COMPUTATIONAL BENCHMARK CALCULATIONS RELEVANT TO THE NEUTRONIC DESIGN OF THE SPALLATION NEUTRON SOURCE (SNS)

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ABSTRACT

The Spallation Neutron Source (SNS) will provide an intense source of low-energy neutrons for experimental use[1]. The low-energy neutrons are produced by the interaction of a high-energy (1.0 GeV) proton beam on a mercury (Hg) target and slowed down in liquid hydrogen or light water moderators[2,3].

Computer codes and computational techniques are being benchmarked against relevant experimental data to validate and verify the tools being used to predict the performance of the SNS. The LAHET Code System (LCS)[4,5], which includes LAHET, HTAPE and HMCNP (a modified version of MCNP[6] version 3b), have been applied to the analysis of experiments that were conducted in the Alternating Gradient Synchrotron (AGS) facility at Brookhaven National Laboratory (BNL). In the AGS experiments, foils of various materials were placed around a mercury-filled stainless steel cylinder, which was bombarded with protons at 1.6 GeV. Neutrons created in the mercury target, activated the foils. Activities of the relevant isotopes were accurately measured and compared with calculated predictions[9]. Measurements at BNL were provided in part by collaborating scientists from JAERI[10] as part of the AGS Spallation Target Experiment (ASTE) collaboration. To date, calculations have shown good agreement with measurements.

Recently available nuclear cross-section data[11], at energies up to 150 MeV, have been provided to the SNS design team by the Accelerator Production of Tritium (APT) project at Los Alamos National Laboratory (LANL). Calculations using this data have been compared to calculations using the physics models in LAHET[4,5] and MCNPX[7,8] and found to make differences in the prediction of low-energy neutrons created in a mercury target. The impact on the predicted moderator output of SNS is found to be small, although there may be other implications, such as increased target heating, that have not been investigated to date.

I. INTRODUCTION

Calculations have been carried out to evaluate the implications of the recently available MCNP nuclear cross-section data to the design of the Spallation Neutron Source. The new data is evaluated to a maximum energy of 150 MeV, while the majority of previously available cross-section data, has generally been limited to energies less than 20 MeV. The physics models implemented in LAHET and MCNPX are most accurate above 150 MeV. Below 150 MeV, quantum effects and nuclear structure details become important and are not accurately represented by the physics models[11]. Extending the range of evaluated cross-section data to 150 MeV should give improved accuracy in calculations. Many of the reactions that occur in the range of energies between 20 MeV and 150 MeV are threshold reactions, which are not represented as accurately in the physics models, as in the measured data. This may result in an inaccurate prediction of some reactions. Neutrons in the SNS target and moderators span the range of energies covered by the new 150 MeV cross section library, making it important to evaluate the impact of this data on predictions of SNS performance.

We are concerned here with the comparison of two sets of calculations, which use the same geometrical model but different cross-section libraries and different calculational techniques in different energy ranges. In the two cases under consideration, one case makes a transition from using physics models to using tabulated cross-section data at 150 MeV and the other at 20 MeV.

a) Above 150 MeV the calculations both use identical physics models of nuclear interactions.

b) Between 150 MeV and 20 MeV, one calculation uses tabulated cross-section data and one uses physics models of nuclear interactions.

c) Below 20 MeV both calculations use tabulated cross-section data, although from different libraries. The two libraries are very similar, but not identical.

II. COMPUTER CODES

Several codes were used in this comparison, including LAHET, HTAPE and HMCNP (from the LAHET Code System: LCS[4,5]) and MCNPX[7,8]. LAHET performs high-energy transport and uses only physics models in its calculations. Residual nuclei, generated by high-energy

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neutrons, are written to a file by LAHET, and translated by HTAPE into a readable format. Low energy neutrons are written to a file and read by HMCNP, which performs the low-energy neutron transport below 20 MeV, using tabulated cross-section data. MCNPX combines the capabilities of LAHET, to perform high-energy particle transport calculations, and MCNP[6], to perform low-energy neutral particle transport. MCNPX uses tabulated nuclear cross-section data below a specified "cross-over" energy, appropriate for the particular cross-section data set, and uses physics models above the cross-over energy. In these calculations the cross-over energy was set to either 20 MeV or 150 MeV. Above the cross-over energy, the same physics models were used by LAHET and MCNPX for all calculations. Calculations using the LAHET-HMCNP calculation sequence cannot use cross-section data from the LA150 library, because the data format is incompatible with HMCNP.

