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Neutron Beam-Line Shield Design for the Protein Crystallography Instrument at the Lujan Center

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Abstract

We have developed a very useful methodology for calculating absolute total (neutron plus gamma-ray) dose equivalent rates for use in the design of neutron beam line shields at a spallation neutron source. We have applied this technique to the design of beam line shields for several new materials science instruments being built at the Manuel Lujan Jr. Neutron Scattering Center. These instruments have a variety of collimation systems and different beam line shielding issues. We show here some specific beam line shield designs for the Protein Crystallography Instrument.

1. Introduction

Shielding of neutron beam lines at spallation neutron sources can present different (and challenging) shielding issues compared to neutron beam lines at a fission reactor. *For this paper, we define neutron beam line shielding to include shielding of collimators, T_0-Choppers, frame overlap choppers, experiment-caves, beam stops, etc.* Each of these beam line shield components may require a different neutron beam line shield composition and thickness.

Until recently, calculational capabilities have been "lacking" for computing ***absolute*** neutron and gamma-ray dose equivalent rates at the surface of neutron beam line shields at spallation neutron sources. What has now made this problem tractable is the computing power of modern workstations, and enhancements in the Monte Carlo codes used to perform spallation calculations.

As mentioned above, shielding at a spallation neutron source is much more difficult than shielding at a nuclear reactor. This is because at a spallation source you not only have to shield against "fast" neutrons (i.e., evaporation neutrons with a "fission-like" spectrum) but also against high-energy neutrons (i.e., neutrons with energies up to the energy of the incident protons). The former neutrons are more-or-less isotropic in angle, while the latter neutrons have a strong angular dependence. At the Manuel Lujan Jr. Neutron Scattering Center (Lujan

Center) located at the Los Alamos National Laboratory, the proton energy is 800 MeV, so neutrons can have very high energies. Characterizing the neutron source in energy and angle for neutron beam line shielding calculations is a difficult and challenging problem.

At Los Alamos, as part of the Accelerator Production of Tritium (APT) project, selected neutron cross section libraries have been extended to 150 MeV [1]. Also, the MCNPX [2] code, which is a merger of the widely used MCNP [3] and LAHET [4,5] codes, has been developed to use these libraries. The MCNPX code has the full complement of variance reduction techniques that can be utilized in shielding calculations. We have used the MCNPX code to develop a technique for designing neutron beam line shielding at the Lujan Center.

We have applied this computational technique to design neutron beam line shields for several new materials-science instruments being built at the Lujan Center. These instruments, which have different beam line shielding requirements, include the Protein Crystallography instrument, the **H**igh-**P**ressure **P**referred **O**rientation (HIPPO) instrument, the **S**pectrometer for **Ma**terials **R**esearch **A**t **T**emperature and **S**tress (SMARTS) instrument, and the **D**etector for **A**dvanced **N**eutron **C**apture **E**xperiments (DANCE) instrument. These scientific instruments present different shielding issues because of dissimilar sample positions (ranging from ~9 m to ~27 m), distinctly different collimation systems (continuous and discrete), the presence or absence of a T_0-chopper and other choppers such as frame overlap choppers, and the presence or absence of a neutron guide.

We have looked at a variety of laminated shields of polyethylene and iron (as well as polyethylene and magnetite concrete) around different neutron beam line components. We calculate ***absolute*** values of the total (neutron plus gamma-ray) dose equivalent rates at the surface of the beam line shields.

Figure 1 shows a plan view of the Experiment Room 1 (ER-1) and Experiment Room 2 (ER-2) areas at the Lujan Center, and the present instrument layout. The **performance criterion** for neutron beam line shielding in ER-1 is 2 mrem/hr for the peak total dose equivalent rate at the outside surface of the beam line shield with the Lujan Center operating at 200 μA. The square-shaped ER-1 roughly extends from the bulk shield with a radius of ~4.72 m from the proton beam centerline to about 10-12 m. The corresponding **performance criterion** for beam line shielding in ER-2 is 1 mrem/hr. To assure ourselves that we can achieve these performance goals, we design our beam line shields to **calculational design criteria** of 1 mrem/hr and 0.5 mrem/hr peak total dose equivalent rates in ER-1 and ER-2, respectively. We will discuss why we chose these (reduced) **calculational design criteria** later.

The physical layout of ER-1 imposes height constraints for our neutron beam line shielding because of the presence of a radial crane and the need to move equipment around the area. There are also limits on the floor loading capacity. Consequently, we have consciously looked at minimizing the thickness of beam line shielding in ER-1, that is, we try to maximize the efficiency of the beam line shielding in ER-1. We do not have similar constraints on crane height for neutron beam line shielding in ER-2, but we do have floor-loading restrictions.

For neutron flux-to-dose equivalent rate calculations, we use neutron flux-to-dose equivalent conversion factors from the 10CFR835 & NCRP-38 publications. For gamma-ray flux-to-dose equivalent rate calculations, we use gamma-ray flux-to-dose equivalent conversion factors from the ANSI/ANS-6.1.1-1977 document.

In this paper, we describe how we generate the neutron source-terms for our neutron beam line shield calculations. We give examples of calculations we have performed for designing the neutron beam line shielding for the new Protein Crystallography instrument at the Lujan Center. In particular, we discuss our calculations for the beam line shield in ER-1 (including the T_0-chopper shield) and the beam stop shield in ER-2 for this instrument. For all the calculations discussed here, we use cylindrical geometry. Thus, our computations are two-dimensional.

2. Calculational Method

The thermal-neutron/high-energy-neutron collimation system for the Protein Crystallography instrument is B_4C/Fe inside the Lujan bulk shield (i.e., for distances < ~4.72 m from proton beam center). Outside the bulk shield and within ER-1 (i.e. from ~4.72 m to ~11.5 m) the collimation system is BN/Fe. In ER-2 (i.e. from ~11.5 m to ~25 m), the collimation system is BN/CH_2(R), where CH_2(R) means regular density polyethylene without boron. The B_4C/Fe segments inside the bulk shield, the BN/Fe segments outside the bulk shield (but inside ER-1), and the BN/CH_2(R) segments in ER-2 are uninterrupted. That is, the collimation system for the Protein Crystallography instrument is "*continuous*" along the complete length of the beam line from the Lujan target crypt to the location of the experiment cave. For example, the diameters of the "thermal neutron" collimators for this instrument at 1.16 m and 27 m from the moderator viewed surface are ~11.5 cm and ~1.0 cm, respectively.

