PROOF OF PRINCIPLE
Unfold an Angle-Energy Dependent Source From Forward and Adjoint Calculations

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Presentation Overview

- Introduction
- Unfolding Theory
- Codes
- Proof-of-Principle Procedure
- Initial Results
- Recommendations

Introduction

- 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 decides that it does not matter exactly what happened when the weapon exploded (since one knows the results, i.e. one has measurements), and if sufficient information exist about those results, one should be able to unfold a source.

Introduction (Cont'd)

- The technique of source unfolding is used extensively in the laboratory, e.g. one might unfold the flux from known detector foil measurements.
- This study will create a known source and then calculate the answer of interest. Succeeding calculations will be made in the adjoint mode to determine the adjoint flux. Finally, an unfolding of the forward source will be attempted.
- If the 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.

General Unfolding Theory

- Consider the following:
  - » S(E)dE = Point source spectrum, i.e. the number of particles emitted by the point source with energy between E and E+dE.
  - » $R_i(E)$ = response of the detector, i.e. the probability that a particle emitted by the source with energy E will contribute to the measured response i. By careful consideration, this term can be expressed as an adjoint energy-dependent flux.
  - » M_i = measured response i.
- These three functions are related by

$$M_i = \int_0^\infty R_i(E)S(E)dE$$

General Unfolding Theory (Cont'd)

- If $S_j = S(E)\Delta E_j$, where S_j is constant over ΔE_j , and
- If $\int_0^\infty$ is replaced with $\sum_{j=1}^{J}$, for J = number of energy groups, then
- $M_i = \sum_{j=1}^{J} \frac{S_j}{\Delta E_j} \int_{E_j}^{E_{j-1}} R_i(E)dE = \sum_{j=1}^{J} R_{ij} S_j$,

  where $R_{ij} = \frac{1}{\Delta E_j} \int_{E_j}^{E_{j-1}} R_i(E)dE$.
- Thus for energy dependent data, the following matrix notation holds, where

  N = number of measurements,

  M = **RS**

General Unfolding Theory (Cont'd)

- or

$$\begin{pmatrix} m_1 \\ m_2 \\ . \\ . \\ . \\ m_N \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} & . & . & . & R_{1J} \\ R_{21} & R_{22} & . & . & . & R_{2J} \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \\ R_{N1} & R_{N2} & . & . & . & R_{NJ} \end{pmatrix} \begin{pmatrix} S_1 \\ S_2 \\ . \\ . \\ . \\ S_J \end{pmatrix}$$

- Thus, the matrices **M**, **R**, **S,** and their uncertainties are fed into an unfolding code to obtain the output spectrum and its uncertainties

General Unfolding Theory (Cont'd)

- Assume now 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. Again, by carefully considering the input adjoint source, this term is the energy-angular dependent adjoint flux.
- 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

General Unfolding Theory (Cont'd)

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

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

- 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

General Unfolding Theory (Cont'd)

- $$\begin{pmatrix} M_1 \\ M_2 \\ \cdot \\ \cdot \\ \cdot \\ M_N \end{pmatrix} = \begin{pmatrix} R_{111} & R_{112} & \cdots & R_{11K} & R_{121} & R_{122} & \cdots & R_{12K} & \cdots & R_{1J1} & R_{1J2} & \cdots & R_{1JK} \\ R_{211} & R_{211} & \cdots & R_{212} & R_{221} & R_{222} & \cdots & R_{22K} & \cdots & R_{2J1} & R_{2J2} & \cdots & R_{2JK} \\ \cdot & \cdot & \cdots & \cdot & \cdot & \cdot & \cdots & \cdot & \cdots & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot & \cdot & \cdot & \cdots & \cdot & \cdots & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot & \cdot & \cdot & \cdots & \cdot & \cdots & \cdot & \cdot & \cdots & \cdot \\ R_{N11} & R_{N12} & \cdots & R_{N1K} & R_{N21} & R_{N22} & \cdots & R_{N2K} & \cdots & R_{NJ1} & R_{NJ2} & \cdots & R_{NJK} \end{pmatrix} \begin{pmatrix} S_{11} \\ S_{12} \\ \cdot \\ \cdot \\ \cdot \\ S_{JK} \end{pmatrix}$$
- Thus, the three matrices are preserved, with the response and source matrices being expanded by adding the angular data.
- This will be accomplished in the STAY'SL code by increasing the number of groups.

