective fission-product poisoning. The two-group poisoning indicates discrepancies of 10 percent and 20 percent associated with the split between the thermal and epithermal parts of the total fission-product poisoning. In Reference VIII-3 these discrepancies are attributed to library errors that, for want of energy-dependent information for some fission product cross sections, behave as $1/v$ over the entire energy range. For such fission products that really have resonances, the assumption of $1/v$ behavior gives thermal and epithermal cross sections that are too high and too low respectively. Calculations using such cross sections overestimate the thermal absorption and underestimate the epithermal absorption. This is consistent with the observations as illustrated typically in the c and d plots of Figure VIII-1.

4. Measured and Calculated Decay Heat

The decay heat captured inside a calorimeter has been measured as a function of cooling time for highly irradiated Th^{232} , U^{233} , U^{235} , and Pu^{239} . The results, together with calculations of decay heat using the COMBO program, are compared in Reference VIII-4. The comparisons cover cooling times from 14 to 4500 hours after irradiation. Comparisons of measured and calculated decay heats show agreements that are generally within 2 or 3 percent.

5. Conclusion

The results presented in References VIII-2 through VIII-4 and discussed above show remarkably close agreements between measured and calculated results, generally in the range of 1 to 5 percent. Such results are all the more remarkable in view of the wide variety of experimental results that are compared with calculations. The comparisons attest to the accuracy of the programmatic calculations embodied in both the COMBO and CINDER programs.

B. Core Reactivity

1. Experimental Core Program

An extensive experimental core program was completed as part of the LWBR Development Program and documented in References VIII-5, VIII-6, and VIII-7. The critical assemblies analyzed in the 3 references are referred to as the S-B series, the BMU series, and the Detailed Cell series. For the qualification of the nuclear analysis model only the latter 2 series are considered since these are the more recent of the experiments and are more representative of the LWBR fuel system and geometry.

The BMU series consisted of 3 single module and 3 multi-module experimental configurations of the seed-blanket type with small diameter seed rods and large diameter blanket rods, both containing mixtures of UO_2 and ThO_2 . The uranium oxide enrichment varied from 2 to 12 w/o of which approximately 98 w/o was U^{233}O_2 . The active fuel lengths were approximately 28 inches for seed rods and 42 inches for blanket rods. Five of the experiments were performed at ambient temperature conditions while the sixth was performed at 410°F . The information obtained from these experiments included the demonstration of criticality for the various configurations as well as a detailed core power traverse for the BMU-2-4 (power flattened) which was a 4-module configuration.

The Detailed Cell series consisted of 7 similar experiments involving a single module, seed-blanket core surrounded by a varying number of additional fuel rods known as the driver. The seed was positioned at a different height relative to the blanket in each case and the amount of driver was varied with seed height to maintain criticality. The single module very closely approximated a type II LWBR module as to fuel enrichments, fuel distribution, and overall geometry. Six of the Detailed Cell experiments were conducted at ambient temperature conditions while the seventh was performed at 477°F . The use of driver material around the module tended to provide an in-core surrounding for the single module. Both criticality and detailed power distribution information were provided by this experiment.

2. Monte Carlo Calculation of Experiments

Three-dimensional Monte Carlo calculations of all the Detailed Cell experiments and 3 of the BMU experiments were performed to qualify the Monte Carlo method as a calculational standard. Section III.B discusses the strategy of this approach. Descriptions of the calculational techniques of the RCP program, which solves the neutron transport equation using Monte Carlo techniques, and the RCPL1 program, which provides detailed full energy range neutron cross section data, are contained in References III-2 and III-12. The detailed cross section data were consistent with the nuclear data discussed in Section IV.B in all cases.

The core geometry was described in great detail in all calculations. Fuel pellet stacks, clad, water, grids, and other supporting structures were explicitly represented as well as end caps and fuel rod plenum regions. In some cases the fuel clad was homogenized with the small fuel-clad gap. Structural members such as posts, shells, control rods, and base plates were described exactly as to position and volume, although with slight geometrical modifications in some cases for calculational convenience.

The procedure in the analysis of each critical configuration was to provide at least 3 independent calculations of approximately 100,000 histories each. The initial source guess for each calculation was based on either a PDQ calculation or a previous RCP calculation for some configuration. Different random number sequencing in each of the 3 calculations was employed to assure independence. The calculated eigenvalues from the independent calculations were combined statistically to provide a single value for each configuration. The gross power sharing data for each detailed cell configuration for which detailed experimental results were obtained was also determined and statistically combined.

