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ASSESSMENT OF SHIELDING ANALYSIS METHODS, CODES, AND DATA FOR SPENT FUEL TRANSPORT/STORAGE APPLICATIONS

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ABSTRACT

This report provides a preliminary assessment of the computational tools and existing methods used to obtain radiation dose rates from shielded spent nuclear fuel and high-level radioactive waste (HLW). Particular emphasis is placed on analysis tools and techniques applicable to facilities/equipment designed for the transport or storage of spent nuclear fuel or HLW. Applications to cask transport, storage, and facility handling are considered. The report reviews the analytic techniques for generating appropriate radiation sources, evaluating the radiation transport through the shield, and calculating the dose at a desired point or surface exterior to the shield. Discrete ordinates, Monte Carlo, and point kernel methods for evaluating radiation transport are reviewed, along with existing codes and data that utilize these methods.

A literature survey was employed to select a cadre of codes and data libraries to be reviewed. The selection process was based on specific criteria presented in the report. Separate summaries were written for several codes (or family of codes) that provided information on the method of solution, limitations and advantages, availability, data access ease of use, and known accuracy. For each data library, the summary covers the source of the data, applicability of these data, and known verification efforts.

Finally, the report discusses the overall status of spent fuel shielding analysis techniques and attempts to illustrate areas where inaccuracy and/or uncertainty exist. The report notes the advantages and limitations of several analysis procedures and illustrates the importance of using adequate cross-section data sets. Additional work is recommended to enable final selection/validation of analysis tools that will best meet the U.S. Department of Energy's requirements for use in developing a viable HLW management system.

EXECUTIVE SUMMARY

Within the DOE Waste Management Program there is a definitive need for calculating radiation doses from shielded spent fuel and other high-level waste (HLW). This report documents a review of existing calculational methods, together with a preliminary assessment of shielding analysis software conducted by the Oak Ridge National Laboratory for the U.S. Department of Energy's Office of Civilian Radioactive Waste Management. Criteria used in the assessment of the codes were (1) the physics model(s), (2) solution capability and flexibility, (3) geometric model restrictions, (4) availability of quality data, (5) validation efforts, (6) efficiency, (7) documentation and ease-of-use, (8) availability and compatability, and (9) existing maintenance program.

The interaction of codes and data for a complete radiation shielding analysis is shown in Fig. S.1. Depletion and decay codes either directly supply the needed radiation source specifications or the isotopics can be used in auxiliary codes to provide the required source strength and spectra. The isotope generation codes (and auxiliary codes) shown in Table S.1 were reviewed to assess the current capabilities regarding generation of radiation source strength and spectra. The ORIGEN2 and ORIGEN-S codes are the most widely used codes for generating spent fuel and HLW radiation sources. The isotope generation code selected by the DOE Waste Management Program should include a complete and versatile scheme for producing radiation source strength and spectra and for interfacing with selected radiation transport codes.

The major calculational tools currently employed for radiation transport (shielding) analyses rely on point kernel, discrete ordinates, and Monte Carlo methods. Point kernel techniques are approximate methods that employ Green's functions to solve the problem of line-of-sight radiation transport from source point to detector point. Quadrature or stochastic methods of integration are used for surface and volumetric sources, and semi-empirical approximations are added to account for scattering and finite boundary effects. The method is computationally fast, making the technique especially well suited for scoping studies and estimations. The relative speed of the method enables greater geometric complexity, including three-dimensional representations using flexible combinatorial geometry (CG) descriptions. Unfortunately, the point kernel method may not achieve acceptable accuracy in complex geometries, especially if non-line-of-sight scattering sources are important or if the shields contain multiple layers of materials with distinctly different radiation attenuation characteristics. The latter limitation results from discontinuities in the material-dependent buildup factors which are used to correct for non-exponential attenuation of the flux. Also, point kernel techniques typically provide very poor results for neutron transport and are limited to applications of gamma-ray transport. Table S.2 provides the prominent point kernel codes. The QAD-CGGP code is recommended for use in further assessment and/or validation work.

Discrete ordinates codes solve the Boltzmann transport equation for discrete values of the space, angle, and energy variables. The method is more accurate for general applications than point kernel, but requires more computational effort. Also, a greater user involvement is required in order to properly manipulate the greater sophistication of the method. Presently, discrete ordinates codes require the geometry to be described on a regular mesh, although one code allows for multiple sets of spatial mesh within a single problem. The mesh restriction can become severe in geometries where intricate detail or diagonal boundaries are important. Another disadvantage is that "ray effects" can result when computing the transport of radiation from localized sources through low-density (air) regions. The use of auxiliary codes and the proper selection of spatial mesh and angular quadrature help to mitigate these effects. A tremendous advantage of the discrete ordinates method is that the flux solution is computed at every location within the problem boundaries. This capability is especially significant when detailed flux mappings are required in a large region.

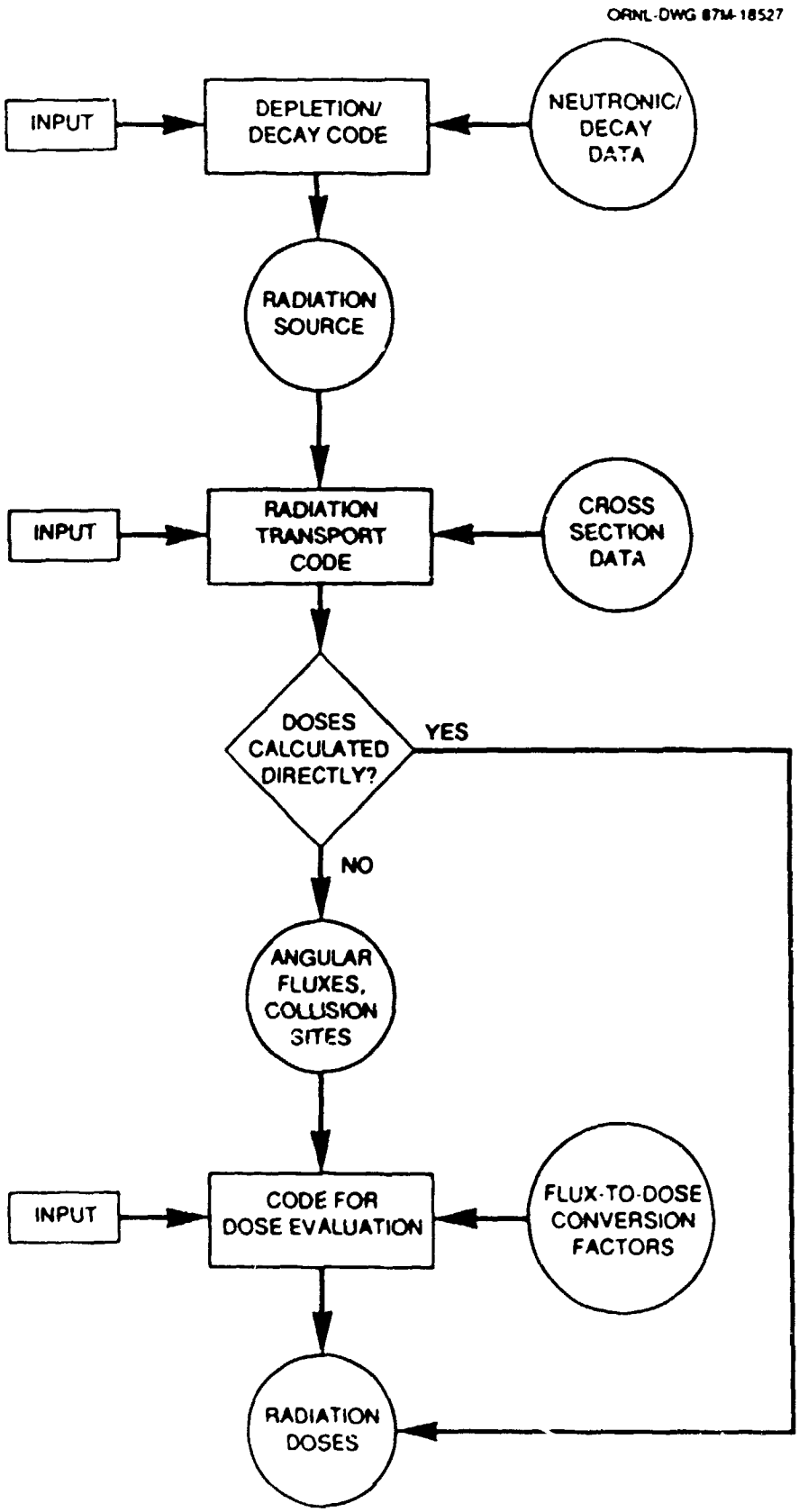

Fig. S.1 Analysis procedure for evaluating doses

Table S.1. Computer programs utilized for generation of radiation source terms

Code (RSIC CCC No.)/ developer	Language	Known computer implementation	Description and comments
DCHAIN2 (CCC-370) Japan Atomic Energy Research Institute	FORTRAN IV	FACOM 230-75	Point calculation of nuclide transmutation via Batemann equations. Nuclear data library for 1170 fission products. Gamma source spectrum computed by FPGAM auxiliary code (CCC-386). Good documentation.
EPRI-CINDER (CCC-309) Los Alamos National Laboratory	FORTRAN IV	CDC-6600	Point depletion code for computing actinide and fission product atom densities. Solution via Bateman equations. Auxiliary codes required for generating radiation source spectra and strengths. Other code versions are CINDER2, CINDER3, CINDER7, and CINDER10. Data libraries and availability vary between versions.
FISPIN (CCC-413) United Kingdom Atomic Energy Authority	FORTRAN IV	ICL 2982	Point depletion code for evaluating fission product, actinide, and structural material inventories. Data libraries for each group of nuclides. Gamma energy spectrum (fixed groups) and total neutron source generated.
KORIGEN (CCC-457) Karlsruhe Nuclear Research Center, Federal Republic of Germany	FORTRAN IV assembler	IBM 3033	Point depletion code for actinides, fission products, and light elements. Solution by matrix exponential method. Substantial update of original ORIGEN code and data libraries. Good documentation. Photon spectra (fixed groups) and neutron source strength provided.
ORIGEN (CCC-217) Chemical Technology Division, Oak Ridge National Laboratory	FORTRAN IV	IBM 360/370 CDC 6600	Point isotope generation and depletion code. Solution by matrix exponential method. Actinide, fission product, and light element libraries available. Photon source spectra (fixed groups) and neutron source strength generated using outdated data and/or analytic functions.
ORIGEN-JR (CCC-399) Japan Atomic Energy Research Institute	FORTRAN IV	FACOM 230-75	Update of ORIGEN code with burnup-dependent cross sections allowed. Substantial improvement to generate neutron and gamma source strengths and spectra (fixed groups) for ANISN, DOT-II, and QAD-P5 shielding codes.

Table S.1. (continued)

Code (RSIC CCC No.)/ developer	Language	Known computer implementation	Description and comments
ORIGEN2 (CCC-371) Chemical Technology Division, ORNL	FORTRAN IV	IBM 360/370 CDC, VAX PRIME, UNIVAC, IBM PC	Significant update of the ORIGEN code to remove deficiencies, improve input features, provide new and better data libraries (actinide, fission product, and light elements). Photon source spectra (fixed groups) and neutron source strength improved over ORIGEN code. Well documented and widely used.
ORIGEN-S (CCC-466) (CCC-475) Nuclear Engineering Applications Department at ORNL	FORTRAN IV FORTRAN 77	IBM 360/370 CDC CRAY-XMP	Significantly updated version of the ORIGEN code developed for the SCALE system. Decay data and photon data same as for ORIGEN2. Radiation source (n and γ) strength and spectra provided in user-specified or default multigroup energy structure. Well documented.
PEPIN (CCC-285) Centre d'Etudes Nucleaires de Saclay, France	FORTRAN IV	IBM 360/370	Point code that solves appropriate differential equations to obtain fission product concentrations, activities, photon spectra, and decay heat. Poorly documented in English.
RASPA (CCC-352) INTERATOM, Federal Republic of Germany	FORTRAN IV	CDC CYBER 172 CDC 6600	Point code for calculation of buildup and decay of fission products and actinides. Data tailored to SNR 300 reactor. Gamma source spectra generated for any multigroup format.
RIBD-II (CCC-79) Pacific Northwest Laboratories	FORTRAN IV	IBM 360/370 UNIVAC 1108	A subroutine within the ISOSHLD II and III point kernel codes. Performs a reactor point depletion analysis to produce gamma source spectra for fission products. Fission product data libraries available for generic thermal and fast reactors.
RICE-CCC (CCC-348) Central Electricity Generating Board, United Kingdom	FORTRAN IV	IBM 370/65 UNIVAC	Point depletion code for evaluating fission product and actinide inventories. Data libraries available. Photon energy spectrum generated. Neutron source strength from spontaneous fission only.

Table S.2. Computer programs based on point-kernel techniques utilized for radiation dose evaluation

Code (RSIC CCC No.)/ developer	Language	Known computer implementation	Description and comments
G33-GP (CCC-494) S3 (CCC-322) Original code from Los Alamos National Laboratory	FORTRAN 77 FORTRAN IV	IBM 360/370 IBM PC Data General	Gamma-ray scattering code using point kernel techniques. Based on a calculated single-scatter source, doses at detectors are evaluated with and without buildup. Direct beam responses (without the single-scatter) are also evaluated with and without buildup. Non-trivial geometric input specifications. Up-to-date buildup factor data in G33-GP. S3 is Westinghouse updated version of original G33.
ISOSHLD* (CCC-79) Pacific Northwest Laboratories	FORTRAN IV	IBM 360/370 UNIVAC IBM PC	Code uses direct point kernel techniques to generate gamma doses for common geometric models. Source may be input directly or calculated via the RIBD routine (see Table 5.1). An extremely user-friendly, for-sale version called MICROSHIELD is available for the PC.
MERCURE 4-V5 (CCC-142) CEA Centre d'Etudes Nucleaire de Saclay France	FORTRAN IV	IBM 360	Gamma-ray kernel integration code for straight line attenuation in three-dimensional geometries defined by planes and quadric surfaces. Stochastic integration of point sources as volume, simplified geometry input, and utilization of multigroup ANISN-formatted photon data are new features over MERCURE-3.
PATH GA Technologies, Inc.	FORTRAN	CDC, CRAY, IBM, UNIVAC, VAX	Proprietary point kernel code available from GA. Buildup factor specification can vary with source and dose point. Claims to be "fully validated and suitable for nuclear licensing applications."
QAD* (CCC-48, 307, 346, 396, 401, 448, 493) Original code from Los Alamos National Laboratory	Version-dependent	IBM 360/370 CDC 6600, CDC CYBER, IBM PC UNIVAC, PRIME Data General	The QAD family of codes make up seven different code packages in the RSIC code collection. All use direct point kernel techniques and differ principally in the available geometry package, source integration method, buildup factor interpolation scheme, and ease-of-input. Latest buildup factor data and attractive geometry in new QAD-CGGP (CCC-493). Most widely used of point kernel codes.
SCAP (CCC-418) Westinghouse Advanced Reactors Division	FORTRAN IV	CDC-7600	Single-scatter or albedo scatter point kernel methods. Numerical integration of point source results over source volume. Anisotropic or isotropic point source representation allowed.

*Code summary provided in Appendix A.

Table S.3 shows the major radiation transport codes, based on discrete ordinates methods. The one-dimensional discrete ordinates code ANISN is probably the most widely used radiation shielding code. Often the shield configuration can be reasonably approximated in one dimension (plane, cylinder, or sphere), and ANISN provides the accuracy of discrete ordinates with the speed of point kernel techniques. For two-dimensional discrete ordinates calculations, the DOT code has become the international standard. The latest DOT release (version 4.3) represents a significant advancement in computing efficiency and speed; however, most problems of reasonable size still require substantial computer resources. Three-dimensional (3-D) discrete ordinates has become practical only since the evolution of vector operation computers. However, recent development efforts have produced viable 3-D codes that could be considered for production work if the need for this type analysis was identified. The current recommendation is to pursue further assessment and validation efforts with ANISN and DOT IV.

Whereas the deterministic method used by discrete ordinates codes is viewed as providing "the exact solution to an approximate geometry," the stochastic approach used in Monte Carlo codes provides "an approximate solution to the exact geometry" because of the statistical nature of the solution scheme. Indeed, Monte Carlo codes allow for fully generalized geometries, limited only by the creativity and perseverance of the user. The Monte Carlo method tracks individual particles through the shield configuration using random numbers and probability distributions to determine particle reactions and their consequences. This approach is most advantageous when a detailed geometry description is important, and when the flux or response is required at only a few select points. The method can become cumbersome (and expensive) if a large number of response locations are desired, or if the system is physically large with highly absorbing regions. In the latter case, appropriate biasing of the particle histories is required to achieve acceptable statistics at a reasonable cost.

