ISOSHLD 4.0

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ISOSHLD 4.0

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ABSTRACT

ISOSHLD (in version 4.0) has been updated and revised and includes fission product inventory, Bremsstrahlung and related source term calculations.

INTRODUCTION

ISOSHLD was developed to carry out routine shielding calculations that would otherwise be very laborious (Ref. 1). More sophisticated methods exist, but there is still need for easy-to-use reliable computer codes. The code has been revised several times including PC (Ref's. 2, 3, 4) and mainframe-based versions (Ref. 5). These versions generally represent different objectives and differ in code, data, and supported features.

The current version includes all features. It has a 30 group energy range from 10 keV to 10 MeV. Bremsstrahlung is included, MODE 1 capability is retained (fission product inventories from decay and transmutation), and the libraries now fully support the actinides.

There were several design objectives in this latest revision; modernization, state-of-the-art nuclear data, and full capability including source generation and time dependent calculations.

WINDOWS INTERFACE

The objective of adapting ISOSHLD to a modern PC operating system was achieved via a Microsoft Windows\(^1\). This interface is a Windows front end program for ISOSHLD which provides the user friendly environment depicted in Figures 1 and 2. The interface translates the entered data into an ISOSHLD/ISOCALC file, runs ISOCALC and ISOSHLD in sequence, and displays the results in a window.

STANDARDIZED FORTRAN

Contemporary computer codes require rigorous standards of validation, configuration control, and maintainability. These objectives were addressed by rewriting ISOSHLD to standard FORTRAN conventions and structure. This

\(^{1}\) Microsoft Windows is a registered trademark of Microsoft Corporation.
ensures the code can be run on any existing or expected computer architecture including personal computers and workstations.

STANDARD DATA LIBRARIES

State of the art nuclear data was achieved via maximum use of standard data libraries. ISOSHLD contains extensive data libraries including buildup factors, attenuation coefficients, and photon data that are impossible to exhaustively check by running test cases. Data quality is ensured by reliance on the broad base of testing and use of these standardized electronic sources. Documentation and traceability is also enhanced by the use of standard data sources.

Photon Library

The new photon library is based on the Evaluated Nuclear Data File (Version VI), ENDF/B-VI (Ref. 6). This data file was funded by the Department of Energy for nuclear reactor and related activities. It has undergone extensive, formal, phased review.

There are several advantages for applications such as ISOSHLD: The nuclide list is far more extensive than previously in ISOSHLD including actinides, fission and activation products, and it represents a single, consistent, source of data. The use of ENDF/B reduces the chance for missing data or incorrect data for less routine tasks (e.g., thin-shield applications involving isotopes such as $^{239}$Pu, $^{241}$Am, and others).

Buildup Factor Library

The new buildup factor library is based on ANSI-6.4.3, "Geometric Progression Gamma-ray Buildup Factor Coefficients" (Ref. 7). For most geometries, this library supersedes the combination of Taylor coefficients and tabular values previously used. The truncated cone and sphere geometries retain the older methods because the analytical form of the Taylor coefficients is required.

A new routine GPFUNC was added to the code to read the buildup coefficient library and to construct buildup factors from the buildup coefficients. Given a photon energy $E$, an effective atomic number $Z$, and the number of mean free paths, buildup coefficients are first calculated for the two nearest $Z$ values, each interpolated on log-energy using four-point polynomial interpolation. The final value is then found by linear interpolation on $Z$.