The RCP eigenvalues for the 10 experimental cores discussed above and the reciprocal variance weighted average are shown in Table VIII-1. The eigenvalue corrections shown are for small reactivity effects not included in the calculations, such as U^{235} fission. The uncertainty quoted (0.0036) represents the standard deviation of the individual λ values about $\bar{\lambda}$, not the standard deviation of the distribution of $\bar{\lambda}$. This uncertainty includes RCP statistics, the variable response of the 10 calculations to whatever cross section errors are in the input data libraries, and the variability of how well the core is represented in the RCP calculations. Considering RCP statistics alone gives a standard deviation of 0.0005. The gross power sharing data for 6 of the Detailed Cell configurations as shown in Table VIII-2 will be discussed later.

3. Development of Reactivity Bias for the Computational Model

In Section III.B.1, the reactivity bias for nuclear analysis model calculations is defined as the sum of 2 components. The first of these is the reactivity difference between the analytical standard, RCP, and experiment based on the analyses of all the experimental configurations discussed in the preceding section. The second is the reactivity difference between nuclear analysis model calculations for the complete LWBR configuration and a corresponding calculation using RCP. PDQ calculations of selected experiments were done with the present model, as discussed below in Section VIII.C.2, and more were done with an earlier version of the model. The multiplication factors are given in Table VIII-1 and show that the range of PDQ multiplication factors is about the same as with RCP. Nevertheless, it was judged that a better approach to obtaining a bias is to use the calculations of the full LWBR core at full power.

For conditions early in core life the reactivity bias was developed as follows: using the data summarized in Table VIII-1 the RCP-Experiment component was determined. In addition, 2 calculations were done of the as-built core at zero EFPH, with the movable seed bank at 14 and at 21 inches below the aligned

position, using consistent nuclear analysis model PDQ and RCP representations of the core to determine the PDQ-RCP component. The RCP-Exp component was 0.0011, as contained in Table VIII-1, while the PDQ-RCP component was 0.0014 (cf., Figure IV-11), resulting in an initial reactivity bias of 0.0025.

To determine later in life bias values the full core PDQ analysis model-RCP comparisons are repeated with fuel and mocked-up poison distributions that simulate these lifetime conditions. This contribution is then adjusted with lifetime to compensate for lifetime variations in reactivity bias. The RCP-Experiment contribution is the same as used for the bias early in core life.

C. Power Distributions

1. Experimental Core Power Distributions

For 6 of the 7 Detailed Cell experiments, detailed three-dimensional power distributions were obtained by fuel rod scanning and foil normalization techniques (Reference VIII-7). Gross region power as reported in Reference VIII-7 is listed in Table VIII-2. Similar results based on RCP analysis of these experiments, as discussed in Section VIII.B.2, and PDQ results, as discussed later, are also listed. Reference VIII-7 (Figures 29-32) contains maps of other more detailed radial power data for 4 of the experiments. These distributions are by rod row except near the center of the seed. Detailed axial power shapes were also measured for many of the fuel rods as indicated by Figures 21 through 28 of Reference VIII-7. Individual rod power distributions were also determined for these cores.

2. PDQ Calculations of Experiments

The analysis model as described in Chapters IV and V above was applied in the calculation of several of the Detailed Cell and BMU experiments. The purpose of these calculations was to test the ability of the analysis model to predict detailed power distributions and develop power uncertainty allowance factors for LWBR based on these predictions. All of the BMU and Detailed Cell cores were calculated with earlier versions of the analysis model. Using the final model, 4 of the configurations were analyzed. These included the BMU-2-4 power flattened configuration and 3 of the Detailed Cells with seed positions of -14, +3.5 (HOT), and +14 inches. It was not necessary to repeat the remaining configurations since analysis of the 4 analysis model calculations revealed that the power distributions were not sensitive to differences between the present and previous models. The Detailed Cell gross power distributions are shown in Table VIII-2 for the 3 Detailed Cell analysis model calculations. A more detailed comparison

of power fractions by fuel rod is shown in Figure VIII-2 for the hot Detailed Cell (+3.5 inch seed position). Similar comparisons were made for the other Detailed Cell configurations.