Table S.4 lists the prominent Monte Carlo shielding codes. MORSE and MCNP are the premier codes available in the United States. MORSE relies on handling the energy and angle dependence in a discrete fashion. Although MORSE remains widely accepted and used, there is an increased recognition of the advantages of the MCNP kinematics treatment which handles energy and angular dependence in a continuous fashion. For this reason, MCNP is recommended as the code of choice for analysis of problems with complex geometries and calculational benchmark analyses. However, if a hybrid software system is desired where the point kernel, Monte Carlo, and discrete ordinates codes use comon data and interface files, then consideration must be given to MORSE because of its common ties with DOT (discrete energy and angle dependence) and QAD-CGGP (geometry model).

The three radiation transport methods discussed above are in some respects competitors since they are different approaches to the same problem. However, the methods also complement each other and, in combination, provide a powerful analysis capability. This is especially true when considering the complete design evolution of a facility since the accuracy criteria vary as the design evolves, which implies the use of a range of computational methods for a cost-effective analysis.

Data libraries required by the three different code methods also differ. State-of-the-art gamma-ray buildup factor data are available with QAD-CGGP while the MCNP developers have provided a point cross-section library based on the latest evaluated nuclear data file (ENDF/B-V). Standard flux-to-dose conversion factors can be found in ANSI/ANS 6.1.1-1977. However, there is a large assortment of existing multi-energy-group libraries. Unlike the point data libraries used by MCNP, multi-energy-group libraries are sensitive to the processing performed to obtain final group-average values from the ENDF/B files. Appropriate weighting functions (approximation of final flux spectrum), adequate group structure, and proper resonance treatment are major application-specific considerations that are crucial to preparing a multigroup library that gives accurate results for a set of applications. Existing and/or enhanced multigroup libraries based on ENDF/B-V need to be further evaluated in comparing multigroup shielding analysis with measured dose data and/or identical (geometrically) point Monte Carlo calculations.

Table S.3. Computer programs based on discrete ordinates techniques utilized for radiation dose evaluation

Code (RSIC CCC No.)/ developer	Language	Known computer implementation	Description and comments
ANISN[a] (CCC-82,253-255,314,514) Oak Ridge National Laboratory	FORTRAN IV FORTRAN 77	IBM/360/370 IBM PC CDC 7600	General 1-D discrete ordinates coupled neutron-gamma radiation transport code. Most popular version is ANISN-ORNL (CCC-254). Flux or activities at a detector site can be evaluated. The Westinghouse version, ANISN-W (CCC-255), and a recent version from EG&G (CCC-514) are available for an IBM PC.
DOT[a] (CCC-89,209,252,276, 319,320,429) Oak Ridge National Laboratory	FORTRAN IV	IBM 360/370 CDC UNIVAC CRAY	General 2-D discrete ordinates coupled neutron-gamma radiation transport code. Latest and best version is DOT 4.3 (CCC-429) although DOT 3.5 (CCC-276) still heavily used. Earlier versions are obsolete. DOMINO II (PSR-162) couples DOT IV to the Monte Carlo MORSE-CG code (CCC-203). Fluxes and activities calculated. Excellent documentation of theory and techniques.
FALSTF (CCC-351) Oak Ridge National Laboratory	FORTRAN IV Assembler	IBM 360/370 CDC	Calculates doses exterior to a shield based on DOT 3.5 calculated fluxes in cylindrical geometry. Doses evaluated as sum of last flight contributions from shield regions. Eliminates potential ray effects in air or void outside cylinder. Only available for DOT 3.5.
ONEDANT[b] (CCC-428) Los Alamos National Laboratory	FORTRAN IV FORTRAN IV/Assembler FORTRAN 77	CDC 7600, UNIVAC IBM 370 VAX, CRAY	General 1-D discrete ordinates coupled neutron-gamma radiation transport code. Modular program developed to be very user-friendly. Fluxes and/or activities provided at detector points.
SPACETRAN (CCC-120) Oak Ridge National Laboratory	FORTRAN IV	IBM 360/370	Evaluates dose for detectors at various distances from the surface of a cylinder. Integrates ANISN leakage or DOT 3.5 flux data. Eliminates potential ray effects in air or void outside a cylinder. Not accurate for detector points near the cylindrical surface.
TWODANT[b] (CCC-456) Los Alamos National Laboratory	FORTRAN IV FORTRAN IV/Assembler FORTRAN 77	CDC 7600 IBM 370 VAX, CRAY	General 2-D discrete ordinates coupled neutron-gamma radiation transport code. TWODANT is basically the ONEDANT package with the one-dimensional SOLVER module replaced with a two-dimensional SOLVER module.

Table S.3. (continued)

Code (RSIC CCC No.)/ developer	Language	Known computer implementation	Description and comments
XSDOSE[a] (CCC-466) Oak Ridge National Laboratory	FORTRAN IV FORTRAN 77	IBM 370 CDC CRAY	Used in conjunction with XSDRNPM (or ANISN) to compute the neutron/photon flux and the resulting dose rate at various points outside a finite cylinder, sphere, rectangular slab, or circular disc. Uses direct line-of-sight integration of surface angular flux over the surface. Eliminates potential ray effects from discrete ordinates outside shield. Extremely easy to use.
XSDRNPM[a] (CCC-466) Oak Ridge National Laboratory	FORTRAN IV FORTRAN 77	IBM 370 CDC CRAY	1-D discrete ordinates coupled neutron/gamma-ray transport code based on ANISN. Extends ANISN capabilities to provide user-friendly features, automatic quadrature generation, and flexibility in weighting cross sections. Easily coupled to XSDOSE for doses exterior to shield.

[a]Code summary provided in Appendix A.
[b]Combined ONEDANT/TWODANT summary provided in Appendix A.

Table S.4. Computer programs based on Monte Carlo techniques utilized for radiation dose evaluation

Code (RSIC CCC No.)/ developer	Language	Known computer implementation	Description and comments
MCNP[a] (CCC-200) Los Alamos National Laboratory	FORTRAN 77	CDC 7600 CRAY, VAX IBM 3033	General-purpose Monte Carlo code for coupled neutron/photon particle transport. Capable of handling point energy and discretized cross-section data. New features for automatic generation of importance functions. Flexible geometry capabilities. Source and response estimator specification flexible and easy to use. Well-supported program with constant improvements and updated. Well documented.
MORSE[a] (CCC-127,203,258 261,277,368,394, 466,471,474) Oak Ridge National Laboratory	FORTRAN IV	FACOM M-200 IBM 360/370 CRAY, VAX UNIVAC CDC	General-purpose multigroup Monte Carlo code for coupled neutron/photon particle transport. Most widely used of Monte Carlo codes. Latest versions from ORNL in CCC-466 and CCC-474 have a popular, easy-to-use geometry package capable of generating multiple arrays within arrays. Flexibility in specifying source, response estimator, and biasing mode easy via wide variety of user-supplied routines.
SAM-CE (CCC-187) Mathematical Applications Group, Inc.	FORTRAN IV	CDC 6600 IBM 360/370	General-purpose code for coupled neutron/photon particle transport. Excellent geometry package available as proprietary option. Excellent treatment of physics using Monte Carlo techniques. Limited availability of cross sections in required format and limited user community.
TRIPOLI 2.2 (CCC-272) CEA Centre d'Etudes Nucleaires de Saclay, France	FORTRAN IV Assembler	IBM	General-purpose code for neutron or photon particle transport. Handles point energy or discretized cross-section data. Coupled neutron/photon problems cannot be treated. Secondary gamma sites generated and subsequent transport treated with MERCURE (CCC-142). Excellent biasing techniques available for deep penetration problems.

[a]Code summary provided in Appendix A.

With the possible exception of the multigroup libraries (which need further evaluation), the software identified above should be technically sufficient to meet the vast majority of waste management applications. However, the assessment did find the software lacking in the validation and quality assurance areas. The problems and recommendations are listed below.

High-quality integral experiments adequate for code and data validation have often been limited to very simple systems or in support of specialized shielding programs (i.e., specific reactor designs). Although dose measurements from casks loaded with spent fuel have been made, no concerted effort has been undertaken to use the available measured data for validating any particular codes and/or data library. However, each of the codes has probably been evaluated through the use of the limited integral experiment data at some time or another. These comparison efforts have typically been performed by various users and often were never formally documented.

Thus, a software validation program needs to be initiated. The initial objectives of the program should be to (1) determine the accuracy of the selected codes and data libraries in comparison to the existing measured data applicable to shielded spent fuel and HLW and (2) identify and/or design integral or benchmark experiments that are needed to supplement the existing experimental data in order to show compliance with licensing and/or quality assurance requirements.

The services of the Radiation Shielding Information Center (RSIC) as a central site for the existing documentation and software have been invaluable for publicizing new shielding software and keeping many useful codes and data libraries from being lost to the user community. Although the viable code versions are normally available from RSIC, many of the code packages and data libraries no longer have a principal technical contact who has a mandated (funded) responsibility for software maintenance (including documentation changes) with a QA plan that would allow complete compliance with current interpretations of ANSI/ASME NQA-1 or NUREG-0856. Historically, software developers have often passed QA and maintenance responsibility onto the users, particularly as funding support for the code development was reduced or deleted by the sponsoring organization.

An overall quality assurance plan for a project is concerned with ensuring that the analytic results are adequate. Unfortunately, accurate evaluation of neutron and gamma-ray doses from shielded spent fuel or HLW is a difficult task that requires a large amount of user expertise to correctly identify appropriate modeling assumptions, provide adequate input data (source specification, code input data, and cross-section data), and interpret/verify the final results. A validated, high-quality code in the hands of an inexperienced user is often less reliable than an approximate, poor-quality code in the hands of an experienced radiation shielding analyst.

To address the software QA concerns and the potential lack of shielding expertise within the various waste management projects, it is recommended that a "shielding support center" be established to

1. serve as the technical contact for the DOE various waste management projects to answer questions or provide guidance regarding software capabilities, appropriate use (input, modeling assumptions, etc.) of the software, accuracy of results, and the numerical and/or theoretical models employed in the software;
2. maintain and document the validated codes and data libraries under quality assurance guidelines that meet the requirements of ANSI/ASME NQA-1 and NUREG-0856; and
3. serve as the technical interface between the projects and developers for providing/obtaining enhancements that may be required to meet specific project needs.

To provide consultation in a complete, efficient, and readily available fashion requires that the center be established at an institute with recognized capabilities in software development and analysis for shielding applications.

1. INTRODUCTION

The Nuclear Waste Policy Act of 1982 mandates the final disposal of spent nuclear fuel and high-level radioactive waste (HLW) in geological repositories. In support of this effort, the U.S. Department of Energy (DOE) Office of Civilian Radioactive Waste Management (OCRWM) is interested in assessing the analytic methods and available software (codes and data) applicable to the design and licensing of the required facilities and/or equipment. This report provides a review and preliminary assessment of current radiation shielding methods, codes, and data to serve as a basis for determining if existing capabilities are adequate for DOE/OCRWM applications involving shipment and/or storage of spent nuclear fuel and HLW.

Carrying out the directive of the Nuclear Waste Policy Act requires that DOE/OCRWM take responsibility for design and licensing of (1) geological repositories for final disposal, (2) a cask transport fleet for movement of fuel or HLW, and (3) interim storage facilities to supplement utility storage prior to completion of the initial repository. In terms of the geometry specification, shield materials, and licensing criteria, the above areas cover a wide spectrum of analysis applications. The criteria of 10CFR60 (repositories), 10CFR71 (transport casks), and 10CFR72 (independent storage installations) indicate the types of analyses required for license submittals.

Analyses for a repository or interim storage facility [such as the proposed Monitored Retrievable Storage (MRS) facility] will be needed to demonstrate that radiation doses in and around hot cells or fuel handling areas will allow safe operation within the criteria of 10CFR20. Analyses of this type often require the use of codes and methods appropriate for evaluating potential radiation streaming caused by mandated shield penetrations. Also, to show compliance with the regulations on dose to the public, accurate calculations of doses several thousand feet up to several miles from the facility are often needed. Regulations governing spent fuel shipping cask allow a very low exterior surface dose relative to the large radiation source. To analyze the very large reduction in radiation particle density (typically source/leakage particle ratios of 10^5 to 10^7) often requires special codes and/or techniques. In summary, the "best" code or technique to employ for **accuracy** often varies from problem to problem. In addition, computing **efficiency** (ease of use, running time) will be the main requirement for large amounts of scoping and/or preliminary design analyses required by DOE/OCRWM. The varying requirements for accuracy and efficiency imposed by different applications often mandate the use of several codes or methods for a complete systems analysis.

Evaluation of existing radiation shielding methods and software is necessary as a first step in ensuring that adequate and consistent software is used by OCRWM and their contractors in the areas of licensing calculations and safety/ALARA (as low as reasonably achievable) concerns. Establishing uniform software could avoid multiple validation efforts, reduce the cause for discrepancies in similar analyses performed by various ORCRWM programs, and, hopefully, make the review process easier for license evaluators (less codes and methods to review). There is also a cost/benefit consideration that may call for choosing between less-accurate/less-expensive techniques or more-accurate/more-expensive techniques. For example, the first choice may decrease analytic costs, but may cause more expensive designs (forced by conservatism) to accommodate analytic inaccuracies. Without well-defined applications, the cost/benefit of such choices cannot be made in a quantitative fashion.

This report attempts to meet the following primary objectives:

(1) review the basic methods and techniques employed in calculating radiation doses;

(2) provide a brief summary description of selected computer codes and data libraries applicable to shielding analyses for spent fuel and HLW sources;

(3) present a limited comparative assessment of the techniques and tools using applicable computational models for spent fuel casks; and

(4) illustrate potential advantages and/or limitations of various codes and techniques.

Spent fuel cask problems are used in this report for most quantitative assessments because (1) the general designs are currently better defined and (2) design optimization is highly dependent on having accurate shielding methods.

A generic flow chart indicating the procedure and software requirements for calculating radiation doses is shown in Fig. 1.1. The current methods and techniques used for shielding analyses are provided in Sects. 2-4. This review provides a basis for later comments regarding the attributes of the various computational tools. The three sections, respectively, cover the three areas that require the knowledge and attention of a shielding analyst--radiation source generation, radiation transport, and physics data (e.g., cross sections, buildup factors). Section 2 provides an overview of the procedures used to obtain radiation source strengths and spectra. Both gamma and neutron sources are covered.

Section 3 reviews the three major calculational techniques for analyzing radiation transport of source particles through a shield. Discrete ordinates techniques are most often used to solve the one-dimensional or two-dimensional Boltzmann transport equation to obtain a flux/dose distribution. Based on the calculated flux distribution, any number of responses can subsequently be obtained. The majority of problems require that an approximate model of the exact geometry be used by the discrete ordinates code used in the calculation. Monte Carlo techniques typically allow an exact representation of the problem geometry, but uses the integral Boltzmann transport equation as the basis to generate and track particles through a shield in order to obtain a statistical estimation of isolated responses (dose at a point, flux at a point, etc.) While the discrete ordinates and Monte Carlo methods are applicable to neutron, primary gamma, and secondary gamma radiation (gammas produced by neutron interaction with shield materials), the point kernel method is typically restricted to primary gamma radiation. The point kernel method is an approximate technique that involves the use of empirical buildup factor data integrated into the codes for a variety of shielding materials. The buildup factor data is normally obtained from experiment or one-dimensional discrete ordinates calculations. Point kernel codes use exact or approximate geometric models to evaluate the uncollided component transported through the shield and then use buildup factors to obtain the total gamma component. The point kernel codes are the simplest group of codes, but they are the most limited in their range of applications.

Section 4 reviews the determination and selection of appropriate physics data for a shielding problem. Point kernel codes usually have the buildup factor and attenuation (cross section) data integrated into the codes. Coupled neutron-gamma cross-section libraries are used for the discrete ordinates and Monte Carlo codes. An extensive amount of work must be done in going from the raw data measured in a laboratory to an acceptable library of cross sections processed for input to radiation transport codes. This section provides a brief description of the entire process, but deals more specifically with the collapse of a general library with a large number of energy groups (fine group library) to one with fewer groups (broad group library) using a flux weighting that is appropriate for the intended application. Typically, broad group libraries are prepared using an analytic flux spectrum (for neutrons the flux is often Maxwellian for the thermal range in low energy, $1/E$ or $1/\sigma E$ for the mid-range, and a fission spectrum for the high energy range). Ideally, however, the cross sections should be prepared using the flux spectrum most applicable to the problem class to be solved.

Using a literature review and specified criteria, a cadre of codes and data libraries were selected as appropriate tools to be included in this assessment. Section 5 contains a discussion of these software tools; Appendices A B provide separate summaries written for the premiere codes (or family of codes) and data libraries that were reviewed. Each summary provides information on the method of solution, limitations and advantages, availability, data access, ease of use, and known accuracy. For each data library, a summary is included that covers the source of the data, its applicability, and known verification efforts. The selected codes used for radiation transport and dose evaluation are summarized in Appendix A. Descriptions of cross-section libraries that are commonly used for waste management applications are included in Appendix B. Section 5 also describes an existing modular code system called SCALE which provides "automated" shielding sequences using some of the codes and data libraries described in the Appendices. All of the codes and data libraries summarized in the Appendices and the SCALE system are available from the Radiation Shielding Information Center at Oak Ridge National Laboratory.