Using the B_4C/Fe collimation system for the Protein Crystallography instrument inside the bulk shield, we generated an energy- and angle-dependent neutron source at ~2.8 m from proton beam center. Figure 2 shows a plan view of the Lujan target station showing the beam line penetration through the bulk shield. Figure 3 depicts an elevation view of the calculational geometry. Details of the Lujan Center spallation target system can be found in Reference 6. We start the source-term calculation with 800-MeV protons incident on the spallation target system. We defined a tally surface at ~2.8 m from proton beam center to insure appropriate source-term modeling when we perform neutron beam line shielding problems near the outer surface of the bulk shield. To carry out the neutron source-term calculation, we employed a pair of DXTRAN spheres to improve the computational efficiency of the MCNPX calculation. We placed a cell of zero importance inside the beam line collimation immediately following the tally surface to restrict the current tally to outward-directed neutrons (i.e., neutrons heading toward the instrument). We used the APT 150-MeV cross section library [1] to allow the DXTRAN spheres to operate up to 150 MeV. This enhances, but does not solve, our ability to adequately predict the high energy part of the neutron spectrum. We used this calculated source term in our neutron beam line shield calculations for the Protein Crystallography instrument.

We performed initial scoping calculations to determine an appropriate binning scheme to obtain the angular distribution of the neutrons. The calculated angular distribution of neutrons integrated over all energies (for the angular binning scheme used in the results we report here) is shown in Figure 4. We selected 20 fine angular bins in the forward direction ($\cos\theta > 0.999$) with a coarser bin structure for larger angles. We chose the angle $\cos\theta = 0.999$ because neutrons starting at the tally surface (~2.8 m) with this angle will be within the collimation before they reach the outer edge of the bulk shield at ~4.72 m for nearly any starting point on the tally surface. (We have since altered our angular binning scheme and improved our ability to predict the higher-energy part of the neutron source. We are in the process of evaluating how these improvements affect our neutron beam line shield performance predictions for the Protein Crystallography instrument.)

Figure 5 shows the angular distribution of the neutron source in the forward direction ($\cos\theta > 0.999$). There is about a factor of two difference in the beam intensity just in these forward-directed neutrons. Accurately modeling this angular variation is important when trying to minimize the thickness of a neutron beam line shield. Assumptions of a flat parallel beam with an average intensity can result, for example, in an experimental cave or beam stop with too little shielding (i.e., missing the peak neutron beam intensity). Also, with the assumption of a flat parallel beam, one could end up with a neutron beam line with generally more shielding than necessary because the angular distribution of neutrons is not being taken into consideration properly.

We also generated neutron energy spectra as a function of angle. Figure 6 shows some of the angle-dependent energy spectra. The energy spectra for angles with $\cos\theta > 0.999$ are very similar in shape, although there is some difference in the absolute intensity of the spectra. For angles with $\cos\theta < 0.999$, the energy spectrum seems to be less "thermalized" with an increased high-energy neutron component as is evidenced by the change in slope of the lines in Figure 6. This level of detail is important for beam line shield design near the bulk shield. Note that the source term extends only to 150 MeV, as that is the limit of our evaluated nuclear data. Over this energy range (0 to 150 MeV), ~99.5% of the neutrons have energies < 20 MeV.

Neutrons with energies greater than 150 MeV may contribute significantly to the calculated dose equivalent rate. We account for this uncertainty by designing the beam line shield to achieve a calculated dose equivalent rate that is **half the shield performance criterion**.

We used the tallied neutron current to create an angle- and energy-dependent MCNPX neutron source. We used this neutron source term and the B_4C/Fe, BN/Fe, and BN/CH_2(R) collimation systems, to perform both the unperturbed and perturbed neutron beam-line shield calculations discussed below.

3. Results

We have performed numerous calculations of neutron beam line shields in both ER-1 and ER-2 as well as shielding for the experiment cave and beam stop. We will only describe here the calculations for the ER-1 beam line shield and the beam stop.

3.1 ER-1 Beam Line Shield Calculations

As mentioned earlier, because of crane access requirements in ER-1 and floor loading issues in both ER-1 and ER-2, we consciously try to reduce the thickness of our beam line shields. We studied the following five composite Fe/CH_2 shields in ER-1 for the Protein Crystallography instrument:

CH_2(5%)/Fe/CH_2(R)/Fe/CH_2(5%)/CH_2(R)/CH_2(5%)

2/6/2/9/1/4/1 (overall thickness 25 inches),

$CH_2(5\%)/Fe/CH_2(R)/Fe/CH_2(5\%)/CH_2(R)/CH_2(5\%)$
2/6/2/12/1/4/1 (overall thickness 28 inches),

$CH_2(5\%)/Fe/CH_2(R)/Fe/CH_2(5\%)/CH_2(R)/CH_2(5\%)$
2/6/2/15/1/4/1 (overall thickness 31 inches),

$CH_2(5\%)/Fe/CH_2(R)/Fe/CH_2(5\%)/CH_2(R)/CH_2(5\%)$
2/6/2/18/1/4/1 (overall thickness 34 inches), and

$CH_2(5\%)/Fe/CH_2(R)/Fe/CH_2(5\%)/CH_2(R)/CH_2(5\%)$
2/6/2/21/1/4/1 (overall thickness 37 inches),

where the 2 inch $CH_2(5\%)$ shield is the innermost part of the shield adjacent to the collimation system and beam pipe - $CH_2(5\%)$ refers to polyethylene with 5 w% boron.

You will note above that we varied the overall shield thickness by changing the thickness (in 3-inch increments) of the outermost Fe layer just before the final CH_2 laminate. Our intention is to establish a basic laminate structure for Lujan ER-1 beam-line shielding using 3-inch-thick Fe as a basis.

