INTEGRAL TARGET FUEL IN A
WATER COOLED GRAPHITE LATTICE:
THEORY-EXPERIMENT CORRELATION

JULY 31, 1968

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THEORY-EXPERIMENT CORRELATION

by

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July 31, 1968

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ABSTRACT

A complete multi-group Sn transport theory analysis and comparison with experiment has been made for an integral target fuel in a water-cooled graphite lattice, including the investigation of the leakage effect on k_{∞} . Emphasis has been placed on the magnitude, relative importance, and recommended improvements of errors in the theory-experiment comparisons due to either the models or methods used in this study.

The improved techniques give results that are in reasonably good agreement with most of the measured lattice parameters.

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1. Introduction and Scope

Recently, ⁽¹⁾ experiments were performed in the Physical Constants Testing Reactor (PCTR) at Battelle-Northwest Laboratory on rod-in-tube integral target assemblies in an 8" x 9" graphite lattice.

This report describes the methods and results of a theoretical study performed in conjunction with, and in addition to, these experiments. The purpose of this study is to provide theoretical support to the experimental effort by developing a theoretical description of the neutronics of the integral target assemblies studied in the PCTR. Extensive comparisons are made between theoretical results and various measured and/or inferred experimental results. The magnitude and relative importance of certain errors in the theoretical model are assessed, and various improvements to this model are investigated. Areas of difficulty encountered in the theoretical analysis and recommended improvements are also outlined.

2. Summary and Conclusions

A standard calculational technique using THERMOS, ⁽²⁾ HRG, ⁽³⁾ and Program S ⁽⁴⁾ proved adequate in calculating cold lattice parameters for the primary integral target cell of interest; i.e., the wet-unpoisoned base target cell. A summary of the calculated lattice parameters of main interest for this cell compared to the corresponding experimental values, when available, is presented below in Table I.

TABLE I

Summary of Calculated Lattice Parameters for Base Target Assembly

	<u>Calc. Program S</u>	<u>Experiment⁽¹⁾</u>
k (air atmosphere)	1.0868	1.098 $\pm$.005
k (vacuum atmosphere)	1.0894	1.101 $\pm$.005
Target thermal utilization	0.1696	0.1671 ($\pm$.0013) ^a
Fuel thermal utilization	0.7319	0.7423 ($\pm$.0056) ^a
²³⁸ U to ²³⁵ U fission ratio	0.0658	0.0530 $\pm$.0027
Target initial conversion ratio	0.269	0.264 $\pm$.002
Fuel initial conversion ratio	0.473	0.451 $\pm$.002
Neutron density thermal disadvantage factor	3.074	2.685 ($\pm$.027) ^b
Average ²³⁵ U capture-to-fission ratio in fuel	0.2184	

^a 3/4% standard error only.

^b 1% error assumed, statistical error only.

Calculations of the just critical wet-poisoned base target cell underpredicted the experimentally determined mass of copper poison by 1.2%. Less detailed calculations of additional cell variations (no coolant, natural target, etc.) were in reasonable agreement with experiment. However, neglecting the axial effect caused by the vertical and horizontal gas vents in forming the geometric model proved to be poor assumption. This effect and the assumption of isotopic scatter in the water coolant in the thermal calculation resulted in a consistent ~15% overestimate of the thermal neutron density disadvantage factors for all lattices. Less noticeable but more directly relatable to the multiplication, these assumptions also cause the predicted thermal utilization to be about 1% high. Including the additional gas vents in the model and using Honeck's suggested isotropic transport approximation for hydrogen scattering, ⁽⁵⁾

$$\sum_{\text{Tr}}(E' \rightarrow E) = \sum_{S_0}(E' \rightarrow E) - \sum_{S_1}(E' \rightarrow E)\delta(E' - E)$$

in the THERMOS calculations gives a marked improvement in the theoretical disadvantage factors and thermal utilizations. This improvement reduces the mean error to a more reasonable 5% for the disadvantage factor and ~1/2% for the thermal utilization for the cases modified.

This calculational method (suggested improvements included) is recommended with reservation for similar graphite moderated, non-plutonium fuel and/or target systems. The assumptions necessary to generate the epithermal spectra were the weakest links in the theoretical chain. For this purpose, the grossly heterogeneous cell was assumed to be composed of only two regions: (1) target, fuel, process tube, clad, and water; (2) air gap, graphite, and gas vents, which were then treated independently as infinite and homogeneous. The resulting two decoupled epithermal energy distributions were then considered to represent, at least to first order, the spatial average of the actual spectra over the above defined

regions. The difficulties encountered in generating epi-thermal region averaged cross sections demonstrate a definite need for the development of a one-dimensional slowing down code. The effects of the various assumptions used to handle resonance species should be considered before using this method; i.e., resonances are widely separated, resonances are either NR or NR1A, interference scattering can be neglected, heterogeneous resonance absorption can be handled by homogeneous equivalence principles, to name a few. This last point is doubly important for plutonium and/or multi-region fueled systems.

3. Lattice Description

The 8" x 9" lattice studied was graphite moderated and water cooled. The integral target fuel had a rod-in-tube configuration. The "base target" was depleted lithium (3.14 wt% Li^6) in the form of lithia aluminate at 74% theoretical density of 1.075" diameter, clad alternately in aluminum of 100 mil thickness and 30 mil thick zirconium. The tubular fuel of 1.767" I.D. and 2.327" O.D. was 2.1 wt% enriched metallic uranium with 25 mil inner and 35 mil outer zirconium cladding. The assembled length of the composite element was nominally 24 inches. A unit cell with respect to the graphite moderator only, showing positions and dimensions of the process hole, and horizontal, vertical, and axial gas vents is depicted in Figure 1. The fuel is shown in Figure 2. The H/U and C/U atom ratios were, respectively, 1.69 and 48.3 for the experimental lattice. All materials were at room temperature. An alternate target rod (same dimensions and cladding) containing natural rather than depleted lithium, called the "natural target," was also studied. See the Appendix for the densities of the various lattice materials and the compositions of the two target rods.

