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Reckoning THOR

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RECKONING THOR

by

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ABSTRACT

Theoretical computation of the Los Alamos National Laboratory's critical assembly THOR (a thorium-reflected plutonium sphere) yields a high eigenvalue when compared to the experimentally measured eigenvalue. Several calculational improvements are investigated in an effort to reduce the discrepancy. Finally, the experimental procedure of reducing the raw configuration to clean specifications is reviewed.

I. THE PROBLEM

Over the years, Los Alamos National Laboratory has constructed several small fast critical assemblies. Numerous experimental measurements of various reactor parameters provide an opportunity to test nuclear data and computational methods. Such testing has been facilitated by the recent publication¹ of simplified specifications (benchmarks) for nine of the Los Alamos critical assemblies.

These specifications have been used to compute the multiplication factor for each of the nine benchmarks. The ratios of the computed eigenvalue to the experimental eigenvalues (C/E) are shown in Table I. These results were obtained with S_{16} transport theory (computer code ONETRAN²) using 70-group, P_3 , infinitely dilute cross sections from LIB-V³ as input.

As Table I reveals, the problem is that the reflected assemblies generally have significantly higher calculated eigenvalues than the bare assemblies. Because the THOR benchmark exhibits one of the highest computed eigenvalues, it was selected for further study in an effort to reduce the discrepancy.

TABLE I

LOS ALAMOS NATIONAL LABORATORY BENCHMARK EIGENVALUES

Benchmark	Brief Description	C/E
THOR	^{232}Th -reflected ^{239}Pu -sphere	1.0152
BIGTEN	^{238}U -reflected 10%- ^{235}U -sphere	1.0157
FLATTOP-Pu	^{238}U -reflected 95%- ^{239}Pu -sphere	1.0119
FLATTOP-25	^{238}U -reflected enriched-U-sphere	1.0092
FLATTOP-23	^{238}U -reflected ^{233}U -sphere	1.0055
JEZEBEL	bare sphere of ^{239}Pu	1.0094
GODIVA	bare sphere of enriched U	1.0013
JEZEBEL-Pu	bare sphere of 80%- ^{239}Pu	1.0008
JEZEBEL-23	bare sphere of ^{233}U	0.9947

II. P_5 CROSS SECTIONS?

The benchmark specifications for THOR are very simple. It is a spherical 5.31-cm-radius core surrounded by a reflector shell of outer radius 29.88 cm. In terms of atoms/b-cm, the composition of the core is 0.03618 ^{239}Pu , 0.00194 ^{240}Pu , and 0.00133 gallium, whereas the reflector is composed of 0.03005 ^{232}Th . These specifications will be used to assess the effects of some calculational improvements.

Let " P_i eigenvalue" refer to the multiplication factor one computes by utilizing P_i cross sections. Then, compared to the P_0 through P_3 bare critical eigenvalues (not shown here), the THOR P_0 through P_3 eigenvalues displayed a much larger variation.

This fact suggests that for the reflected assemblies maybe P_3 calculations are not sufficiently close to P_∞ . Therefore P_4 and P_5 cross sections were also tested on the THOR assembly. All of the THOR P_i eigenvalues are shown in Table II.

TABLE II
THOR EIGENVALUES

<u>Order</u>	<u>Eigenvalue</u>
P_0	1.1514
P_1	0.9917
P_2	1.0265
P_3	1.0152
P_4	1.0189
P_5	1.0178

Obviously, neither the P_5 eigenvalue, nor any other higher order eigenvalue, will solve the high eigenvalue problem of THOR. In fact, the problem is now worse because a P_∞ eigenvalue estimate from Table II is about 1.0180. At any rate, it appears one does have to use P_5 cross sections on the reflected assemblies to get the comparable approach to P_∞ that one gets using P_3 cross sections on the bare assemblies.

III. FISSION SOURCE MATRIX?

Until now, only a single 70-group vector has represented the fission source in all regions in the calculations. Even though this chi vector was obtained by weighting isotope chi vectors with their reactor-wide neutron production rates, a fission source matrix for each region of the reactor would better represent reality.

