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CALCULATIONAL METHODS AND HIGH ENERGY CROSS SECTIONS FOR SPALLATION SOURCE SHIELDING

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SUMMARY

The features of the calculational methods being used at KFA for SNQ target shield design studies are discussed. The existing high-energy cross section data base is checked against the requirements of these calculations. The two available libraries, HILO and LANL, are intercompared by calculation of neutron fluxes in an iron sphere as a simple benchmark. This benchmark problem was also used to compare codes. A fast running, easy to operate shielding layout and assessment code called CASL is described, which uses approximate, semi-empirical physics treatment.

1 INTRODUCTION

Shielding problems of high proton current spallation neutron sources are unique in terms of calculational requirements because of the combination of a relatively high-energy source, large shielding dimensions, and geometric complexities. Presently there does not exist a computer code system and furthermore only few data suitable for high energy neutron transport calculations are available. There is little experience with the type of calculations needed and the influence of the presently available data bases are not known.

Therefore, we checked the data and computer codes available, whether they are suitable to meet the difficult requirements of this predominately deep penetration problem and proposed a "high-energy neutron shielding benchmark", as neutrons are the main particles in this context. The benchmark allows both comparison of cross-section data libraries and different methods of calculation.

2 CROSS SECTION DATA BASE

The shielding code system suggested here requires high-energy multigroup cross section data for the discrete ordinates transport calculations. Much of the needed cross section data are available, but present data base is not completely compatible with SNQ application requirements because the maximum neutron energy considered is 800 MeV. Also, there are other approximations in the present data base whose accuracy is questionable for the very thick shields of interest for the SNQ.

The approach suggested here is to make ad hoc modifications to the present data to allow "Phase I" calculations to be made, which would include transport calculations to test the importance of present approximations.

2.1 Status of Present High-Energy Transport Cross Section Data Base

A multi-energy group cross section library (called HILO /1/) for coupled neutron/γ-ray transport has recently been developed at ORNL in a format compatible with ANISN and DOT input requirements. Features of this library are summarized in Table I. These data have been obtained by using experimental data at low energies (< 14.9 MeV) and theoretical models at high energies (14.9 - 400 MeV).

Table I

Features of the HILO Library

- Energy Range

  Neutrons: thermal to 400 MeV
  γ rays: 10^{-2} MeV to 14 MeV

- Group Structure

  66 neutron groups
  21 γ-ray groups

- Angular Expansion

  P_5 expansion for E>14.9 MeV
  P_3 expansion for E<14.9 MeV

- Elements Available

  H,B,C,N,O,Na,Mg,Al,Si,
  S,K,Ca,Cr,Fe,Ni,W,Pb

Some work has also been done at Los Alamos /2/ to obtain a high-energy cross section set which extends for neutrons to 800 MeV. These cross sections were obtained in a manner similar to that of the HILO library -- i.e., ENDF data at low energies (<20 MeV) and optical model and intranuclear-cascade-evaporation model calculations for higher energies. The features of the LANL library are given in Table II.

Table II

Features of the LANL Library

- Energy Range

  Neutrons: thermal to 800 MeV

- Group Structure

  41 neutron groups
  (8 groups above 50 MeV)

- Angular Expansion

  P_3 expansion

- Elements Available

  H,C,O,Al,Si,Fe,Mo,W,Pb

It should be noted that the Los Alamos cross section library does not include elastic scattering for nuclides other than H at high energies. This may have implications for the SNQ bulk shielding calculations in comparing iron vs. cast-iron since cast-iron contains nominally 20 atom per cent C and Si.

2.2 Approximations in Present Data Base

The main restriction in using directly the HILO library is that the maximum neutron energy allowed is 400 MeV, whereas for the SNQ we have neutrons up to the proton beam energy of 1100 MeV.

Other considerations for present applications of the HILO data base include:

1) The high-energy neutron production is based on intra-nuclear-cascade-evaporation model calculations where the spectra were tabulated in rather broad angular intervals(0-30°, 30-60°, 60-90°, and 90-180°) The radiation penetrating deeply in thick shields is mainly high-energy neutrons with peaked angular distributions. Therefore, it is not clear that these few broad angular intervals are adequate for very deep penetration problems.

2) The cross sections represent neutron production by neutron induced collisions. Thus, if neutrons actually produce charged particles (protons or pions) in collisions, and these charged particles produce neutrons, these latter neutrons are not accounted for.

3) The γ-rays produced by low-energy (<14.9 MeV) neutron collisions are included, but γ-ray production by higher-energy neutron collisions is neglected.