Codes

- DORT
  - » The two-dimensional discrete-ordinates radiation transport code DORT will be used in the forward and adjoint modes.
  - » DORT solves large neutron and photon transport problems in the forward and adjoint mode.
  - » Output from DORT will include the forward and adjoint fluxes, respectively, and will be both scalar and angular.

Codes (Cont'd)

- STAY'SL
  - » The least-squares dosimetry unfolding code, STAY'SL, will be used to attempt to unfold the angle-energy dependent source.
  - » The output spectrum (in our case, the source) is obtained by minimizing chi-square.

Proof-of-Principle Procedure

- Run a forward DORT calculation with a KNOWN (my choice) polar-angle-energy distributed point source at a certain distance above an air-ground interface.
- At selected ground ranges, the cobalt, europium, sulfur, chlorine, etc. doses will be calculated from the DORT forward fluxes using the response functions.

Proof-of-Principle Procedure (Cont'd)

- Adjoint calculations from adjoint sources at those ground ranges will be made.
- The angular-energy dependent adjoint fluxes at the forward point-source spatial location will become the STAY'SL input dosimetry cross sections; the forward calculated doses at the selected ground ranges will become the STAY'SL input measurements.
- STAY'SL iterations will be made to unfold the forward angular-energy dependent source with which the forward calculations were made.

Proof-of-Principle Procedure (Cont'd)

- Table 1 shows the activation cross sections to be used in the unfolding procedure.
- Figure 1 shows the geometries for the forward calculation (upper figure) and the adjoint calculations (lower figure).
- One forward calculation and one adjoint calculation for each activation cross section are required.

Table 1. Neutron Reaction Products Measured in Samples From Hiroshima*

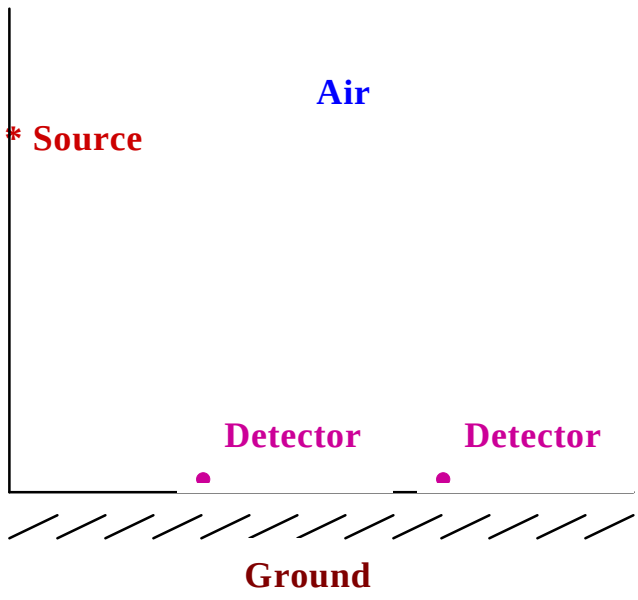
Neutron reaction	Threshold energy	Half-life	Sample type	Ground range (m)	Measurement
$^{32}S(n,p)^{32}P$ **	2.5 MeV	14.3 d	Sulfur in electrical insulators	76-1025	Beta particle
$^{59}Co(n,\gamma)^{60}Co$ **	Thermal	5.271 y	Steel, granite, roof tiles	0-1295	Gamma ray
$^{151}Eu(n,\gamma)^{152}Eu$	Thermal	13.33 y	Roof tiles, granite, concrete	0-1370	Gamma ray
$^{153}Eu(n,\gamma)^{154}Eu$	Thermal	8.6 y	Granite	107	Gamma ray
$^{35}Cl(n,\gamma)^{36}Cl$	Thermal	3.01E+5 y	Granite, concrete	107-1606	AMS
$^{40}Ca(n,\gamma)^{41}Ca$	Thermal	1.03E+5 y	Granite	107	AMS
$^{62}Ni(n,\gamma)^{63}Ni$	Thermal	100 y	Steel	163	Beta particle
$^{63}Cu(n,p)^{63}Ni$ **	1 MeV	100 y	Copper wire, lighting rods, etc.	132-1450	AMS, beta particle

* Table provided by G. D. Kerr, ORNL.
** Used in the POP study.