We performed two different types of calculations for the ER-1 beam line shields:

> ***Unperturbed calculations*** where we assumed the beam-line shield surrounding the neutron beam pipe containing the Protein Crystallography instrument BN/Fe collimation system in ER-1 was continuous with no interruptions.
>
> ***Perturbed calculations*** where we assumed the beam line shield surrounding the neutron beam pipe containing the BN/Fe collimation system in ER-1 was interrupted (perturbed) in several ways such as: a) by the outer magnetite concrete layer of the Lujan bulk shield; b) by the magnetite concrete zone that transitions from the round bulk-shield geometry to a flat-surface beam line geometry; c) by the Hg shutter zone that holds the Hg shutter components; and d) by the T_0-chopper hardware.

Unperturbed Calculations – In Figs. 7-8, we show the results of our unperturbed calculations for two laminated shields with a thickness of 28 inches and 37 inches, respectively. In these figures, we show the gamma-ray, neutron, and total dose equivalent rates along the beam line for the Lujan Center operating at 200 μA. We used a spatial resolution increment along the beam-line shield of 25 cm. From these results, we make the preliminary observations that we can use the 28-inch thick shield after ~6.5 m, and the 37-inch shield right up to the Lujan bulk shield surface at ~4.72 m.

Perturbed Calculation for Single Shield Thickness – In reality, our neutron beam line shields are perturbed because shield material must be removed to accommodate Hg shutter reservoirs, T_0-choppers, etc. In order to study this effect, we perturbed the 37-inch beam line shield described above with the necessary features to support the Hg shutter system in use at the Lujan Center and the Lujan T_0-chopper design. Figure 9 shows the results of our perturbed calculation for this 37-inch laminated shield. Again, we used a spatial resolution increment along the beam-line shield of 25 cm. However, we varied our spatial resolution in the vicinity of the Lujan bulk shield to account for major perturbations in the beam line shielding. From this perturbed calculation, we conclude that we can use the 37-inch laminated shield only after ~5.25 m. For distances less than ~5.25 m, the shield must be thicker than 37 inches. Note for the unperturbed case shown in Fig. 8, the 37-inch unperturbed shield could be used right up to the bulk shield surface at ~4.72 m.

Perturbed Calculation for a 3-Step Shield – Based on the results of the above computations, we performed a calculation for a 3-step perturbed ER-1 laminated shield for the Protein Crystallography instrument. The first step from the bulk shield at ~4.72 m to 5.25 m was 46 inches thick. The second step from 5.25 m to 6.5 m was 37 inches thick. The third step from 6.5 m to the ER-1 wall at ~11.5 m was 28 inches thick. We show this 3-step shield in Fig. 10, and the results of our calculation in Fig. 11. In Fig. 11, we can see that our calculated design goal of 1 mrem/hr is exceeded at around a distance of 6.5 m.

As a result of the above calculations, we recommended a beam-line shield in ER-1 for the Protein Crystallography instrument with three steps in it. The Fe sections of the three shields adjoin at ~5.25 m and ~7.0 m from proton beam center. The first shield extends from the Lujan bulk shield at ~4.72 m to ~5.25 m. This shield covers the magnetite concrete transition region and the Hg shutter zone, and reaches to a height of at least 46 inches from the o.d. of the neutron beam pipe. The second shield is a composite beam-line shield starting from the juncture at ~5.25 m and extending to ~7.0 m. The thickness of this second step is ~37 inches as measured from the o.d. of the neutron beam pipe. The third shield is also a composite beam-line shield starting from the juncture at ~7.0 m and extending to the transition shield at the ER-1/ER-2 wall. The thickness of this third step is ~28 inches as measured from the o.d. of the neutron beam pipe.

All shields are "capped" with a 6-inch composite CH_2 layer (the thickness of this CH_2 layer is included in the above shield dimensions). The downstream surface of the 46 inch shield is also "faced-off" with this CH_2 laminate, extending the portion of this region above the 37 inch shield from ~5.25 m to ~5.40 m. The two composite beam-line shields "wrap" completely around the beam line with the outer CH_2 laminated zone replaced by a regular concrete base extending to the ER-1 floor. Around the T_0-chopper area (from ~9.25 m to ~10.25 m, i.e., underneath the T_0-chopper), we are recommending that the regular concrete base be altered to accept the 28 inch laminated shield with the outer CH_2 laminate replaced by magnetite concrete. This enhanced shield underneath the T_0-chopper area is to help address ground-shine issues in ER-1.

For the Protein Crystallography instrument, the T_0-chopper is located at ~9.5 m. The component of the chopper that blocks the beam is essentially a 12-inch-long by 4-inch-diameter cylinder of Inconel. With the T_0-chopper blocking the beam, the calculated total dose equivalent rate from neutrons plus capture gamma rays, averaged over a 6-inch diameter cylindrical surface area and the length of the Inconel beam block, is **~150 rem/hr**. This dose equivalent rate neglects the contribution from gamma rays in the Protein Crystallography extracted beam, as well as neutrons in the extracted beam with energies less than 1 eV.

3.2 Beam Stop Shield Calculations

We have completed the design of a beam stop for the Protein Crystallography instrument based solely on personnel radiation protection in ER-2. We have not specifically optimized the design of the beam stop for minimizing instrument backgrounds. However, we have qualitatively considered reducing instrument backgrounds by employing the concept of a laminated core for the beam stop and in the overall design of the beam-stop shield.

The “core” of the beam stop has square lateral dimensions of 8 inches by 8 inches. The length of the core is ~26.3 inches in the direction of the neutron beam. The core of the beam stop is surrounded on the top, bottom, sides and downstream surface by 8 inches of laminated polyethylene, forming (in the lateral direction) an overall square cross section for the beam stop of 24 inches by 24 inches. For the results shown here, the upstream “snout” (that portion of the beam stop shield extending from the front surface of the beam-stop core toward the Protein Crystallography experiment cave) is 36 inches. The downstream side of the beam-stop shield (the back-end) will be positioned ~96 inches from the downstream wall of the experiment cave. This was the farthest downstream distance that we were comfortable accepting. Our desire is to get the beam stop as far from the Protein Crystallography experiment cave as possible. With the 36 inches snout, the overall length of the beam stop (from the front of the snout to the back of the beam stop) is ~70.3 inches.