4) For the very heavy elements (W and Pb) elastic scattering is neglected because the P_5 order expansion is not adequate to describe the angular distributions.

5) The high-energy neutron cross sections were generated using a version of the intranuclear-cascade-evaporation model that existed in the early 1960's. There have been several improvements to the model (and the input data used) since then. The Los Alamos library was also generated using old versions of the model -- MEÇC-3 and EVAP-3. There is not much documentation about the Los Alamos library. However the approximations given above are similar also in this library.

2.3 Library Comparison by Benchmark Calculations

Requirements to the Benchmark:

- It is thought of a bulk shielding problem only
- Geometry should be simple that one-dimensional transport codes can run without approximations and results can be compared directly with Monte Carlo.
- Only neutron are considered as they are dominant particles and most radiation transport codes work only on neutral particles.
- Source energy of those neutrons should be sufficiently high and identical in all calculations.

With the above requirements the following modell was defined:

- Iron sphere of 200 cm radius density of the iron: ρ=8 g/cm^3
- no impurities
- a homogeneous and isotropic neutron source is located in the center as a sphere of radius 5 cm. The energy spectrum of that source is a flat distribution from 300 to 400 MeV, comprising exactly the first 4 energy groups of the HILO library and the fifth group of the LANL library, the highest groups that are common to both of the two existing libraries in the high energy region.

The Monte-Carlo-Code considered was the HETC program, and for one-dimensional transpt calculations ANISN. For the calculations here the energy range was taken from 50 to 400 MeV, because onyl high-energy neutrons are of interest to deep penetration and both libraries have group limits at 50 and 400 MeV, respectively.

The iron sphere was radially subdivided into 40 meshes of 5 cm, to perform the following 4 ANISN calculations:

with library	to expansion
HILO	P_0 (HILOP$_0$)
HILO	P_5 (HILOP$_5$)
LANL	P_0 (LANLP$_0$)
LANL	P_3 (LANLP$_3$)

In addition a HETC calculation was made and evaluated with the auxiliary code SIMPEL /3/. SIMPEL produces mesh fluxes for primary and secondary neutrons, the sum of which was compared with the ANISN results.

Results of the Benchmark Calculations

Fig. 1 shows the neutron flux of the source group for ANISN calculations HILOP$_0$ and HILOP$_5$. It is seen, that the flux in the surface mesh (at 200 cm) is higher by orders of magnitude in the HILOP$_5$ than in the HILOP$_0$ calculation. This, however, was to be expected, but leads to the question whether a P_5 expansion of the cross-section is already sufficient to describe transport of high energy neutrons adequately.

Fig. 2 shows the neutron flux of the source group for ANISN calculations LANLP$_0$ and LANLP$_3$. Unlike the results of the HILO calculations the flux in the surface mesh is for LANLP$_3$ only twice that of LANLP$_0$. This somewhat surprising result is due to the fact that there is no elastic scattering cross-section for high energies in the LANL library and on the other hand elastic cross sections in HILO are much too high in this energy region.

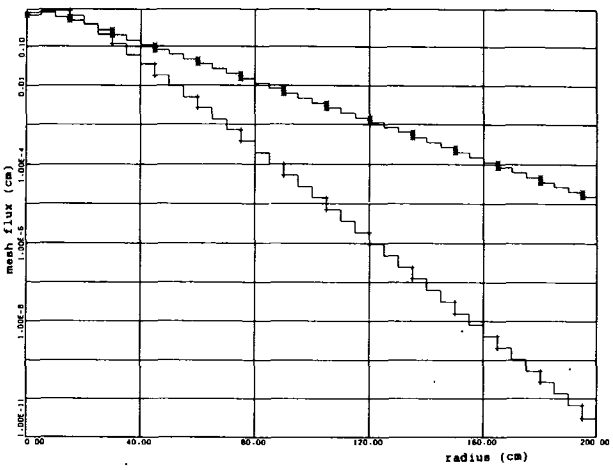

Fig. 1 Neutron Flux (300-400 MeV) per Source Neutron (Integrated over Mesh and Time) + HILOP0 * HILOP5

