PROOF-OF-PRINCIPLE TO UNFOLD AN ANGLE-ENERGY DEPENDENT SOURCE FROM FORWARD AND ADJOINT CALCULATIONS

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ABSTRACT

For many years there has existed a discrepancy between the measured and calculated responses from the Little Boy weapon in Hiroshima. A myriad of solutions have been proposed, but to no avail. If one can rationalize to himself that it does not really matter exactly what happened with the weapon when it exploded, and if sufficient information exist about the measurements, one should be able to unfold the source. Moreover, if a source can be unfolded in a controlled environment, then it should be possible to unfold a more complicated source, for example, the Little Boy source. This report records the findings of a proof-of-principle test to unfold a source in the controlled environment.

I. INTRODUCTION

Since the completion of DS86,[1] it has been known that the neutron measurements did not agree with the calculated values, especially at Hiroshima, Japan. The measured values have consistently indicated a larger relaxation length than the calculated values can produce; so much larger that at a ground range of 1500m, the measured values have been as high as an order of magnitude greater than the calculated. Many solutions to this problem have been suggested, but to no avail. One widely postulated scenario has been that the neutron spectrum from the weapon was more energetic than calculated because the weapon's case broke apart during the explosion. This type of speculation is not something that can ever by resolved by the current physics.

Since no one knows exactly what happened physically to the weapon at the time of burst, one should be able to unfold a source if sufficient information exist about the measurements. Source-unfolding techniques[2-10] are used extensively in the laboratory, e.g. one might unfold the fluence from known detector foil measurements.

This proof-of-principle study was undertaken to determine if it was possible to unfold a previously conceived source. An angle-energy dependent source was fabricated and then used to calculate the answers of interest. Succeeding calculations were made in the adjoint mode to determine the adjoint fluence - these values were equivalent to the dosimetry cross sections. Finally, an unfolding of the forward source will be attempted. If the source could be unfolded in a controlled environment, then it should be possible to unfold a more complicated source, for example, the source from the Little Boy device.

II. THEORY

a. Adjoint notation

Using operator notation, the Boltzmann transport equation[11] is represented as

$$LF = Q, \tag{1}$$

where L denotes the linear time-independent Boltzmann transport operator; F is the forward fluence and is a function of energy E, direction vector **d**, and position vector **r**; and Q is the source, also a function of E, **d**, and **r**.

If R is a given response function dependent on E, **d**, and **r**; and F is the forward neutron fluence as before, then the answer of interest, A, is given by

$$A = \langle R,F \rangle , \tag{2}$$

where <> denotes the inner product notation and indicates integration over the common domains of all independent variables E, **d**, and **r**.

The adjoint transport operator L* is defined by

$$\langle F^*,LF \rangle = \langle L^*F^*,F \rangle , \tag{3}$$

where the adjoint fluence, F*, satisfies the adjoint transport equation

$$L^*F^* = R . \tag{4}$$

The mathematically equivalent formulations using the adjoint fluence F*, and eqs. 1, 2, 3, and 4 follows from the following:

$$
\begin{aligned}
A &= \langle R,F\rangle = \langle R,F\rangle + \langle F^*,(Q - LF)\rangle \\
&= \langle R,F\rangle + \langle F^*,Q\rangle - \langle F^*,LF\rangle \\
&= \langle R,F\rangle + \langle F^*,Q\rangle - \langle F,L^*F^*\rangle \\
&= \langle (R - L^*F^*),F\rangle + \langle F^*,Q\rangle \\
&= \langle F^*,Q\rangle \qquad (5)
\end{aligned}
$$

Equations 2 and 5 are seen to be equal.

Thus, the answer of interest, A, can be determined in two ways:

1. Using the forward source, Q, one can calculate the forward fluence, F, using (Eq. 1); then determine A from Eq. 2, or

2. Using the adjoint source, R, one can calculate the adjoint fluence, F*, using (Eq. 4); then determine A from Eq. 5.

In both 1 and 2 above, the forward source, Q, must be known.

If Q is unknown, then one can calculate the adjoint fluence, F*, using Eq. 4 and the adjoint source, R. Then, if one knows a sufficient number of answers of interest (cobalt, europium, sulfur, etc., activations), and has calculated the proper adjoint fluence, one can unfold the source using unfolding techniques.