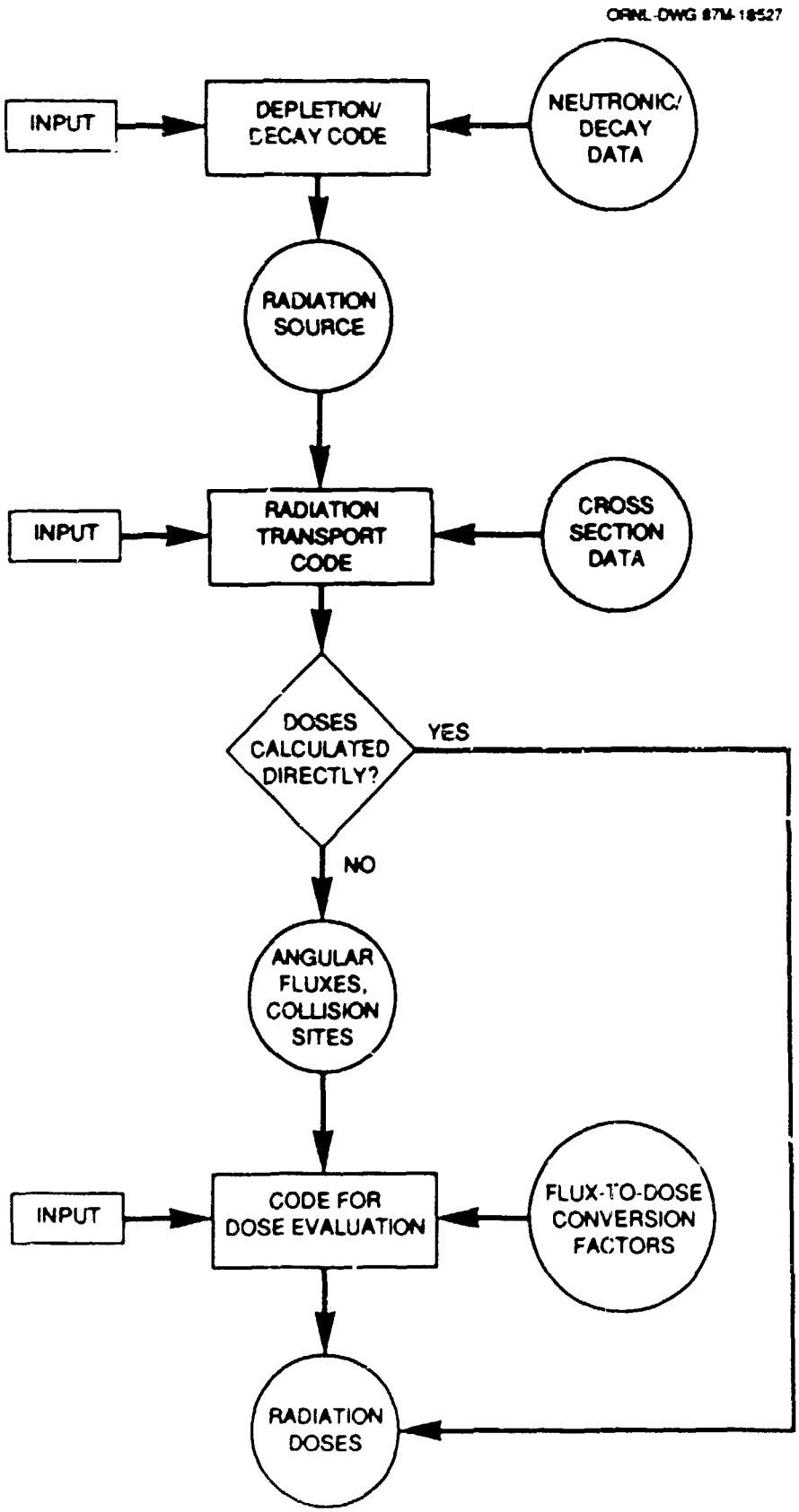

Fig. 1.1 Analysis procedure for evaluating doses

Section 6 provides a discussion of the available methods for assessing codes. A brief summary of available experimental data appropriate for verifying or benchmarking spent fuel shielding analyses is presented. The usefulness of comparative calculations using different tools and/or data is discussed. Section 7 presents a comparison of various calculational results that provides preliminary indications of the advantages, disadvantages, and discrepancies found in several techniques, codes, and data libraries noted in Sects. 2–5. Calculational models of casks are used for the analytic comparisons performed with several codes and data libraries. The importance of a qualified user in obtaining a reliable answer is also illustrated.

Finally, Sect. 8 uses the information from the previous sections as a basis for discussing the acceptability of using the current methods and software to address the needs of DOE/OCRWM. The recommended software for further use in validation or detailed assessment activities are listed together with recommended improvements in the software or its implementation that will aid the mission of DOE/OCRWM.

2. METHODS FOR CALCULATING RADIATION SOURCES

Equations used in particle transport theory contain a source term to simulate the emission of the particles (photons, neutrons, atoms, etc.) being transported. Once the isotopic concentrations for radioactive waste is calculated (or known), the basic techniques for generating the radiation sources do not usually depend on the waste type. Since the shielding computation typically covers a wide energy range, the sources must be cast in units of emission rate per unit volume as a function of energy. Methods of calculating these gamma and neutron source spectra are discussed in this section.

2.1 GAMMA SOURCE STRENGTHS AND SPECTRA

Isotopic concentrations generated by a depletion and decay code are sometimes used within the same code to determine, as a function of energy, the intensity of the gamma (or photon) rays emitted from the radioactive waste. Some depletion and decay codes rely on auxiliary codes to actually evaluate the gamma source strength and spectra. In either case, for completeness, five different types of photon production processes should be considered in generating gamma sources:

- gamma rays and x-rays from radioactive decay,
- gamma rays from (alpha,n) reactions,
- prompt fission gamma rays from spontaneous fission,
- delayed gamma rays from spontaneous fission, and
- bremsstrahlung radiation from positron and electron deceleration.

The extent to which these photon production processes are considered in the creation of the gamma-ray source terms is important to a spent fuel shielding analyst. The following discussion of analytic techniques for evaluating these processes is based on the procedures used in the ORIGEN2[1,2] and ORIGEN-S[3] codes. The primary variation likely to be seen between these procedures and that of other codes that include these production processes lies with the data employed.

The predominant part of the photon source spectrum from spent fuel is from the gamma rays produced by the decay of fission and activation products. The energy-dependent photon intensities for both the gamma rays and x-rays need to be included in the photon data base (a good data source is the Evaluated Nuclear Structure Data File or ENSDF[4,5]). Photon intensities, I, in the data base and their associated energy, E_I, are typically converted to energy group intensities, G, by conserving energy. The following equation is applied for this adjustment:

$$G = I(E_I/E_G),$$

where E_G is the arithmetic average of the energy group boundaries. These procedures maintain the conservation of energy rather than photon intensity and provide a more accurate computation of dose rates in multigroup shielding analyses.

Many of the isotopes in the spent fuel emit alpha particles that may interact with the ^{17}O and ^{18}O atoms in oxide fuel, producing neutrons and prompt gamma rays during the process. The measured gamma-ray spectrum produced by the reaction of alpha particles from ^{238}Pu with ^{18}O atoms are typically used for developing[6-8] approximate spectra for the various alpha emitters in the data library. The spectral distribution of the prompt and delayed spontaneous fission photons can be computed from equations fit to the photon spectrum from neutron-induced fission of ^{235}U.[9] The intensities of the spontaneous fission product gamma rays can be assumed to be 0.75 times that from prompt fission photons.[10] The photons from (alpha,n) reactions and spontaneous fissions normally are a very insignificant part of the source in spent fuel. However, essentially all of the low-intensity gammas above 4 MeV in the spent fuel spectrum are due to spontaneous fission.

A significant source of photons in spent fuel is the bremsstrahlung radiation, which is generated as a continuous spectrum when electrons or positrons are decelerated in the Coulomb field of nuclei. The theory indicates that only a relatively small bremsstrahlung intensity is derived from alpha particles, and so this contribution is typically not included. First, in the determination of bremsstrahlung data, the continuous energy-dependent electron and positron spectra of the nuclide are computed from the Log-f Tables derived[11] from the theory of beta decay. This model, also, is used in producing average beta energies for ENSDF.[4,5] Then, a model for computing the bremsstrahlung spectrum from the beta emission spectrum is applied. (For example, see ref. 12.)

The bremsstrahlung radiation is an important part of the total photon source spectrum from long-cooled spent fuel. It has significant intensities for the energy range from 0 to 4 MeV. As the photon energy increases, the intensity from bremsstrahlung usually decreases more rapidly than that from delayed nuclei decay. Calculations that compared the bremsstrahlung source with the total photon source indicated about one-third of the photons and from 7 to 10% of the total energy are from bremsstrahlung. By observing these spectra and the energy-group dose rates of a somewhat typical shielding problem, it was indicated that 10 to 20% of the total photon dose rate was due to bremsstrahlung radiation.

2.2 NEUTRON SOURCE STRENGTHS AND SPECTRA

As with the calculation of gamma sources, calculation of neutron production is highly dependent on the availability and use of reliable data. The neutron source for spent fuel and other HLW is a result of spontaneous fission of heavy nuclides and interaction of energetic alpha particles with a wide variety of light elements. The other potential source of neutrons is from photofission or photoneutron processes, neither of which are typically considered in codes used for radioactive sources from spent fuel or other HLW. During the first hour, or possibly several hours, after a reactor shutdown there is a significant neutron source from photoneutron reactions. At longer cooling times only insignificant fractions (<0.1%) of the neutron source are caused by the usual photoneutron target materials, the uranium fuel and the tritium in a water coolant.

Methods for computing a neutron source and spectrum emitted from the radioactive waste require data of the following types:

- decay half-lives and energies,
- neutron yields per fission and half-lives for spontaneous fission,
- thick target neutron yields per (α,n) reaction in the waste medium (e.g., UO_2 for spent fuel) as a function of alpha energy,
- neutron spectra from spontaneous fission, and
- neutron spectra from (α,n) reactions caused by alpha decay from heavy nuclides.

The following paragraphs provide reliable (but not necessarily unique) sources for the above data. The reference sources are those employed by the ORIGEN-S code,[3] although other sources for the required data can be found (see ref. 2).

Data required to compute the neutron production rate from spontaneous fission include the spontaneous fission half-life, the average neutron yield per spontaneous fission, ν_{sf}, and the concentration for each contributing nuclide. Spontaneous fission half-lives are available from ENSDF[4] and from Kocher's compilation of decay data,[5] both of which contain evaluated measured data. For several less important nuclides, unmeasured half-lives are available from ref. 13. These data were estimated with a correlation between measured data and so-called fissility parameters.[14] Measured values for ν_{sf} are available in ref. 13 for 21 nuclides, including the most significant. An equation, derived[13] to compute ν_{sf}, produces values which are within two experimental standard deviations for all except three nuclides. This equation can be applied for nuclides that do not have measured data.

As noted above (α,n) neutrons are produced by light elements in the waste. The principal (α,n) sources for most waste in the commercial nuclear fuel cycle are ^{17}O and ^{18}O. Thin target cross sections for $^{17}O(\alpha,n)$ and $^{18}O(\alpha,n)$ reactions and alpha stopping power data may be applied to compute neutron yields of spent fuel material. Measurements[15] of thin target cross sections for the $^{17}O(\alpha,n)$ and $^{18}O(\alpha,n)$ reactions produced improvement over earlier data.[16,17] Additionally, thick target energy-dependent (α,n) yields for $^{238}U^{NAT}O_2$ were computed,[15] having estimated accuracies within 10%. Yield data from ref. 15 can be applied to weighted energy averages of alpha energy-intensity data[5] of nearly all nuclides. Data for nuclides such as ^{214}Bi, ^{241}Pu, and ^{249}Bk, which have very small alpha branching fractions, can be found in ref. 18. Decay constants and alpha decay branching fractions are also required to compute the (α,n) source and can be obtained from refs. 4 and 5.

The isotopes ^{242}Cm and ^{244}Cm characteristically produce all except a few percent of the spontaneous fission and (α,n) neutron source in spent PWR fuel over a 10-year decay time. The next largest contribution is usually from the (α,n) reaction of alphas from ^{238}Pu, which is approximately 1 to 2% of the source. Neutron energy spectra of both the spontaneous fission and (α,n) reactions have been determined for the curium isotopes[19,20] and ^{238}Pu.[7] The measured spontaneous fission neutron spectrum of ^{244}Cm was found to be quite similar to that from ^{235}U and ^{252}Cf. Thus, the spectrum for ^{242}Cm was computed[19] from these measurements. The (α,n) neutron spectra were determined by extrapolating the neutron spectrum from Po-α-O source measurements[21] to the alpha energies of ^{242}Cm, ^{244}Cm, and ^{238}Pu. The energy distribution of the spontaneous fission neutron spectrum can be computed from the spectra for ^{242}Cm and ^{244}Cm by using the calculated concentrations of those two isotopes and then renormalizing to include the total neutron source from all isotopes capable of spontaneous fission. A similar approach using the data for all three isotopes can be performed for the (α,n) neutron spectrum. The spectra must be collapsed from the energy group structure of the data to the desired group structure. One procedure is to assume uniform distribution within each group and simply sum the quantities based upon energy fractions common to both groups in the two group structures. The total neutron source spectrum is then computed as the sum of the spontaneous fission and (α,n) spectra.

The relative importance of the spontaneous fission and (α,n) sources for PWR and BWR fuel at different burnups is well illustrated by the neutron radiation sources shown in Figs. 2.1-2.4.[22] It is important to notice that the total neutron source at discharge increases almost exponentially with burnup. However, the long half-life of the ^{244}Cm causes the neutron source to decrease slowly with cooling time. Since the gamma source changes linearly with burnup (following the fission product trend), it follows that the overall importance of the neutron source relative to the gamma source increases with burnup and cooling time.

Finally, it should be noted that for applications involving vitrified HLW, light elements present in the glass can yield a significant (α,n) source that should be accounted for, and additional (α,n) yield data and spectrum data besides that for oxygen must be obtained.[23]

2.3 RANGE OF APPLICABILITY

As evidenced from Sects. 2.1-2.2, the reliability of the radiation sources produced by a code is primarily dependent on the number and accuracy of the given isotopic concentrations and the completeness and accuracy of the data employed. This section briefly discusses facets of spent fuel source terms that an analyst should be aware of prior to the use and/or selection of a source term generation procedure.[4,5]

2.3.1 Source Strength

One of the major contributors to uncertainty in the radiation sources can be the uncertainty in the calculated isotopic inventory. The calculation of isotopic inventories for spent fuel is more sensitive to cross sections for heavy metals than it is for fission products. Cross-section processing in the depletion

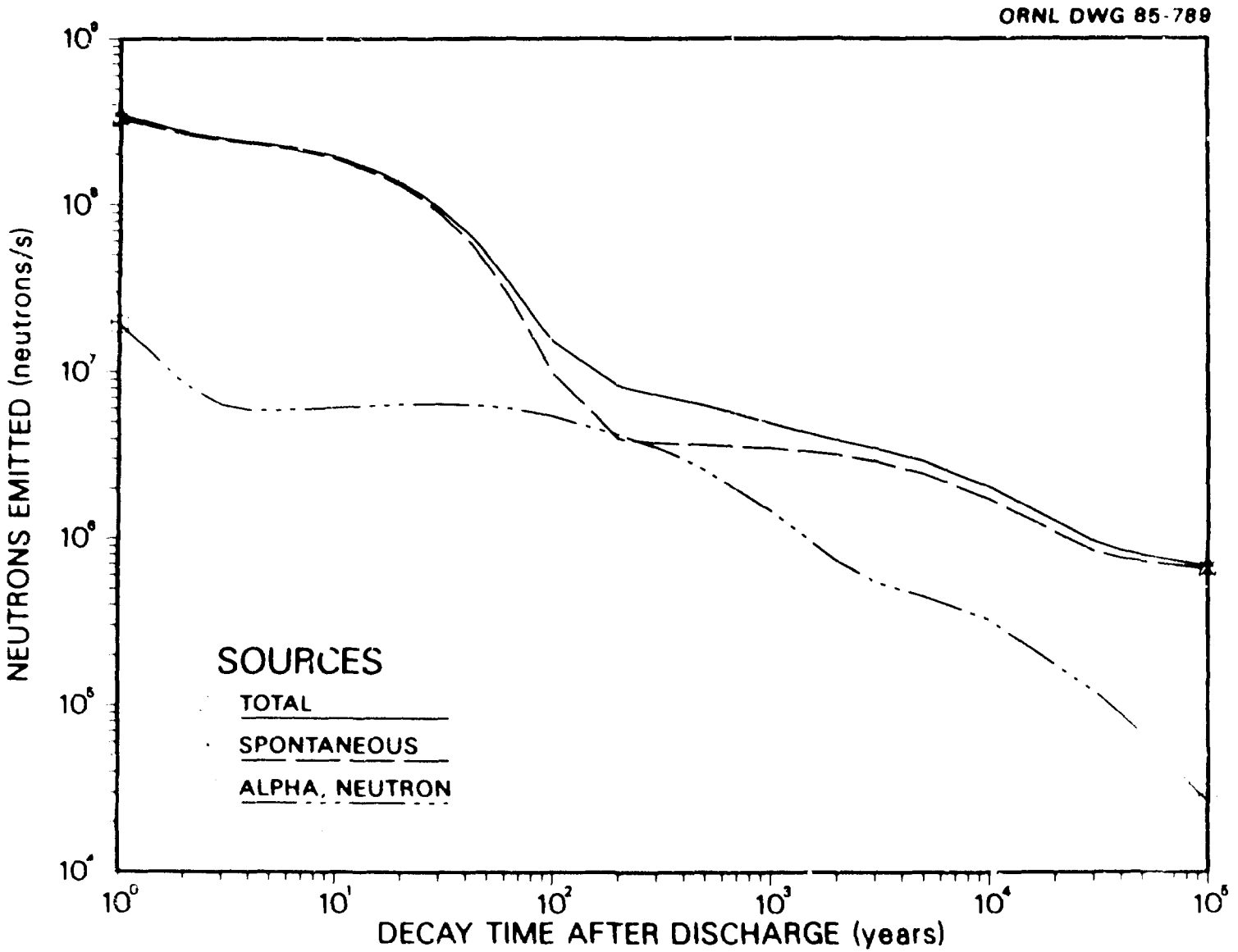

Fig. 2.1. Neutrons emitted by 1 metric ton of initial heavy metal. PWR, 60,000 MWd (from ref. 22).