III. MERCURY CROSS-SECTION DATA

To isolate the effect of the mercury cross-section data, only mercury and void space were used in the simple target model. For the comparison, natural mercury cross-section data (80000.40c), evaluated below 30 MeV, was used from the ENDL92 library[10] and the appropriate mix of mercury isotopes (80196.23c, ... , 80204.23c) were used from the new 150 MeV LA150 library[11]. Although the ENDL92 library was evaluated below 30 MeV, it has been used, in our calculations, with a cross-over energy of 20 MeV to be consistent with the cross over energies of other isotopes that were used in similar cases. Hereafter in this report, we will refer to these cross section libraries as the ENDL92 library and the LA150 library, implying associated cross-over energies of 20 MeV and 150 MeV respectively. The ENDL92 mercury cross-section data has been used in many previous transport simulation calculations for SNS. Comparing total neutron cross-section data for mercury from the ENDL92 library and the LA150 library we see very little difference below 20 MeV, except in the resonance region where the two libraries agree only qualitatively.

IV. SIMPLE MERCURY TARGET MODEL

A. Geometric Model

A simple geometrical model of a cylindrical mercury target was constructed to evaluate the differences in predicted neutron flux in calculations with tabulated cross-section data from the ENDL92 and LA150 Libraries. In this comparison, the Monte Carlo radiation transport code, MCNPX was used for all calculations. Above the cross-over energy, the LAHET physics models were used. The geometric model consists of a cylindrical target of mercury and an axially impinging beam of 1 GeV protons. The proton source in this case is a uniform, circular cross-section, monoenergetic beam of 1-cm radius. Cases were evaluated with mercury target radii of 2, 5, 10 and 20-cm. The mercury target was segmented axially, for tallying of the neutron flux, to obtain an axial profile. Tallies of volume averaged neutron flux in each axial segment of the target were compared.

B. Simple Target Simulation Results

The predicted total neutron flux, as a function of axial position in the mercury target, for various target radii, is shown in Fig. 1. At the smallest target radius, the predicted differences in neutron flux are insignificant. As the mercury target radius is increased, the predicted flux differences increase. The percentage increase in total neutron flux using tabulated cross-section data from the LA150 library, ranged up to 30% and is shown in Fig. 2.

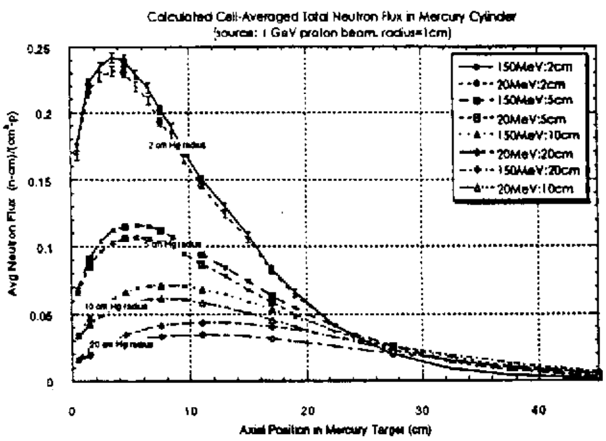

Fig.1. Axial profile of neutron flux in simple cylindrical mercury targets of various diameters.

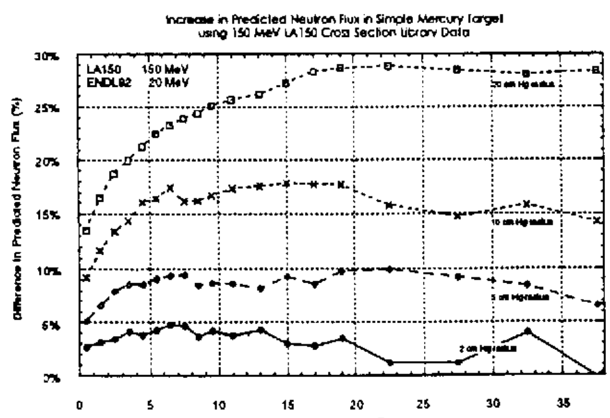

Fig.2. Increase in total neutron flux using data from the LA150 library compared to physics models.

C. Summary of Simple Target Simulations

In geometric models with small dimensions, neutrons produced by the initial collisions of protons with mercury atoms escape almost immediately from the system without undergoing additional interactions. Since only a relatively small number of the neutrons undergo secondary reactions, the differences between calculations using tabulated cross section data and using physics models are expected to be of the order of the statistical uncertainty. As the radius of the mercury target is increased, neutrons produced in the center of the mercury travel longer distances before escaping from the system, thereby increasing the number of secondary reactions. For these cases the model for nuclear interactions in the range of energies of 20–150 MeV becomes more important.