This research will use the "minimum chi-square" procedure of the STAY'SL code[10].

b. Angle-Energy Unfolding Theory

Expand the measured response equation[2] by assuming that the source and the response are angular dependent, i.e.

$$M_i = \int_E \int_\Omega R_i(E,\Omega) S(E,\Omega) d\Omega dE$$

where $R_i(E,\Omega)$ = probability that a particle leaving the source with energy E in direction Ω contributes to the measurement M_i. By carefully considering the input adjoint source, one deduces that this term is the energy-angular dependent adjoint fluence.

$$\text{Let } S_{jk} = \int_{E_j}^{E_{j-1}} \int_{\Omega_k}^{\Omega_{k-1}} S(E,\Omega) d\Omega dE$$

For S(E,Ω) constant over dΩ and dE, then

$$S_{jk} = S(E,\Omega)\Delta\Omega_k\Delta E_j$$

and

$$M_i = \sum_{j=1}^{J} \int_{E_j}^{E_{j-1}} \sum_{k=1}^{K} \int_{\Omega_k}^{\Omega_{k-1}} R_i(E,\Omega) \frac{S_{jk}}{\Delta\Omega_k\Delta E_j} d\Omega dE$$

$$= \sum_{j=1}^{J}\sum_{k=1}^{K} \frac{S_{jk}}{\Delta\Omega_k\Delta E_j} \int_{E_j}^{E_{j-1}} \int_{\Omega_k}^{\Omega_{k-1}} R_i(E,\Omega) d\Omega dE$$

$$\text{Letting } R_{ijk} = \frac{1}{\Delta\Omega_k\Delta E_j} \int_{E_j}^{E_{j-1}} \int_{\Omega_k}^{\Omega_{k-1}} R_i(E,\Omega) d\Omega dE$$

gives

$$M_i = \sum_{j=1}^{J}\sum_{k=1}^{K} R_{ijk} S_{jk}$$

or in matrix notation

$$\begin{pmatrix} M_1 \\ M_2 \\ . \\ . \\ . \\ M_N \end{pmatrix} = \begin{pmatrix} R_{111} & R_{112} & \cdots & R_{11K} & R_{121} & R_{122} & \cdots & R_{12K} & \cdots & R_{1J1} & R_{1J2} & \cdots & R_{1JK} \\ R_{211} & R_{211} & \cdots & R_{212} & R_{221} & R_{222} & \cdots & R_{22K} & \cdots & R_{2J1} & R_{2J2} & \cdots & R_{2JK} \\ . & . & \cdots & . & . & . & \cdots & . & \cdots & . & . & \cdots & . \\ . & . & \cdots & . & . & . & \cdots & . & \cdots & . & . & \cdots & . \\ . & . & \cdots & . & . & . & \cdots & . & \cdots & . & . & \cdots & . \\ R_{N11} & R_{N12} & \cdots & R_{N1K} & R_{N21} & R_{N22} & \cdots & R_{N2K} & \cdots & R_{NJ1} & R_{NJ2} & \cdots & R_{NJK} \end{pmatrix} \begin{pmatrix} S_{11} \\ S_{12} \\ . \\ . \\ . \\ S_{JK} \end{pmatrix}$$

Thus, a three-matrix equation (required in the STAY'SL code) is preserved, with the response and source matrices being expanded by adding the angular data.

IV. TECHNICAL APPROACH

This effort was broken into 7 steps:

a. Select activation measurements. The two reactions chosen for the initial calculations were the thermal $^{40}Ca(n,\gamma)^{41}Ca$ and the fast $^{63}Cu(n,p)^{63}Ni$.

b. Determine cross-section group structure. The ENDF/B-VI BUGLE-96 cross-section set with no upscatter[15] was chosen for the calculations. This broad-group set has sufficient high energy resolution, yet a low number of groups (47 neutron).