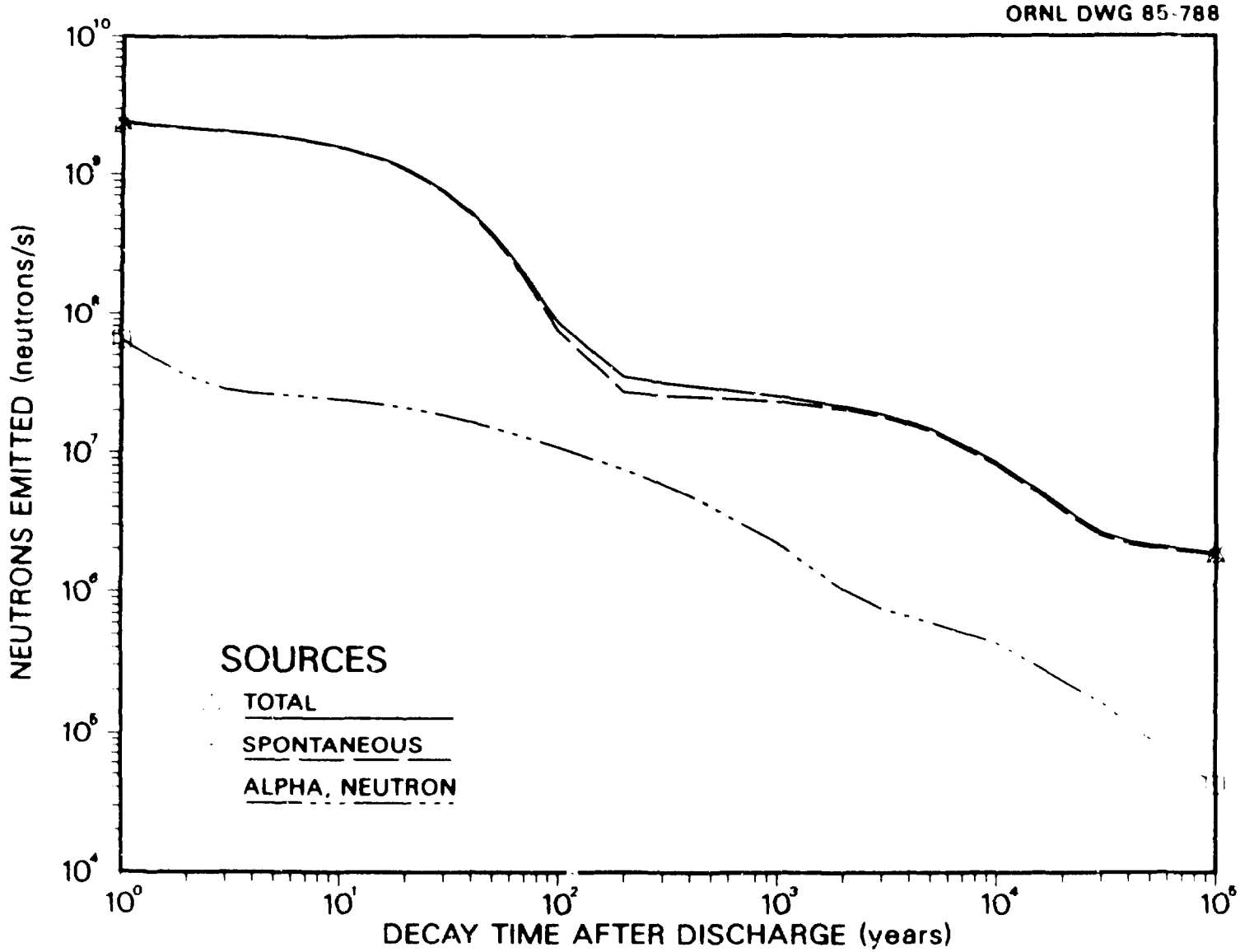

Fig. 2.2. Neutrons emitted by 1 metric ton of initial heavy metal: PWR, 33,000 MWd (from ref. 22).

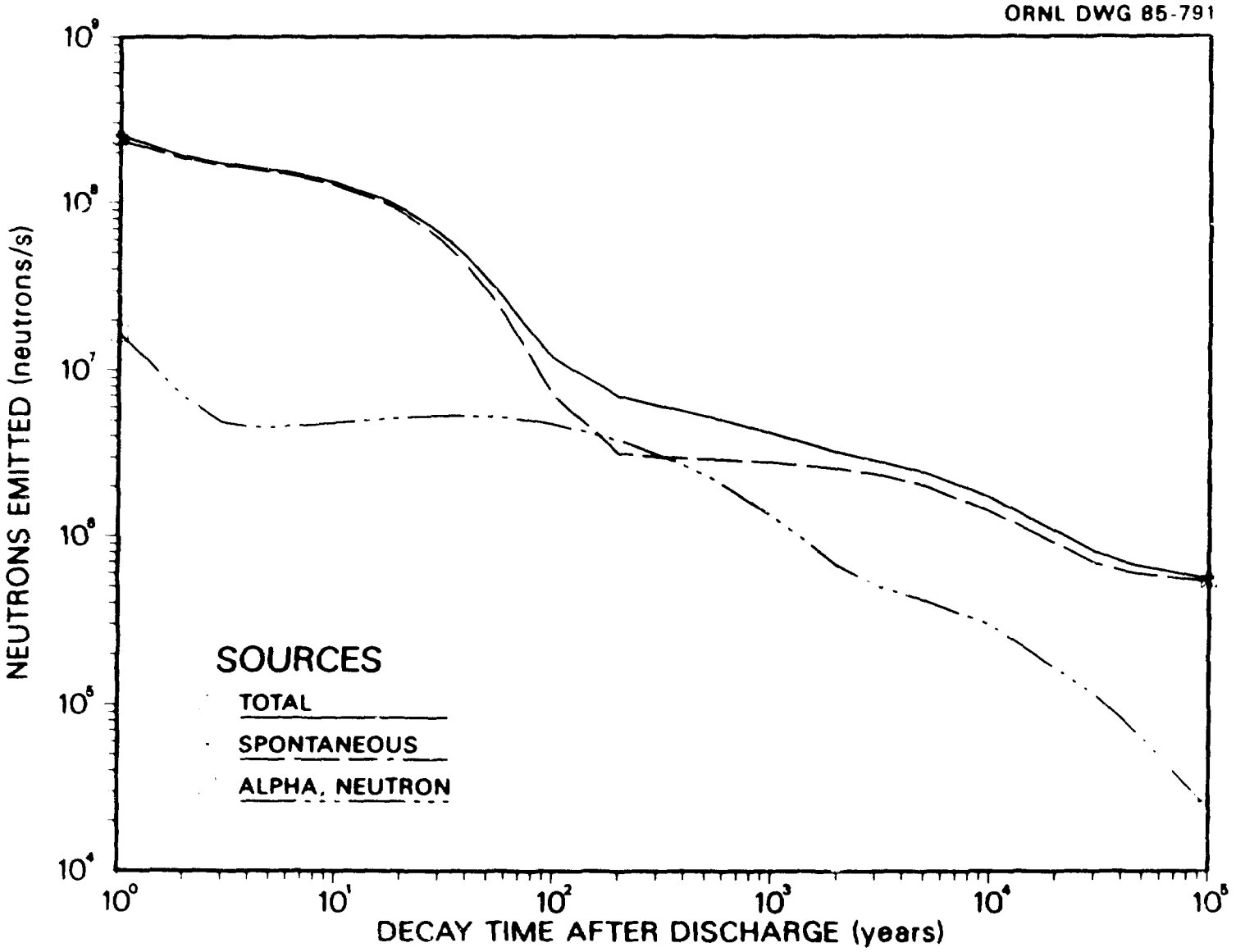

Fig. 2.3. Neutrons emitted by 1 metric ton of initial heavy metal: BWR, 40,000 MWd (from ref. 22).

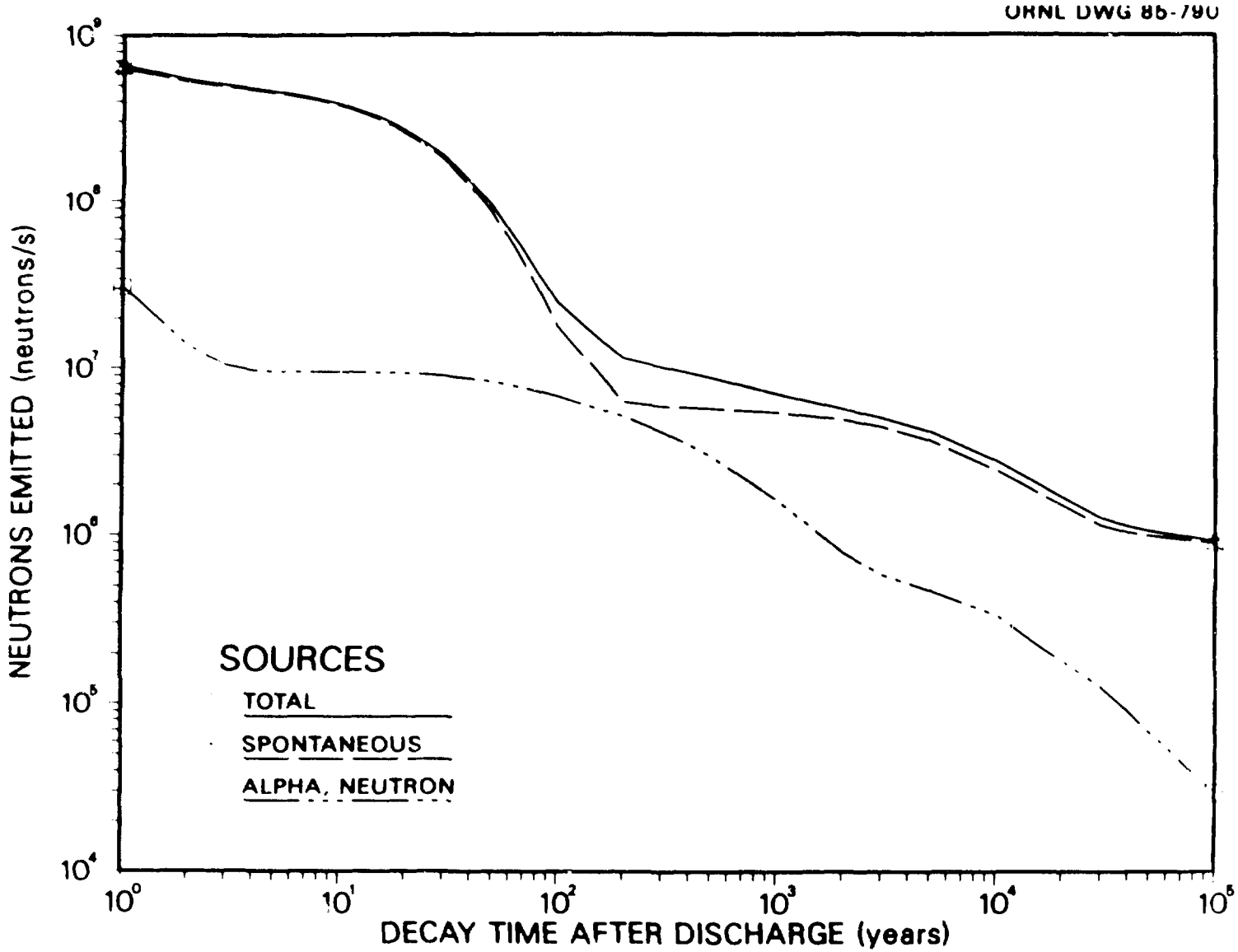

Fig. 2.4. Neutrons emitted by 1 metric ton of initial heavy metal: BWR, 27,500 MWd (from ref. 22).

analyses are typically performed with a point depletion model instead of a more representative multidimensional model. The high sensitivity of spent fuel actinides to the burnup-dependent cross-section set used and the lack of spatial treatment in the point depletion calculation, cause the radiation sources from actinides to have higher **potential** inaccuracy than either the fission or activation products. Thus, as the importance of the actinide contribution to the total radiation source increases with burnup and cooling time, the shielding analyst needs to be aware of this potential inaccuracy and seek to verify the accuracy of the actinide inventory or investigate its importance (sensitivity study) on the final dose results.

The photon source from high-level radioactivity is usually dominated by the contributions from fission products, and possibly one or two activation products. However, for shielding applications, it is often the energy of the emitted gamma rays rather than the intensity that is important. Thus, such activation products as ^{60}Co in spent fuel assembly structures can produce a relatively small proportion of the overall assembly source strength, but be a dominant factor in the dose rate outside a shield. The reason for this is the relatively high (1.17 and 1.33 MeV gammas/disintegration) gamma rays emitted by ^{60}Co. The shielding analyst needs to be aware of the importance of this activation product and seek accurate information on the ^{59}Co content in the unactivated assembly.

Note that shortly after discharge and thereafter, the photon emission rates in the higher-energy range are dominated by actinides. Typically, this is true at energies above 4 MeV at all cooling times and at energies above 3.5 MeV after 10 years. The major part of this higher range of the spectrum is contributed by ^{244}Cm after 90 days and at least 90% appears to be from ^{244}Cm during the range of 10 to 50 years cooling time.[27] The low intensity from high energy photons from the heavy metal isotopes can contribute a dose rate fraction comparable to that of activation and fission products for long cooling times and extremely thick shields.

Given accurate concentrations of heavy element nuclides in spent fuel, the major uncertainty in the computed neutron source strength is in the neutrons produced by spontaneous fission of ^{242}Cm and ^{244}Cm. At discharge, the neutron source is almost equally produced by ^{242}Cm and ^{244}Cm. The half-lives of ^{242}Cm and ^{244}Cm are about 163 d and 18 years, respectively. The neutron emission is mainly from ^{242}Cm at shorter cooling times and from ^{244}Cm at longer times. The source computed from a given quantity of ^{244}Cm is more accurate due to less uncertainty in its spontaneous fission half-life. For the data referenced in Sect. 2.2, it has been estimated that over a 10-year cooling time, the combined uncertainty in the computed neutron source from the spontaneous fission is in the range 4 to 8%, with a decrease as a function of time resulting from the 163.2-d half-life of ^{242}Cm. The total source strength uncertainty, for given isotopic concentrations, is assessed as being <10%.[25]

As noted in Figs. 2.1-2.4, the neutrons from spontaneous fission most often dominate the neutron source strength. However, for lower burnups and intermediate cooling times the (α,n) contribution to the neutron source can be extremely important and should not be ignored simply because (α,n) processes are not considered in generating the source.

The above discussion, together with that of Sect. 2.1, points out that computer programs that omit one or more of the isotopic categories (activation products, fission products, and actinides) or production processes may cause an incomplete source to be obtained. The importance of the missing isotopes and/or production processes should be determined by the user for the application at hand.