Table VIII-2 also shows ratios of the gross power sharing to experiment for the present model, as well as a complete set for the previous model, and for RCP calculations. As mentioned earlier it can be seen that the previous model (PDQ) results are very similar to the present model, where comparisons can be made. It can be seen that the model is much better for predicting the gross power sharing for some cores than for others. It can also be seen in Table VIII-2 that PDQ and RCP agree well. This was also demonstrated for the full LWBR core in Figure IV-11, discussed in Section IV.F. Figure IV-3 of Section IV.E demonstrated with the BMU-2-4 core that PDQ can calculate accurately a detailed power traverse across the full width of the LWBR core. The question arises as to why there should be significant errors in certain of the Detailed Cell power distributions.

It may be observed from Table VIII-2 that PDQ does much better compared to experiment when the seed is at +17.8 inches than when the seed is at +14 inches. These two cases should be virtually the same core. The +14 inch core was disassembled and the grids were welded for use in the hot experiment and the second series of cold experiments producing a slightly smaller pitch. The core was reassembled for the second series of cold experiments after the hot experiments were done. The PDQ model and RCP should be able to calculate one of these cores about as well as the other. There are only 3 potential reasons for the discrepancies, namely, cross section errors, lack of eigenfunction convergence, or misrepresenting the experimental configuration in the RCP (and PDQ) because of not knowing that configuration precisely. There are no other reasons because RCP solves the neutron transport equations "exactly," within the statistical error bands known to the user.

Cross section errors could not produce such a large discrepancy in the +14 inch core when they don't produce that discrepancy in the +17.8 inch core. Eigenvalue convergence in RCP could not be the cause either, because PDQ and RCP behave in a similar way. A similar conclusion results from comparing the -3.5 inch core and the -2 inch core, which again should be virtually the same core. The conclusion is that the physical representations of the +14 inch core and -3.5 inch core in PDQ and RCP may be inaccurate.

Since the PDQ and RCP are independent calculations, and they agree with each other, this lends confidence that the calculations are accurate.

3. Development of Experiment/Calculation Factors for Power Distributions

Based on detailed comparisons of power distributions calculated using the analysis model with those measured in the experimental configurations, allowance factors were generated for application to the power distribution within LWBR calculated with the analysis model. The factors based on these comparisons are designated as Experiment-to-Calculation (E/C) factors and are in addition to other allowance factors arising from (1) manufacturing uncertainties, (2) instrumentation errors, (3) fuel misalignment, and (4) operation with less than equilibrium xenon and protactinium.

E/C allowance factors were generated for each of the 4 basic regions of the core: seed, regular blanket, power flattening blanket, and reflector blanket. In addition, individual factors are selectively applied to different fuel regions within the larger basic regions. Separate E/C factors were obtained for application to whole rods and to axial peak powers along rods. The E/C factors were based on comparisons of gross power sharing, row-by-row power sharing within the gross regions, individual rod-to-rod row power shapes, and detailed axial shapes.

D. Core Breeding

In Section III.B.3 the factors that affect breeding are discussed. The breeding parameters CR and FIR are defined there and in Section VI.A. The factors that affect breeding are the value of η of U^{233} and the competition between neutron capture in thorium and in parasitic materials. The qualification of these factors is described below. An overall test of the breeding predictions is planned at the completion of the core life by assaying the fissile content of the core.

1. η of U^{233}

The data for η of U^{233} and the sources of the data are discussed in Section IV.B.2. The value $\eta = 2.2972$ used at 0.0253 eV is in good agreement with detailed Monte Carlo analyses of direct measurements of η . Analysis of the experiment of Smith, et al, gives $\eta = 2.2993 \pm 0.0082$ (Reference IV-18); analysis of the experiment of Macklin, et al, gives $\eta = 2.3019 \pm 0.0086$ (Reference IV-19). Thus the value of η used is only 0.15 percent lower than the average of the experimental analyses and is well within the statistical uncertainty. The shape of $\eta(E)$ is based on matching the capture and fission

cross section shapes of Weston, et al (Reference IV-20 and IV-21), and comparison to experimental η data shows good agreement (Reference IV-16).