The recommended laminated core of the beam stop is as follows (from front to back):

- Pb/Gd/Flex-Panel(30%)/B_4C/CH_2(30%)/Cu/CH_2(5%)/Cu/CH_2(5%)/Cu @

  1/0.002/0.25/1/3/5/3/5/3/5 inches.

The front part of the beam-stop core has been heavily-ladened with boron to reduce back-streaming of neutrons into the Protein Radiography experiment cave. In the lateral and downstream dimensions, the laminated polyethylene shield is CH_2(5%)/CH_2(R)/CH_2(5%) at 2/5/1 inches. This beam-stop (core/shield) reduces the total dose equivalent rates in ER-2 to below the calculational design value (for ER-2) of 0.5 mrem/hr with a proton beam current of 200 μA incident on the Lujan target system at all locations accessible by personnel. The beam stop design is depicted in Fig. 12.

We compared Fe to Cu for the beam-stop core and, from a personnel radiation viewpoint, either material is acceptable. However, a Cu-core produces ~20% lower axial total dose equivalent rates towards the back of the beam stop than does a Fe-core. Similarly, a Cu-core is better than a Fe-core by ~25-50% at the downstream beam-stop surface. Copper purportedly produces fewer gamma rays than Fe, but we could not discern a difference between the two materials from a dose perspective. Therefore, the choice between the two materials comes down to cost and instrument background issues. However, we recommended a Cu-core for the Protein Crystallography beam stop.

The calculated total dose equivalent rate in the primary (incident) beam of the Protein Crystallography instrument at 29 m is **~78 rem/hr** with the Lujan Center operating at 200 μA. This is only for primary incident neutrons with energies >1 eV, no primary gamma rays, and no T_0-chopper in the incident beam.

4. Conclusions

We have developed a very useful methodology for calculating absolute total dose equivalent rates for use in the design of neutron beam line shields at a spallation source. We have applied this technique to the design of beam line shields for several new materials-science instruments being built at the Lujan Center. We showed a specific beam line shield design for the Protein Crystallography instrument for ER-1 as well as the design for the beam stop.

The ER-1 beam line shield design described above for the Protein Crystallography instrument should result in the shield meeting the performance criterion of 2 mrem/hr peak total dose equivalent rate, with the Lujan Center operating at 200 μA.

We also studied composite CH_2(5%)/magnetite-concrete shields in ER-2 for the Protein Crystallography instrument. The composite shields we studied begin with a 2-inch-thick inner layer of CH_2(5%) followed an outer layer of magnetite concrete. For completeness, we show here the thickness of the composite shield in ER-2. The shields start at the outside of the void zone surrounding the beam pipe for the Protein Crystallography instrument. The following composite CH_2(5%)/magnetite-concrete shields meet the calculated design criterion for beam line shield in ER-2 of 0.5 mrem/hr peak total dose equivalent rate with the Lujan Center operating at 200 μA:

- From the ER-1/ER-2 wall at ~11.5 m to ~12.5 m, a 28-inch-thick shield of
  - ✓ CH_2(5%)/Magnetite-Concrete
  - ✓ 2/26 inches

- From ~12.5 m to ~16.0 m, a 24-inch-thick shield of
  - ✓ CH_2(5%)/Magnetite-Concrete
  - ✓ 2/22 inches

- From ~16.0 m to ~20.0 m, a 20-inch-thick shield of
  - ✓ CH_2(5%)/Magnetite-Concrete
  - ✓ 2/18 inches

- From ~20.0 m to ~25.0 m (the start of the experiment-cave), a 16-inch-thick shield of
  - ✓ CH_2(5%)/Magnetite-Concrete
  - ✓ 2/14 inches

The Experiment cave for the Protein Crystallography instrument starts at ~25 m. We have specified the experiment cave shield design as follows:

- 8 inches of CH_2(5%) contained in Fe
  - ✓ Fe/ CH_2(5%)/Fe
  - ✓ 0.375/8/0.75 inches (8.75 inches overall).

Acknowledgements

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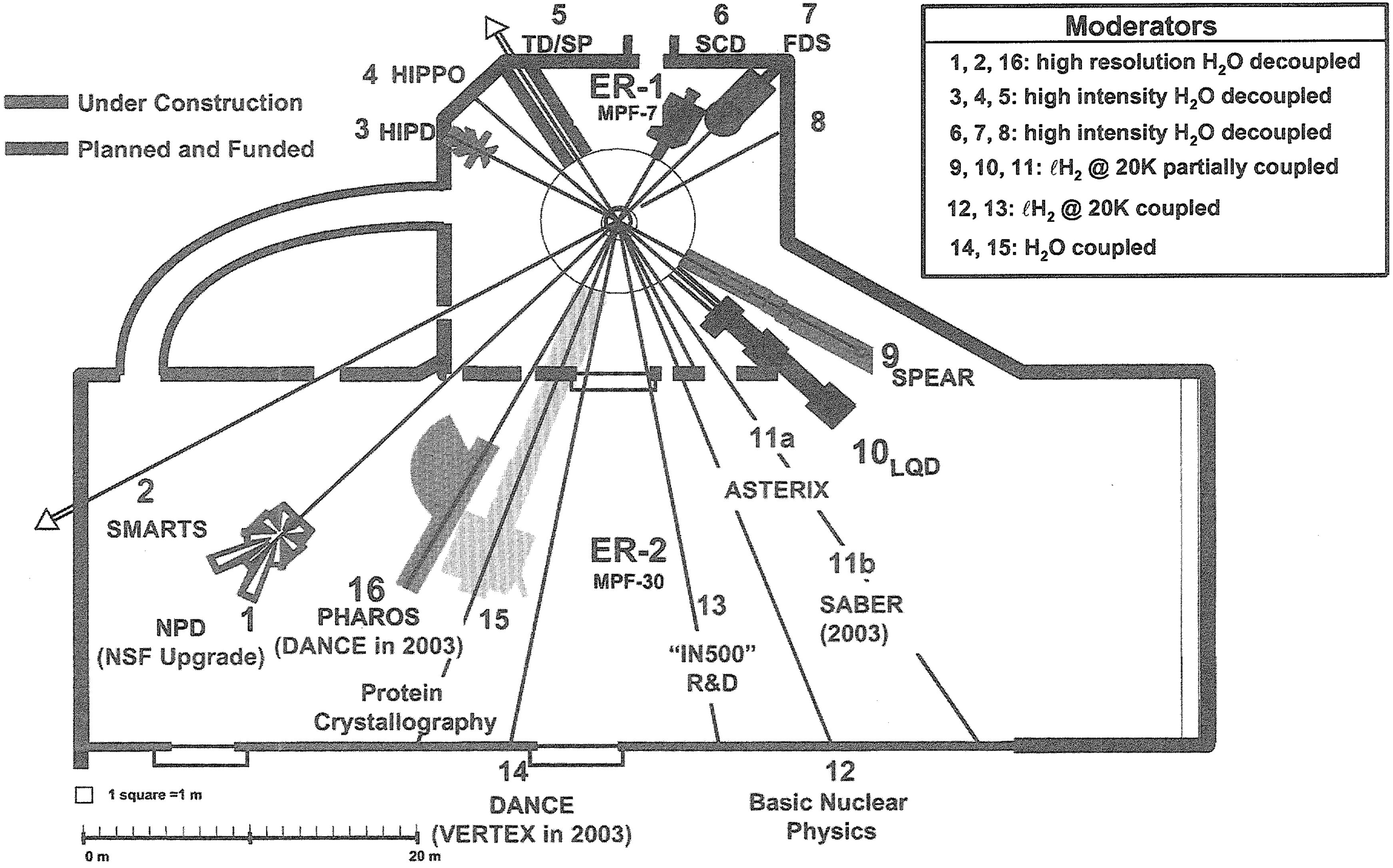