FIGURE 1

Graphite Moderator Lattice

4. Experimental Procedure

The detailed PCTR experimental procedure has been described elsewhere,^(6,7) but a brief outline pertinent to the calculational procedure is presented herein for completeness.

The central cell is surrounded by a buffer region of identical cells. Poison in the form of copper strips is gradually added to both the central cell and the buffer cells until a central cell multiplication of unity is obtained. This condition is determined to be fulfilled when, upon removal of the central cell, a reactor null reactivity worth is measured. Simultaneously, a spectral match between the buffer cells and the test cell is maintained by appropriate manipulations of special driver and absorber elements surrounding the buffer regions. When measured cadmium ratios of corresponding gold foils in the central cell and buffer cells are equal, this second condition is assumed to be fulfilled. A spectral match with the same test cell without any copper poison in any of the cells (test or buffers) is similarly obtained and checked. After a spectral match has been obtained in each case (poisoned and unpoisoned), extensive foil activation traverses are taken throughout the test cell. Relative cell reaction rates are inferred from the activation data and are used with the measured mass of copper required to poison the cell multiplication to unity, to calculate k_{∞} and other lattice parameters.

5. Geometric Models

A Wigner-Seitz unit cell in cylindrical geometry (axial effects ignored) was used as the basis for the theoretical calculations. The rectangular portions of the experimental cell were described by the standard equivalent radius technique. The axial gas vents (parallel to the process tube) and associated outer portion of the graphite moderator were then homogenized by a simple volume weighting. When a poisoned cell was being considered, an additional

homogenized annular region composed of copper and graphite was introduced by conserving the mass, thickness, and position of the copper.

The actual cell geometry, including the position of the two 3-inch by 24-inch strips of variable thickness copper poison, is compared with the above described basic cell model in Figure 2. The dimensions and descriptions of these geometric models are outlined in Tables A-1 and A-2 in the Appendix.

Since all calculations were performed in zero or one-dimensional geometry with various code limitations in degree of spatial detail and number of allowable material mixtures, several variations of this basic geometric model were used.

FIGURE 2

Heterogeneous Geometric Model

5.1 HRG

To form a model compatible with the geometric limitations of HRG, the cell was divided at the outer boundary of the process tube into two macro-regions; a core region and a moderator region. The fine geometric detail was homogenized within each of these regions by simple volume weighting. Each homogeneous macro-region was then treated separately as being infinite in extent.

5.2 THERMOS

The basic model also had to be modified to be usable in the THERMOS code. The degree of geometric detail was adequate, but unfortunately, the number of materials allowable was limited to six. Therefore, with additional region smearing a semi-heterogeneous model had to be used (Figure 3). The method differed depending upon whether or not the poisoned cell was being considered. In general, the procedure was to homogenize the following: target and aluminum clad; water and zirconium clad; air gap, inner and outer graphite.

5.3 Program S

The basic model was unmodified for Program S use, except for the addition of a radial leakage region outside the equivalent cell. The description and use of this artifice is discussed in Section 7.2.

FIGURE 3

Semi-Heterogeneous Geometric Model

6. Calculational Methods

Epi-thermal energy spectra and the resulting averaged microscopic group constants for three fast groups (lower energy boundaries at 11.7 KeV, 2.38 eV, and 0.683 eV) were obtained from HRG, a consistent Pl slowing down code, by treating the two macro-regions (core and moderator) separately as homogeneous and infinite in extent for each cell configuration. The ^{238}U resonance integral and effective resonance absorption cross sections were calculated internally by HRG using resonance parameters. In determining the parameters, a correction was obtained using the COLPRO-I Monte Carlo Collision Probability Code⁽⁸⁾ to fit, at least on the average, the rational approximation to the exact fuel escape probability for the actual tubular fuel region (including Dancoff effects). Space energy thermal neutron flux and density distributions and region averaged thermal group constants were calculated with the integral transport neutron thermalization code, THERMOS (a 30 energy, 30 space point version) with semi-heterogeneous geometric detail for each cell configuration. The scattering kernels used were: the Nelkin kernel for hydrogen in water, the Parks kernel for carbon in graphite, and the perfect gas kernel for the remaining materials. The HRG and THERMOS cross section information was derived from the Battelle Master Library.⁽⁹⁾ The group absorption for the copper poison was formed from a $1/v$ (1 barn at 2200 m/sec) cross section, averaged over the appropriate THERMOS and HRG spectra and normalized to 3.85 barns at 2200 m/sec. The excess resonance contribution of $\bar{\sigma}_2^{\text{ex}}(\text{eff}) = \text{RI}^{\text{ex}}/\Delta u_2$ was added to group two, where $\text{RI}^{\text{ex}}(40 \text{ mil Cu}) \simeq 1.03 \text{ barns}^{(a)}$ and $\Delta u_2 = 8.5$. A similar treatment was used for the 10 mil thick copper detector foils, but with an excess resonance integral of 1.37 barns.^(b) Complete four-group cross section foil sets were formed only for the wet base target cell configurations. Due to the widely

(a) Inferred from revised⁽¹⁴⁾ reference 10 data.