Further confidence in the η function used for LWBR was obtained by the analysis of critical experiments. The homogeneous spheres and cylinders of Gwin and Magnuson (Reference IV-22) provided tests of η in simple geometric configurations without the presence of thorium. As discussed in Section IV.B.2, the average error in predicting the multiplication factor was less than 1×10^{-4} and the range of errors was essentially within the experimental uncertainty. The LWBR critical assemblies discussed in Section VIII.B are more complex in geometry and material content than the spheres and cylinders and all contain thorium. Although the effect of η cannot be truly separated from other effects in the LWBR critical assemblies, the behavior of the Detailed Cell reactivities goes against any significant bias in η . It is concluded that the cross section measurements, direct measurements of η , and criticality testing demonstrate the adequacy of the LWBR η function for breeding calculations.

2. Competition Between Thorium and Parasitic Materials - Cross Sections

The competition between neutron capture in thorium and in parasitic materials is affected by both the basic cross section data and the model for calculating the neutron distribution in space and energy. The cross section data for each isotope are qualified by being based directly on measured data and by being tested in integral experiments. Section IV.B summarizes the sources, testing, and relative importance of the cross section data.

Overall tests of the cross section data which are important prior to depletion are obtained by calculating LWBR critical assemblies with RCP. The results have been discussed in Sections VIII.B and VIII.C. The RCP reactivity data indicate an average error of 0.1 percent. The RCP gross power distribution data in the second series of cores were within 2 percent of measurement. The larger errors in the first series of cores were attributed to a suspected inaccurate representation of the core in the calculation.

Section VIII.A describes special irradiation experiments which permit testing the calculation of fission-product poison in long-term irradiations. The results given there show that the predicted total effective fission-product cross section is in good agreement with experiment as illustrated in Part b of Figure VIII-1. The discrepancies in the two-group cross sections are attributed

in Reference VIII-3 to library errors involving assumptions of $1/v$ behavior which enhance thermal cross sections at the expense of epithermal cross sections. These errors tend to cancel in their overall effect, especially for spectra similar to those of the irradiation experiments. Despite such compensation, the harder spectra in LWBR mean that the total fission-product poison would be underestimated; but there is an additional compensation. The harder spectra deplete the epithermal absorbers more and the thermal absorbers less than do the softer spectra. This is shown in Reference VIII-3 where both the quantity I and the discrepancy in I are smaller for harder spectra. The net effect of cancellation of thermal errors with epithermal errors and cancellation of harder spectra with fewer epithermal absorbers is that the total fission product poison in LWBR spectra might be underestimated by a few percent.

Recent comparative studies of fission product poison have been done with the LWBR cross section library, which was used to analyze the irradiation experiments, versus the current ENDF/B-IV fission product data files. These studies show that the ENDF/B-IV data yield lower epithermal and total fission product poisons than the current LWBR library yields in an LWBR spectrum. Thus, either the ENDF/B-IV data set is worse than the current LWBR fission product data set or the interpretation of the irradiation experiments needs to be modified.

Any small underestimate of fission product poisoning in LWBR resulting from the spectral effects discussed above are overshadowed by the fact that fission product poison resonances are shielded by resonances of thorium and other heavy atoms in LWBR fuel rods. The above irradiation experiments did not include these effects because very small highly enriched U^{233} samples were irradiated.

In summary the cross section data have undergone extensive testing, both special tests for individual isotopes and overall tests in LWBR critical experiments and other reactor environments. Most of the tests show good agreement with experiment. Some of the discrepancies have been attributed to inaccurate calculational representations of the tests and some uncertainties in the data still require further work. The data as a whole are qualified for accurate calculations of the distribution of absorptions among the isotopes.

3. Competition Between Thorium and Parasitic Materials - Flux Distribution

In addition to the cross section data, the model for calculating the neutron flux distribution in space and energy has been qualified for accurate breeding predictions. Since the Monte Carlo analytical standard RCP is essentially exact,

as discussed in Section III.B.1, the calculation of the neutron flux distribution can be tested against RCP.

Tests of the nuclear analysis model within the unit fuel rod cell were described in detail in Section IV.C.5. Results are given in Tables IV-8 through IV-13. At operating temperature total thorium capture fractions calculated by the analysis model are demonstrated to be accurate to at least 0.4 percent and are virtually within the Monte Carlo statistics.

Tests of space-energy corrections to the unit cell environment were described in Section IV.F.6. It was demonstrated that the use of these factors accounts for a large fraction of the influence of neighboring regions on the flux spectrum.