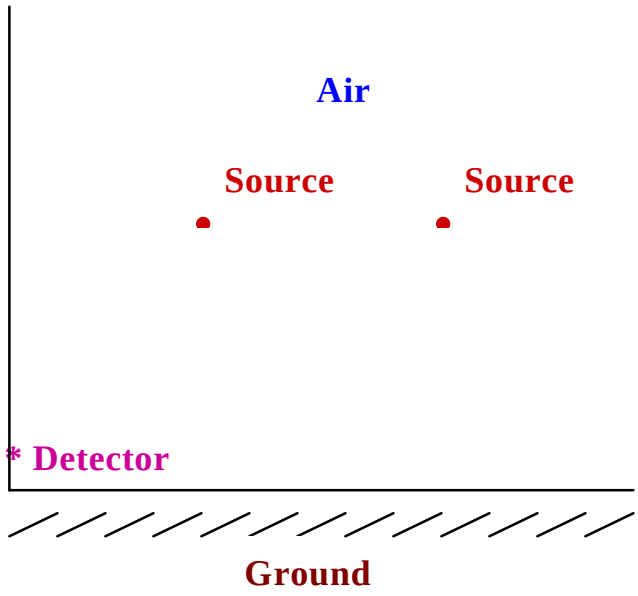
Note: Other potential neutron reaction products that can be measured in granite close to the hypocenter include $^{39}K(n,p)^{39}Ar$ with a threshold energy of about 0.2 MeV and a half-life of 269 years.

Fig. 1. Forward and Adjoint Calculational Illustration

Forward Calculation



Adjoint Calculation



Initial Results

- The initial set of calculations used only the Ca(n,g) and the Cu63(n,p) reactions.
- Figures 2 and 3 show the comparisons of the Ca and Cu responses as a function of isotropic and anisotropic sources versus ground range.
- The anisotropy has essentially disappeared by the time the neutrons reach the ground, thus implying the test source should have been more anisotropic in the horizontal direction.
- Figures 4 and 5 show the comparisons of the Ca and Cu responses as calculated in the forward and adjoint modes. Agreement is quite good.