2.3.2 Source Spectra

As will be discussed in Sects. 3.4, many radiation transport codes require the radiation source to be input in a multienergy-group format that corresponds to the multigroup cross-section set being utilized for the radiation transport analysis. Figure 2.5 is a plot comparing three broad groups of a PWR spent

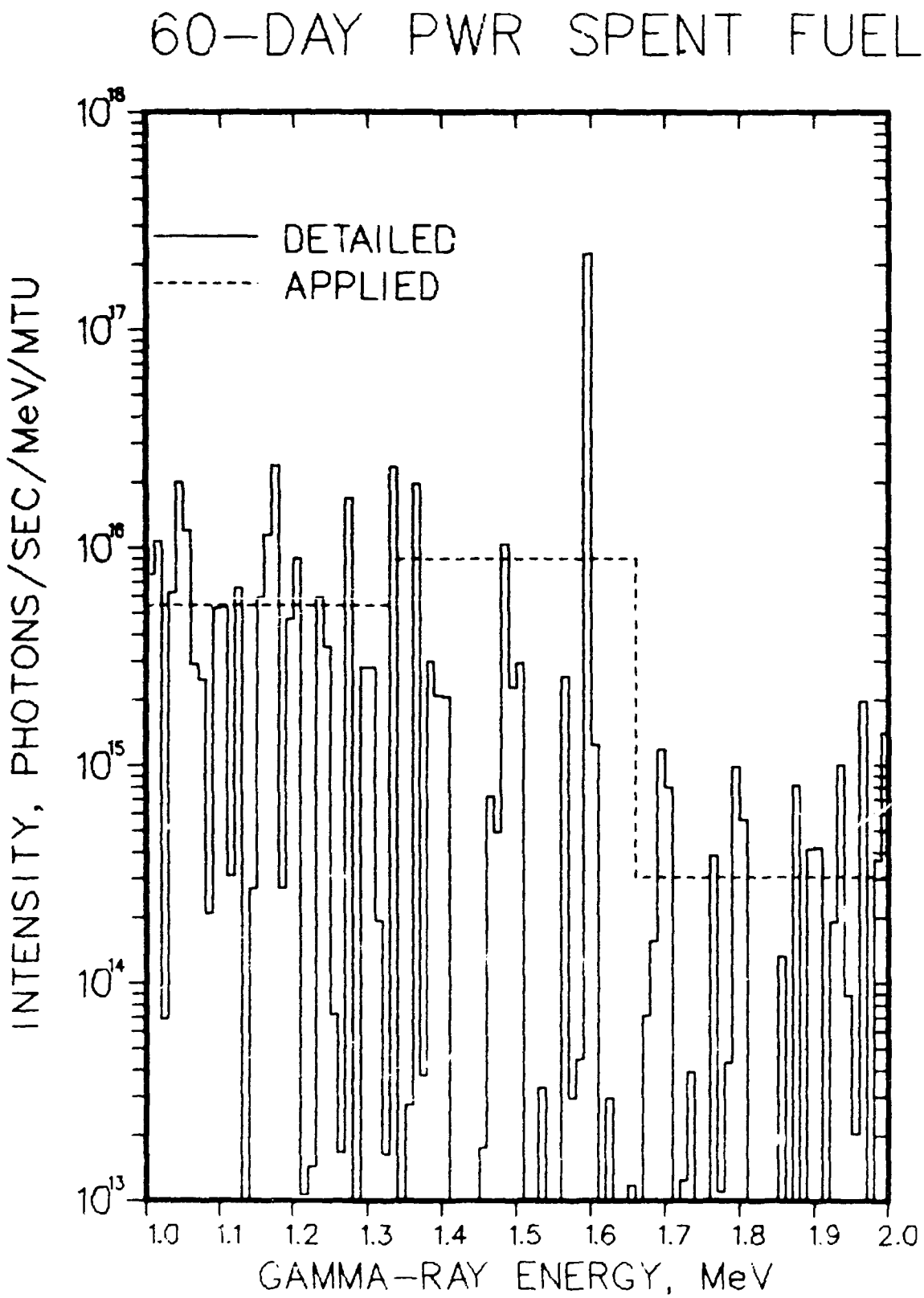

Fig. 2.5. Part of spectrum, comparing intensities for different energy-group widths (from ref. 26).

fuel spectrum with that for the same source in 0.01-MeV group intervals. It illustrates the pronounced variations of the intensities in the detailed spectrum. As described in Sect. 2.1, the best technique for calculating the intensity associated with each energy group is to conserve the total energy of the gammas produced. Thus, for the graphical representation of Fig. 2.5, the area under each of the applied broad groups times the group average energy should equal the sum of the products of the area and average energy of each fine group within the broad group. Attempts to conserve only the intensity when allotting particles to a group can cause either an overprediction or underprediction of the results depending on the procedure used. For example, 1.1-MeV gamma rays of intensity I binned directly into an energy group with limits 1.0-1.5 MeV would have an effective energy of 1.25 MeV (group average) which would result in a higher dose than if the energy was conserved, i.e., use of a modified intensity $I_{mod} = I(1.1)/1.25$. A sample comparison of dose results for an intensity or particle-conserved source vs an energy-conserved source is shown in Sect. 7.1.1.

The dose rates computed for two monoenergetic photon sources shielded with a typical shield thickness are highly dependent on the two photon energies. Adjoint flux calculations have indicated that the ratio of the importance of photons in two adjacent energy groups may be as great as a factor of 2 or 3, for significant groups in a typical 18-group structure. Thus, the benefit of finer group intervals should be properly balanced against computer cost in selecting an appropriate energy group structure. Also, due to the importance of using a correct energy-intensity combination, the conversion of one photon spectrum having a broad group structure to a spectrum of another group structure may significantly reduce its quality.

For the references of Sect. 2.2, there are no reported uncertainties in the data applied for conversion to the neutron source spectrum. However, the use of measured spectral data should be an improvement over the use of standard fission spectrum formulae (e.g., Watt fission spectrum) that are often employed by shielding analysts when a spectrum is not provided with the neutron strength (see Sect. 7.1.1).

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3. METHODS OF RADIATION TRANSPORT AND DOSE EVALUATION

The behavior of radiation particles in a material is modeled by the Boltzmann equation for radiation transport. In order to calculate radiation doses outside a shield (e.g., a cask), a solution to the Boltzmann transport equation must be obtained. There are a number of methods for solving the Boltzmann transport equation for shielding applications. However, in the past two decades two methods have received the most development in the United States and have been used extensively for radiation transport problems. They are the discrete ordinates method and the Monte Carlo method. In this section, along with the derivation of the Boltzmann equation, these two methods will be described with respect to their applications to spent fuel storage/transport problems. In addition, the point kernel technique, which is an approximate approach for calculating radiation doses, will be presented because it is relatively easy and inexpensive to use and produces reasonable results for certain limited problems. References 1–3 are good resources for a more extensive review of shielding methods.

3.1. BOLTZMANN EQUATION FOR RADIATION TRANSPORT

The derivation of the Boltzmann transport equation can be found in many textbooks on transport theory or radiation shielding.[1–4] Nevertheless, the time-independent Boltzmann transport equation is presented here in order to facilitate the discussion in this section.

The Boltzmann transport equation is a particle balance equation that describes the distribution of particles in terms of a flux density $\phi(\mathbf{r},E,\Omega)$ that is differential in space, energy, and direction variables. This quantity, when combined with appropriate macroscopic cross sections, can be used to define R(r), the interaction rate per unit volume and time as

$$R(\mathbf{r}) = \int_E dE \int_\Omega d\Omega \, \Sigma_R(\mathbf{r},E)\phi(\mathbf{r},E,\Omega) \ , \tag{3.1}$$

where Σ_R is a macroscopic reaction cross section.

The flux density, also known as angular flux, is defined such that $\phi(\mathbf{r},E,\Omega)dEd\Omega$ is the number of particles at point r in solid angle $d\Omega$ about Ω, with energy in interval dE about E, per unit area perpendicular to Ω, per unit time. The population balance (assuming no net change as a function of time) states that for an elemental spatial volume at r, the net loss of particles of energy E going in direction Ω is equal to the net gain. The net loss is due to (1) outflow plus (2) interactions that remove particles completely or change their energy and/or direction. The net gain is due to (3) interactions in the elemental volume of particles at different energies/directions whose interactions result in particles of energy E and direction Ω, and (4) sources in the spatial volume at r (external sources). The resulting equation is as follows:

$$\underset{(1)}{\Omega\cdot\nabla\phi(\mathbf{r},E,\Omega)} + \underset{(2)}{\Sigma_t(\mathbf{r},E)\ \phi(\mathbf{r},E,\Omega)} = \underset{(3)}{\int_E dE' \int_\Omega d\Omega' \Sigma_s(\mathbf{r},E'\rightarrow E,\Omega'\rightarrow\Omega)\phi(\mathbf{r},E',\Omega')} + \underset{(4)}{s(\mathbf{r},E,\Omega)} \ . \tag{3.2}$$

This is the Boltzmann transport equation in integrodifferential form.

In general, the differential operation $\Omega\cdot\nabla$ is a complicated function of the spatial coordinate system in which the radiation transport problem is expressed. The quantity Σ_s is the differential scattering cross section and is defined such that $\Sigma_s(r,E'\rightarrow E,\Omega'\rightarrow\Omega)\phi(r,E',\Omega')dEd\Omega$ is the probable number of particles produced per unit volume and time in dE and dΩ due to interactions of particles of energy E' and direction Ω'. The integration over E' and Ω' is required to account for all possible contributions. The term $s(r,E,\Omega)$ is the external source per unit energy, angle, and volume; that is, particles that are not produced by interactions of the radiation field itself.

Exact solutions of the Boltzmann equation, Eq. (3.2), exist only for simplified cases of little practical use for spent fuel shielding applications. However, the use of digital computers has allowed satisfactory numerical solutions using deterministic (discrete ordinates) as well as stochastic (Monte Carlo) techniques.

An integral form of the Boltzmann transport equation can be derived by considering the contribution, from all other points in the system, to the particle flux at a given point in a system. This can be expressed as

$$\phi(r,E,\Omega) = \int_r dr' P(E,r'\rightarrow r)\chi(r',E,\Omega) \quad , \tag{3.3}$$

where $\chi(r',E,\Omega)dEd\Omega$ represents the emission of particles from point r' per unit volume and time with energies in interval dE about E and directions in solid angle interval dΩ about Ω, and $P(E,r'\rightarrow r)$ is the probability that a particle emitted in unit volume at r' with energy E in dE will not have a collision between r' and r. Thus, $P(E,r'\rightarrow r)$ is the transmission probability from point r' to r at energy E. The emission density $\chi(r',E,\Omega)$ consists of particles from scattering and external sources, and it can be expressed as

$$\chi(r',E,\Omega) = \int_E dE' \int_\Omega d\Omega' \Sigma_s(r',E'\rightarrow E,\Omega'\rightarrow\Omega)\phi(r',E',\Omega') + s(r'E,\Omega) \quad , \tag{3.4}$$

where Σ_s and s have been previously defined. Substitution of Eq. 3.4 into Eq. 3.3 yields the equation for the flux φ as follows:

$$\phi(r,E,\Omega) = \int_r dr' P(E,r'\rightarrow r) \left[\int_E dE' \int_\Omega d\Omega' \Sigma_s(r',E'\rightarrow E,\Omega'\rightarrow\Omega)\phi(r',E',\Omega') + s(r',E,\Omega)\right] \quad . \tag{3.5}$$

The transmission probability P is given by

$$P(E,r'\rightarrow r) = e^{-\int_{r'}^{r} \Sigma_t(E,r''\rightarrow r'')dr''} \quad , \tag{3.6}$$

where the integral is the number of mean free paths that the particle with energy E is required to travel from point r' to r.

Both the integral and integrodifferential forms of the Boltzmann transport equation involve the same fundamental quantities φ, s, Σ_s, and P and are equivalent. In fact, the integral form can be derived directly from the integrodifferential form by integrating Eq. (3.2), with an exponential integrating factor, over space.[1,4] Shielding analyses typically involve solving the Boltzmann transport equation,

Eqs. (3.2) or (3.5), and evaluating doses at various exterior locations using Eq. (3.1). Most numerical deterministic methods used for shielding applications start from the integrodifferential form, but a few are based on the integral form. The Monte Carlo approach, which is stochastic in nature, proceeds in a manner which follows the logical development of the integral equation.

The widespread use of discrete ordinates and Monte Carlo applications has led to solutions of the "adjoint" Boltzmann equation,[3-5] which are more appropriate to some systems than the "forward" equation in Eq. (3.2). The adjoint or "backward" equation is a purely mathematical entity, similar to Eq. (3.2) with Σ_R in Eq. (3.1) and $s(r,E,\Omega)$ in Eq. (3.2) being interchanged, and constituting an "effect-and-cause" concept rather than a physical "cause-and-effect" relationship. For an adjoint problem, the response of interest (e.g., detector dose rate) defines the source for the problem and adjoint particles flow from this source back towards the radiation source region of the forward problem. The adjoint form of Eq. (3.2) is used for two main purposes:

1. The adjoint flux is an importance function that provides information on the relative importance of the forward flux particles as a function of space and energy. Knowledge of this importance allows reliable biasing parameters to be obtained for complex Monte Carlo calculations.
2. Using an adjoint source corresponding to one detector location, an analyst can use one adjoint solution to obtain the detector dose from several different radiation sources.

3.2. DISCRETE ORDINATES METHOD

The discrete ordinates, or S_n, method provides solutions to the Boltzmann transport equation by using deterministic numerical techniques to obtain satisfactory results. The S_n method is based on expressing the continuous form of the Boltzmann equation, Eq. 3.2, in terms of discrete variables (i.e., the spatial variables are expressed as finite intervals, the energy variable as energy groups, and the direction variables as discrete directions). Whereas the continuous transport equation represents a particle balance over differential intervals ($dV,dE,d\Omega$), the discrete ordinates equation represents a particle balance over finite intervals. The direction variables are specified in terms of a finite number of discrete directions and corresponding weights (representing solid angles) to replace integration over direction variables by a summation (quadrature) over discrete directions. The energy domain is divided into a finite number of ranges called groups. This "multigroup" approach is also used in many other deterministic methods and even in some Monte Carlo methods.

For the spatial variables, a coordinate system most appropriate to the physical system is chosen and the operator $\Omega\cdot\nabla$ is expressed in terms of the appropriate spatial and angular partial derivatives. The physical system is then divided into a number of spatial cells or intervals, and flux densities are evaluated at boundaries and midpoints of these intervals. For systems which can be represented in one spatial dimension, there are models for slab, spherical, and cylindrical geometries. For two-dimensional systems there are X-Y, R-Z, R-θ, and hexagonal geometries. Both one- and two-dimensional geometry applications are routinely handled in today's computing environment. For spent fuel cask problems, one-dimensional slab and cylindrical geometries and two-dimensional R-Z geometry are commonly used to calculate radiation levels inside and outside of the casks.

The above discussion addresses the way that the spatial, angular, and energy variables are treated by the discrete ordinates method in computing the fundamental quantity of interest, namely the flux density $\phi(r,E,\Omega)$. Implied in the approach are corresponding treatments of the energy and angular dependence of cross sections, scattering kernels, and source distributions. Consider a multigroup form of the transport equation, Eq. (3.2).

$$\Omega\cdot\nabla\phi_g(r,\Omega) + \Sigma_t(r)\phi_g(r,\Omega) = \sum_{g'=1}^{G}\int_{\Omega} d\Omega'\,\Sigma_s^{g'g}(r,\Omega'\cdot\Omega)\phi_{g'}(r,\Omega') + s_g(r,\Omega)\,, \tag{3.7}$$

where ϕ_g and s_g represent the angular flux and external source, respectively, in group g, that is, the integrals of those quantities over the energy group interval. This implies a definition for the multigroup cross sections and scattering kernels that requires a prior knowledge of ϕ. For example, the above equation implies

$$\Sigma_t^g(r) = \frac{\int_{E_g} dE \int_{\Omega} d\Omega \; \Sigma_t(r,E)\phi(r,E,\Omega)}{\int_{E_g} dE \int_{\Omega} d\Omega \, \phi(r,E,\Omega)} , \tag{3.8}$$

and, of course, ϕ is the quantity which is to be calculated. In practice, multigroup cross sections are computed prior to their application as

$$\Sigma_t^g(r) = \frac{\int_{E_g} dE \; \Sigma_t(r,E) \; W(E)}{\int_{E_g} dE \; W(E)} , \tag{3.9}$$

where W(E) is a weighting function chosen in such a way as to closely represent the energy dependence of the flux for the problem at hand. For the scattering cross section, the angular dependence is represented as truncated Legendre polynomials of the scattering angle μ_o. That is,

$$\Sigma_s(r,E' \rightarrow E, \Omega' \rightarrow \Omega) = \sum_{m=0}^{m=n} \frac{2m+1}{2} \; \sigma_m(r,E' \rightarrow E) \; P_m(\mu_o) ,$$

where n is the order of expansion and σ_m are the expansion coefficients. The multigroup scattering cross section is obtained as follows:

$$\Sigma_s^{g g'} (r,\Omega' \rightarrow \Omega) = \frac{\int_{E_{g'}} W(E') \int_{E_g} \Sigma_s(r,E' \rightarrow E, \Omega' \rightarrow \Omega) dE' dE}{\int_{E_{g'}} W(E') dE'} .$$

Theoretically, the proper weighting function should have an angular dependence W(E,Ω); however, in practice, the angular dependence is hardly ever considered.

The task of selecting a multigroup cross-section library with the appropriate W(E) for a particular system is quite important and must not be overlooked (see Sect. 7.2.4). For example, the appropriate flux spectrum for a spent fuel cask can change dramatically from application to application due to the presence of water in the cavity or differing shielding materials in the cask body. Nevertheless, the multigroup approach is the method most often used, and with considerable success, for shielding calculations.