Figure 1. Layout of the two Lujan Center Experimental areas and arrangement of materials science instruments.

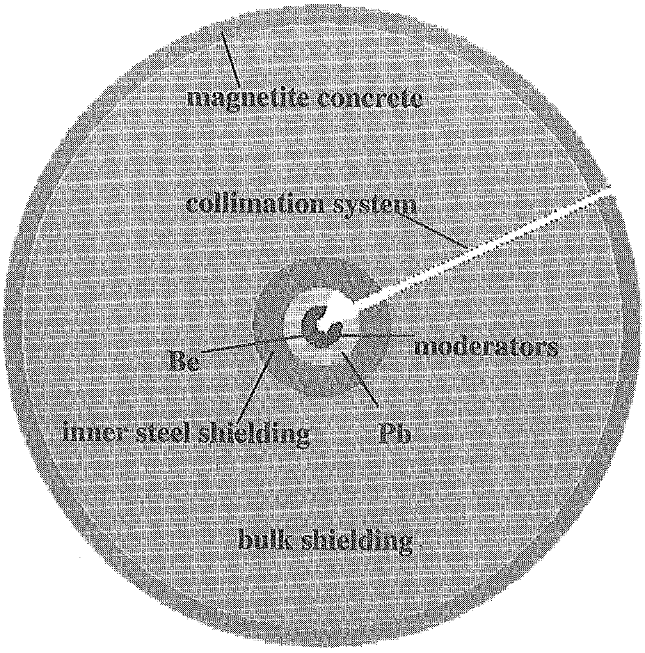

Figure 2. Plan view of the Lujan Center target station model used to calculate the beam line shielding source term.

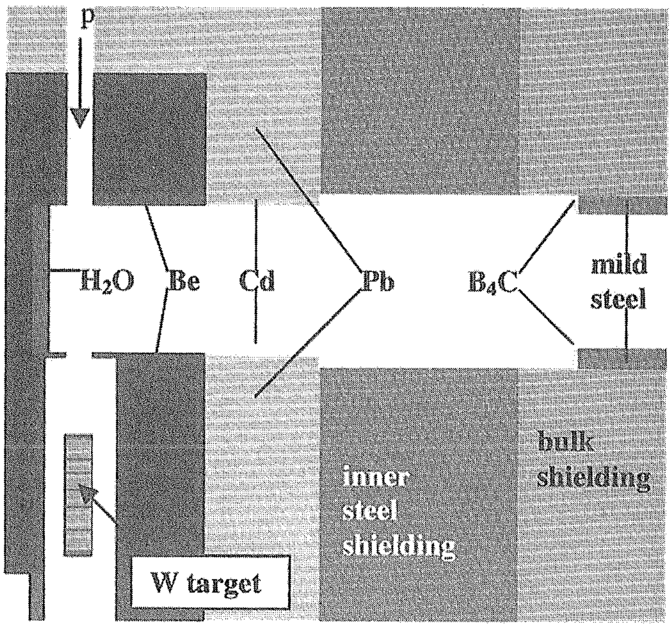

Figure 3. Elevation view of the Lujan Center target station model used to calculate the beam line shielding source term. The dimensions of the above figure are 80 cm long by 30 cm high.

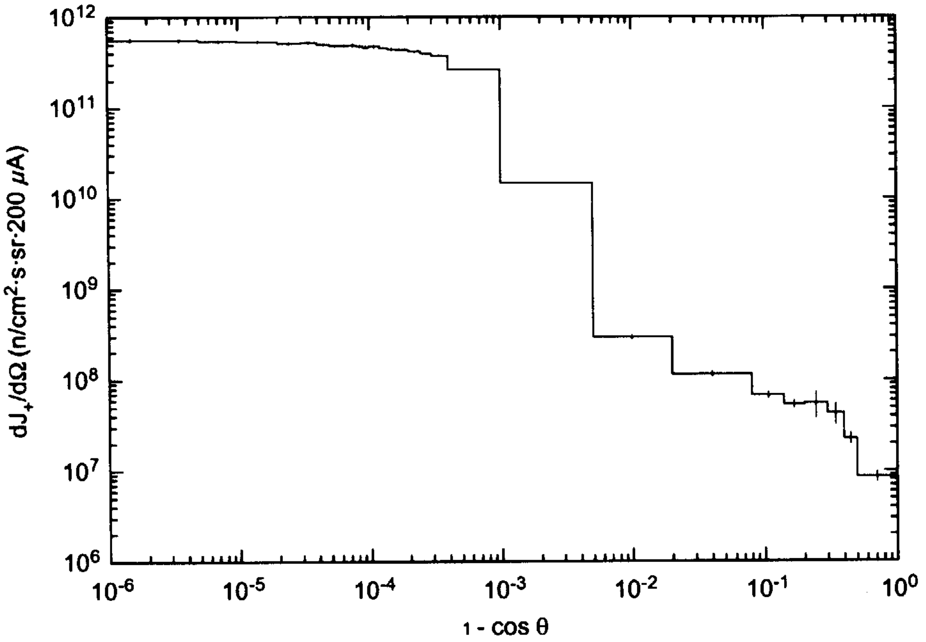

Figure 4. Calculated neutron angular distribution of the source for the flight path 15 (Proton Crystallography instrument) beam line shielding calculations.