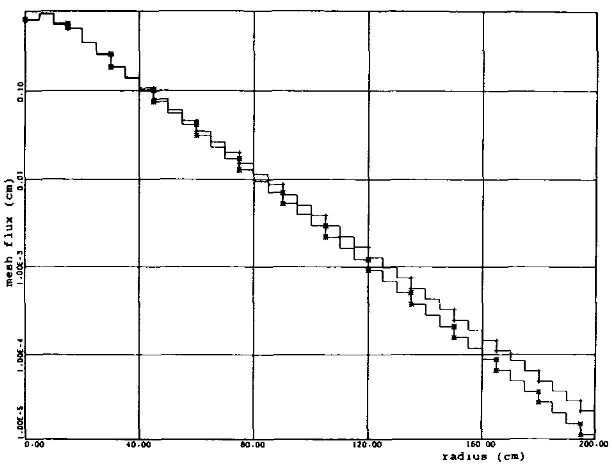

Fig. 2 Neutron Flux (300-400 MeV) per Source Neutron (Integrated over Mesh and Time) * LANLP0 + LANLP5

Because naturally the calculations in the higher P orders give higher fluxes in the surface mesh, the results of these calculations were compared. Fig. 3 shows the flux in the whole energy range from 50 to 400 MeV. The general trend, which is stated here is that using higher P expansion of neutron cross sections leads to higher fluxes in the surface mesh. Thus the question arises whether the current available expansions (P_3 for LANL, P_5 for HILO) are sufficient. To clarify this the ANISN $LANLP_3$ calculation which results in the highest flux was compared to an according HETC-Monte-Carlo calculation.

In general can be stated, that flux values of $LANLP_3$ are lower in the vicinity of the surface than those of the HETC calculation. The discrepancies are, however, with standard deviation of about 30 % marginal in the case of HETC and should therefore not be overemphasized.

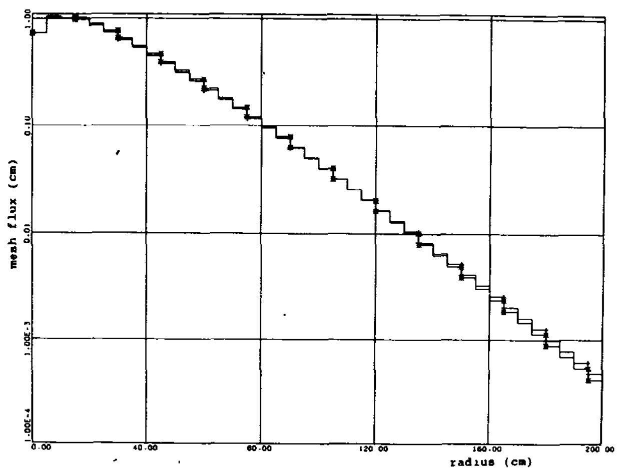

Fig. 3 Neutron Flux (50-400 MeV) per Source Neutron (Integrated over Mesh and Time) + HILOP5 * LANLP3

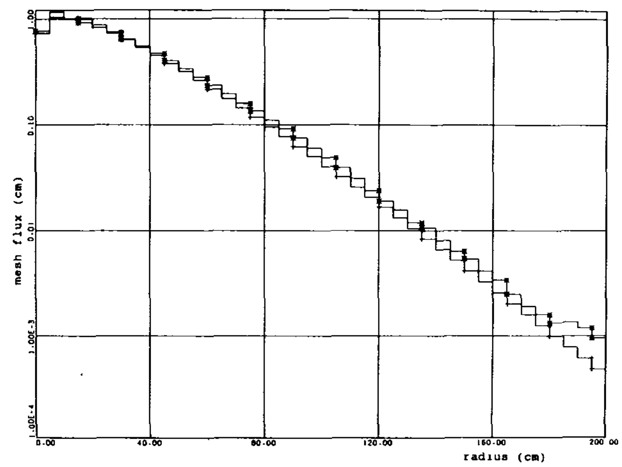

Fig. 4 Neutron Flux (50-400 MeV) per Source Neutron (Integrated over Mesh and Time) * HETC + LANLP3

How insufficient the representation of the forward peaked cross section data might be, may be judged from Fig. 5 in which the angular distribution of certain LANL data is compared to a HETC calculation.