The overall analysis model, except for temperature feedback, was tested against RCP. The reactivity and power distribution results are displayed in Figure IV-11 and discussed in Sections IV.F.6 and VIII.B.3. The isotopic distribution of absorptions is given in Table VIII-3. If we neglect the small amount of U^{234} fission, the conversion ratio may be calculated as

$$CR = \frac{Th^{232} \text{ capture} + U^{234} \text{ absorption}}{U^{233} \text{ absorption} + U^{235} \text{ absorption}}$$

The results are shown in Table VIII-3. To get a best estimate bias in CR an adjustment must be made for the differing multiplication factors. This corresponds physically to moving the seeds to attain a critical position. A detailed adjustment of isotopic absorptions is made during the PDQ depletion calculation as described in Section VI.A. Approximately the adjustment is

$$CR' = CR - 2\Delta\lambda$$

where CR' is the conversion ratio corrected to the RCP multiplication factor and $\Delta\lambda$ is the difference in multiplication factors between PDQ and RCP. The best estimate bias in conversion ratio is then 0.0027, a value which is within the statistical uncertainty of the RCP calculation.

Studies of the bias in CR' as a function of lifetime, done with the procedure described in Section III.B.1, indicate that the conversion ratio bias does not shift appreciably during core lifetime. If the above CR' bias

persists throughout core lifetime, the resulting bias in the fissile inventory ratio may be determined from Section VI.A as

$$\frac{\bar{A}_f}{N_o} T (0.0027) = 0.001$$

where T is the core lifetime. Thus the FIR predicted by PDQ must be reduced by 0.001 to agree with the analytical standard. This bias and the statistical uncertainty are accounted for in core performance predictions.

REFERENCES

- VIII-1. T. R. England, "CINDER - A One-Point Depletion and Fission Product Program," WAPD-TM-334 (Revised), June 1964. Also, T. R. England, R. Wilczynski, and N. L. Whitmore, "CINDER-7: An Interim Report for Users," LA-5885-MS, April 1975.
- VIII-2. S. B. Gunst, J. C. Connor, and D. E. Conway, "Measurements and Calculations of Heavy Isotopes in Irradiated Fuels and of U²³³ Fission-Product-Poisoning," WAPD-TM-1182, July 1974.
- VIII-3. S. B. Gunst, J. C. Connor, and D. E. Conway, "Measured and Calculated Fission-Product Poisoning in Neutron-Irradiated Uranium-233," Nuc. Sci. Eng. 58 (1975) 387.
- VIII-4. S. B. Gunst, D. E. Conway, and J. C. Connor, "Measured and Calculated Rates of Decay Heat in Irradiated U²³⁵, U²³³, Pu²³⁹, and Th²³²," Nuc. Sci. Eng. 56 (1975) 241.
- VIII-5. S. Milani and S. H. Weiss, "Small Uranium-233 Fueled Seed-and-Blanket Critical Experiments," WAPD-TM-614, November 1967.
- VIII-6. J. A. Mitchell, editor, "BMU Series of U²³³ Fueled Critical Experiments," WAPD-TM-1117, January 1975.
- VIII-7. G. G. Smith, J. P. Semans and J. A. Mitchell, editors, "U²³³ Oxide-Thorium Oxide Detailed Cell Critical Experiments," WAPD-TM-1101, October 1974.

TABLE VIII-1. EIGENVALUES FROM CRITICAL ASSEMBLIES

	<u>RCP λ</u>	<u>Corrections to RCP λ</u>	<u>Corrected RCP λ (1σ)</u>	<u>PDQ λ</u>	<u>Previous PDQ λ</u>
<u>BMU CORES</u>					
BMU1C (410°F)	1.0061	+0.0000	1.0061 (0.0017)		
BMU-2-4 (power flattened)	1.0048	+0.0000	1.0048 (0.0018)	1.0055	1.0015
BMU1B	1.0069	+0.0000	1.0069 (0.0019)		
<u>DETAILED CELLS</u>					
Seed Position (inches)*					
+14.0	1.0015	+0.0006	1.0021 (0.0017)	1.0037	1.0046
-3.5	0.9978	+0.0012	0.9990 (0.0017)		1.0032
-26.35	0.9985	+0.0003	0.9988 (0.0015)		1.0024
+3.5 (477°F)	0.9969	+0.0007	0.9976 (0.0015)	0.9961	0.9947
+17.8	1.0026	+0.0010	1.0036 (0.0017)		1.0024
-2.0	1.0006	+0.0009	1.0015 (0.0018)		1.0014
-14.0	0.9948	+0.0008	0.9956 (0.0015)	1.0002	1.0020
Average, $\bar{\lambda}$ (see text)			1.0011 (0.0036)		

*The seed position is with respect to the position where the seed is aligned with the blanket (Figure II-4).