Figs. 3-6 show the neutron spectra in each of the four cases at a location roughly corresponding to the axial peak in neutron flux for all cases which were evaluated. Only results up to 100 MeV are plotted since above this range the two calculations give virtually identical results.

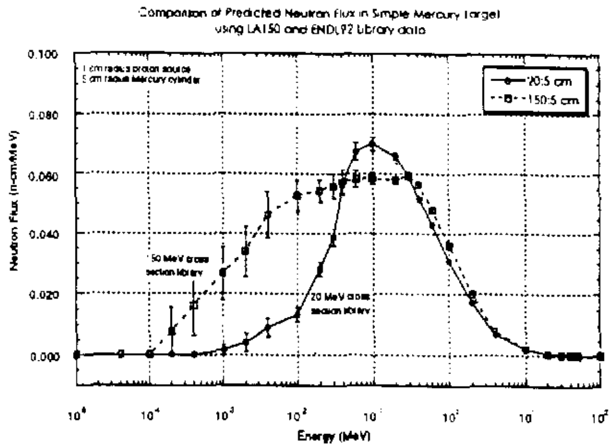

Fig.3. Neutron flux in 2-cm radius mercury target.

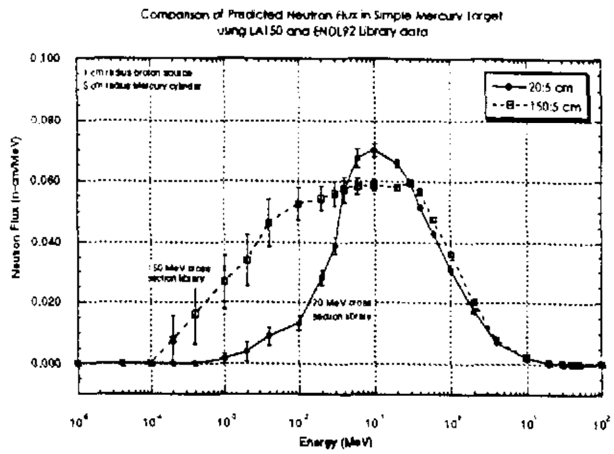

Fig.4. Neutron flux in 5-cm radius mercury target.

We see that most of the differences in predicted neutron flux occur at energies between about 100 eV and 100 keV. Above 10 MeV differences are within the statistical uncertainty, regardless of the cross-section data used. We see also that the differences between predictions are principally on the low-energy side of the peak in the spectrum. Depending on the diameter of the mercury target, using the new cross-section data resulted in predictions of up to 30% higher total neutron flux, and up to a factor of 6 higher flux at particular energies, than was predicted using physics models and cross-section data limited to 20 MeV. To further quantify the differences predicted by using the 150 MeV cross-section data, additional tallies of neutron flux, leakage or heating would be needed in other regions of the geometrical model.

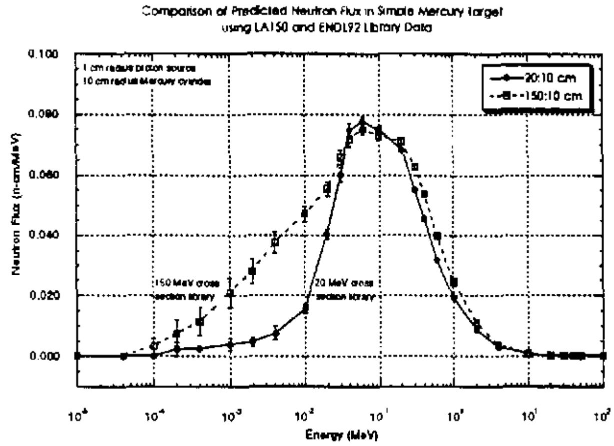

Fig.5. Neutron flux in 10-cm radius mercury target.

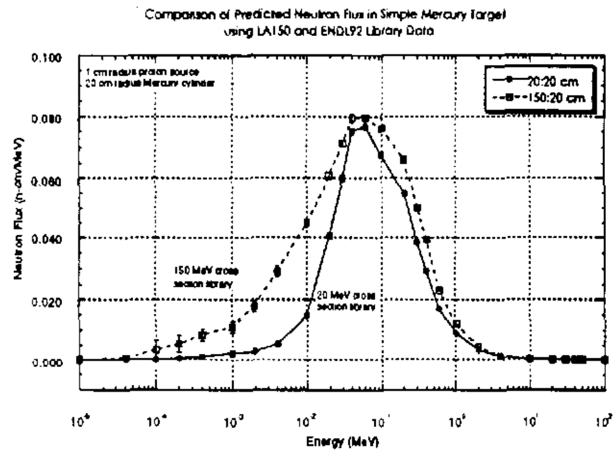

Fig.6. Neutron flux in 20-cm radius mercury target.