2.4 Data Base Modifications for Temporary Usage

The high energy cross section library HILO has the advantage of containing γ-cross-sections, but it has the disadvantage that the maximum energy is 400 MeV and that furthermore the elastic scattering seems to be incorrect. The LANL library has the advantage that the maximum energy is 800 MeV, but has the disadvantage that γ-ray-cross-sections are neglected. So we decided to generate a library which combines the advantages of both libraries:

We combined the libraries LANL and HILO in a way, that LANL-data are used for the neutron cross sections in the energy range from 800 MeV to 50 MeV and that HILO-data are

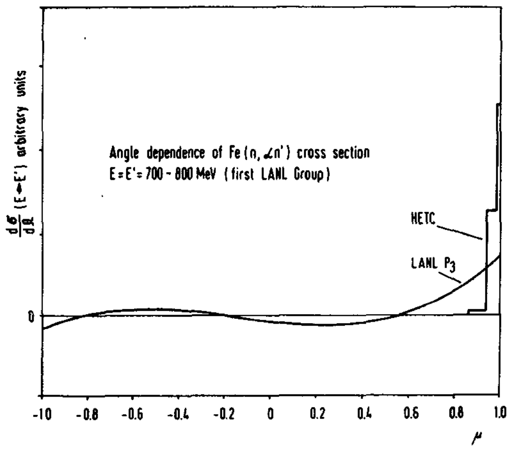

Fig. 5 Comparison of Angle Dependence of LANL P_3 Data with HETC Calculation

used for neutron energies less than 50 MeV and for γ-groups. The new library contains the following eight elements as ANISN-formatted data in Legendre expansion P_3:

H, C, O, Al, Si, Fe, W, Pb

The library consists of 53 neutron groups and 21 γ-groups.

Some provision has to be made for neutrons in the range from 800 MeV (present upper limit) to 1100 MeV (SNQ source energy). One simple method would be to assign all neutrons in this energy range to the midpoint of the energy group (700-800 MeV) presently allowed by the cross section set, but with an increased neutron multiplicity to conserve energy. That is, the statistical weight of a source neutron with energy E>800 MeV would be multiplied by E/750. This is somewhat justified because the neutron total cross sections are approximately constant in this energy range. However, the partial inelasticities (fraction of energy carried away from a collision by secondary particles) varies.

2.5 Data Updates for High-Energy Shielding Codes

We suggest that new cross sections be generated for at least one shielding material (Fe) with the energy range extended to 1100 MeV and with finer angular resolution than the four broad intervals in the present HILO data base. This will allow transport calculations to be made to see the difference in shield attenuation prediction by the present and updated data for the case of an Fe shield. A decision can then be made as to whether new cross sections should be generated for other materials.

One way of obtaining these updated cross sections is to use the same procedure as used in generating the HILO cross section set, which consisted of: (a) calculating differential particle emission spectra and nonelastic cross sections using the Monte Carlo intranuclear-cascade-evaporation model, (b) fitting these histogram data with continuous analytic functions for interpolation and to reduce the influence of statistical fluctuations, and (c) applying these analytic representations to put the data in the multigroup, Legendre expansion format needed by the transport codes. In the HILO library, a 1/E flux weighting factor was used for averaging the cross sections over energy group.

To account for the extreme forward peaking of the new data it is necessary to use very high P order expansion. To give an impression Fig. 6 shows several P approximations of a certain neutron production cross section of protons (the situation for neutrons is very similar). As can be seen, only P_{19} seems to be adequate. This may cause difficulties in using those data by the transport codes.

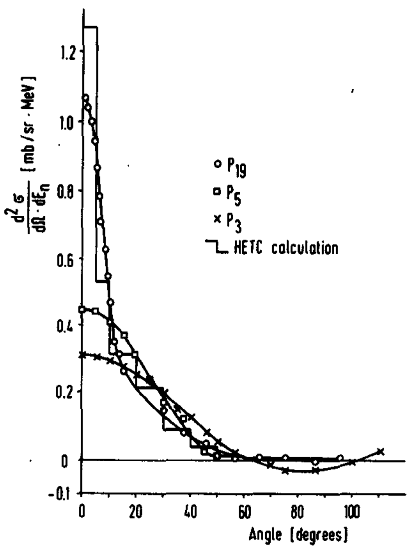

Fig. 6 Legendre Expansion of the Neutron Production Cross Section for Protons on Iron: E_p=1100 MeV, E_n=500-550 MeV

Nuclear elastic scattering at high energies (> 15 MeV) is a mechanism which is often neglected in high-energy radiation transport calculations because the energy loss and angular deflections from such interactions are small. However, there are several situations related to SNQ shielding estimates and heating where elastic scattering effects may be important. For example, small angular changes can effect shield attenuation for very deep penetrations.

Assessment of Elastic Cross Sections

Elastic cross sections for neutrons have been collected from several sources for comparison. For example, Figure 7 compares several sets of data for iron including: (a) Cross sections from the low-energy (< 19.6 MeV) DNA library /4/, which is based on ENDF data. (b) Cross sections from the ORNL high-energy (< 400 MeV) HILO library. (c) Cross sections from NASA compilation for the energy range 100 MeV to 22.5 GeV /5/. (d) The measurents of Schlimmerling et al. /6/ in the 400-1000 MeV range, and the measurements of Bellettini, et al., /7/ at 20 GeV.