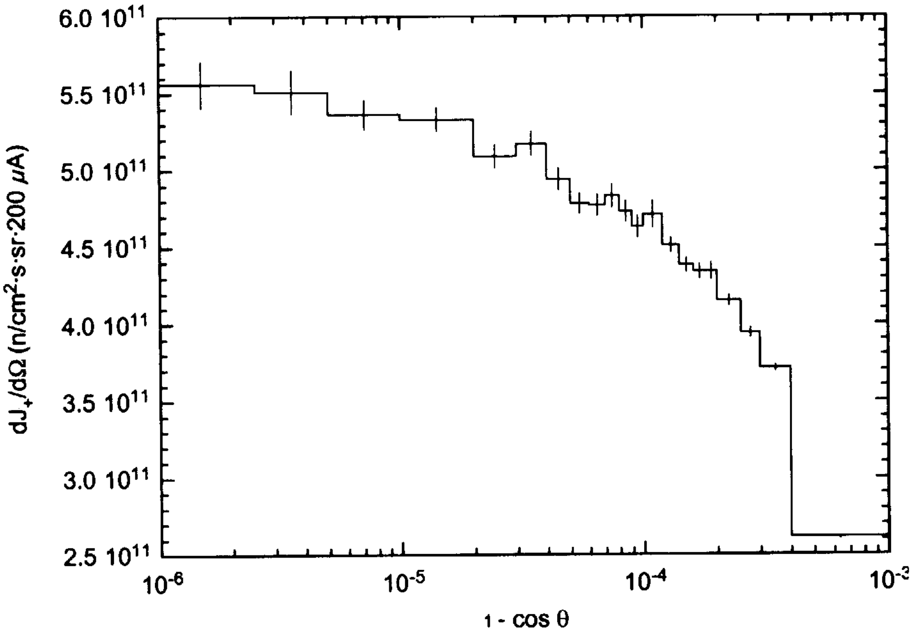

Figure 5. Calculated neutron angular distribution of the neutron source for the Protein Crystallography instrument showing the small angle details.

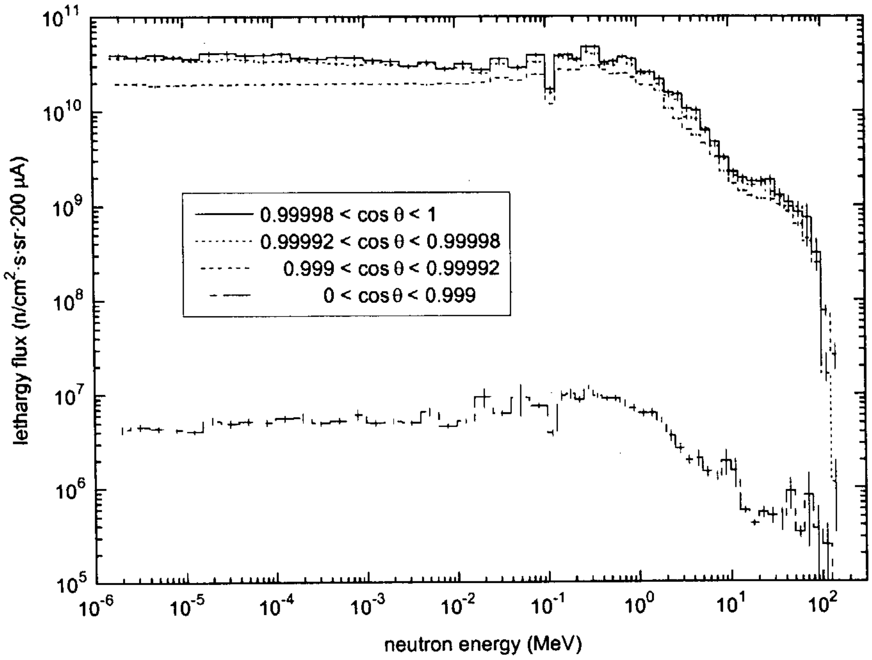

Figure 6. Calculated neutron energy spectra of the source for the flight path 15 beam line shielding calculations as a function of source angle.

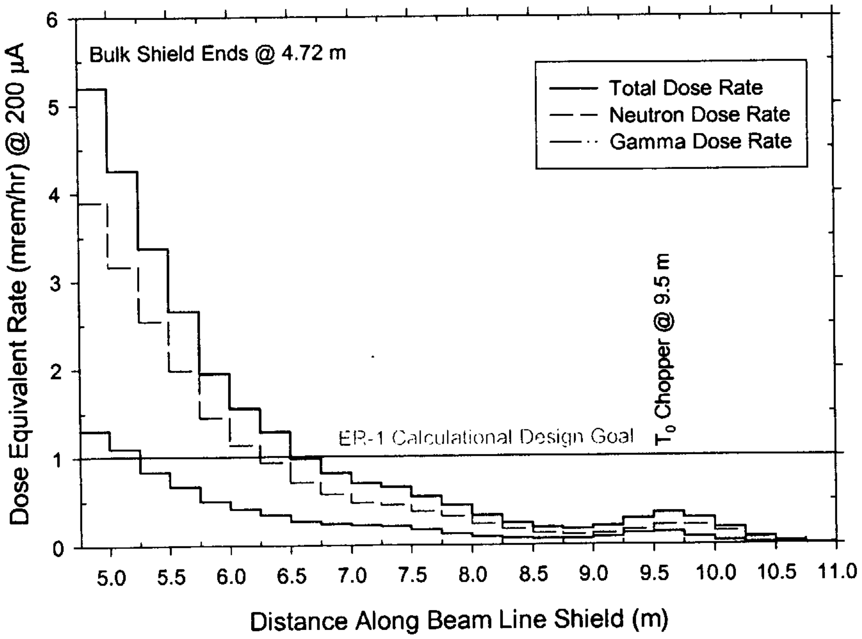

Figure 7. Dose equivalent rate for the 28-inch unperturbed laminated ER-1 beam line shield as a function of distance along the beam line shield.