Fig. 2. Ca(n,g) Response from Isotropic and Anisotropic Source

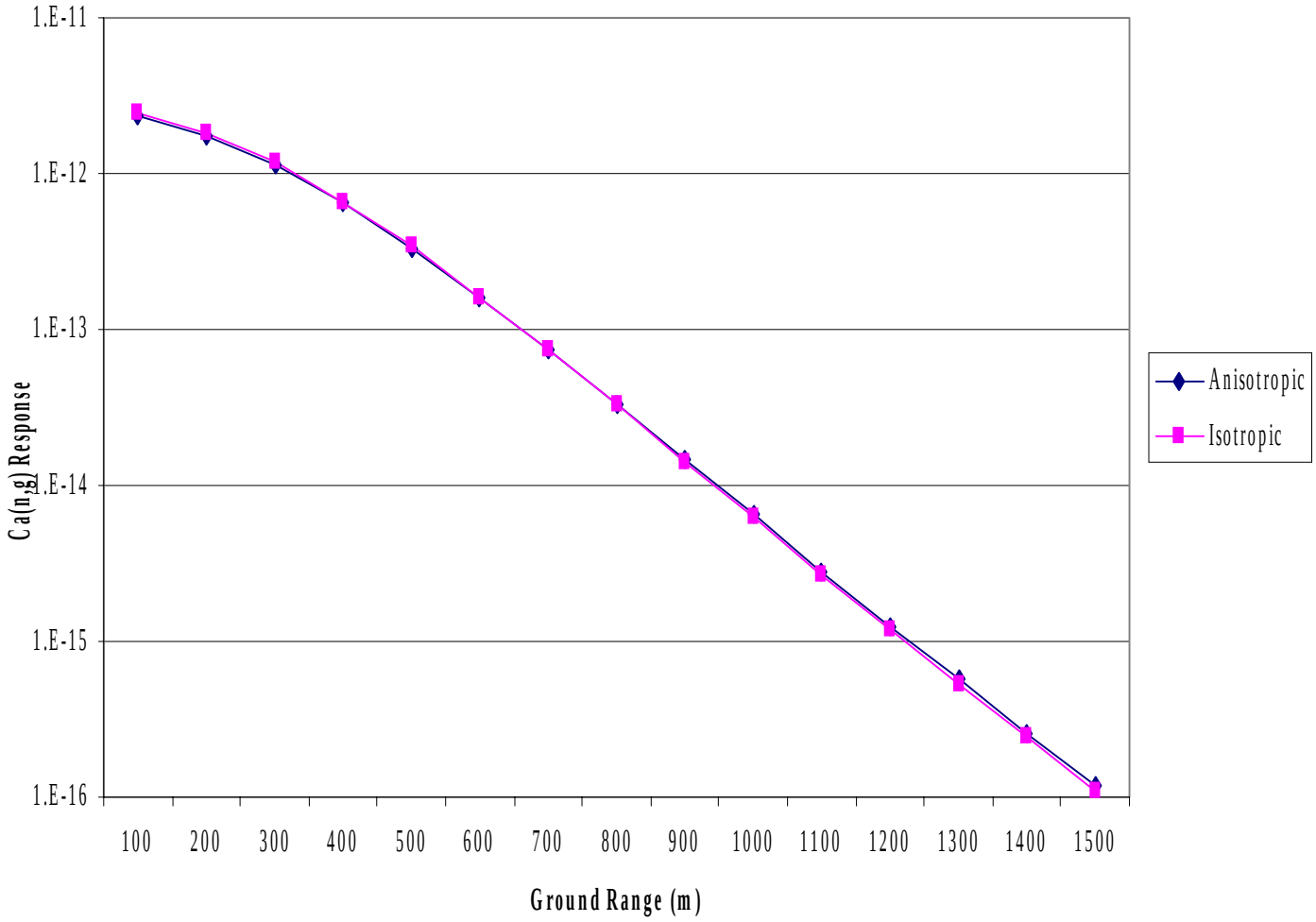