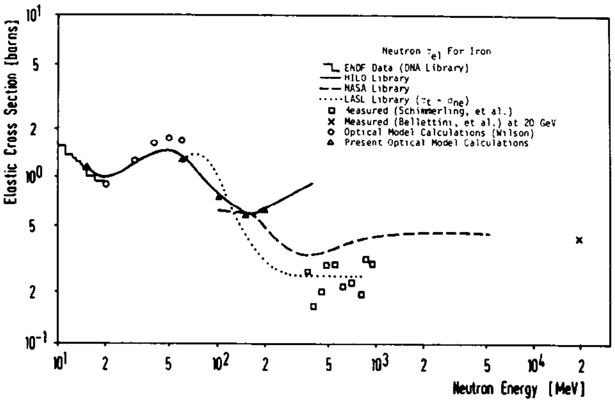

Fig. 7 Elastic Scattering Data

The main conclusion from Fig. 7 is that there are large differences in the data in the 10^2 - 10^3 MeV range. In particular, the HILO values appear incorrect > 150 MeV. (This is also the case for other elements, e.g. the reason for the apparent error in the HILO cross sections at > 150 MeV is probably that the optical model parameters used based on fits to dat < 50 MeV) are not applicable at high-energies.

The A dependence of the HILO elastic scattering cross section at high energies also differs substantially from the NASA values. For example, at 400 MeV, σ_{el} $A^{2/3}$ for the HILO library, whereas σ_{el} $A^{.94}$ for the NASA library. (The NASA values are in good agreement with the measured /7/ dependence of σ_{el} $A^{1.04}$ for energies >10 GeV.)

3 COMPUTER CODES

We have considered different calculational methods for deep penetration problems showing us the following:

The Monte-Carlo code HETC faces difficulties with statistics at depths of 1 m and more. On the other hand this code can treat protons and other charged particles and is capable of complex geometries.

The one-dimensional transport program ANISN can calculate deeply into the shielding if suitable cross-section data is available. The main disadvantage is that it can treat only very simple geometry and no protons.

3.1 HETC/ANISN Coupling

We draw the conclusion that the combined advantages of the two types of codes could be helpful for deep-penetration problems:

Near the source (within the target, the moderators and inner part of shield) calculation is done with HETC as deep into the shield as secondary proton become negligible. In this area a coupling surface is defined at which the angle dependent neutron flux towards the outer surface of the shield is recorded by the auxiliary code SIMPEL. This flux is fed as a surface source into ANISN. Thus, the neutron fluxes within the shield beyond the coupling surface can be calculated in simple geometry (sphere or slab). A "coupled" calculation was performed as a test for the above mentioned benchmark of an iron sphere of 2 m radius. The neutron source was 5 cm volume source in the center with a flat energy distribution between 300 and 400 MeV. A spherical coupling surface was chosen at radius 50 cm. After computing the surface source with HETC/SIMPEL the ANISN calculation was started in spherical geometry with black boundary conditions at the inner side of the coupling sphere.

The LANL library was used in Legendre order P_3. The result of the calculation was compared with an ANISN only calculation starting again with a 5 cm thick volume source in the center of the sphere. The comparison is given in Fig. 8 and shows reasonable agreement.

It is thought of providing coupling also to the 2-D transport code DOT to allow collimator calculations.

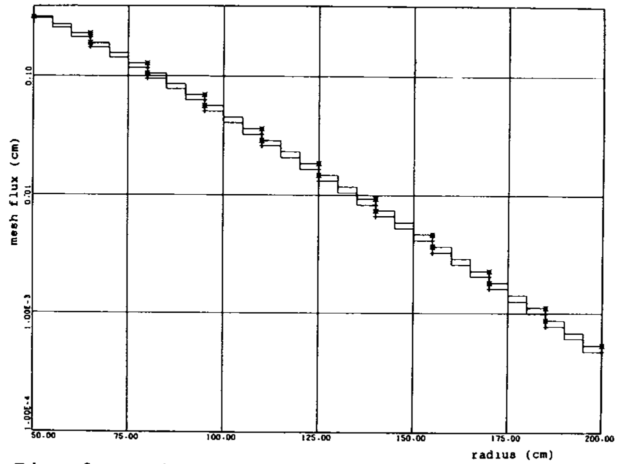

Fig. 8 Neutron Flux (50-400 MeV) per Source Neutron beyond coupling surface (Integrated over Mesh and Time)
* ANISN only + ANISN/HETC Coupling