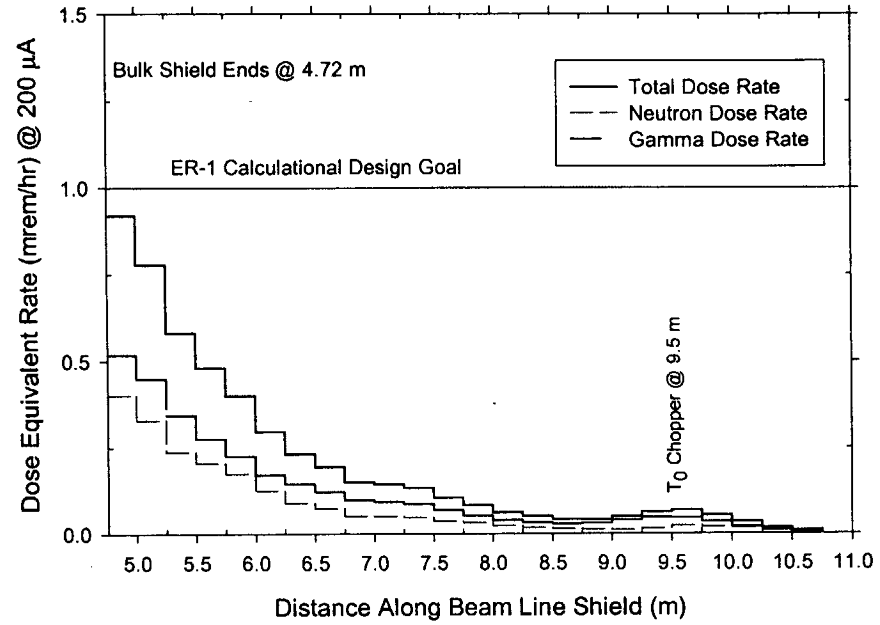

Figure 8. Dose equivalent rate for the 37-inch unperturbed laminated ER-1 beam line shield as a function of distance along the beam line shield.

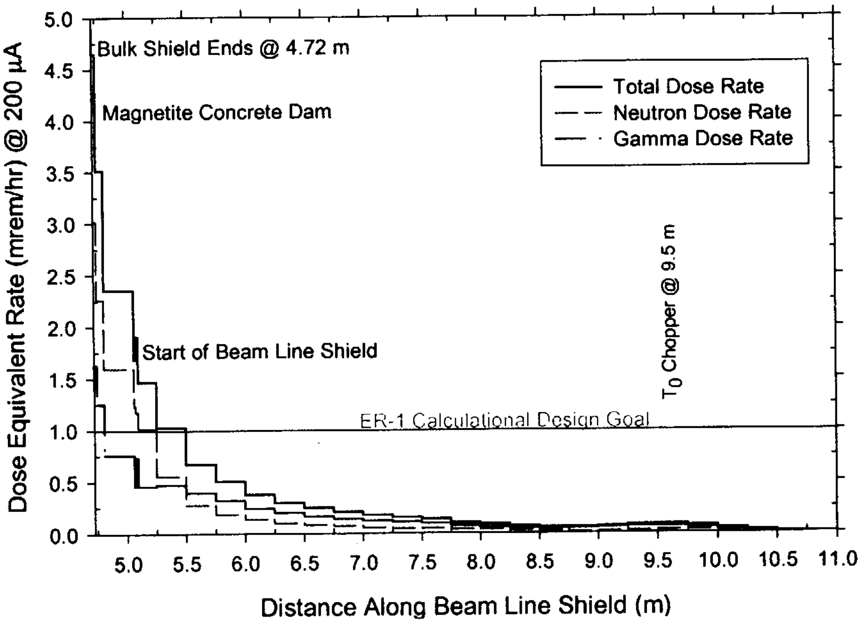

Figure 9. Dose equivalent rate for the 37-inch perturbed laminated ER-1 beam line shield as a function of distance along the beam line shield. The magnetite concrete transition zone and the Hg shutter region (but not the T_0-chopper zone) perturbed the shield.

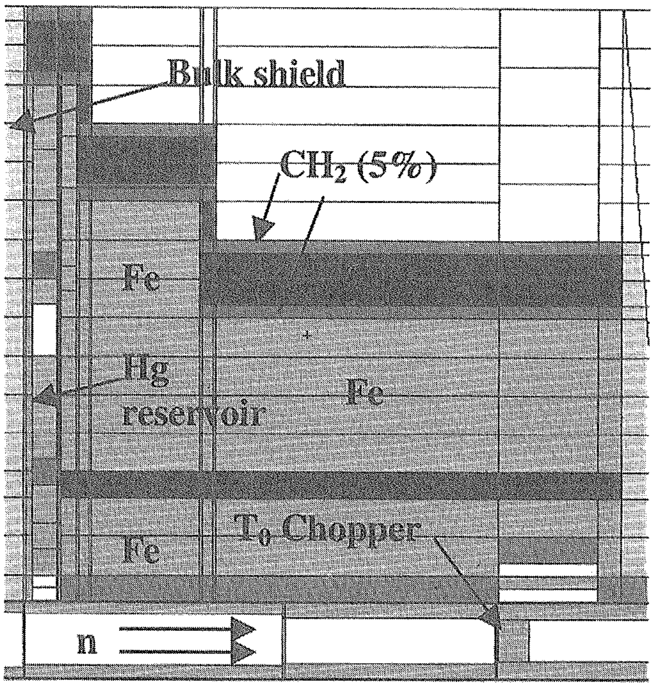

Figure 10. Illustration of the 3-step beam line shield for the Protein Crystallography instrument in ER-1 of the Lujan Center. The neutron beam enters as indicated. The dimensions of the above figure are ~5 m long by ~1.3 m high.