A fission source matrix is available from LIB-V for any isotope that has a fission cross section. However, even though ONETRAN can handle a fission source matrix for each region, it cannot mix the isotope fission source matrices to form the region matrices. This capability has been programmed into SUPERX, which is an overhauled $1DX^4$ code containing many improvements. The SUPERX self-shielded P_0 transport-corrected cross sections were fed into ONETRAN first with the vector chi and then with the SUPERX region-dependent chi matrices. In spite of the fact that there were substantial differences between the single chi vector and the region chi vectors obtained by volume-flux-averaging the region chi matrices (see Table III), the region dependent fission source matrices lowered the THOR eigenvalue by only 0.0017.

IV. REDUCTION TO CLEAN CRITICAL?

Because the discrepancy does not yield to the above calculational improvements, the process of reducing the actual THOR assembly to clean benchmark specifications will be reviewed.

The experimental⁵ THOR consisted of a plutonium metal core centered in a 53.34-cm equilateral cylinder of metallic thorium. The plutonium core consists of three nickel-coated pieces as described in Fig. 1.* Subcritical measurements were made on two configurations. The first configuration, located in a 634.8-cm³ thorium cavity, had a 0.10668-cm (0.042-in.) gap between the lower cap and center section and a 2.54-cm (1-in.) plutonium plug centered in the otherwise empty glory hole and was 23 ± 5 cents subcritical. The second configuration, without the gap and plug, was located in a 629.9-cm³ thorium cavity and was 32 ± 5 cents subcritical.

Reduction to clean specifications involves volume integrating measured worth curves of thorium, nickel, gallium, and plutonium to effect the replacement of voids and nickel with thorium and plutonium, and to adjust the thorium-plutonium radius and/or plutonium density to achieve criticality.

To accurately carry out the involved geometric, worth weighted volume integrations, the measured worth curves were approximated with the following analytic functions.

$$W_{\text{thorium}}(r) = (0.55)(5.330571^4)/r^4 \text{ } \$/\text{g};$$

$$W_{\text{gallium}}(r) = -0.578 + 0.314r \text{ } \$/\text{g};$$

$$W_{\text{plutonium}}(r) = 6.4438 + 0.004268r - 0.1707r^2 \text{ } \$/\text{g};$$

$$W_{\text{alloy}}(r) = 0.009796W_{\text{Ga}} + 0.990204W_{\text{Pu}} = 6.372111 + 0.007300r - 0.170633r^2 \text{ } \$/\text{g};$$

$$W_{\text{nickel}}(r) = -0.82 + 0.38r \text{ } \$/\text{g}.$$

The total mass of alloy in all three major pieces is 9548.40 g, of which 93.54 g (or 0.9796%) are gallium and 9454.86 g (or 99.0204%) are plutonium. The gallium and plutonium worths were weighted with these weight fractions to form the alloy worth.

* Private communication with G. E. Hansen who kindly searched the records for the data.