V. SNS TARGET AND MODERATOR MODELS

Given that the simple mercury target model predicted differences in neutron flux and spectrum, when using the 150 MeV cross-section data compared to physics models, another set of test cases were evaluated using a recent model of the SNS target and moderator region, shown in Fig. 7. The cases represent possible moderator options for SNS and were evaluated to assess the potential impact in a realistic geometry. In the SNS model there are four moderators, two in the upstream position, closest to the proton beam source ('Upstream' designation), and two in the downstream location ('Downstream' designation). Moderators located above the path of the proton beam ('Top' designation) are liquid hydrogen moderators and moderators located below ('Bottom' designation) are ambient water moderators. For each of these, cases were evaluated with de-coupling and poison layers included ('De-coupled' designation) and with the de-coupling and poison materials replaced by void space ('Coupled' designation). In this comparison, the only measure of difference between calculations is the tabulation of leakage from the moderator face into a beam tube. Additional tallies of neutron flux or heating would be desirable to quantify differences.

A. De-Coupled Moderator Output

De-coupled moderators are surrounded by cadmium sheets (de-coupler) and divided by gadolinium foils (poison), for which there are no cross sections available in the LA150 library. In this comparison, they were both replaced with ^{199}Hg, which also has a large thermal neutron absorption cross-section, very similar to cadmium. The density was increased to compensate for differences in neutron thermal absorption cross-section between ^{199}Hg and the normal de-coupling and poison materials. A density increase factor of 1.96 was applied to ^{199}Hg. However, ^{199}Hg has a much smaller thermal absorption cross-section than gadolinium and in this case the number density was increased by a factor of 21 to equate the macroscopic thermal neutron capture cross-section.

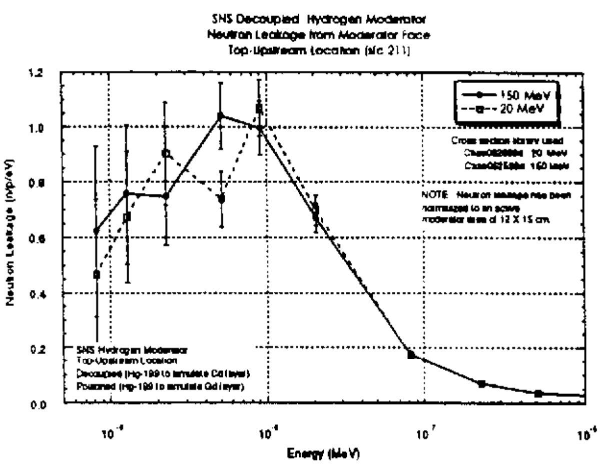

Fig. 8. Comparison of predicted neutron leakage from a de-coupled hydrogen moderator.

Figs. 8 and 9 show the predicted leakage from a de-coupled hydrogen moderator, in the top-upstream location, and a de-coupled water moderator, in the bottom-upstream location, using the LA150 and ENDL92 libraries. For both cases, the largest difference was 10% or less in regions where the statistical uncertainty was small. The additional low-energy neutrons, predicted in the simple mercury target model, are likely produced here also but are lost through absorption in the mercury. They may however, contribute to heating or other effects in the target, even though they do not appear in the leakage from the moderators.

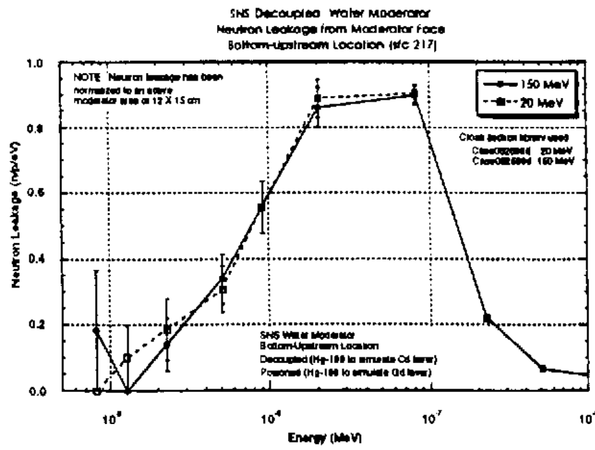

Fig. 9. Comparison of predicted neutron leakage from a de-coupled water moderator.