(b) Revised⁽¹⁴⁾ reference 10.

varying spatial behavior of the copper average thermal cross section, thirty each of these foil cross section sets were needed for the poisoned and the unpoisoned cells. Full energy range (4 groups) neutronics calculations for the wet base target cells only were made using the one-dimensional, discrete ordinate, transport theory code, Program S, with the full radial heterogeneous geometric detail. Twelve discrete angular ordinates were used to describe the angular detail (within a quarter sphere) of the directed flux; two polar angles and six azimuthal angles with double precision at the 90° azimuthal angle.

7. Results and Discussion

7.1 Discussion of the Discrepancy Between Calculated and Measured Amounts of Copper Poison Required to Poison Cell Multiplication to Unity

The nuclear density of copper used in the Program S calculation of the wet poisoned base target cell was that corresponding to an estimated mass of 843.4 grams.⁽¹¹⁾ A calculated copper eigenvalue of 1.1482 resulted from the transport theory solution in this poisoned cell case. Correspondingly, without a $(1.15)^{-1}$ reduction in copper, a fission eigenvalue or cell multiplication of 0.9882 was obtained. This estimated amount of copper was determined experimentally to be too large and the final value was quoted at 776 grams.⁽¹⁾ Correcting for this difference gave a K_{cu} of 1.0558. The multiplication of the cell corresponding to an unreduced 776 grams of copper then became .9931, which means that the calculated cell was still overpoisoned by 6.9 mk. Also the end caps and horizontal and vertical gas vents were not accounted for in the cell model, and the true cell, as determined by first order perturbation theory, was actually 5.6 mk less reactive than the model cell. The calculated multiplication of the poisoned cell, therefore, was 0.9875, as compared to the experimental value of 1.000.

This final discrepancy can be attributed to several related causes. The relative thermal flux in the graphite moderator with respect to the fuel as calculated by Program S; i.e., the thermal disadvantage factor, is overpredicted as seen in Table IV. The cause of the thermal disadvantage factor overprediction in Program S is a direct result of the similar overprediction by THERMOS. This error is carried, so to speak, into Program S from THERMOS via the THERMOS determined average thermal cross sections. The causes of this error in the THERMOS results are discussed in Section 7.6.

7.2 Discussion of Boundary Conditions for Unpoisoned Cell Calculations

The calculation of the wet unpoisoned base target cell was not as straight forward as the poisoned one. The difficulty was in defining the boundary

conditions at the edge of the central cell. The cell multiplication was known to be greater than one with the excess neutrons being lost by radial leakage, but there was no experimental evidence as to the energy dependance of that leakage. The standard and simplest approach of simply ignoring any spectral shift caused by leakage was used first by setting the albedos at the outer cell boundary to one. This assumes $k_{\infty}^* = k_{\infty}$ to use Weinberg and Wigner's notation.⁽¹²⁾ In order to get a first order estimate of $k_{\infty}^* - k_{\infty}$, the boundary condition $\nabla\phi(E, r_b)/\phi(E, r_b) = C$ was assumed.⁽¹³⁾ As this condition could not be used explicitly with the methods at hand, it was approximated by adding a non-moderating region to the outer boundary with an absorption cross section $CD(E)$, where $D(E)$ is the diffusion constant of the graphite moderator. Outer albedos of one were then used and the stationary value of the constant C was found by iteration. k_{∞}^* was then determined by effectively removing this pseudo leakage by perturbation techniques.

Comparison with the non-leakage multiplication then gave the magnitude of the spectral shift $(k_{\infty}^* - k_{\infty})$ to be -4 mk. The resulting albedos at the equivalent cell boundary were also determined and are listed below:

<u>Group</u>	<u>Outer Albedos</u>
1	.9889
2	.9948
3	.9955
4	.9930

The resulting four group radial flux distributions for this just critical leakage cell are shown in Figure 4.

Quantitatively, this "spectral shift" effect was calculated to be relatively "small" as generally expected; however, no direct experimental evidence of sufficient accuracy was available to verify the magnitude of this effect. From

a theoretical standpoint, the accuracy of applying a diffusion theory derived boundary condition to a discrete ordinate transport theory solution is equally in doubt. Therefore, use of this boundary condition as outlined above is not generally recommended.

FIGURE 4

Calculated Multigroup Radial Flux Distributions with Leakage (Program S)

7.3 Fast Spectra Calculations

The inadequacy of any attempt to define a single best epi-thermal cell spectrum for such complicated geometry is illustrated, in a broad group sense, in Figure 4. For instance, note the change of the group one flux relative to that of group two; $\bar{\phi}_1$ to $\bar{\phi}_2$ is 1.83 in the target, 2.16 in the fuel, 1.42 in the process tube, 1.06 in the inner graphite, and 0.91 in the outer graphite. Such broad-group spatial variations are an indication of the magnitude of the epi-thermal energy distribution variations.

In obtaining average cross sections, this effect may be minimized by a careful selection of broad group boundaries such that the energy shape within each broad group is roughly spatially constant; i.e., $\phi_i(E,r) \simeq \phi_i(E)A_i(r)$, where the subscript i denotes the broad group and therefore the energy domain. The spatial variation then becomes only a scaling factor which cancels out in the energy averaging process; i.e., $\bar{\phi}_i(E) \simeq \bar{A}_i \phi_i(E)$.

Within the limitations of allowing only homogeneous zero-dimensional geometry, the method of calculating fast spectra by splitting the cell into two regions, as discussed previously in Section 5.1, appears to be an improved recipe as seen in Table II below:

TABLE II

Relative Fast Spectra (n/cm²/sec/unit lethargy)

<u>Group</u>	<u>Core Region</u>		<u>Moderator Region</u>	
	<u>Program S</u>	<u>HRG</u>	<u>Program S</u>	<u>HRG</u>
1	.5414	.5689	.3886	.3251
2	.2468	.2345	.3158	.3391
3	.2119	.1876	.2956	.3358

This comparison is not completely unbiased, however, since the Program S results were obtained with average epi-thermal cross sections from HRG using this recipe. These difficulties demonstrate a definite need in this type of study for a one-dimensional slowing down code to generate few group epi-thermal cross sections for each region, averaged over the appropriate spectra.