TABLE III

THOR FISSION FRACTIONS

Group	Energy Boundary (eV)	Lethargy Width	Original Average chi	From the Core Matrix chi	From the Reflector Matrix chi
1	2.0000E+07	1.9315E-01	0.18982E-04	9.0622E-06	2.9298E-05
2	1.6487E+07	2.5000E-01	0.26099E-03	1.6158E-04	3.6481E-04
3	1.2840E+07	2.5000E-01	0.19230E-02	1.4129E-03	2.4423E-03
4	1.0000E+07	2.5000E-01	0.83700E-02	6.9082E-03	9.7942E-03
5	7.7880E+06	2.5000E-01	0.23972E-01	2.1417E-02	2.6318E-02
6	6.0653E+06	2.5000E-01	0.49383E-01	4.6576E-02	5.1788E-02
7	4.7237E+06	2.5000E-01	0.78707E-01	7.7018E-02	8.0052E-02
8	3.6788E+06	2.5000E-01	0.10293E+00	1.0320E-01	1.0270E-01
9	2.8650E+06	2.5000E-01	0.11574E+00	1.1777E-01	1.1414E-01
10	2.2313E+06	2.5000E-01	0.11607E+00	1.1895E-01	1.1360E-01
11	1.7377E+06	2.5000E-01	0.10681E+00	1.0957E-01	1.0388E-01
12	1.3533E+06	1.2500E-01	0.48201E-01	4.9205E-02	4.6635E-02
13	1.1943E+06	1.2500E-01	0.44195E-01	4.4973E-02	4.2894E-02
14	1.0540E+06	1.2500E-01	0.40028E-01	4.0586E-02	3.8951E-02
15	9.3014E+05	1.2500E-01	0.35917E-01	3.6263E-02	3.5199E-02
16	8.2085E+05	1.2500E-01	0.31975E-01	3.2108E-02	3.1522E-02
17	7.2440E+05	1.2500E-01	0.28174E-01	2.8177E-02	2.7597E-02
18	6.3928E+05	1.2500E-01	0.24679E-01	2.4584E-02	2.4444E-02
19	5.6416E+05	1.2500E-01	0.21473E-01	2.1314E-02	2.1475E-02
20	4.9787E+05	1.2500E-01	0.18557E-01	1.8365E-02	1.8620E-02
21	4.3937E+05	1.2500E-01	0.15957E-01	1.5752E-02	1.6128E-02
22	3.8774E+05	2.5000E-01	0.25334E-01	2.4957E-02	2.5839E-02
23	3.0197E+05	2.5000E-01	0.18281E-01	1.7984E-02	1.8942E-02
24	2.3518E+05	2.5000E-01	0.13023E-01	1.2822E-02	1.3728E-02
25	1.8316E+05	2.5000E-01	0.91859E-02	9.0602E-03	1.0012E-02
26	1.4264E+05	2.5000E-01	0.64336E-02	6.3728E-03	7.0261E-03
27	1.1109E+05	2.5000E-01	0.44825E-02	4.4612E-03	4.9853E-03
28	8.6517E+04	2.5000E-01	0.31057E-02	3.1073E-03	3.4681E-03
29	6.7379E+04	2.5000E-01	0.21388E-02	2.1509E-03	2.3667E-03
30	5.2475E+04	2.5000E-01	0.14698E-02	1.4857E-03	1.6114E-03
31	4.0868E+04	2.5000E-01	0.10090E-02	1.0250E-03	1.0975E-03
32	3.1828E+04	1.2500E-01	0.37852E-03	3.8592E-04	4.0963E-04
33	2.8088E+04	1.2500E-01	0.31340E-03	3.2025E-04	3.3817E-04
34	2.4787E+04	1.2500E-01	0.25946E-03	2.6571E-04	2.7921E-04
35	2.1875E+04	1.2500E-01	0.21479E-03	2.2043E-04	2.3057E-04
36	1.9304E+04	1.2500E-01	0.17780E-03	1.8283E-04	1.9042E-04
37	1.7036E+04	1.2500E-01	0.14718E-03	1.5164E-04	1.5729E-04

TABLE III (cont)
THOR FISSION FRACTIONS

Group	Energy Boundary (eV)	Lethargy Width	Original Average chi	From the Core Matrix chi	From the Reflector Matrix chi
38	1.5034E+04	1.2500E-01	0.12183E-03	1.2575E-04	1.2994E-04
39	1.3268E+04	1.2500E-01	0.10085E-03	1.0428E-04	1.0736E-04
40	1.1709E+04	1.2497E-01	0.83460E-04	8.6442E-05	8.8698E-05
41	1.0333E+04	1.2503E-01	0.69122E-04	7.1706E-05	7.3342E-05
42	9.1188E+03	1.2500E-01	0.57205E-04	5.9433E-05	6.0606E-05
43	8.0473E+03	1.2500E-01	0.47358E-04	4.9272E-05	5.0103E-05
44	7.1017E+03	1.2500E-01	0.39206E-04	4.0846E-05	4.1424E-05
45	6.2673E+03	1.2500E-01	0.32460E-04	3.3861E-05	3.4253E-05
46	5.5300E+03	1.2500E-01	0.26876E-04	2.8069E-05	2.8327E-05
47	4.8809E+03	1.2500E-01	0.22253E-04	2.3268E-05	2.3429E-05
48	4.3074E+03	1.2500E-01	0.18427E-04	1.9288E-05	1.9381E-05
49	3.8013E+03	1.2500E-01	0.15259E-04	1.5988E-05	1.6034E-05
50	3.3546E+03	1.2500E-01	0.12636E-04	1.3253E-05	1.3265E-05
51	2.9604E+03	1.2500E-01	0.10465E-04	1.0985E-05	1.0976E-05
52	2.6126E+03	1.2500E-01	0.86670E-05	9.1061E-06	9.0835E-06
53	2.3056E+03	1.2500E-01	0.71785E-05	7.5482E-06	7.5178E-06
54	2.0347E+03	1.2500E-01	0.59456E-05	6.2566E-06	6.2223E-06
55	1.7956E+03	1.2500E-01	0.49249E-05	5.1862E-06	5.1507E-06
56	1.5846E+03	1.2500E-01	0.40794E-05	4.2988E-06	4.2637E-06
57	1.3984E+03	1.2500E-01	0.33795E-05	3.5635E-06	3.5294E-06
58	1.2341E+03	1.2500E-01	0.27996E-05	2.9538E-06	2.9221E-06
59	1.0891E+03	1.2500E-01	0.23194E-05	2.4485E-06	2.4196E-06
60	9.6112E+02	2.5000E-01	0.35135E-05	3.7119E-06	3.6629E-06
61	7.4852E+02	2.5000E-01	0.24119E-05	2.5505E-06	2.5123E-06
62	5.8295E+02	2.5000E-01	0.16560E-05	1.7526E-06	1.7236E-06
63	4.5400E+02	2.5000E-01	0.11370E-05	1.2042E-06	1.1826E-06
64	3.5357E+02	2.5000E-01	0.78081E-06	8.2751E-07	8.1117E-07
65	2.7536E+02	2.5000E-01	0.53625E-06	5.6865E-07	5.5680E-07
66	2.1445E+02	2.5000E-01	0.36831E-06	3.9076E-07	3.8225E-07
67	1.6702E+02	2.5000E-01	0.25298E-06	2.6853E-07	2.6200E-07
68	1.3007E+02	2.5000E-01	0.17378E-06	1.8453E-07	1.7991E-07
69	1.0130E+02	5.0000E-01	0.20140E-06	2.1396E-07	2.0841E-07
70	6.1442E+01	1.7500E+00	0.18011E-06 1.00000E+00	1.9151E-07 1.0000E+00	1.8621E-07 1.0000E+00