To illustrate the basic ideas of the discrete ordinates method, the simplest case of one-dimensional slab geometry is presented below. The same principles are applicable to other geometries even with more than one spatial dimension. The multigroup Boltzmann transport equation, Eq. (3.7), in x-dimension is

$$\mu\frac{\partial\phi_g(x,\mu)}{\partial x} + \Sigma_t(x)\phi_g(x,\mu) = \sum_{g'=1}^{G} 2\pi\int_{-1}^{1} d\mu'\,\Sigma_s^{g'g}(x,\mu'\rightarrow\mu)\phi_{g'}(x,\mu') + s_g(x,\mu) \quad . \quad (3.10)$$

where μ is the cosine of a direction with respect to the x axis. Integrating the above equation over a spatial interval i bounded by $(x_i,\ x_{i+1})$ and representing the scattering source as a summation over the angular quadrature set $\{\mu_m,\ w_m\}$, m = 1,...,M lead to the following set of finite difference equations:

$$\mu_m\left[\frac{\phi_{gm}(x_{i+1}) - \phi_{gm}(x_i)}{x_{i+1} - x_i}\right] + \Sigma_t(\hat{x}_i)\phi_{gm}(\hat{x}_i) =$$

$$\sum_{g'=1}^{G} 2\pi \sum_{m'=1}^{M} w_{m'}\,\Sigma_{s,m'm}^{g'g}(\hat{x}_i)\phi_{g'm'}(\hat{x}_i) + s_{gm}(\hat{x}_i) \qquad (i=1,...,I;\ m=1,...,M), \quad (3.11)$$

where μ_m is a discrete direction and w_m is the corresponding quadrature weight. The size of a quadrature set is designated by S_n. For a S_n quadrature set, there are n+1 directions for a slab geometry and n(n+4)/4 directions for a one-dimensional cylindrical geometry. For spatially dependent quantities, the general notation $f(x_i)$ refers to a function f evaluated at point x_i whereas the notation $f(\hat{x}_i)$ refers to the function f evaluated at some point internal to the interval. The latter quantities arise because the mean value theorem is invoked in evaluating the integrals over spatial intervals. The quantity $\Sigma_{s,m'm}^{g'g}$ represents the probability of scattering from group g' and direction m' into group g and direction m. In order to obtain solutions to the above set of equations, additional equations are needed. These expressions are obtained by relating the internal fluxes for a spatial interval with its boundary values using various flux extrapolation techniques and can be expressed as:

$$\phi_{gm}(\hat{x}_i) = A\phi_{gm}(x_{i+1}) + (1-A)\phi_{gm}(x_i) \qquad \text{for } (\mu>0) \ , \quad (3.12)$$

and

$$\phi_{gm}(\hat{x}_i) = (1-A)\phi_{gm}(x_{i+1}) + A\phi_{gm}(x_i) \qquad \text{for } (\mu<0) \ , \quad (3.13)$$

where A is a constant between 1/2 and 1. These additional equations allow the solution of the boundary and internal flux density values. One of the most common choices for A is 1/2, which results in the so-called ordinary diamond difference equations. However, selection of A = 1/2 can lead to negative fluxes for too coarse a spatial mesh. A variety of methods have been developed to ensure positivity of the fluxes, and a good discussion is provided in refs. 6–7.

For fission systems such as water-flooded spent fuel casks, an extra term to include fission neutrons must be added to the right-hand side of Eq. (3.11) so that Eq. (3.11) becomes

$$\mu_m\left[\frac{\phi_{gm}(x_{i+1}) - \phi_{gm}(x_i)}{x_{i+1} - x_i}\right] + \Sigma_t(\hat{x}_i)\phi_{gm}(\hat{x}_i) = Q_{gm}(\hat{x}_i) \ (i=1,...,I;\ m=1,...,M) \ , \quad (3.14)$$

where

$$Q_{gm}(\hat{x}_i) = \frac{f^g(\hat{x}_i)}{2} \sum_{g'=1}^{G} \nu^g(\hat{x}_i)\Sigma_f^{g'}(\hat{x}_i) \sum_{m'=1}^{M} w_{m'} \phi_{g'm'}(\hat{x}_i)$$

$$+ \sum_{g'=1}^{G} 2\pi \sum_{m'=1}^{M} w_{m'} \Sigma_{s,m'm}^{g'g}(\hat{x}_i)\phi_{g'm'}(\hat{x}_i) + s_{gm}(\hat{x}_i) , \qquad (3.15)$$

where f^g is the fraction of the fission neutrons that are produced in group g, ν^g is the number of fissioned neutrons resulting from a fission in group g', and $\Sigma_f^{g'}$ is the macroscopic fission cross section in group g'.

Substituting Eq. (3.12) with A = 1/2 into Eq. (3.14) gives

$$\phi_{gm}(x_{i+1}) = \frac{(2\mu_m - \Delta x_i \Sigma_g)}{(2\mu_m + \Delta x_i \Sigma_g)} \phi_{gm}(x_i) + \frac{2\Delta x_i}{(2\mu_m + \Delta x_i \Sigma_g)} Q_{gm}(\hat{x}_i) \qquad \text{for } (\mu_m > o) \qquad (3.16)$$

where $\Delta x_i = x_{i+1} - x_i$.

Similarly, substituting Eq. 3.13 into Eq. 3.14 gives

$$\phi_{gm}(x_i) = \frac{(2\mu_m + \Delta x_i \Sigma_g)}{(2\mu_m - \Delta x_i \Sigma_g)} \phi_{gm}(x_{i+1}) - \frac{2\Delta x_i}{(2\mu_m - \Delta x_i \Sigma_g)} Q_{gm}(\hat{x}_i) \qquad \text{for } (\mu_m < o) . \qquad (3.17)$$

Equations (3.12)–(3.17) form the basis for the iterative procedure used in discrete ordinates codes. With an assumed initial value for $Q_{gm}(\hat{x}_i)$, the iterative solution starts from the first energy group g = 1 and sweeps over all spatial intervals for each direction μ_m. Flux densities $\phi_{gm}(x_i)$ at all spatial boundaries and directions are solved using Eqs. (3.16) and (3.17). Then the interval flux densities $\phi_{gm}(\hat{x}_i)$ are computed by Eqs. (3.12) and (3.13) and used in Eq. (3.15) to update the values of $Q_{gm}(\hat{x}_i)$. For each energy group, one sweep over all directions and spatial intervals is known in discrete ordinates calculations as an **inner iteration**. The inner iteration is continued until the within group scatter source converges to an acceptable accuracy. Similarly, the procedure is repeated for all energy groups. This completes the so-called **outer iteration**. After each outer iteration, the scattering and fission sources in Eq. (3.15) are updated, and a new outer iteration is begun. The outer iteration is continued until the scalar flux densities converge. Note that problems requiring only gamma-ray transport need only one outer iteration for an accurate solution.

For spent fuel problems, several outer iterations may be required in order to correctly take into account the fission neutrons produced in the fuel and, possibly, a depleted-uranium shield. The outer iterations increase the cost of discrete ordinates calculations, but they are often necessary (for neutron transport) in order to correctly treat the physics of the problems. It is sometimes a practice by analysts to exclude fission neutrons from the transport process and, instead, add them initially to the fixed source using various techniques. This approach is an approximation, and although it may perhaps save some computing cost, the practice is discouraged since the correct treatment of fission is straightforward and is a standard option in most radiation transport codes. A secondary reason for outer iterations is to

consider upscatter between thermal neutron groups. Thermal neutron groups may be important in calculating secondary gamma sources as well as obtaining accurate fission sources for wet systems which have much higher neutron multiplication than dry systems. Most shielding cross-section libraries significantly limit (often to one) the number of thermal neutron groups in order to limit or avoid iterations due to upscatter.

The computational cost of the discrete ordinates method is directly related to the rate of convergence of the iterative process. Various techniques have been used to accelerate the convergence so as to reduce the number of iterations. The rate of convergence is particularly important for large problems involving many energy groups, spatial meshes, and discrete directions as would be encountered in large multidimensional systems. Fortunately, with today's computing environment one- and two-dimensional analyses can be performed routinely at an affordable cost. The decision on which applications require a multidimensional treatment as opposed to a one-dimensional treatment can be difficult, but very important, from both a cost and accuracy standpoint. For example, it has been found that one-dimensional cylindrical calculations generally provide reasonable results for radiation doses radially outward from casks. However, for axial dose calculations, one-dimensional geometry results are much too high because the radiation leakage through the side is not accurately accounted for, and a two- or three-dimensional analysis is required for computing axial doses. Various techniques exist and are available to approximate radial leakage in a one-dimensional axial calculation, but their approximate nature requires each application be verified against measurement or multidimensional "benchmark" calculations.

Compared to other methods, the discrete ordinates method appears to have the following advantages for shielding applications:

1. The method is deterministic in nature such that errors in calculated results are systematic rather than statistical (as in stochastic or Monte Carlo approaches).
2. A series of problems having similar characteristics benefit from knowledge of flux densities calculated for a similar case. That is, the starting flux guess for the iterative process can be obtained from a previous calculation of similar problems leading to faster convergence of the present calculation.
3. Neutrons and photons (including neutron-capture photons) can be treated simultaneously or separately without any real restrictions.
4. One-dimensional calculations are much faster than similar Monte Carlo calculations. However, in two dimensions, the S_n method has no clear advantage over Monte Carlo in computational speed.
5. Results are obtained throughout the entire system in contrast to Monte Carlo methods where reliable results are restricted to only selected portions of the geometry.

The following are some disadvantages of the discrete ordinates method:

1. The problem geometry must be one of the three basic geometries (rectangular, cylindrical, or spherical) with boundaries placed along coordinate planes. The importance of the geometry approximations that are required vary with the application and must be either evaluated (via other methods) or rationalized by the user.
2. In multidimensional geometries, the discrete ordinates method often produces nonphysical oscillations in the spatial flux distribution (the so-called ray effect) for radiation transport through void or low scattering media. The ray effect is primarily a result of localized sources and particle propagation in discrete directions, and it is most serious for radiation transport through a void. Special techniques must be employed in order to correctly compute doses at external detector points.

One technique is the last flight approach which computes the flux density at each point detector due to particle scattering from all spatial cells in the system to each detector. Another technique is to calculate the scalar flux at each detector from the angular flux on the outside surface of the shield.

3. There are no basic ground rules to define the best angular quadrature set, space mesh, multigroup structure, and polynomial expansion order for a particular problem. Unfortunately, these user input quantities can be very important to the final dose result. As for angular quadrature sets, at least S_8 or above is recommended for cask calculations. Finally, for the Legendre expansion order of scattering distributions, P_3 is normally sufficient for neutron shielding problems. For photon transport, a higher expansion order is preferable but is not always used (or available) in practice.

3.3. MONTE CARLO METHOD

The Monte Carlo method has been very important to shielding analysis and has received a great deal of attention along with the discrete ordinates method in the last two decades. For a more formal and detailed development of Monte Carlo techniques, the reader is referred to one of the texts devoted to the subject.[8-10] In this section the Monte Carlo method of solving radiation transport phenomenon is developed, and variance-reduction techniques applied to Monte Carlo shielding analysis of spent fuel casks are discussed. The variance of a Monte Carlo calculation is a measure of the statistical uncertainty associated with the results due to the random (stochastic) nature of the method of solution.

In Sect. 3.1 it was suggested that the integral Boltzmann transport equation provides a logical basis for applying Monte Carlo techniques to radiation transport analysis. This logic becomes even more apparent when the integral form is represented in terms of the collision density, ψ, or the emission density, χ. The collision density is defined such that $\psi(\mathbf{r},E,\Omega)dEd\Omega$ is the number of particles entering (having) collisions at point $\mathbf{r}$ per unit volume and time with energies in interval dE about E and directions in $d\Omega$ about Ω. The integral equation for $\psi(\mathbf{r},E,\Omega)$ is obtained by multiplying the total cross section in Eq. (3.3), that is,

$$\psi(\mathbf{r},E,\Omega) = \Sigma_t(\mathbf{r},E)\phi(\mathbf{r},E,\Omega) = \int_r d\mathbf{r}'\Sigma_t(\mathbf{r},E)P(E,\mathbf{r}'\to\mathbf{r})\chi(\mathbf{r}',E,\Omega) .$$

Substitution of χ from Eq. (3.4) into the above equation gives

$$\psi(\mathbf{r},E,\Omega) = \int_r d\mathbf{r}'\Sigma_t(\mathbf{r},E)P(E,\mathbf{r}'\to\mathbf{r})\left[\int_E dE' \int_\Omega d\Omega'\Sigma_s(\mathbf{r}',E'\to E,\Omega'\to\Omega)\phi(\mathbf{r}',E',\Omega') + s(\mathbf{r}',E,\Omega)\right]$$

$$= \int_r d\mathbf{r}'T(E,\mathbf{r}'\to\mathbf{r})\left[\int_E dE' \int_\Omega d\Omega' \frac{\Sigma_s(\mathbf{r}',E'\to E,\Omega'\to\Omega)}{\Sigma_t(\mathbf{r}',E')} \Sigma_t(\mathbf{r}',E')\phi(\mathbf{r}',E',\Omega') + s(\mathbf{r}',E,\Omega)\right]$$

$$= \int_r \int_E \int_\Omega d\mathbf{r}'dE'd\Omega' \; T(E,\mathbf{r}'\to\mathbf{r})C(\mathbf{r}',E'\to E,\Omega'\to\Omega)\psi(\mathbf{r}',E',\Omega') + s_c(\mathbf{r},E,\Omega) , \qquad (3.18)$$

where we have introduced: (1) the transport kernel

$$T(E,\mathbf{r}'\to\mathbf{r})d\mathbf{r} = \Sigma_t(\mathbf{r},E)P(E,\mathbf{r}'\to\mathbf{r})d\mathbf{r} ,$$

which is the probability that a particle emitted in unit volume at $\mathbf{r}'$ with energy E in dE will enter a collision at r in dr, (2) the collision kernel

$$C(\mathbf{r}',E'\rightarrow E,\Omega'\rightarrow\Omega)dEd\Omega = \frac{\Sigma_s(\mathbf{r}',E'\rightarrow E,\Omega'\rightarrow\Omega)}{\Sigma_t(\mathbf{r}',E')}\, dEd\Omega ,$$

which is the probability that a particle entering a collision in unit volume at $\mathbf{r}'$ with energy E' and direction Ω' will emerge with energy E in dE and direction Ω in $d\Omega$, and (3) the first collision source density

$$s_c(\mathbf{r},E,\Omega) = \int_{\mathbf{r}'} d\mathbf{r}' T(E,\mathbf{r}'\rightarrow\mathbf{r})s(\mathbf{r}',E,\Omega) . \tag{3.19}$$

The integral equation for χ is obtained by substituting Eq. (3.3) into Eq (3.4), that is,

$$\chi(\mathbf{r},E,\Omega) = \int_{E'}\int_{\Omega'}\int_{\mathbf{r}'} dE'd\Omega'd\mathbf{r}' \; C(\mathbf{r},E'\rightarrow E,\Omega'\rightarrow\Omega)T(E',\mathbf{r}'\rightarrow\mathbf{r})\chi(\mathbf{r}',E',\Omega') + s(\mathbf{r},E,\Omega) . \tag{3.20}$$

The quantities ψ and χ can also be represented as a sum over the number of collisions as

$$\psi(\mathbf{r},E,\Omega) = \sum_{n=1}^{\infty} \psi_n(\mathbf{r},E,\Omega) , \tag{3.21}$$

and

$$\chi(\mathbf{r},E,\Omega) = \sum_{n=0}^{\infty} \chi_n(\mathbf{r},E,\Omega) , \tag{3.22}$$

where ψ_n is the number of particles per unit volume at r with energy E per dE and direction Ω per $d\Omega$ that have undergone (n-1) collisions and are entering the n^{th} collision at r, and χ_n is the number of particles per unit volume emerging from the n^{th} collision with energy E per dE and direction Ω per $d\Omega$, with $n = 0$ referring to the external sources. Then

$$\chi_0(\mathbf{r},E,\Omega) = s(\mathbf{r},E,\Omega) , \tag{3.23}$$

$$\chi_n(\mathbf{r},E,\Omega) = \int_{E'} dE' \int_{\Omega'} d\Omega' \; \psi_n(\mathbf{r},E',\Omega')C(\mathbf{r},E'\rightarrow E,\Omega'\rightarrow\Omega) \;\; (n = 1,2,...) , \tag{3.24}$$

and

$$\psi_n(\mathbf{r},E,\Omega) = \int_{\mathbf{r}'} d\mathbf{r}' \; T(E,\mathbf{r}'\rightarrow\mathbf{r})\chi_{n-1}(\mathbf{r}',E,\Omega) \;\; (n = 1,2,...) . \tag{3.25}$$

The Monte Carlo method simulates an "analog" random walk process governed by the above equations. This process is created in a computer code by random variable techniques in which r, E, and Ω are randomly chosen (sampled) from the source, transport, and collision kernels in a manner that mathematically simulates the physical properties of the particles. The initial position, energy, and

direction of a source particle are selected from the source density $\chi_o(r,E,\Omega)$. Then the source particle is transported to its first collision site by the transport kernel T. At the collision site the collision kernel C is sampled to identify the interaction type and, if a scattering event occurs, a new direction and energy are selected. Then the distance to the next collision is determined from the transport kernel. This "analog" process is repeated until the particle is absorbed or leaves the system. Quantities such as the number of collisions occurring in particular regions of interest are tabulated during the process, and estimates of responses of interest are computed. The sequence is continued until enough particles have been sampled to reduce the statistical uncertainty in the results to an acceptable level, usually on the order of 10% of the sample mean. The square of the uncertainty is inversely proportional to the number of sampled particles.