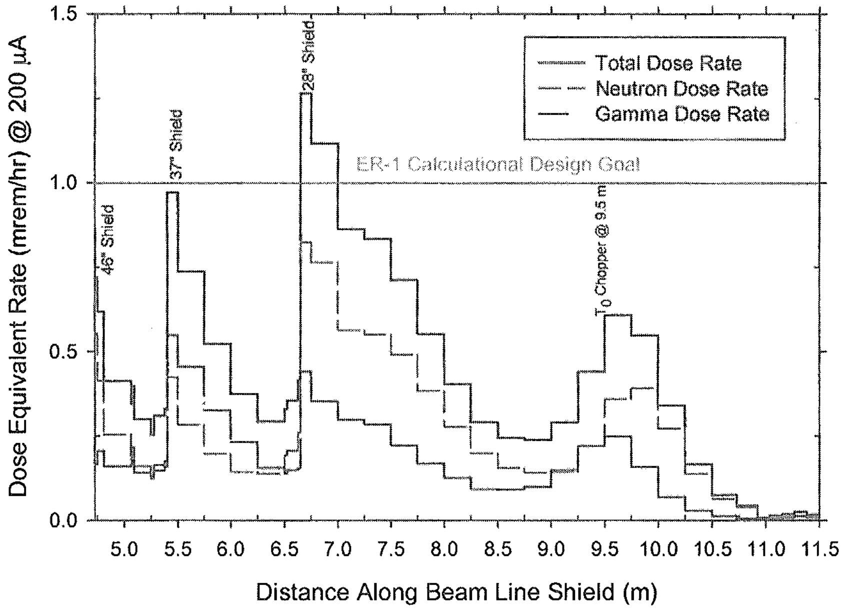

Figure 11. Dose equivalent rate for the 3-step perturbed laminated ER-1 beam line shield as a function of distance along the beam line shield. The magnetite concrete transition zone, the Hg shutter region, and the T_0-chopper zone perturbed the shield

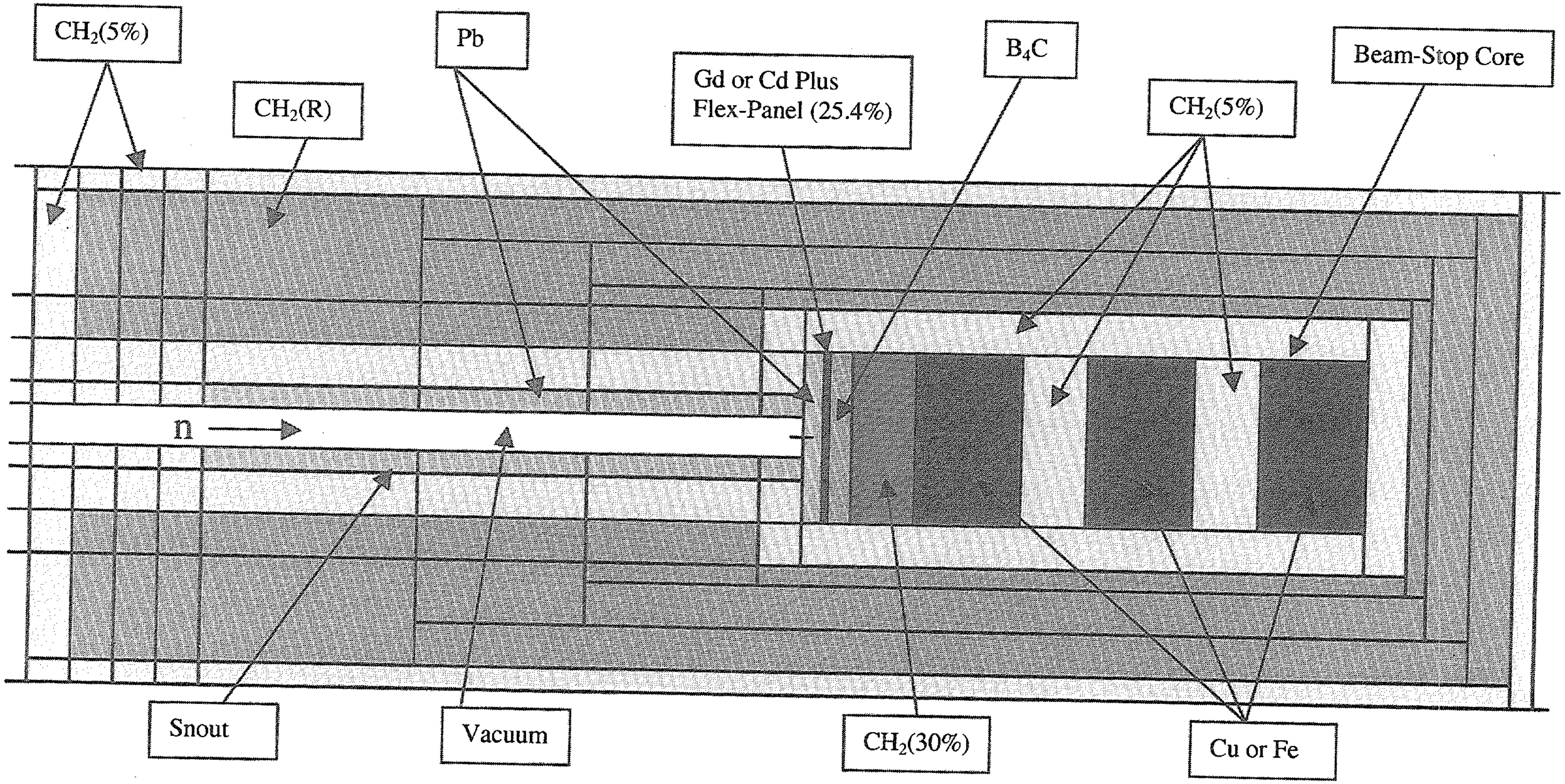

Figure 12. Monte Carlo mockup of the beam stop for the Protein Crystallography instrument (Run #INP70) with an overall snout length of 36 inches. The length of the Pb snout is 28 inches from the surface of the beam-stop core.