dimensions in inches
(nickel coated dimensions)

Ni mass = 49.35 g
Ga mass = 33.87 g
Pu mass = 3191.48 g
Alloy volume = 203.974 cm³
Pu composition = 94.47 at.% Pu-239
5.17 at.% Pu-240
0.36 at.% Pu-241

Ni mass = 31.85 g
Ga mass = 41.27 g
Pu mass = 4085.88 g
Alloy volume = 259.096 cm³
Pu composition = 94.66 at.% Pu-239
5.02 at.% Pu-240
0.32 at.% Pu-241

Ni mass = 20.85 g
Ga mass = 18.40 g
Pu mass = 2177.5 g
Alloy volume = 137.048 cm³
Pu composition = 94.64 at.% Pu-239
5.04 at.% Pu-240
0.38 at.% Pu-241

Totals

Ni mass = 100.95 g
Ga mass = 93.54 g
Pu mass = 9454.86 g
Alloy mass = 9548.40 g
Alloy volume = 600.118 cm³

Averages

Alloy density = 15.911 g/cm³
Alloy composition = 99.0204 w/o Pu
0.9796 w/o Ga
Pu composition = 94.591 at.% Pu-239
5.075 at.% Pu-240
0.334 at.% Pu-241

Fig. 1.
THOR pieces.

The proposed method of reducing either configuration to clean specifications represents a relatively severe macroscopic use of supposedly zero sample size worth curves, which were obtained from configurations different from those to be passed through during the reduction process. Therefore the method and worth curves will first be tested on a much less severe case that has experimental results available for verification--changing configuration 1 into configuration 2!

Recall that configuration 2 has a 2.54-cm (1-in.) plug centered in the glory hole. If one assumes the plug has 47 g of alloy,* has an alloy density equal to the three-piece average of 15.911 g/cm^3 , is coated with 0.0127 cm (0.005 in.) of nickel, and has an outside diameter of 1.27 cm (0.5 in.) then its alloy dimensions are $r_a = 0.6223 \text{ cm}$ and $h_a = 2.4280 \text{ cm}$; and its plated dimensions are $r_p = 0.6350 \text{ cm}$ and $h_p = 2.4534 \text{ cm}$.

With these plug dimensions and the piece dimensions shown in Fig. 1, and assuming average densities of 11.580, 15.911, and 8.9 g/cm^3 for thorium, alloy, and nickel, one can proceed with changing configuration 1 into configuration 2. The results of individual steps are shown in Table IV. The total result is -34.77% , which is only 2.77% different from the configuration 2 measured excess reactivity of $-32 \pm 4\%$. Because the result is well within the measurement error, one is encouraged to proceed.