B. Coupled Moderator Output

Another set of cases simulated the SNS with coupled moderators by replacing the de-coupling material (cadmium) and poison material (gadolinium) by void space. Figs. 10 and 11 show the predicted leakage from a coupled hydrogen moderator, in the top-upstream location and a coupled water moderator, in the bottom-upstream location. As in the de-coupled moderator cases, coupled moderators showed only small differences, when simulated using the LA150 library rather than physics models. In coupled moderator cases, the overall leakage is higher than in de-coupled moderator cases due to the absence of the absorbing cadmium and gadolinium layers.

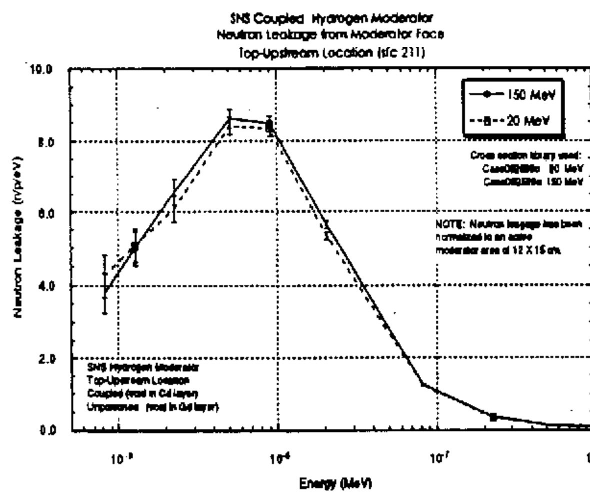

Fig. 10. Comparison of predicted neutron leakage from a coupled hydrogen moderator.

Over the majority of the energy spectrum below 1.0 GeV, the moderator leakage calculations, using the LA150 cross-section data rather than the physics models, are nearly identical. Virtually no differences are seen in moderator leakage above 1 eV and generally the differences are within the statistical uncertainty. In other simulation situations, or with other energy ranges of interest, the LA150 cross section library may, however, result in differences that are quite important.

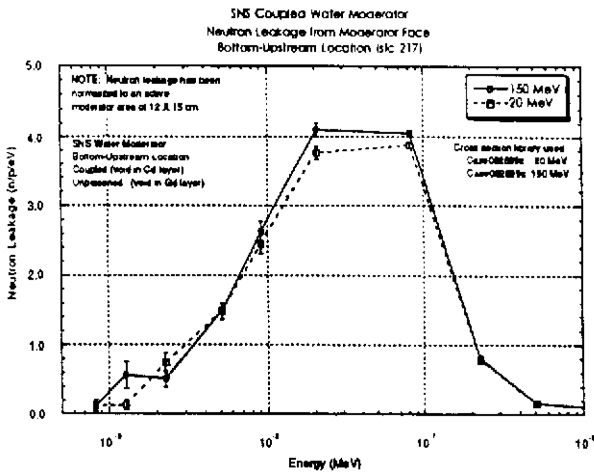

Fig. 11. Comparison of predicted neutron leakage from a coupled water moderator.

C. Summary of SNS Simulation Results

VI. AGS EXPERIMENTS

A. Introduction

At the Alternating Gradient Synchrotron facility at Brookhaven National Laboratory experiments have been carried out to measure the radioactive nuclei formed in a set of foils irradiated by neutrons generated in a mercury spallation source[9,10]. The results of these experiments have been used to benchmark the calculational techniques being used in the design of the Spallation Neutron Source. In the AGS experiments, foils of various materials were placed around a mercury-filled stainless steel cylinder, which was bombarded with protons at 1.6 GeV. Neutrons created in the mercury target activated the foils. Activities of the relevant isotopes were accurately measured and compared with calculated predictions[9]. The AGS experimental team used multiple methods to determine the proton beam intensity and profile[10]. After irradiation, the foils were analyzed with gamma ray spectroscopy to determine the number of nuclei generated in each foil during the experiment. In the benchmarking calculations, the LAHET Code System was used to predict the number of specific reactions in each metal foil due to neutron bombardment.

B. Benchmark Calculations of AGS Experiments

The AGS geometrical model consists of a stainless steel cylinder, 10-cm in radius, filled with natural mercury. The incident proton beam is 10-cm in radius with a parabolic radial intensity profile at an energy of 1.6 GeV. Metal foils 2-cm x 2-cm x 0.1 cm are located near the surface of the target along its length. Simulations were done with foils represented discretely and also with foils represented as annular rings around the target. The annular model gave much better statistical results because the foils experienced about 30 times more neutron flux for the same incident proton beam. The 1.6 GeV proton beam in the experiment was estimated to contain 3.7×10^{13} protons. Schematic, transverse cross-sections of the two geometry options are shown in Figs. 12a and 12b. An axial cross section is shown in Fig. 13.