c. Model forward/adjoint geometries. The geometries consisted of air and ground only. The air/ground data was taken DS86.[1] The maximum height of the system was 1810 m, the maximum ground range was 1810 m, and the maximum ground thickness was 50 cm. In the forward calculation, the source was placed at a height of 580 m,

and detector locations were 1 m above the ground at every 100 m to a ground range of 1500 m. In the adjoint calculation, the adjoint source was placed at 1 m above the air/ground interface.

d. Select the directional source. The energy-angle dependent source was derived as a subset of the Whalen-SAIC source, initially produced by Paul Whalen, and later modified by Steve Egbert of SAIC.[1] It was first reduced to the BUGLE-96 47-energy group structure, and finally made angle dependent using a standard S8 quadrature by placing 50% of the neutrons in the 2 polar angles nearest the horizontal, 30% in the next 2 polar angles, 15% in the next 2 polar angles, and 5% in the most upward and downward polar angles.

e. Calculate forward fluences and responses. The forward directional source was used in this step. A forward first-collision source was calculated and input into the DORT code,[13] which then calculated the collided fluences using a high-order quadrature composed of 240 angles. The total fluence was produced by adding the uncollided and collided fluences, and then the responses were calculated by folding the responses with the total fluences.

f. Calculate adjoint directional fluence. The response functions were input as the adjoint sources in this step. An adjoint first-collision source was calculated and input into the DORT code, which then calculated the adjoint collided directional fluences using the 240-angle high-order quadrature. The total adjoint directional fluence was calculated by adding the uncollided and collided adjoint directional fluences and then averaged over the azimuthal directions and collapsed into the polar angles of the S8 quadrature. These final adjoint directional fluences were a function of the 8 polar angles and 47 energy groups, and were now the energy- and angle-dependent dosimetry cross sections for the STAY'SL code.

g. Unfold the source spectrum. The activation data, dosimetry cross sections (adjoint directional fluence at the source position), the input guess spectrum, and their uncertainties (covariance matrices) were input to the STAY'SL code. The solution was the most likely value, given the uncertainties in the input data and the important correlations in those uncertainties. The code is capable of producing a solution even when the input data are highly unlikely. However, when chi-square per degree of freedom is > 2.0, the output should be viewed with great caution.

V. RESULTS

The STAY'SL calculations unfolded a 47-energy-group, 8-angle-per-group source from the 2 activities at 10 ground ranges (equivalent of 20 measurements). Figure 1 shows a table of the energy group structure and a plot of the ratio of the angle-integrated—unfolded-source to the angle-integrated-original-source. In a perfect world, all the raitos would be 1.0 . As shown in the figure, 2 groups have ratios of nearly 5, which can be expected since only 2 activations were used in the unfolding.

Even though only one thermal and one fast response were used in the analysis, the unfolded source reproduces the data for the 2 responses at the 10 ground ranges to within 10%.

VI. RECOMMENDATIONS

FALSTF,[14] the last-flight code, should be modified to produce angle-dependent fluence information as input data to the STAY'SL code. This will mitigate any ray effects.

The anisotropic source chosen for the study provided activation results that were not significantly different than the activation results from the isotropic source. Therefore, a radical anisotropic source should be tested.

Although 6 thermal and 2 fast responses were measured in Hiroshima and were available for the analysis, only one of each could be used. The reason for this is that each additional thermal response and each additional fast response supply no new information to the unfolding code. If there were epithermal and intermediate responses, then their adjoints would contribute. However, in the real world, the local shielding around each response should alter the spectrum such that more activations could be used in the unfolding process. Thus, local shielding similar to that found at Hiroshima sample sites should be used in a final calculation to determine if its use will sufficiently alter the spectrum to allow additional data to be used.

Once all the unfolding data is prepared and/or calculated, the STAY'SL code is run. The new output source must be manually input to a new calculation, then that result re-input until an accepted convergence is reached. Therefore, the STAY'SL code should be changed to incorporate automatic source iteration.

Once the above steps have been proven to work, then the full effort to unfold the Little Boy source should be undertaken, and Monte Carlo should be used to generate the angle-dependent adjoint functions for the more complicated geometries.