For shielded spent fuel problems, analog Monte Carlo is inadequate and inefficient in calculating radiation responses with acceptable accuracy because the events of interest are usually very rare. For example, a shield such as the body of a spent fuel cask will attenuate radiation by several orders of magnitude. From the shielding point of view, the particles that escape the cask are of primary interest for radiation dose evaluation. However, the probability of recording such an event in a Monte Carlo calculation is extremely low ($<10^{-5}$), and an unacceptably large number of histories is required to get good results. For this reason, variance-reduction techniques must be employed for the thick shields typically required to protect the public and workers from spent fuel radiation.

Variance-reduction techniques are procedures for altering the analog Monte Carlo process in order to reduce the variance of the calculated results. They are also loosely called "importance sampling" or "biasing" techniques. The natural distributions in the random walk are modified by some importance function and the particle statistical weights are adjusted from the analog value of unity to remove the bias. The purpose of variance-reduction techniques in Monte Carlo transport analyses is to improve the efficiency of a calculation by reducing the variance of the results without increasing the computing time. The objective is to maintain a reasonable particle population in the regions of primary interest and control the fluctuation of statistic weight of the particles. Variance-reduction techniques are numerous, and their implementations differ depending on the treatments of the random walk and geometry modeling. However, a list of the more commonly used variance-reduction methods is given here, along with a brief description of each technique.

- **Survival biasing**, also known as nonabsorption weighting, prohibits the absorption of particles at collision sites. Instead, the statistical weight of a particle is reduced to account for absorption. Survival biasing is a standard procedure or option in most Monte Carlo codes.
- **Splitting and Russian roulette** are typically used in combination and help to regulate the particle population and/or the associated statistical weight so that a sufficient number of particles reach the important regions of the system without a large dispersion in weights.
- **Path-length stretching** biases the transport kernel so that the path lengths to new collision sites are stretched in a specified preferential direction (towards the response locations) and shrunk in the opposite direction.
- **Collision-biasing** alters the collision kernel so that the energy and/or direction from a collision are selected so as to increase the particle population at preferred energies or directions. This variance-reduction technique has not been used widely because of the difficulty in implementation and choice of biased distributions.
- **Source biasing** is one of the most effective and easily applied variance-reducing techniques available. Energy, angle, and position of source particles can be biased, in combination or separately, to improve the ultimate results.

In applying variance-reduction techniques, the analyst is required to specify the importance (biasing) functions that will hopefully direct particles toward those regions of phase space (position, energy, and direction) which contribute most to the desired results. Theoretically, the adjoint flux is a good, if not optimum, choice of importance function for Monte Carlo biasing.[9,11] From a practical standpoint, however, calculation of the adjoint flux and subsequent selection from the biased distributions usually require more computational expense than an unbiased solution to the original problem. Therefore, in order to achieve a reduction in the cost of the calculation, this optimal biasing function must be approximated.

When a spent fuel cask is analyzed by Monte Carlo, the goal of biasing is to increase the propagation of radiation particles toward the outside of the cask so that better estimates of exterior doses can be obtained. Spent fuel casks generally have long cylindrical shapes, and the characteristics of particle transport radially and axially may be drastically different due to the geometry, the shielding materials, and possibly the radiation streaming in the fuel. Because of these complications, it is difficult to effectively bias particles simultaneously toward all three surfaces of a cask. Hence, separate Monte Carlo calculations with different biasing objectives are recommended for radial and axial external detectors. For radial detectors, the particle random walk should be biased radially toward the side of a cask. For axial detectors, the particle random walk should be biased axially from the midplane and toward the top or bottom surfaces. For spent fuel cask problems, a systematic approach has been developed to bias a Monte Carlo shielding calculation using adjoint functions derived from an adjoint S_n calculation with a one-dimensional model of the cask.[12] In this approach, the particle random walk is biased either radially or axially, depending on the detector locations, and separate Monte Carlo calculations are performed for radial and axial detectors.

The process of extracting response information from particles and their statistical weights is known as estimation. Generally, there are two types of estimations (or estimators): analog and statistical. In analog estimation, particles must reach the detector and/or have collisions inside the detector. Therefore, the computed response is based on particle interactions with the detector by crossing detector boundaries or having collisions inside the detector. In statistical estimation, particles do not reach the detector. Rather the probability of each particle arriving at the detector is calculated and the responses are then computed. In a sense, particles are statistically transported to the detector in order to compute the desired responses. To obtain results for a point detector, one must use statistical estimation since the chance of any particle intersecting the point detector is infinitesimally small. When using (statistical) point detector estimation, one must be sure that no detectors are inside or close to (less than about 2 cm) any scattering material. This is because of the $1/r^2$ factor in the response where r is the distance between the detector and the scattering point. Although there are remedies to this shortcoming,[14-16] it is advisable to avoid the $1/r^2$ singularity when possible.

The primary advantage of Monte Carlo over deterministic methods has been its ability to accurately model complex, three-dimensional geometries without having to employ approximate techniques. The primary disadvantages of the Monte Carlo method are that (1) it is a stochastic method which introduces statistical uncertainty in the results and (2) only selected integral responses are typically evaluated as opposed to distributions. And just as discrete ordinates codes require a certain amount of expertise to define an appropriate spatial and angular mesh, Monte Carlo codes require expertise in specifying biasing parameters, specifying response estimators, and interpreting the results.

In theory, Monte Carlo methods provide a convenient means for treating space, energy, and angular dependence in a continuous fashion. In practice, however, the energy and angular dependence is often treated in a discrete fashion. Historically, this arises from the fact that the cross-section data sets were being prepared in a multigroup format for use in discrete ordinates codes. But, unlike the set of discrete directions fixed in space in the discrete ordinates method, only the scattering angle μ_o is discrete in multigroup Monte Carlo codes, and it is different for each group-to-group transfer. Thus, after several collisions the angular distribution of particle directions is continuous. Some problems may not

be treated well by this approach, including situations with little multiple scattering or highly directionally dependent external sources. For this and other reasons, Monte Carlo codes that use "point" cross-section data and continuous scattering kinematics are again gaining in popularity.

3.4. POINT KERNEL METHOD

Unlike the last two methods, the point kernel method is an approximate but very inexpensive approach for evaluating photon responses in shielding analyses. The relative value of the point kernel method in modern shielding calculations is a matter of individual opinion. Those accustomed to using the more sophisticated methods point to its limitations and lack of rigor. However, the method is still successfully applied by many analysts for both design and safety analysis work. Experience has shown that this method is useful and provides fairly good results for gamma radiation when correctly applied, but it cannot be used to solve all shielding problems.

The basic concept of the method is quite elementary and is based on the kernel, which is a Green's function, between the source and detector points. For distributed sources, the total response is calculated by summing the kernel from each elementary portion of the source. The kernel is constructed by considering the uncollided flux from a point isotropic source with energy E and strength s(E) in a homogeneous medium. The uncollided flux is

$$\phi_o(r,E) = s(E)\frac{e^{-\Sigma_t(E)r}}{4\pi r^2} , \tag{3.26}$$

where r is the distance from the source. This formula accounts only for the particles of a specific source energy which arrive at the detector point having experienced no interaction with the medium. There will also be particles arriving at the point having reduced energies caused by either single or multiple scattering. A buildup factor is introduced to include this scattered portion of the flux density. Hence, the total flux density can be written as

$$\phi(r,E) = B(\Sigma_t r,E)\phi_o(r,E) = B(\Sigma_t r,E)s(E)\frac{e^{-\Sigma_t(E)r}}{4\pi r^2} , \tag{3.27}$$

where B is the buildup factor, which is a function of material, energy, and distance in mean free paths. In shielding analysis, quantities such as dose rate, kerma factors, and energy absorption are usually the desired responses. Therefore, buildup factors have been determined for these quantities for the common shielding materials. For example, the total dose rate from a point source of energy E is given by

$$D(r,E) = B_d(\Sigma_t r,E)s(E)\frac{e^{-\Sigma_t(E)r}}{4\pi r^2} , \tag{3.28}$$

where B_d is the dose buildup factor.

In practice, the radiation source often comprises a volume or surface. Point-kernel codes generate a mesh of source "points" within the source region and integrate over the source region to obtain the total dose. Integration is formed via numerical quadrature or stochastic processes.

Point-kernel codes are of two classes: (1) those that provide the dose on direct line-of-sight attenuation from source to detector, and (2) those that allow consideration of a single-scatter source. Most single-scatter codes also provide the direct line-of-sight dose contribution. The single-scatter techniques are useful for skyshine problems or for consideration of potential scatter "around" a finite shield.

Values of the buildup factor are determined from experiments and transport theory calculations that are based on assuming an infinite homogeneous shield. They are given directly or as coefficients and parameters for fitting functions that facilitate their use. One of the most used forms of the buildup factor is the Taylor form. Others are the Berger form and the geometric progression form. The reader is referred to the text by Chilton et al.[2] for details on application of the point kernel method and buildup factors.

The point kernel method is restricted to photon transport problems. It is very seldom used for neutrons because the neutron cross section generally is a rapidly changing function of energy and nuclide, and no simple tabulation of buildup factors is possible. Also, point kernel results are valid only for integrated responses. Energy-dependent results are usually inappropriate.

The method has been implemented in a large number of computer codes, most of them treating a general three-dimensional geometry and using buildup factor data in some form. The buildup factor data and/or coefficients for a fitting function are usually fixed in the codes. For other materials for which data are unavailable, an approximation must be made.

The integral number of mean free paths must be evaluated even though many materials may be traversed between the source and detector. If this is the case, the computed dose can be in great error because the available buildup factor data are for individual homogeneous materials. Several formulas for combining two or more layers of material are available, but none is employed in the commonly used computer codes. A rule of thumb is to use the buildup factor for the material of the final layer if that layer is several mean-free paths thick. The composite buildup factor is known to asymptotically approach that of the final layer. Otherwise, several calculations should be made with the B_d for different materials, and the largest dose value chosen to be conservative.

The point-kernel method must be used cautiously. If the shield is made of one solid material and the spent fuel can be approximated as one homogeneous material, the method may give reasonable photon responses. But for shields with several layers of materials and geometric complexities that might yield radiation streaming paths, at least one discrete ordinates or Monte Carlo calculation should be performed to establish confidence in the point kernel method or provide correction factors for future calculations on the same or similar designs. The method will not account for radiation scattering from walls, ceilings, floors, or other structures external to the shield. This scattering effect will increase the calculated dose in varying degrees depending on the proximity of these structures to the shield and dose calculation points in question.[17] The buildup factor calculated for an infinite medium, and its use in a finite medium, may overpredict the actual result for a system in which there is no backscatter to the detector. This effect increases for lower source energies. Again, at least one or more discrete ordinates or Monte Carlo calculations should be made to study these effects. However, the point kernel method is usually a reliable and inexpensive means for obtaining photon doses in simple systems consisting of a source, solid homogeneous shield material, and point detector locations.

3.5 APPLICATION OF THE METHODS

A basic review of the principal methods used for radiation transport calculations has been provided in Sects. 3.2–3.4 along with some comments on the advantages and disadvantages of each method. This section attempts to briefly provide an overview of the important aspects of radiation transport calculations for spent fuel shielding problems that should be understood by the analyst. Improper attention to these areas could lead to erroneous results or misleading conclusions. Some of the issues discussed here have already been noted in Sects. 3.2–3.4. Most of the issues will be illustrated by the sample applications of Sect. 7.

3.5.1. Computational Model

When a shielding design has been formulated, one of the first tasks is to determine the proper geometric model to be employed in the analyses. For example, spent fuel casks require a number of decisions involving the modeling detail for the cask internals and cask body areas where radiation streaming could occur. Discrete ordinates codes typically require a homogenization of the cask internals into one or more regions. Homogenization of the radiation source region(s) over the full cask cavity area is the conservative approach that yields the highest radial dose (see Sect. 7.1.2). Modeling the source zone as a homogeneous region with the same cross-sectional area as the fuel elements can produce nonconservative radial results since the actual cask could have assemblies much closer to the cask wall than the outer surface of the equivalent-area model. Input of an appropriate axial or radial profile for the fuel source should also be considered. Because of the uncertainty associated with the profile and the potential for change between assemblies, safety analysts often use a flat profile and assume a peaking factor to ensure maximum dose rates.

When concerned about axial dose rates from spent fuel, the different source zone homogenization techniques noted above will again vary the results depending on the relative spent fuel locations and the type calculation (one- or two-dimensional). Of particular importance to an axial or corner dose evaluation is the ^{60}Co gamma source from the assembly end-fittings and plenum regions. Although the total source in these hardware regions is low in comparison to the fuel region, they can be of major significance to the doses from spent fuel casks because (1) the homogenized hardware regions consist of low-density light element materials that provide virtually no self-shielding (as opposed to the fuel region where self-shielding is significant), and (2) the hardware regions are very near the end walls of the cask.

As noted above, the code selected for the analysis can limit the level of modeling detail allowed. The geometry packages available in Monte Carlo codes allow far more geometric detail to be included in the computational model than discrete ordinates codes. There are situations where the geometric detail of the shield, source region, or surrounding environs can be important to the evaluated dose.

Another aspect of the computational model development for discrete ordinates codes lies with the specification of the discrete angles and spatial mesh. For example, for one-dimensional anlaysis an angular quadrature less than S_8 or a spatial mesh larger than that recommended in Sect. 3.2 can result in the calculation of nonconservative dose rates.[18] For all important energy groups, it is desirable for the flux to not change more than about 30% from one mesh interval to the next. For all multigroup codes, the selection of an appropriate cross-section energy group structure is also required. Improper energy group detail in important energy ranges can lead to erroneous results. Employing too few or inappropriate energy groups can sharply deteriorate the reliability of the calculations.[19]

As noted in Sect. 3.2, "ray effects" are often seen in discrete ordinates calculations involving the transport of radiation from localized sources through low-density (e.g., air) regions. The use of auxiliary codes and the proper selection of the spatial mesh and angular quadrature help to mitigate these effects. Calculation of fluxes more than a meter or so from a cask or transport of radiation from spent fuel within a large hot cell could be unreliable unless ray effects are removed.

3.5.2. Consideration of the Physics

Erroneous results can be produced if the radiation transport code and cross sections employed are not suitable for the physics of the applied problem or if the user does not adequately understand the physics of the problem. A prime example as illustrated in Sect. 7.2.3 is the sensitivity of the dose results to the selected cross-section set and/or group structure (also see Sect. 4). A good code using poor cross sections will yield poor results. For deep-penetration problems where the flux attenuation is between 10^{+5} and 10^{+7}, it can be easily illustrated that the uncertainty in the surface flux or dose is at

least an order of magnitude greater than the cross-section uncertainty.[20,21] Other areas that need to be considered prior to their dismissal from an analysis is (1) the effect of neutron and secondary gamma doses, (2) scattered radiation from the surroundings (e.g., the ground, nearby structural walls or buildings), and (3) the importance of subcritical multiplication to radiation doses for both wet and dry configurations.

For 10-year-old-cooled fuel it is often thought that the neutron and secondary gamma contribution is relatively small. However, cask designs exist where the secondary gamma dose accounts for 85% of the total gamma dose even though the neutron source is a factor of 10^{+7} smaller than the gamma source. This is caused by having an effective primary gamma shield followed by a neutron shield that produces the secondary gammas via neutron capture. Different source characteristics and/or different cask designs can cause primary gamma rays to dominate. In either case, the role of both neutrons and secondary gammas to the total dose becomes increasingly important for high burnup spent fuel. The gamma dose contribution from secondary gamma rays is not provided by point kernel codes.

Consideration of increased dose rates due to scatter from the ground, air, or adjacent nonshielding structures could be of prime importance from an operational and/or ALARA analysis viewpoint. This scattered radiation can significantly increase the dose over that coming directly from the shield. However, consideration of this possible contribution can also greatly increase the complexity of the geometric model and the calculational time of the analysis. Also, point kernel codes may be unreliable in situations where scattered radiation beyond the shield or returned from the shield (e.g., within a hot cell) is important.

Another contributor to the total dose that is sometimes overlooked is the neutrons generated from subcritical multiplication. Even for dry systems, the dose due to subcritical multiplication can be >25% of the total neutron dose. The radiation dose importance increases with the value of k-effective and, as the importance of the fission source grows, so does the importance of being sure an accurate k-effective value is obtained and used for the analysis (see Sect. 7.1.3). If k-effective is calculated within the shielding analaysis itself, an appropriate geometry model and cross-section set must be used.