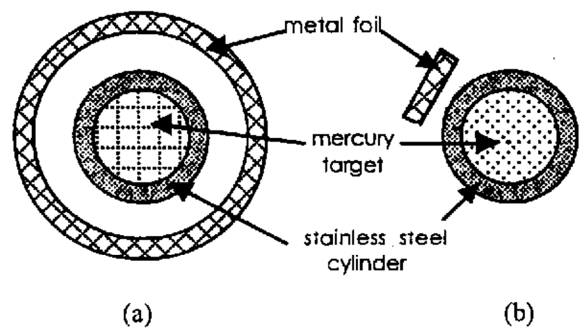

Fig. 12 Schematic transverse cross-sections of (a) annular and (b) discrete AGS foil models.

C. Analysis Technique

Calculations were done, using the LAHET Code System to predict activation products in the foils. MCNP reaction cross section data did not exist for all reactions which were studied experimentally. To obtain sufficiently good statistics, 500,000 particle histories were used in the final calculations using the annular model, giving average uncertainties of a few percent.

LAHET was used to calculate high-energy reactions from the proton beam interaction in the mercury and the high-energy neutron reactions in the metal foils resulting in the creation of radioactive nuclei. Residual nuclei, generated by high-energy neutrons, are written to a file by LAHET, and translated by HTAPE into a readable format. Low energy neutrons are written to a file by LAHET and read by HMCNP, which performed the low-energy neutron transport calculations. After completion of the calculations, the high-energy contribution to the residual nuclei, from LAHET, and the low-energy contribution from HMCNP, were combined manually to obtain the total foil activation for each foil material, in each location.

LAHET calculates the total number of residual nuclei for each cell (nuclei / source particle). MCNP calculates the production rate of specific isotopes in each cell (nuclei/cm^3/source particle). To combine the results of the low- and high-energy parts of the calculation, we divide the LAHET result by the volume of the foil in the model to put it into the same terms at the MCNP result. These two parts are summed to obtain the total isotope production rate / source particle. The proton beam source was determined experimentally[10]. The total number of 1.6 GeV protons delivered to the target during the experiment is estimated to be 3.7 x 10^{13} protons. The total isotope production rate is multiplied times the actual foil volume times the source (total number of protons) and multiplied by the decay constant of the particular isotope to get the activity of the foil in Becquerels.

D. AGS Simulation Results

For the purposes of this study, selected foil materials and nuclear reactions were compared. The principal materials that were compared, were cobalt and nickel, although iron and bismuth were also simulated early in the study. Figs. 14-15 show the comparison of predicted and measured activities for (n,p) and (n,d) reactions in nickel foils. Differences in predictions and measurements were generally less than a factor of 2. The comparison of results for (n,p) and (n,2n) reactions in cobalt foils are shown in Figs. 16-17, respectively. Cobalt foils showed somewhat less agreement than nickel, although the general behavior was reproduced well.

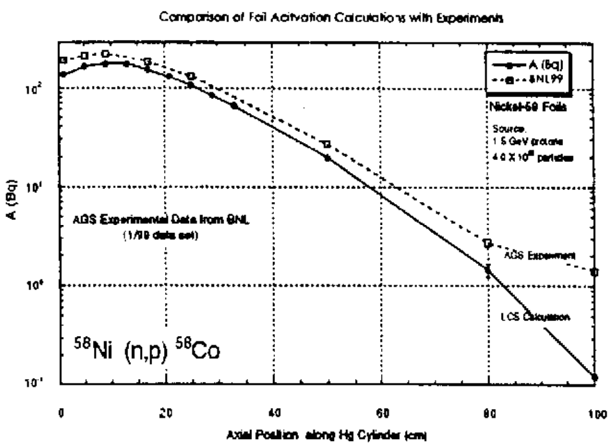

Fig. 14. Comparison of predicted and measured activity in a nickel foil due to (n,p) reactions.