Fig. 3. Cu63(n,p) Response from Isotropic and Anisotropic Source

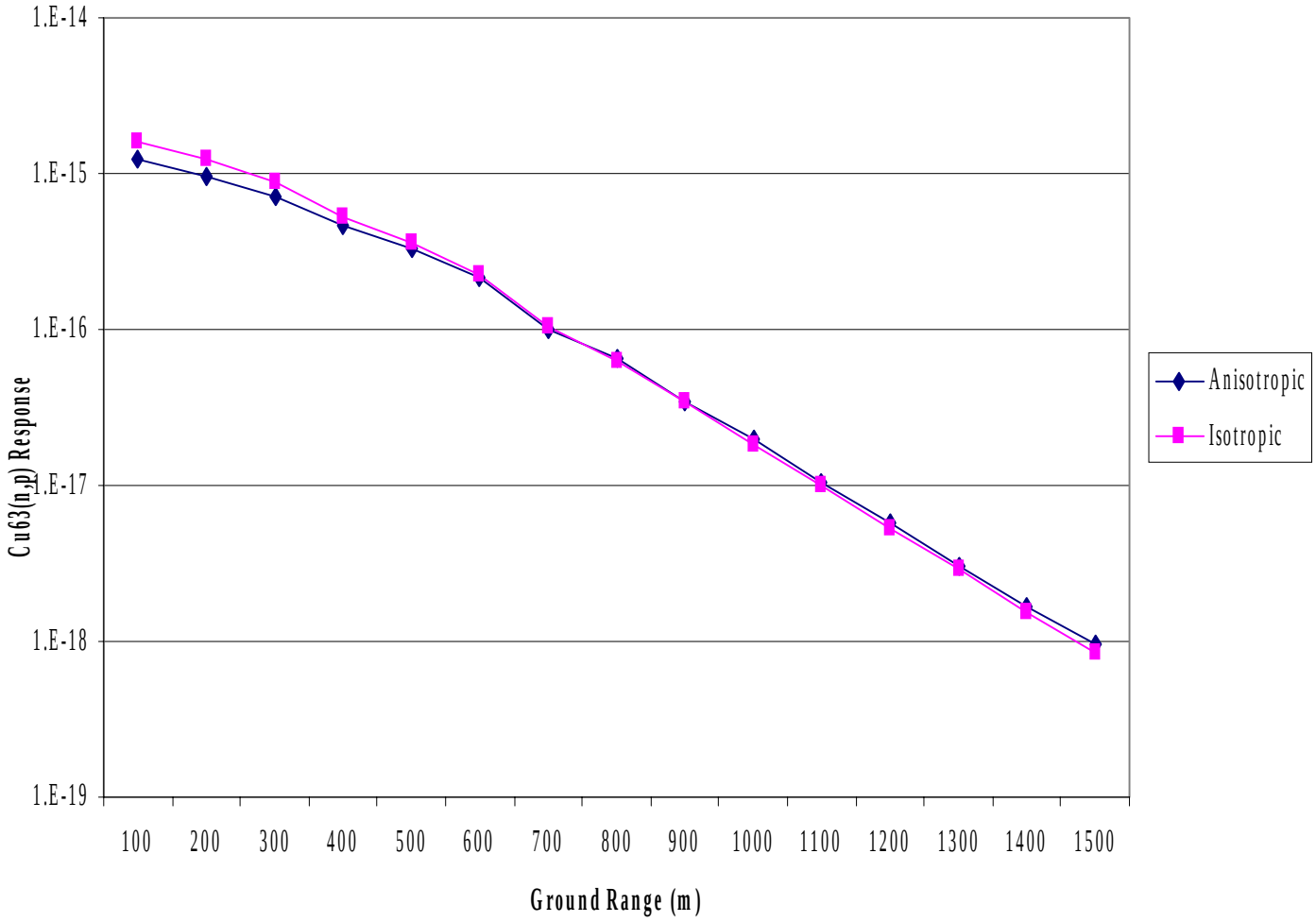


Fig. 4. Ca(n,g) Response from