7.4 Partial Currents

The calculated spatial distributions of the total and the four group partial neutron currents are displayed in Figures 5 through 9 for the water cooled base target cell with neutron leakage. The partial currents are:

$$\underline{J}^{\text{out}}(\underline{r}) = \int \underline{\Omega} \phi(\underline{r}, \underline{\Omega}) d\Omega^+, \text{ and}$$

$$\underline{J}^{\text{in}}(\underline{r}) = \int \underline{\Omega} \phi(\underline{r}, \underline{\Omega}) d\Omega^-$$

where, $d\Omega^+$ and $d\Omega^-$ are the differential solid angle elements of outward and inward domains. The effect of introducing the radial leakage constraint at the equivalent cell boundary can also be seen in these figures.

It is also of interest to compare the net current $J^{\text{net}}(r) = J^{\text{out}}(r) - J^{\text{in}}(r)$ obtained from Figures 7 through 9, to the gradients of the fluxes in Figure 4, and note that contrary to the diffusion approximation, the net current is not necessarily zero when $\frac{\partial \phi}{\partial r} = 0$. This is due to both the current source from the first moment energy transfer scattering and the flux anisotropy.

FIGURE 5

Calculated Total Partial-Current Distribution with Leakage (Program S)

FIGURE 6

Calculated Group 1 Partial-Current Distribution with Leakage (Program S)

FIGURE 7

Calculated Group 2 Partial-Current Distribution with Leakage (Program S)

FIGURE 8

Calculated Group 3 Partial-Current Distribution with Leakage (Program S)

FIGURE 9

Calculated Group 4 Partial-Current Distribution with Leakage (Program S)

7.5 Thermal Absorption Rates

7.5-1 Wet-Base Target Lattice

Comparisons of calculated and experimental relative thermal absorption rates in the various cell components are summarized in Tables III and IV for wet-base target-poisoned (WPBT) and unpoisoned (WUBT) configurations. "Wet" or "dry" refers to whether or not there was any water in the coolant channels.

The relative absorption rates of primary interest are those in the target, fuel, and poison. The correlations of the target and fuel rates are quite good, while that of the poison is not. A small error is introduced by the homogenization of a small amount of graphite with the poison in defining the geometric model. This effectively enhances the worth of the copper in the poison region. A major source of error, however, is a direct consequence of the 10 to 20% overprediction of the moderator to fuel flux ratio. Causes of this error are discussed in Section 7.6.

TABLE III

Theoretical/Experimental Relative Thermal Absorption Rate Comparison
WUBT Case

Region	Material	Relative Thermal Absorption Rates						
		Program S	(I)		THERMOS	(II)		Experimental (III) ($\pm 3/4\%$)
1	Target	0.1696	0.1718	0.1740	0.1643	0.1663	0.1671	0.1688
2	Al Clad	0.0022			0.0020		0.0017	
3	Zr Clad	0.0005	0.0125	0.0123	0.0004	0.0126	0.0002	0.0123
4	Water	0.0114			0.0116		0.0116	
5	Zr Clad	0.0006	0.0309	0.0328	0.0006	0.0342	0.0005	0.0289
6	Fuel	0.7319			0.7311		0.7423	
7	Zr Clad	0.0015	0.0260	0.0273	0.0017	0.0275	0.0013	0.0228
8	Water	0.0294			0.0325		0.0276	
9	Process Tube	0.0260	0.0120	0.0125	0.0275	0.0126	0.0228	0.0110
10	Air Gap	0.0001			0.0001		0.0001	
11	Inner Graphite	0.0119	0.0149	0.0157	0.0125	0.0158	0.0109	0.0140
12	Outer Graphite	0.0149			0.0158		0.0140	

I - Semi-heterogeneous geometry (see Figure 3 or Table A-2)

II - Reference geometry (see Figure 2 or Table A-1)

III - Inferred from subcadmium copper activation data⁽⁴⁾

TABLE IV

Theoretical/Experimental Relative Thermal Absorption Rate Comparison
WPBT Case

Relative Thermal Absorption Rates

Region	Material	<u>Program S</u>							
		(I)		<u>THERMOS</u>		(II)		Experimental (III) ($\sim \pm 3/4\%$)	
1	Target	0.1567	} 0.1588	0.1655	0.1557	} 0.1576	0.1572	} 0.1588	
2	Al Clad	0.0021			0.0019		0.0016		
3	Zr Clad	0.0004	} 0.0114	0.0119	0.0004	} 0.0118	0.0002	} 0.0113	
4	Water	0.0105			0.0109		0.0106		
5	Zr Clad	0.0005	} 0.0274	0.0283	0.0005	} 0.0298	0.0005	} 0.0263	
6	Fuel	0.6614			0.6625		0.6766		
7	Zr Clad	0.0014	} 0.0103	0.0097	0.0015	} 0.0106	0.0012	} 0.0099	
8	Water	0.0260			0.0283		0.0251		
9	Process Tube	0.0227	0.0227	0.0233	0.0234	0.0234	0.0208	0.0208	
10	Air Gap	0.0001	} 0.0102	0.0132	0.0001	} 0.0128	0.0001	} 0.0125	
11	Inner Graphite	0.0102			0.0105		0.0098		
12	Poison	0.0955	0.0955	0.0886	0.0914	0.0914	0.0840	0.0840	
13	Outer Graphite	0.0127	0.0127	0.0132	0.0128	0.0128	0.0125	0.0125	

I - Semi-heterogeneous geometry (see Figure 3 or Table A-2)

II - Reference geometry (see Figure 2 or Table A-1)

III - Inferred from subcadmium copper activation data⁽⁴⁾

7.5-2 Additional Cell Variations

In addition to the wet-base target experimental information, there was dry base target and wet and dry natural target experimental data with and without the cell poisoned. "Natural target" refers to a target element with the same dimensions as the base target element but containing natural rather than depleted lithium. The composition of the target is given in Table A.4 of Appendix A.