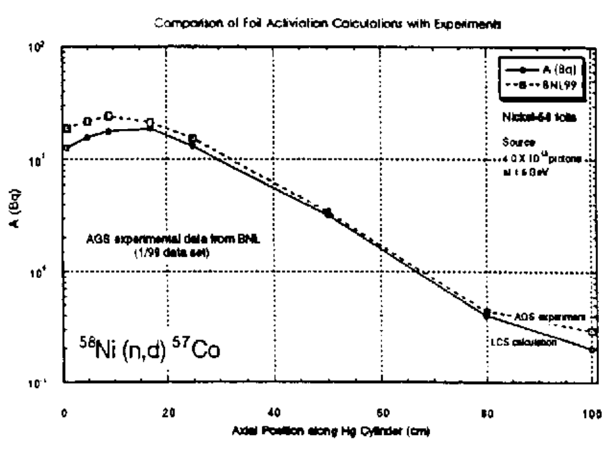

Fig. 15. Comparison of predicted and measured activity in a nickel foil due to (n,d) reactions.

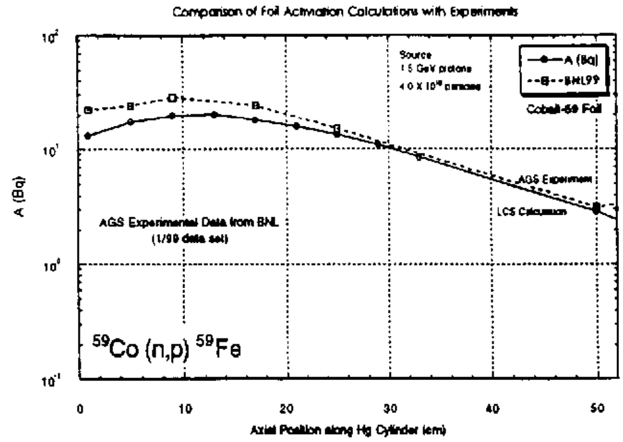

Fig. 16. Comparison of predicted and measured activity in a cobalt foil due to (n,p) reactions.

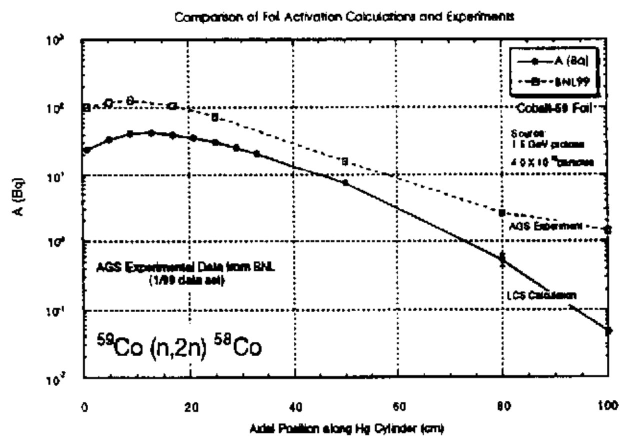

Fig. 17. Comparison of predicted and measured activity in a cobalt foil due to (n,2n) reactions.

E. Discussion of AGS Simulation Results.

The majority of the simulations reproduced experimental results quite well, considering the simplicity of the model. Experimentally measured activities were almost universally somewhat greater than calculated values, but whether this is due to differences in the experimentally-determined proton source term, or due to back-scatter that was not included in the simulations, is not known. For both nickel and cobalt foils, the calculations deviate slightly more from measurements at the furthest downstream foil location, suggesting that the measurement may have been perturbed by 'end effects' in the experimental arrangement. Nearby equipment and structures, which could cause back-scatter, were not included in this simulation model. These include a stainless steel target enclosure, a steel lift-table and nearby concrete floor and walls. The 150 MeV cross-section data, discussed earlier, more accurately represents the interaction events in the critical range of energies for the events of interest and might have improved the agreement of calculations with the experiment. Unfortunately, the partial reaction cross sections, necessary to calculate individual reactions are not available for the LA150 library. It is, however, very encouraging that even this simple model gave reasonable agreement with experimental measurements.

F. Summary of AGS Simulations

A simple model was able to reasonably reproduce experimental results in most cases. Agreement within factors of 1.5 – 1.7 were typical for these cases. All of the essential structure of the behavior of the experimental data was reliably reproduced in the simulations. Inclusion of additional details of the experimental environment will likely improve the agreement by adding scattering, onto the foils, which does not occur in this simple case.