Isotropic Source in Forward and Adjoint Mode

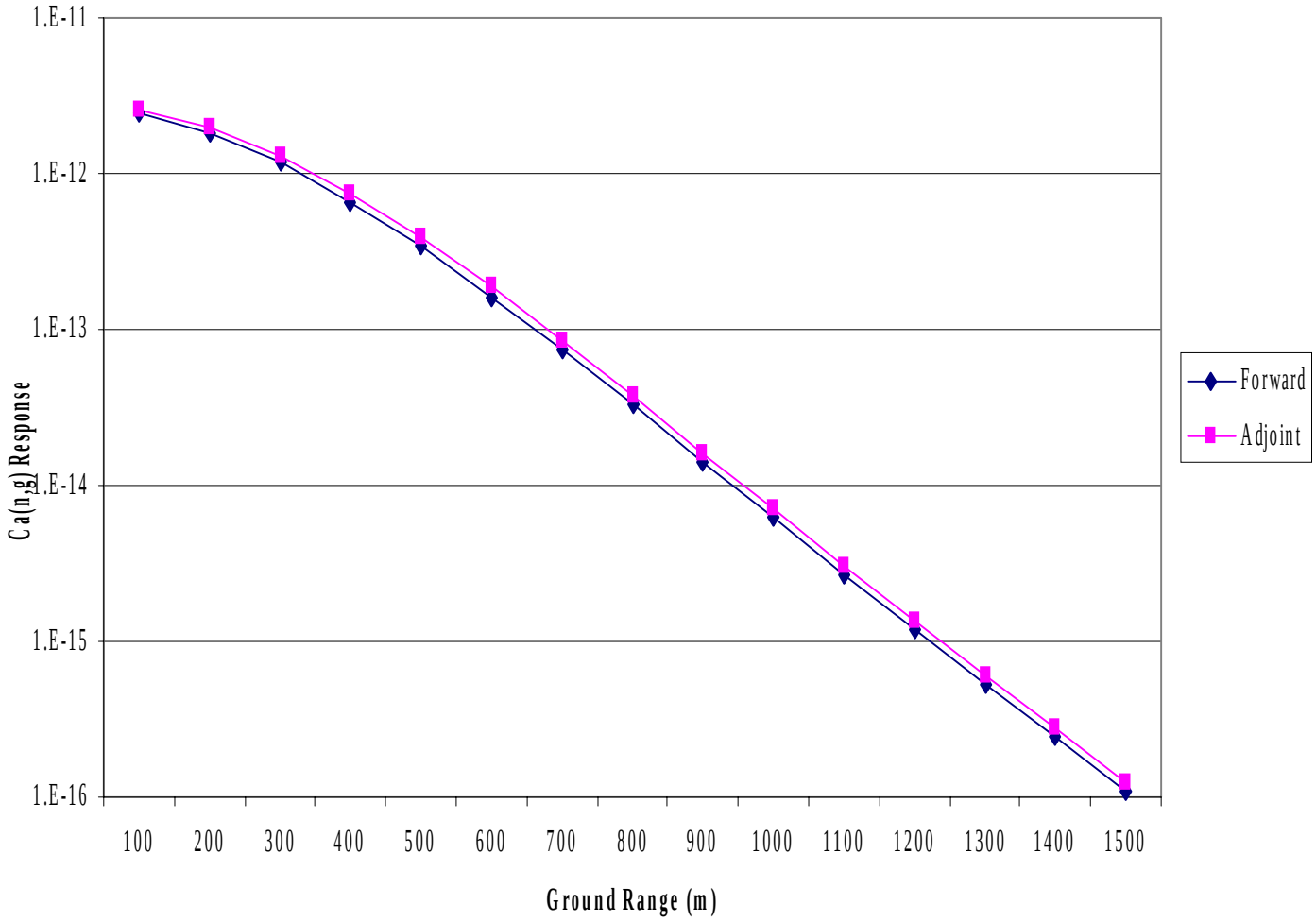
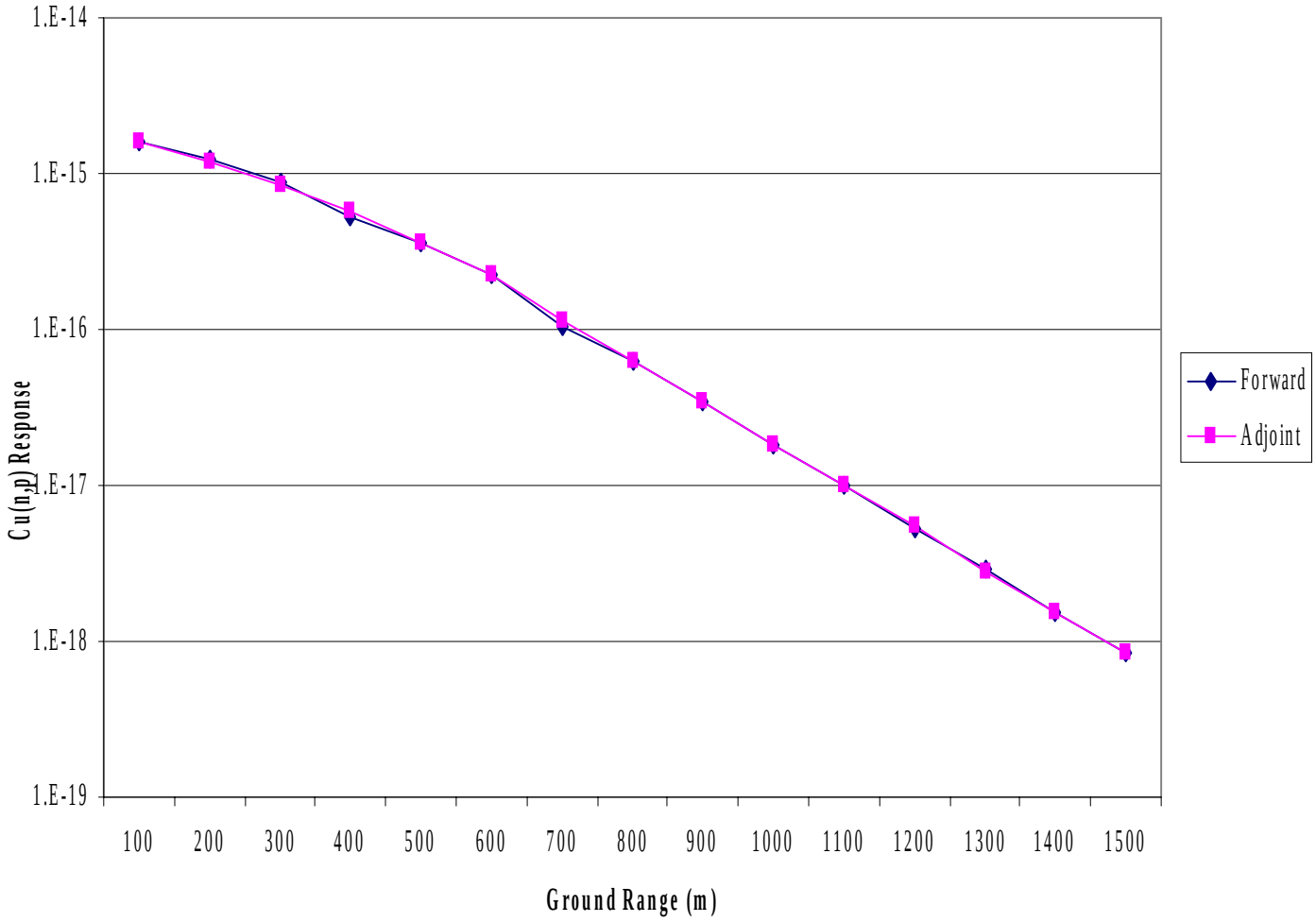