There are three compounds/mixtures in the new library: air, water, and concrete. Since ISOSHLD uses an effective atomic number $Z$ stored with the attenuation coefficients to specify the appropriate buildup factor coefficients, values found by interpolating on $Z$ are used rather than the specific values for the compound/mixture. A value of 8 was chosen for water since the oxygen ($Z=8$) buildup factors provide a good approximation to the explicit water buildup factors.
Attenuation Coefficient Library

The mass attenuation coefficients (without coherent scattering) are also taken from ANS-6.4.3. This provides a standard data source, and enhances consistency between the attenuation coefficients and the buildup factors. In order to minimize the chance of introducing spurious errors, the format of data file ATTNUATE.LIB was left nearly intact from its original electronic form. A minor exception was the insertion, for each material, of two values required by the ISOSHLD code (an effective atomic number EAZ and effective atomic weight EAN) and a one or two character identifier code. The identifier code for all elements is the usual abbreviation, e.g., "H" for hydrogen, "HE" for helium, etc.

ISOCALC

MODE 1 denotes the ability to use the results of a decay and transmutation code; a feature supported in some, ISOSHLD versions by a reduced version of RIBD, (Ref. 8). The current version supports MODE 1 calculations by a transparent interface to a new decay and transmutation code, ISOCALC. This adds the capability of time-dependent calculations (i.e., decay and other transmutations) for specific nuclides not originating as fission products. It also adds a complete burnup calculation; decay and transmutation of all nuclides including activation products and actinides. RIBD was limited to fission products within a simple burnup model.

ISOCALC is a standalone decay and transmutation code. An interface file ISODAT.QQQ is automatically created by ISOCALC and is read by ISOSHLD in MODE 1. Decay, transmutation constants and cross sections are from ORIGENZ (Ref. 9).

Facilities include variable flux irradiation histories, ready access to alternative data sources including ORIGEN2 data, and user-supplied values. Time-dependent cross sections may be supplied by the user. Isotopic amounts can be expressed in grams, gram-atoms, or curies for both input and output. Printed output is generated along with a file that may be used for plotting or as an interface with other codes.

VALIDATION TESTS

Two classes of tests were run to verify and validate ISOSHLD 4.0. The first class is a series of comparisons with MCNP. The MCNP values represent full Monte Carlo transport calculations that provide reliable base values useful to validate ISOSHLD and the underlying point kernel method. The second class were verification examples designed to check ISOSHLD options.

A series of MCNP calculations are documented in Reference 10. They cover a wide range of photon energies, shield materials and thicknesses. A subset of these calculations were compared with ISOSHLD results including water, iron, and lead as shield materials. Shield penetrations from 1 mean free path (mfp) to 20 mean free paths were considered for each material as well as four photon energies from 0.05 MeV to 8.0 MeV.

Figures 3, 4, and 5 depict the results for moderate (5 mfp) and deep (20 mfp) penetration for water, iron, and lead respectively. Both the figures and
the table also show the results of an independent PC version of ISOSHLD. The general agreement is excellent for all three codes and thus validates the ISOSHLD codes and the underlying point-kernel approximation within their expected limitations.

With a minor exception at 8 MeV, ISOSHLD and MCNP gives results within 20% for water (see Figure 1). The PC version of ISOSHLD is discrepant at low energies especially for the deeper penetration case. The improved agreement of the current version of ISOSHLD reflects the new geometric-progression buildup factors. The comparisons for iron (see Figure 2) are similar to those for water.

The lead comparison is again generally in good agreement. An exception is low energies and deep penetration. For high Z materials, attenuation coefficients in this low energy region are subject to discontinuities arising from photo-electric absorption (K-edges). As a consequence, the point-kernel method is very sensitive to a delicate balance between buildup factors and attenuation coefficients.

REFERENCES


Figure 1.

Figure 2.
Figure 3.

Water (MFP=5) \{\text{mrem/hr}\}

Water (MFP=20) \{\text{mrem/hr}\}
Figure 4.
Iron (MFP=5) (mrem/hr)

Iron (MFP=20) (mrem/hr)
**Figure 5.**

Lead (MFP=5) \(\text{mrem/hr}\)

![Graph showing dose vs. energy for lead with MFP=5.]

Lead (MFP=20) \(\text{mrem/hr}\)

![Graph showing dose vs. energy for lead with MFP=20.]

- Isoshid
- Iso-pc
- MCNP