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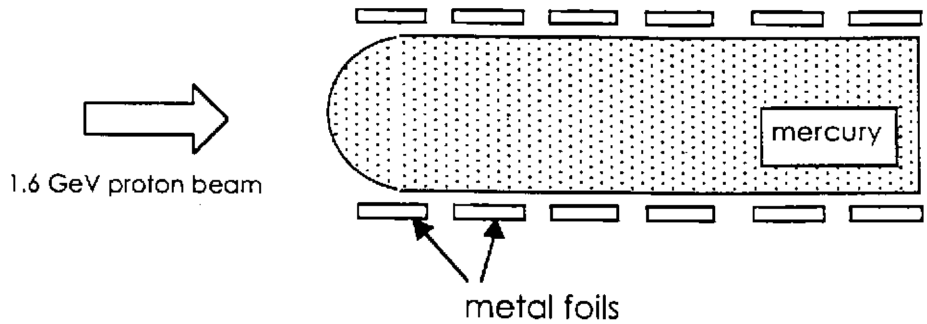

Fig. 13. Schematic axial cross-section of the geometric model used in LAHET, HMCNP and MCNPX to simulate foil activation experiments in the AGS experiments.

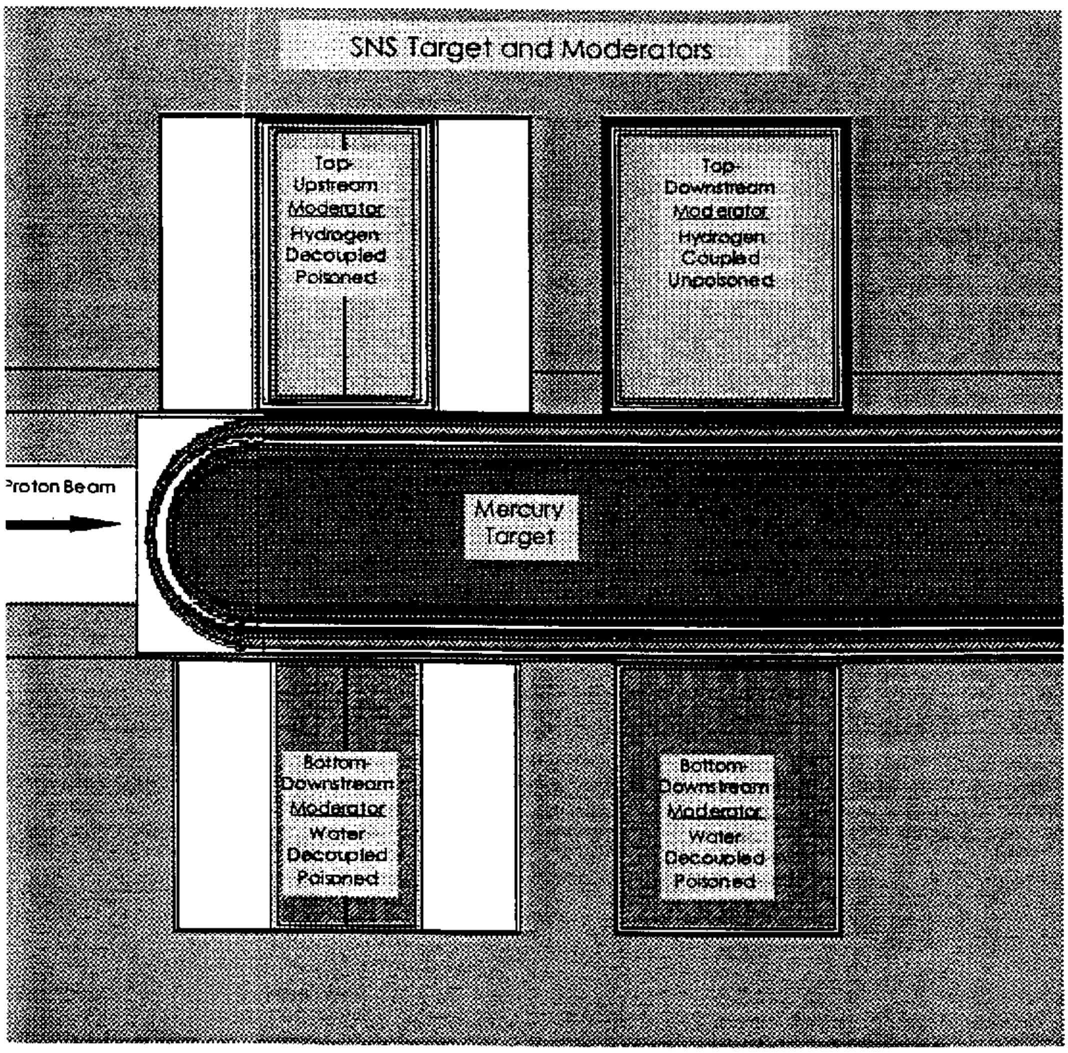

Fig. 7. Cross-section of MCNP geometrical model of SNS target and moderator region.