An attempt to reduce configuration 2 to a clean critical by preserving the average alloy density of 15.911 g/cm^3 is shown in Table V. The resulting core radius is 5.1037 cm. The thorium reflector density and outer radius are 11.58 g/cm^3 and 29.88 cm, respectively.⁵ To compute atom densities, the following data are used: Atomic weight gallium 69.72, atomic weight of thorium 232.038054, atomic weight of ^{239}Pu 239.1096874, atomic weight of ^{240}Pu 240.053809, atomic weight of ^{241}Pu 241.056847, avogadro number $6.02308\text{E}23$, weight fraction of gallium in alloy 0.009796, weight fraction of plutonium in alloy 0.990204, atom percent of ^{239}Pu in plutonium 94.591, atom percent of ^{240}Pu in plutonium 5.075, and the atom percent of ^{241}Pu in plutonium 0.334. The resulting clean specifications are compared to the original⁵ clean specifications in Table VI. The new specifications lower the THOR eigenvalue by only 0.0055.

*Private communication with G. E. Hansen who kindly searched the records for the data.

TABLE IV

CHANGING CONFIGURATION 1 INTO CONFIGURATION 2

<u>Step Description</u>	<u>Worth (cents)</u>
Initial excess reactivity	-23.00 $\pm$ 5
Remove Ni from plug	+ 0.48
Remove plug alloy	-294.31
Move lower cap Ni to closed position	- 0.44
Move lower cap alloy to closed position	+251.30
Replace 4.9 cm ³ of core surface void with Th	<u>+ 31.20</u>
	- 34.77

TABLE V

REDUCING CONFIGURATION 2 TO A CLEAN CRITICAL

<u>Step Description</u>	<u>Worth (cents)</u>
Initial excess reactivity	- 32.00 $\pm$ 5
Replace top cap Ni with alloy	+ 84.72
Replace lower cap Ni with alloy	+ 60.38
Replace Ni with alloy on cylindrical part of middle section	+ 55.73
Replace Ni with alloy on spherical part of middle section	+ 91.20
Replace glory hole Ni and void with alloy	+1091.07
Replace core surface void with Th	+ 46.32
Replace Th with alloy in step part of middle section	+ 72.27
Replace top cap alloy with Th to convert it to middle section radius of 5.3306 cm	- 17.46
Replace Th with alloy to convert lower cap to middle section radius	+184.95
Replace alloy with Th at the core surface until critical	<u>-1637.18</u>
	0.0
Final core radius = 5.1037 cm	

TABLE VI

THOR SPHERICAL BENCHMARK SPECIFICATIONS

		<u>Original</u>	<u>This Report</u>
Core:	radius (cm)	5.310	5.1037
	²³⁹ Pu (atoms/b-cm)	0.03618	0.0375399
	²⁴⁰ Pu (atoms/b-cm)	0.00194	0.0020141
	²⁴¹ Pu (atoms/b-cm)		0.0001326
	Gallium (atoms/b-cm)	0.00133	0.0013465
Reflector:	radius (cm)	29.88	29.88
	²³² Th (atoms/b-cm)	0.03005	0.0300585

V. CONCLUSIONS

This study began by noting that the calculated eigenvalues for the Los Alamos reflected assemblies are relatively high. Selecting THOR ($k = 1.0152$) for further study, it was found that utilizing P_5 instead of just P_3 cross sections increased the eigenvalue by 0.0026 to 1.0178. Then, it was found that utilizing region-dependent chi matrices instead of a single vector chi decreased the eigenvalue by 0.0017 to 1.0161. Finally, an attempt to reduce the experimental THOR to a new set of clean specifications decreased the eigenvalue by 0.0055 to 1.0106.

Several other options (such as varying the group structure, varying the angular quadrature, using self-shielded cross sections) were judged to have negligible effect on the THOR eigenvalue because they had negligible effect on the Jezebel and Godiva eigenvalues.⁶

Thus the THOR eigenvalue discrepancy has not yielded to any general calculational improvement, nor is it likely that improved clean specifications will solve the problem--the eigenvalue remains about 1% high. Only the spectrum of possible causes has been narrowed. Unfortunately, even though cross sections have gone through years of adjustment, it appears that reducing the Los Alamos reflected assembly eigenvalues will require yet another round of delicate, interdependent changes of the involved isotope cross sections.

This study does show that future calculations of the Los Alamos reflected assemblies should involve P_5 cross sections and region-dependent chi matrices.

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