TABLE VIII-2. BINARY FUEL POWER DISTRIBUTION IN DETAILED
CELLS, EXPERIMENT VERSUS RCP AND PDQ

<u>Seed Position (Inches)</u>	<u>Region</u>	<u>Experiment</u>	<u>RCP01</u>	<u>PDQ</u>	<u>RCP/Exp.</u>	<u>PDQ/Exp.</u>	<u>Previous PDQ/Exp.</u>
FIRST SERIES							
+14.0	Seed	0.495	0.5266	0.522	1.064	1.055	1.057
	Blanket	0.162	0.1605	0.159	0.991	0.981	0.981
	PFB	0.343	0.3129	0.319	0.912	0.930	0.927
-3.5	Seed	0.488	0.5196		1.065		1.043
	Blanket	0.191	0.1833		0.960		0.984
	PFB	0.321	0.2971		0.926		0.944
HOT							
+3.5	Seed	0.452	0.4660	0.460	1.031	1.018	1.020
	Blanket	0.174	0.1614	0.160	0.928	0.920	0.920
	PFB	0.374	0.3726	0.380	0.996	1.016	1.016
SECOND SERIES							
+17.8	Seed	0.514	0.5163		1.004		0.996
	Blanket	0.159	0.1601		1.007		1.013
	PFB	0.327	0.3236		0.990		1.000
-2.0	Seed	0.504	0.5041		1.000		0.996
	Blanket	0.192	0.1898		0.989		0.995
	PFB	0.304	0.3061		1.007		1.010
-14.0	Seed	0.430	0.4229	0.424	0.983	0.986	0.988
	Blanket	0.160	0.1620	0.165	1.013	1.031	1.025
	PFB	0.410	0.4151	0.411	1.012	1.002	1.002

TABLE VIII-3. ISOTOPIC ABSORPTIONS IN THREE-DIMENSIONAL
LWBR CORE CALCULATIONS AT BEGINNING OF LIFE

Material	Absorptions**		Absorption Differences	
	RCP $\pm 1\sigma$	PDQ	%	σ Units
Th ²³² Capture	0.48635 $\pm$ 0.00072	0.48669	-0.07	-0.5
Th ²³² Fission	0.01159 $\pm$ 0.00002	0.01153	+0.50	+3.0
U ²³³ Absorption	0.44288 $\pm$ 0.00066	0.44323	-0.08	-0.5
U ²³⁴ Absorption	0.00288 $\pm$ 0.00004	0.00286	+0.70	+0.5
U ²³⁵ Absorption	0.000407 $\pm$ 0.000001	0.000409	-0.50	-2.0
Parasitic Material Absorption*	0.05865 $\pm$ 0.00028	0.05774	-1.60	-3.0
Multiplication Factor (λ)	1.0091 $\pm$ 0.0010	1.0105		
Conversion Ratio (CR)	1.1036 $\pm$ 0.0033	1.1035		
CR'	1.1036	1.1063		

*Hydrogen, oxygen, Zircaloy, and three types of steel.

**Moderator temperature = 550°F. Fuel temperature = 920°F. The absorptions are normalized to one starting neutron in the problem.

Figure VIII-1. Results for Sample Irradiated to 89 Percent U^{233} Depletion Showing (a) Fuel Fraction of the Initial Fuel and Fission Product Barns per Fission in Terms of (b) Effective One-Group σ_{eff} , (c) Thermal σ_{2200} , and (d) Resonance Integral I

Figure VIII-2. Hot Detailed Cell Power Fractions - Experimental
Power Fractions (in Parenthesis) and PDQ/Exp Ratios

IX. CONCLUSION

The preceding chapters have described the calculational model used in the analysis of nuclear performance of LWBR. The model is sophisticated, both in the sense of having many important improvements over a simple few-group diffusion model with infinite media cross sections, and in the degree of detail which it can handle because of automation. The model is also practical and is in current use. The model has been demonstrated to be successful through comparisons of calculation to critical experiments and to an analytical standard. Further qualification of the calculational model will be obtained from following operation of the LWBR core as it is depleted by operation at Shippingport.