The configurations are identified by the following defined abbreviations:

TABLE V - Experimental Configuration Abbreviations

WUNT	Wet unpoisoned natural target
WPNT	Wet poisoned natural target
DUBT	Dry unpoisoned base target
DPBT	Dry poisoned base target
DUNT	Dry unpoisoned natural target
DPNT	Dry poisoned natural target

Complete analysis of all the coproduct experiments was beyond the scope of the present study; however, thermal calculations on all the additional lattice configurations were performed to provide cross section information for the data analysis. Comparisons between the calculated and experimental relative thermal absorption rates for these additional configurations are summarized in Table VI.

Since these calculations were performed prior to the completion of the experimental analysis, the masses of copper used in the poisoned cell calculations were only estimates. The corrected theoretical values as reported in Tables III, IV, and VI, were adjusted using the correct masses of copper and assuming these mass errors produced negligible perturbations in the original space-energy flux solutions.

TABLE VI

Theoretical/Experimental Relative Thermal Absorption Rate Comparison
Additional Cases

Region	Material	Relative Thermal Absorption Rates											
		WUNT		WPNT		DUBT		DPBT		DUNT		DPNT	
		Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.
1	Target	.1854	.1860	.1813	.1874	.1954	.1926	.1908	.1923	.2376	.2234	.2479	.2311
2	Al Clad	.0016	.0014	.0016	.0013	.0022	.0017	.0022	.0017	.0019	.0016	.0020	.0017
3	Zr Clad	.0004	.0002	.0004	.0002	.0004	.0002	.0004	.0002	.0004	.0002	.0004	.0002
4	Coolant	.0107	.0105	.0104	.0103	.0000	.0000	.0000	.0000	.0000	.0000	.0000	.0000
5	Zr Clad	.0006	.0005	.0005	.0005	.0005	.0004	.0005	.0004	.0004	.0004	.0005	.0004
6	Fuel	.7104	.7241	.6770	.6891	.7530	.7607	.7291	.7353	.7127	.7314	.7356	.7537
7	Zr Clad	.0016	.0012	.0015	.0012	.0017	.0014	.0016	.0014	.0016	.0013	.0017	.0014
8	Coolant	.0321	.0279	.0298	.0262	.0001	.0001	.0001	.0001	.0001	.0001	.0001	.0001
9	Zr Process Tube	0.272	.0231	.0251	.0217	.0196	.0183	.0190	.0179	.0190	.0180	.0195	.0185
10	Air Gap	.0001	.0001	.0001	.0001	.0001	.0001	.0001	.0001	.0001	.0001	.0001	.0001
11	Graphite	.0133	.0110	.0121	.0102	.0115	.0102	.0110	.0097	.0112	.0101	.0114	.0104
12	Poison	None	None	0.452	.0387	None	None	.0306	.0276	None	None	-.0343	-.0312
13	Graphite and parallel gas vents	.0167	.0140	.0150	.0131	.0154	.0143	.0146	.0135	.0151	.0127	.0152	.0124

Calc. - Discrete region averaged cross sections and fluxes (THERMOS)

Exp. - Inferred from copper subcadmium activation traverse data⁽¹⁴⁾

7.6 Neutron-Density Thermal Disadvantage Factors

The theoretical methods discussed previously yield the neutron density, $N(\underline{r}, v)$, or flux, $\phi(\underline{r}, E)$, as a function of velocity or energy and position in the lattice. The total thermal neutron density, flux, and first moment of the spectrum are the integral properties of immediate interest,

$$\begin{aligned} N(\underline{r}) &= \int_0^{v_c} N(\underline{r}, v) dv, \\ \phi(\underline{r}) &= \int_0^{v_c} v N(\underline{r}, v) dv, \quad \text{and} \\ v(\underline{r}) &= \int_0^{v_c} v N(\underline{r}, v) dv / \int_0^{v_c} N(\underline{r}, v) dv, \end{aligned}$$

where a thermal cutoff velocity v_c corresponding to a neutron energy of .683 eV was used for all the theoretical calculations. The calculated (THERMOS) and experimental relative thermal neutron density distributions (normalized at the center of the cell) for all cell variations are shown in Figures 10 through 17.

7.6-1 Theoretical Disadvantage Factors

A most sensitive property of $N(\underline{r})$ is the neutron density disadvantage factor,

$$\zeta_N = \frac{1}{V_m} \int_{\text{moderator}} N(\underline{r}) d\underline{r} / \frac{1}{V_f} \int_{\text{fuel}} N(\underline{r}) d\underline{r} = \bar{N}_m / \bar{N}_f$$

where the subscripts "m" and "f" refer to the moderator and fuel, respectively.

A flux disadvantage factor, ζ_ϕ , can be converted to a neutron density disadvantage factor,

$$\zeta_N = \bar{v}_f \zeta_\phi / \bar{v}_m$$

provided the average first spectral moments in the fuel and moderator are known.