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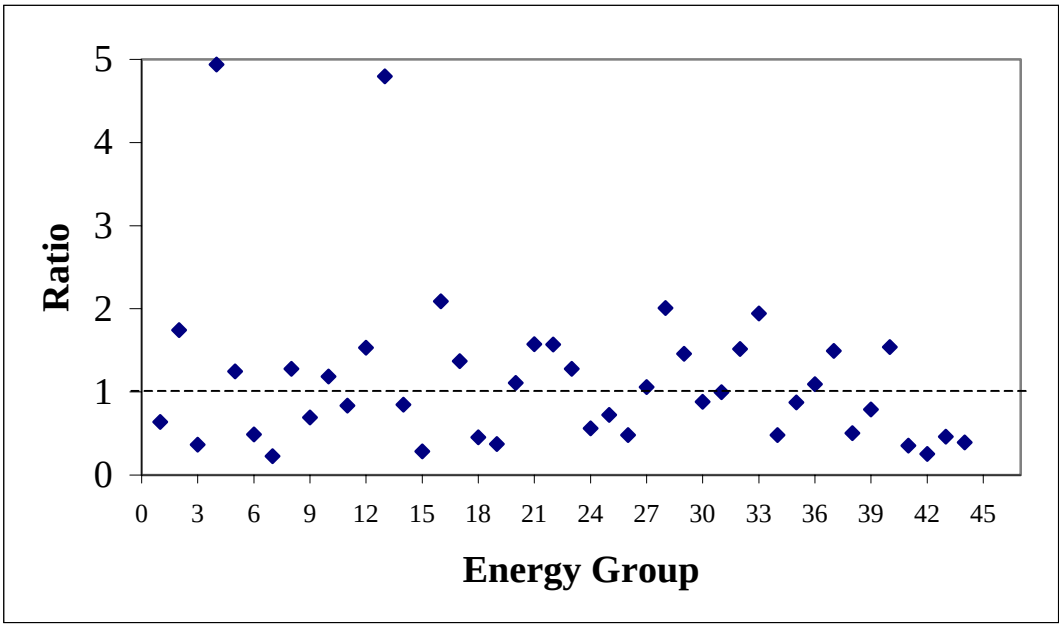

Grp #	Energy Range (eV)			Grp #	Energy Range (eV)		
1	1.733E+07	-	1.419E+07	25	2.972E+05	-	1.832E+05
2	1.419E+07	-	1.221E+07	26	1.832E+05		1.111E+05
3	1.221E+07	-	1.000E+07	27	1.111E+05		6.738E+04
4	1.000E+07	-	8.607E+06	28	6.738E+04		4.087E+04
5	8.607E+06	-	7.408E+06	29	4.087E+04		3.183E+04
6	7.408E+06	-	6.065E+06	30	3.183E+04		2.606E+04
7	6.065E+06	-	4.966E+06	31	2.606E+04		2.418E+04
8	4.966E+06	-	3.679E+06	32	2.418E+04		2.188E+04
9	3.679E+06	-	3.012E+06	33	2.188E+04		1.503E+04
10	3.012E+06	-	2.725E+06	34	1.503E+04		7.102E+03
11	2.725E+06	-	2.466E+06	35	7.102E+03		3.355E+03
12	2.466E+06	-	2.365E+06	36	3.355E+03		1.585E+03
13	2.365E+06	-	2.346E+06	37	1.585E+03		4.540E+02
14	2.346E+06	-	2.231E+06	38	4.540E+02		2.144E+02
15	2.231E+06	-	1.920E+06	39	2.144E+02		1.013E+02
16	1.920E+06	-	1.653E+06	40	1.013E+02		3.727E+01
17	1.653E+06	-	1.353E+06	41	3.727E+01		1.068E+01
18	1.353E+06	-	1.003E+06	42	1.068E+01		5.043E+00
19	1.003E+06	-	8.208E+05	43	5.043E+00		1.855E+00
20	8.208E+05	-	7.427E+05	44	1.855E+00		8.764E-01
21	7.427E+05	-	6.081E+05	45	8.764E-01		4.140E-01
22	6.081E+05	-	4.979E+05	46	4.140E-01		1.000E-01
23	4.979E+05	-	3.688E+05	47	1.000E-01		1.000E-05
24	3.688E+05	-	2.972E+05				

Figure 1. Ratio of Unfolded Source to Original Source.

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