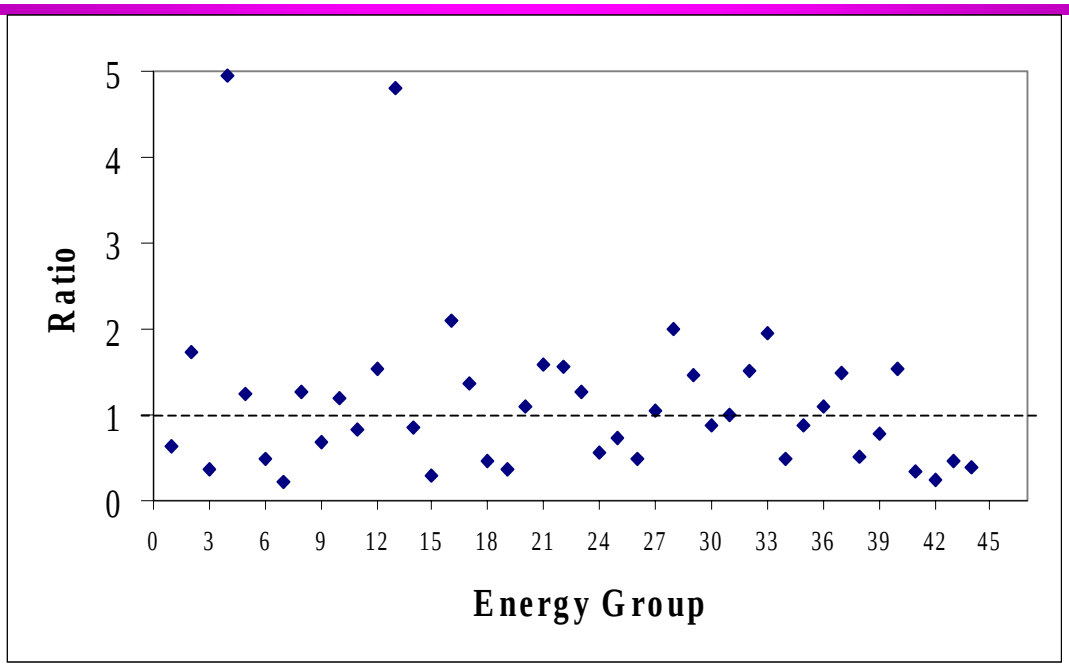
Fig. 5. Cu63(n,p) Response from Isotropic Source in Forward and Adjoint Mode



Initial Results (Cont'd)

- The high-energy Cu63(n,p)-response plots exhibit ray effects, even though a 240-angle quadrature was used. These effects can be mitigated completely by using a last-flight routine, which was not used in these initial calculations.
- The initial STAY'SL calculation unfolded a 47-energy-group, 8-angle-per-group source from 2 activities at 10 ground ranges (equivalent of 20 measurements).
- Figure 6 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.

Fig. 6. Ratio of Unfolded Source to Original Source



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					

Initial Results (Cont'd)

- In a perfect world, all the ratios would be 1.0 . As can be seen, 2 groups have ratios of nearly 5, which can be expected since only 2 activations were used in the unfolding.
- Although the ratios are scattered about 1.0, the unfolded source reproduces the data for the 2 responses at the 10 ground ranges to within 10%. This percentage can be reduced still further with more iterations.
- The next unfolding calculation will use additional activities.

Recommendations

- The STAY'SL code should be changed to incorporate automatic source iteration.
- The last-flight code, FALSTF, should be modified to produce angle-dependent flux information as input data to the STAY'SL code. This will mitigate the ray effects.
- A radical anisotropic source should be tested.
- Upon approval of the Little Boy unfolding work, Monte Carlo should be used to generate the angle-dependent adjoint functions, since the geometries surrounding the measurement locations are probably three dimensional.