FIGURE 10

Theoretical/Experimental Relative Thermal Neutron Density Comparison - WUBT Case

FIGURE 11

Theoretical/Experimental Relative Thermal Neutron Density Comparison - WPBT Case

FIGURE 12

Theoretical/Experimental Relative Thermal Neutron Density Comparison - WUNT Case

FIGURE 13

Theoretical/Experimental Relative Thermal Neutron Density Comparison - WPNT Case

FIGURE 14

Theoretical/Experimental Relative Thermal Neutron Density Comparison - DUBT Case

FIGURE 15

Theoretical/Experimental Relative Thermal Neutron Density Comparison - DPBT Case

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FIGURE 16

Theoretical/Experimental Relative Thermal Neutron Density Comparison - DUNT Case

FIGURE 17

Theoretical/Experimental Relative Thermal Neutron Density Comparison - DPNT

7.6-2 Experimental Disadvantage Factors

The total thermal neutron density $N(\underline{r})$ is proportional to the sub-cadmium activation rate of a $1/v$ detector. Therefore, $N(\underline{r})$ is determined quite clearly from experimental copper activation data,

$$N(\underline{r}) = c \left[A^{\text{bare}}(\underline{r}) - A^{\text{Cd covered}}(\underline{r}) \right]$$

where c is the constant of proportionality and $A(\underline{r})$ is the copper activation rate. The measured data was that obtained by R. A. Bennett et al.⁽¹⁾ The experimental thermal cutoff energy corresponding to 40 mil cadmium covers was .64 eV. $\bar{N}_m$ and $\bar{N}_f$ were obtained by fitting curves to the experimental data and performing a graphic integration over the moderator and fuel regions.

7.6-3 Comparison of Experimental and Theoretical Disadvantage Factors

The experimental and theoretical disadvantage factors, ζ_N , are tabulated in Table VII on the following page, along with the ratio ϵ , where

$$\epsilon \equiv \frac{\zeta_N (\text{theoretical})}{\zeta_N (\text{experimental})} .$$

Table VII

Theoretical/Experimental Neutron Density Disadvantage Factor Comparison

Case	ζ_N		ϵ
	Theory	Experiment ^c	
WUBT	3.256 ^a	2.685	1.213
WUBT	3.074 ^b	2.685	1.145
WPBT	2.983 ^a	2.637	1.131
WPBT	2.933 ^b	2.637	1.112
WUNT	3.332 ^a	2.787	1.196
WPNT	3.170 ^a	2.709	1.170
DUBT	2.764 ^a	2.543	1.087
DPBT	2.726 ^a	2.483	1.098
DUNT	2.851 ^a	2.439	1.169
DPNT	2.812 ^a	2.439	1.153

$$\bar{\epsilon} = \begin{matrix} a \\ b \end{matrix} \begin{matrix} 1.152, \\ 1.129, \end{matrix} \quad \sigma = \begin{matrix} .042 \\ .016 \end{matrix}$$

^aTHERMOS results

^bPROGRAM S results

^cThe average uncertainty was estimated to be somewhat less than $\pm 2\%$

Examination of Table VII shows a large systematic discrepancy between the theoretical and experimental disadvantage factors. On the average, the THERMOS calculations overpredicted ζ_N by about 15% ($\bar{\epsilon}_{\text{THERMOS}} = 1.152$) with a 4% scatter ($\sigma = .042$). No statistically significant trends of the errors in ζ_N (THERMOS) with type of lattice configuration were established.

	<u>Unpoisoned-Poisoned</u>	<u>Wet-Dry</u>	<u>Base target-Natural target</u>
ϵ	1.166 - 1.138	1.177-1.127	1.132 - 1.172
σ	0.048 - 0.27	0.031-0.035	0.049 - 0.048
$ \Delta\epsilon $	0.028	0.050	0.040

7.6-4 Uncertainties in the Calculations and Improvements

No investigation of the sensitivity of the THERMOS results to changes in input parameters or to numerical inaccuracies in the transport theory solutions were made on these lattices. However, an estimated upper limit of about 2 or 3% error due to these causes still failed to explain the large discrepancies between theory and experiment.

An investigation of the effect of neglecting the air filled cross vents (see Figures 1 and 3) in the geometric model was next made. Two configurations, wet-unpoisoned natural target (WUNT) and dry-poisoned base target (DPBT) were considered.

	<u>Theory</u>	<u>ζ_N</u> <u>Experiment</u>	<u>ϵ</u>	<u>Air Filled Cross Vents?</u>	<u>$\Delta\epsilon$</u>
WUNT	3.332	2.787	1.196	Neglected	-.061
	3.164		1.135	Included	
DPBT	2.726	2.483	1.098	Neglected	-.052
	2.598		1.045	Included	

Inclusion of this correction reduced ϵ by about the same amount (-.061 and -.052), which brought the theoretical error in ζ_N of the dry case down to a more reasonable level, but not for the wet case.

An assumption of importance to the wet cases and not to the dry cases is the neglect of anisotropic scattering by hydrogen in water. Using a simple isotropic kernel transport correction as suggested by Honeck⁽⁵⁾ for hydrogen,

$$\sum_{Tr}^H (E' \rightarrow E) = \sum_{S_0}^H (E' \rightarrow E) - \sum_{S_1}^H (E' \rightarrow E) \delta(E-E')$$

where, $\delta(E-E')$ is the delta function, Worden et al^(15,16) showed improvement in the calculated values of η , f , and ζ_N for lattices similar to those studied here. When this correction was made to the WUNT case, the error in its calculated disadvantage factor was also reduced to about the expected level.

	<u>Theory</u>	<u>Experiment</u>	<u>ϵ</u>	<u>Approx. Anisotropic Correction?</u>
WUNT	3.164	2.787	1.135	No
	2.946		1.057	Yes

No similar modifications to the remaining lattice configurations of further attempts to resolve more accurately the remaining errors in the disadvantage factors were made.