3.2 The CASL Code

High-energy radiation transport codes (namely, the discrete ordinates codes ANISN and DOT, and the Monte Carlo codes HETC and MORSE) are being applied at KFA to investigate some of the fundamental shielding problems associated with the SNQ. While these codes have the advantage of containing state-of-the-art physics treatments and cross-section data, they require considerable set-up and computing time. It is not practical to run these large transport codes for detailed calculations to address all of the numerous radiation safety questions and engineering-type design problems associated with target station, experimental area, and accelerator shielding.

Therefore, we are writing a simple, fast-running Shielding Layout and Assessment Code (CASL) which has rather general source, material and geometry capabilities but which requires minimal computer and set-up time, and can operate in an interactive mode. While the CASL code uses approximate, semi-empirical physics treatments, it can provide sufficient accuracy for many practical problems and parameter variation surveys where only approximation estimates are adequate.

The basic calculational approach of the CASL code is to assume a simple, exponential attenuation relation for the shield attenuation of high-energy radiation. The form of this semi-empirical model used here is similar to that used for many years fro accelerator shielding estimates, but with two main differences: (a) the shield attenuation parameters and the neutron production data for proton beams needed for input are generated by detailed radiation transport codes (with options for experimental data input, if available), and (b) the semi-empirical attenuation model is coupled with simple 1-D and general 3-D geometry modules to automate the generation of results for either simple or complicated material/geometry configurations.

Calculational Method of the CASL Code

The form of the attenuation equation used is shown in the Equation, where the notation is as follows:

$$D(\bar{r}) = \frac{\tilde{D}\cdot\dot{S}_n(\bar{\Omega}\cdot\bar{\Omega}_o;E_o,A_t)B(E_o,t)\exp(-t/\lambda(E_o,t))}{\bar{F}_h|\bar{r}-\bar{r}_o|^2}$$

(a) $D(\bar{r})$ is the dose-equivalent rate at location $\bar{r}$ and direction $\bar{\Omega}$ from a proton beam of energy E_o and direction $\bar{\Omega}_o$ bombarding a target material of mass number A_t at location $\bar{r}_o$.

(b) The high-energy neutron flux at material thickness t is $\Phi_h(t)=B\cdot\exp(-t/\lambda)/|\bar{r}-\bar{r}_o|^2$, where B is "buildup factor" and λ is the attenuation length.

(c) The dose rate due only to the high-energy neutrons is then $\Phi_h(t)/\bar{F}_h$, where $\bar{F}_h$ is an average neutron flux-to-dose factor for neutrons >100 MeV.

(d) The dose is determined predominately by the low-energy neutrons whereas the attenuation equation gives only the high-energy dose. Therefore, the dose-ratio factor $\tilde{D}$ (total dose/dose due to neutrons >100 MeV) is applied. (Thus, $\tilde{D}$ depends on the neutron spectra of the particular shield material used, which we obtained from transport code calculations.)

(e) The source term $\dot{S}$ is the rate of high-neutron production, per steradian, in the direction $\bar{\Omega}$ with respect to the beam direction $\bar{\Omega}_o$.

The general capabilities of the CASL code are summarized in Table III. The neutron production data are calculated for thin targets. They can be applied approximately for thick targets by using empirical relations giving the number of collisions in a thick target creating high-energy neutrons; or, more accurately, by using the high-energy neutron leakage for thick targets (e.g., from the SNQ target wheel) calculated by HETC as input.

The parameters Φ_h, λ, B and $\tilde{D}$ are being calculated with ANISN. An advantage of using transport codes for generating shield parameters is that dependence upon shield thickness and source energy (usually neglected in semi-empirical shielding calculations) can be taken into account.

Table III

Capabilities of the CASL Code

- Modes of Operation
  - "Layout": 3-D shield requirements for specified dose rate criterion
  - "Assesment": dose rates at arbitrary locations for specified simple or 3-D configurations
- Beams/Materials/Geometries Allowed
  - proton beams: 100 MeV to 1 GeV
    target materials: arbitrary
    shield materials: those most commonly used
  - geometries: simple 1-D or Com-Geom 3-D
- Source Options
  - protons on thin targets
    protons on thick targets
  - empirical treatment
  - use target leakage neutrons from HETC code calculations

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