7.7 Initial Conversion Ratios

7.7-1 Target Initial Conversion Ratio (ICR_{Target})

The target initial conversion ratio is defined as the number of absorptions in Li^6 per absorption in ^{235}U in "clean" target and fuel.

$$ICR_{Target} = (VN^{Li^6} \sum_{i=1}^4 \sigma_{a_i} \phi_i)_{Target} / (VN^{235} \sum_{i=1}^4 \sigma_{a_i}^{235} \phi_i)_{Fuel}$$

TABLE VIII

Target Initial Conversion Ratio Comparison

<u>Case</u>	<u>ICR_{Target} Calculated</u>	<u>Experiment⁽¹⁾</u>
WUBT	.269	.264 $\pm$.002
WPBT	.273	.270 $\pm$.002

7.7-2 Fuel Initial Conversion Ratio (ICR_{Fuel})

The fuel initial conversion ratio is defined as the number of captures in ^{238}U per absorption in ^{235}U for clean fuel.

$$ICR_{Fuel} = N^{28} \sum_{i=1}^4 \sigma_{c_i}^{28} \phi_i / N^{25} \sum_{i=1}^4 \sigma_{a_i}^{25} \phi_i$$

TABLE IX

Fuel Initial Conversion Ratio Comparison

<u>Case</u>	<u>ICR_{Fuel} Calculated</u>	<u>Experiment</u> ⁽¹⁾
WUBT	.473	.451 $\pm$.003
WPBT	.484	.478 $\pm$.004

7.8 ^{238}U to ^{235}U Fission Ratio (δ^{28})

The theoretical ratio of the fission rate in ^{238}U to that in ^{235}U was calculated from the expression:

$$\delta^{28} = N^{28} \sum_{i=1}^4 \bar{\sigma}_{f_i}^{28} \phi_i / N^{25} \sum_{i=1}^4 \bar{\sigma}_{f_i}^{25} \phi_i$$

using the averaged group constants obtained from HRG and THERMOS and Program S fluxes. ($\bar{\sigma}_{f_i}^{28} = 0$, $i=2$ through 4).

δ^{28} experimental was obtained from R. A. Bennett et al.⁽¹⁾ Their determination of δ^{28} was based on fuel foil fission product analysis.

TABLE X

^{238}U to ^{235}U Fission Ratio Comparison

<u>Case</u>	<u>δ^{28}</u>	
	<u>Calculated</u>	<u>Experimental</u> ⁽¹⁾
WUBT	.0658	.0530 $\pm$.0027
WPBT	.0676	.0545 $\pm$.0027

Without markedly affecting the k_{∞} agreement, this disagreement in δ^{28} with experiment could be explained by either a too large calculated group-one flux with respect to the total flux in the fuel by Program S, or a high energy bias in the HRG fast energy spectra, causing $\bar{\sigma}_f^{28}$ to be too large.

7.9 Cadmium Ratios

Calculated cadmium ratios for 3/4 inch diameter, 10 mil thick copper foils are plotted and compared with experiment at various radial positions for the wet base target poisoned and unpoisoned configuration only in Figures 18 and 19.

While the calculated spatial variation seems to agree quite well with experiment, the absolute magnitude does not, being constantly on the order of 10 to 15% high. However, it is felt that this disagreement could be reduced at least in half by the improvements to the calculational techniques, outlined previously.

FIGURE 18

Theoretical/Experimental Copper Cadmium Ratio Comparison - WUBT Case

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FIGURE 19

Theoretical/Experimental Copper Cadmium Ratio Comparison - WPBT Case

7.10 ^{235}U Capture-to-Fission Ratio

The calculated capture-to-fission ratio in ^{235}U is given by:

$$\alpha^{25} = \left(\sum_{i=1}^4 \sigma_{c_i}^{25} \bar{\phi}_i \right) / \left(\sum_{i=1}^4 \sigma_{f_i}^{25} \bar{\phi}_i \right),$$

where the $\bar{\phi}_i$ are the fuel region averaged total fluxes for each group as computed by Program S.

$$\text{WUBT} \quad \alpha^{25} = 0.2184$$

$$\text{WPBT} \quad \alpha^{25} = 0.2209$$

No experimental determinations of α^{25} were available for comparison with the above calculated values for these lattices.

7.11 Perturbation Calculations

The effects of k on some of the various model improvements, end cap, and other corrections outlined thus far, were calculated indirectly by first order perturbation theory. These perturbation coefficients were obtained from the Program S results of the wet-base target lattice. For instance, a -7.0 mk was determined to be caused by neglecting the "horizontal" and "vertical" gas vents (vacuum atmosphere). A breakdown of the corrections for the wet-base target lattice is as follows: ($k = 1.0$ reference basis)

1. Removing leakage	+ 93.5 mk
2. Including target end cap	+ 5.2 mk
3. Including fuel end cap	- 2.3 mk
4. Including horizontal and vertical gas vents (vacuum)	- 7.0 mk
5. Adding air	- 2.6 mk

Table XI on the following page compares some calculated to experimental replacement effects based on the corrected wet-base target lattice.

TABLE XI

Theoretical/Experimental Replacement Worth Comparison

<u>Explanation</u>	<u>Δk_{∞}</u>	
	<u>Calculated</u>	<u>Experimental</u>
Replacing thick-walled zirconium process tube by a thin-walled aluminum tube	+10.5 mk	~ +11 mk
Total replacement of air by vacuum	+ 2.6 mk	~ + 3.2 mk
Replacing the base target by a natural target	-54 mk	~ -48 mk

Also in Table XII below, the final theoretical values of k_{∞} for the wet-base and natural target cells are compared to experimental in both an air and a vacuum environment.

TABLE XII

Theory/Experiment k_{∞} Comparison

	<u>Base Target</u>	<u>Natural Target</u>	
Air Atmosphere	1.0868	1.0324	Theory
	1.098 $\pm$.005	1.051 $\pm$.010	Experiment
Vacuum Atmosphere	1.0894	1.0351	Theory
	1.101 $\pm$.005	1.053 $\pm$.010	Experiment

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APPENDIX

TABLE A-1: Heterogeneous Model Dimensions

<u>Region #</u>	<u>O.R. (cm)</u>	<u>Description</u>
1	1.365	Lithia Aluminate Target
2	1.619	Aluminum Cladding
3	1.695	Zirconium Cladding
4	2.181	Water Coolant ⁽¹⁾
5	2.244	Zirconium Cladding
6	2.955	Uranium Metal Fuel
7	3.044	Zirconium Cladding
8	3.442	Water Coolant ⁽¹⁾
9	4.135	Zirconium Process Tube
10	4.321	Air Gap
11	8.598	Inner Graphite
12	Variable	Poison ⁽²⁾
13	12.16	Outer Graphite ⁽³⁾

(1) filled with air in "dry" cases

(2) copper and graphite mixture in "poisoned" cases

(3) gas (air) vents and graphite mixture

TABLE A-2: Semi-Heterogeneous Model Dimensions

<u>Region #</u>	<u>O.R. (cm)</u>	<u>Description</u>
1	1.619	Target and Aluminum Clad
2	2.244	H ₂ O ⁽¹⁾ and Zr Clad
3	2.955	Fuel
4	3.442	H ₂ O ⁽¹⁾ and Zr Clad
5	4.135	Zr Process Tube
6	8.598	Inner Graphite and Air Gap
7	Variable	Poison ⁽²⁾
8	12.16	Outer Graphite and Gas Vents

(1) filled with air in "dry" cases

(2) copper and graphite mixture in "poisoned" cases

TABLE A-3: Material Densities

<u>Material</u>	<u>Density (gm/cm³)</u>
Lithia Aluminate	2.62*
Uranium	18.82
Aluminum	2.71
Zirconium	6.55
Water	1.00
Graphite	1.67
Air	1.29×10^{-3} (STP)

* Theoretical density

TABLE A-4: Target Compositions

a) Base Target Composition

- 1) $\text{Li}_2\text{O} (\text{Al}_2\text{O}_3)_a$ assumed molecular formula
- 2) 2.62 gm/cm^3 = theoretical density
- 3) 74% theoretical density
- 4) 9.45 wt% Li in target
- 5) 3.14 wt% Li^6 in lithium
- 6) $a = 1.155$ (inferred from 1 through 5 above)

b) Natural Target Composition

- 1) $\text{Li}_2\text{O} (\text{Al}_2\text{O}_3)_a$ assumed molecular formula
- 2) 2.62 gm/cm^3 = theoretical density
- 3) 71.2% theoretical density
- 4) 7.43 wt% Li in target
- 5) 6.4 wt% Li^6 in lithium
- 6) $a = 1.535$ (inferred from 1 through 5 above)

TABLE A-5: Nomenclature-Cell Configuration Abbreviations

WUBT	wet unpoisoned base target
WPBT	wet poisoned base target
WUNT	wet unpoisoned natural target
WPNT	wet poisoned natural target
DUBT	dry unpoisoned base target
DPBT	dry poisoned base target
DUNT	dry unpoisoned natural target
DPNT	dry poisoned natural target

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D. E. Christensen
R. G. Clark
E. D. Clayton
R. E. Dahl
G. M. Dalen
E. C. Davis
F. G. Dawson
D. R. de Halas
R. F. Dickerson
B. H. Duane
G. W. R. Endres
S. E. DeMyer
E. A. Eschback
E. A. Evans
J. R. Fishbaugh
D. G. Foster
H. A. Fowler
J. J. Fuquay
A. G. Gibbs
D. W. Glasgow
V. W. Gustafson
C. E. Haines
L. E. Hansen
G. E. Hanson
R. W. Hardie
O. K. Harling
R. A. Harris
H. Harty
R. A. Harvey
C. M. Heeb
R. E. Heineman
H. L. Henry
R. J. Hoch
P. L. Hofmann
U. P. Jenquin
R. L. Junkins
E. L. Kelley, Jr.
D. A. Kottwitz
J. W. Kutcher
C. R. Lagergren
D. D. Lanning (5)
J. H. Lauby
B. R. Leonard, Jr.
D. L. Lessor
W. R. Lewis
R. C. Liikala
E. P. Lippincott, Jr.
W. W. Little, Jr.
R. C. Lloyd

Battelle-Northwest (Con't)

C. W. Lindenmeier
L. L. Maas
C. L. Mansius
D. R. Marr
R. P. Matsen
D. D. Matsumoto
D. F. Newman
R. E. Nightengale
T. J. Oakes
D. R. Oden, Jr.
L. J. Page
H. M. Parker
R. E. Peterson
W. W. Porath
W. L. Purcell
W. A. Reardon
J. J. Regimbol
C. R. Richey
W. C. Roesch
C. A. Rogers
J. T. Russell
R. E. Schenter
J. E. Schlosser
L. C. Schmid
J. D. Smith
R. B. Smith
R. I. Smith
K. B. Stewart
W. P. Stinson
J. J. Stoffels
H. J. Svoboda, Jr.
D. H. Thomsen
C. R. Tipton, Jr.
V. O. Uotinen
A. D. Vaughn
E. E. Voiland
A. E. Waltar
J. D. White
O. J. Wick
R. D. Widrig
L. D. Williams
J. R. Worden
D. C. Worlton
H. S. Zwibel
Technical Information Files (5)