Finally, an inexperienced analyst needs to exercise a good deal of caution in performing deep penetration shielding analyses with Monte Carlo codes. Attempting nonbiased (analog) Monte Carlo for deep penetration analyses will result in expensive calculations with very high statistical uncertainty. However, performing the analysis with ineffective biasing parameters can likewise lead to inaccurate results even if the statistical uncertainty is low. Thus, one must have an effective scheme for obtaining biasing parameters and then also be able to determine the adequacy of the dose results from a review of the output provided by the code.

3.6 REFERENCES

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4. SHIELDING ANALYSIS DATA

The primary purpose of this section is to inform the user about the basics of shielding analysis data, particularly cross sections, to summarize the current state of affairs, and to suggest to users that prudence is advised in the selection of an approach to obtaining data for spent fuel transport/storage applications.

4.1. TYPES OF CROSS-SECTION DATA LIBRARIES

4.1.1. Evaluated Cross-Section Data

In the United States there has been a continuing effort for about 20 years to prepare a cross-section library that provides evaluated data that meet the requirements for solving radiation transport problems for a wide range of applications. The resulting library is called the Evaluated Nuclear Data File (ENDF/B). The format for the data is described in ref. 1, and the current version of the library is ENDF/B-V.[2]

Generally data are tabulated as energy, cross-section pairs on a fine energy grid. Cross-section values between the tabulated points can be obtained by interpolation laws that are also given for the entire grid. The interpolation is usually log-log or linear-linear, but the evaluator, the person responsible for recommending what data are appropriate, can choose from several interpolation schemes to describe the energy dependence. The evaluator considers all available experimental data and supplements the measurements with nuclear model calculations. The final product, the "evaluation," provides a unique specification of the cross sections for a given element over the energy range from 1.0E-5 eV to 20.0 MeV.

It is a requirement of ENDF/B that the partial cross sections must sum to the total at every energy point. The evaluator may use parameters to represent the total, elastic, capture, and, if appropriate, the fission cross sections for isotopes with a great deal of structure or resonances. Angular distributions of secondary neutrons from elastic and inelastic scattering and other reactions can be tabulated (at incident neutron energies) as a function of scattering angle cosine or represented as Legendre expansions.

A data testing program is undertaken prior to the release of a new version of ENDF/B, and various subcommittees must approve the results of calculations versus a series of experimental benchmarks. For ENDF/B-V, the disciplines covered were fast reactor, thermal reactor, shielding, fission products, and dosimetry.[3] While all have some relevance to spent fuel casks, no specific benchmarks of that type are included in the CSEWG compilation.[4]

In addition to ENDF/B, there are several other useful evaluated cross-section libraries. These include the Livermore Evaluated Nuclear Data Library (LENDL),[5] the Karlsruhe Evaluated Library (KEDAK),[6] the United Kingdom Nuclear Data Library (UKNDL),[7] the Japanese Evaluated Nuclear Data Library (JENDL),[8] and two recent efforts, the Joint Evaluated File (JEF) and the European Fusion File (EFF).[9]

The National Nuclear Data Center at Brookhaven National Laboratory distributes the official ENDF/B evaluated data library in the United States. The Radiation Shielding Information Center (RSIC) at Oak Ridge National Laboratory distributes other evaluated data and, more importantly, all the processed cross-section data used for radiation transport calculations.

In order to be adequate for "shielding" applications, an evaluation for a given isotope must also include photon production data. The ENDF/B-V version does have a reasonable proportion of isotopes with photon production data, but there are a few exceptions. In those situations, it is usually most convenient to use the LENDL library because all of its entries have photon production data.

Photon interaction data are very well known in comparison to neutron and photon production data. Photon interaction data for atomic numbers 1–100 appear together on a single evaluated library.[10] The current ENDF/B-V library has no photoneutron production data so there need be no connection of photon interaction to neutron data.

4.1.2. Multigroup Cross-Section Data

As was mentioned in Sect. 3.2, the type of data used for analysis of radiation transport by the discrete ordinates methods is "multigroup." One of the main advantages of multigroup data is that the Monte Carlo (three-dimensional) codes are able to use the same sets of multigroup data as used in one-dimensional and two-dimensional discrete ordinates calculations. This feature makes comparisons of results on a common energy grid possible and allows the direct coupling of discrete ordinates and Monte Carlo calculations. Another advantage is the ability to easily perform adjoint calculations, a great difficulty for point Monte Carlo. Many problems, such as those with a large external source region or a small concentrated detector region, are more amenable to solution in the adjoint mode.

Often, however, an analyst simply uses the same set of multigroup cross sections in all calculations, even though the source, geometry, and material compositions may be quite different. There are many pitfalls to this approach, and some will be enumerated later in this section. For most analyses, consideration should be given to the importance of resonance self-shielding, final energy-group structure and collapsing procedure, and temperature correction of the group-averaged cross sections.

As will be described in more detail in Sect. 4.2, a user typically chooses a library from an array of available multigroup cross-section libraries already prepared by other analysts. These available libraries may be application-dependent or pseudo-application independent libraries. The former must be used with great care since they were likely developed for a different application and cannot be further processed to be suitable for the given task. The latter allow correction for temperature and resonance self-shielding effects and can be tailored to the problem at hand. Naturally the analyst must have at hand the appropriate calculational tools to perform this additional processing for the given application.

As noted in Sect. 3.2, a multigroup cross section is obtained by performing a weighted average of the "true" cross section over the energy limits of the group. The average is typically done to preserve the reaction rate over the energy range of the group. Hence, for this situation the definition of a group cross section, σ_g is usually expressed as

$$\sigma_g = \frac{1}{\phi_g} \int_g dE \sigma(E) \phi(E) , \tag{4.1}$$

where $\phi(E)$ is the flux density at energy E, $\sigma(E)$ is the cross section at E, and ϕ_g is the integral of the flux over the energy limits of the group.

It is implied in Eq. (4.1) that the flux is a known quantity. Of course if the flux were already known for a given problem, there would be no need to run a radiation transport code to calculate it! In all calculations of multigroup cross sections, the flux is approximated with a "weighting" function,

W(E), that is expected to have a spatial-averaged energy and dependence that is close to that for the problem to be solved. The expression of Eq. (4.1) is therefore approximated as

$$\sigma_g = \frac{1}{W_g}\int_g dE\,\sigma(E)W(E) \ . \tag{4.2}$$

Thus, an additional "parameter" that determines the application range of a given library is the choice of W(E) used to generate the library.

The quantity $\sigma(E)$ in Eq. (4.2) is the energy-dependent cross section. The best estimate for this function is found in the evaluated cross-section libraries discussed in Sect. 4.1.1.

4.1.3 Point Cross-Section Data

There are cross-section libraries that are known as "point" libraries because the data contained therein are represented by cross sections tabulated at a large number of energy points. These have been processed from the evaluated libraries into forms suitable for further processing into multigroup form or for direct use in a transport code, primarily of the Monte Carlo type.

For a "point" Monte Carlo library, the data typically are represented by values tabulated at energy points selected such that interpolation between points yields values acceptably close to the original evaluated data. Since an evaluated data file for an isotope such as iron may require up to 5000 energy points to represent the total cross section over the energy range from 10^{-5} eV to 20.0 MeV, the point approach involves extensive cross-section data files. The scattering angular distributions are typically represented in a point fashion such that for a given incident particle energy, the scattering kernel is restructured so that values are tabulated at a fixed number (e.g., 30) of equally probable cosine values, making the selection of scattering directions very fast. Of course, use of point libraries avoids having to determine an appropriate weighting function W(E) [see Eq. (4.2)] which is a potential problem associated with multigroup libraries.

Point libraries are typically designed for a particular transport program and are often included in the code package. Multigroup data can often be used in several types of transport codes and as a result there are many more multigroup data packages available.

4.2. PROCESSING CODES

Computer codes or, in some cases, code systems are available for processing the evaluated data into point or multigroup form. These are distributed from the Radiation Shielding Information Center (RSIC) as part of the collection of Peripheral Shielding Routines (PSR).[11] There are a variety available to the ambitious user who wishes to get into the cross-section processing business. Many of the point and multigroup libraries used in current radiation transport calculations in the United States have been generated using PSR-63/AMPX-II,[12] PSR-105/MINX,[13] or PSR-171/NJOY-II.[14] The resonance treatment in AMPX-II is the Nordheim Integral Treatment[15] available via the NITAWL module. The MINX and NJOY programs utilize the Bondarenko[16] method for resonance self-shielding and temperature correction.

Some installations maintain independent processing systems in-house, but this practice has dwindled in recent years due to decreasing budgets and the general availability of systems such as those listed above. To maintain a processing system is a big chore and most analysts prefer to rely on using multigroup libraries generated by others or, in the case of point Monte Carlo, those provided with the codes.

RSIC has acquired, generated, and packaged data libraries as part of its Data Library Collection (DLC)[17] since the late 1960s. These have proved to be popular and useful over the years. Until the late 1970s, the majority of such libraries were inflexible in that they had been generated for a specific project at a fixed temperature and composition, often at infinite dilution (no consideration of self-absorption by the processed nuclide).

4.3. APPROACHES TO USING MULTIGROUP CROSS SECTIONS

4.3.1. Application-Dependent Libraries

A broad-group, application-dependent library is normally ready for direct input into a radiation transport code and are therefore often referred to as "working" libraries. These libraries typically are in ANISN (after the code, see ref. 18) or, more generally, discrete ordinates format. It is recommended that such libraries, which are normally transmitted to users in card image format, be converted to unformatted or "binary" form. A DLC package includes a handling code that will do the conversion. Useful ANISN library manipulations, can be performed using programs such as PSR-48/ALC1[19] or PSR-75/AXMIX.[20] The latter can also be used to mix macroscopic cross sections prior to their input into a multigroup code.

A fine-group ANISN-type library can be used directly once binary conversion is done. It is likely, however, that a collapse to a smaller number of groups would be performed prior to its use in a multi-group transport code. If an appropriate spectrum is known, such a collapse can be done using the AMPX module COMMAND. The weighting spectrum and the description of the "few-group" structure are required input to COMMAND.

Such a spectrum is usually determined by using results from a one-dimensional discrete ordinates calculation. A one-dimensional model of the true geometry of the problem would be devised, and several runs would be performed. If the spectrum in the system shows dramatic variation from zone to zone, it may be prudent to perform several collapses to specify appropriate cross sections for the entire problem. It is possible that a given problem would require several different sets of cross sections for the same material if the material is present in several different zones.

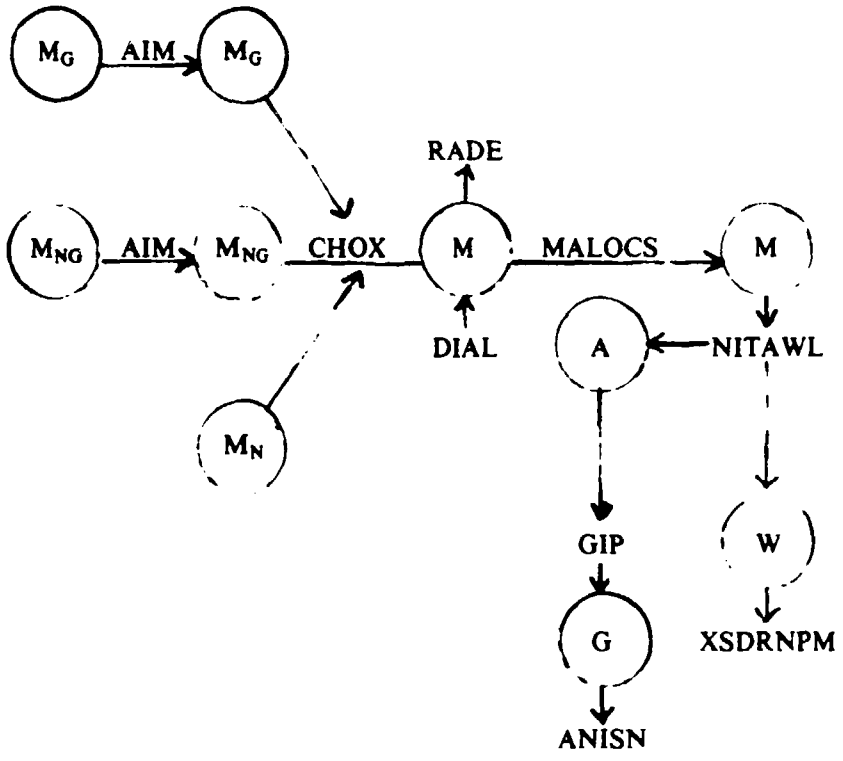
It is not necessary to save the zone-dependent spectral results to be used as input to a code like COMMAND because discrete ordinates codes offer various types of cross-section collapsing options that may be suitable. Thus, one output of such a run could be a collapsed cross-section library in ANISN format ready for subsequent use.

Using an application-dependent library, broad- or fine-group, is relatively straightforward. Using a library in "flexible" format (e. g., the AMPX master library format) is more involved, but can offer distinct advantages in making the library more independent of a specific application.

4.3.2. Application-Independent Libraries

The libraries in AMPX, CCCC, or MATXS formats offer the user a great deal of control over the choice of cross sections for a given problem. Essentially all data that were on the original evaluated data set are present on an AMPX master library, for example. Most importantly, especially if the library has many groups, the user can derive application-dependent sets for different uses (see Sect. 5.3.2 for some examples of the variety of libraries that have been derived from the VITAMIN-C fine-group library[21]). All this flexibility has a price, of course. However, the price is not as dear as that of getting into the business of processing cross sections directly from ENDF/B.

The Controlled Thermonuclear Reactor (CTR) standard blanket sample problem, shown in Fig. 4.1, demonstrates the coupling of neutron and photon production cross sections and energy group



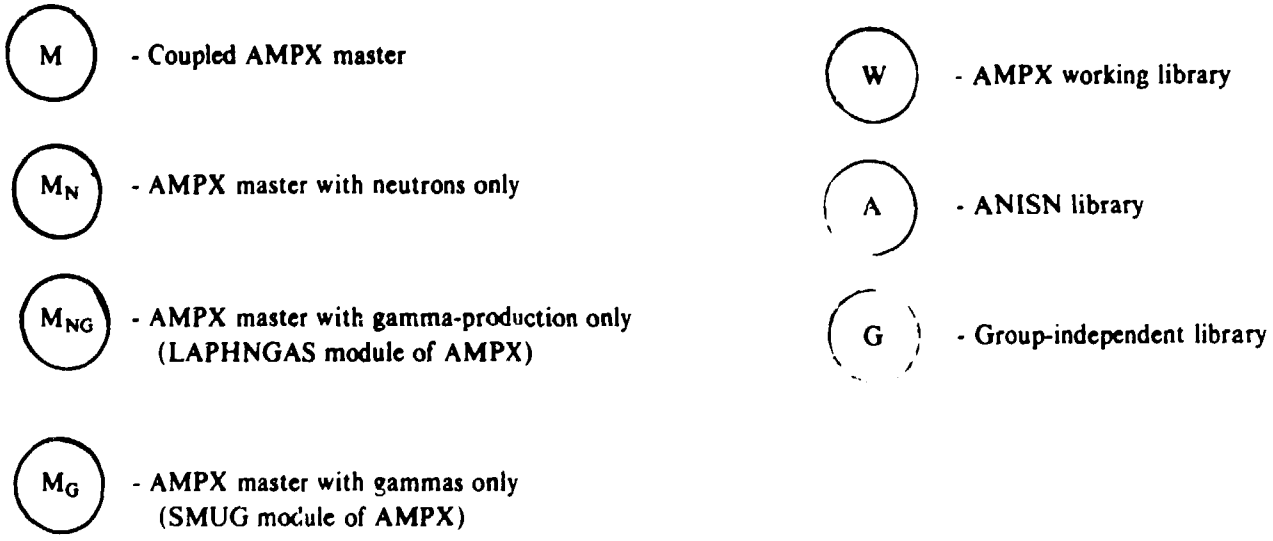


Fig. 4.1. The CTR standard blanket sample problem for DLC-41/VITAMIN-C demonstrating the use of AMPX modules to produce a coupled cross-section library for transport calculations.

collapsing. The various types of AMPX cross-section libraries involved in this process are given in shorthand notation. The running times on an IBM-360/91 for various parts of the calculation are summarized in Table 4.1. Note that the major task was the conversion from card image to binary form. It should be noted that the conversion task needs to be done one time and does not have to be repeated for each problem.

Table 4.1. Running times, region, and I/O requirements for solving the CTR standard blanket sample problem in DLC-41/VITAMIN-C

CTR standard blanket	Name	Maximum region	Total I/O[a]	Total Time	Individual Code	Individual Region	Individual I/O[a]	Individual Time
Job 1	IJB3SAMP	270K	20	3.42 m	AIM	270K	5	1.76 m
					AIM	270K	3	1.23 m
					CHOX	270K	12	25 s
Job 2	IJB4SAMP	310K	11	1.01 m	RADE	300K	5	28 s
					DIAL	268K	2	10 s
					MALOCS	310K	4	23 s
Job 3	IJB5SAMP	420K	18	3.94 m	NITAWL	410K	7	54 s
					XSDRNPM	420K	11	3.03 m
Job 4	IJB5ASAM	308K	16	4.23 m	GIP	236K	7	26 s
					ANISN	308K	9	3.80 m

[a]In thousands.

The developers of SCALE[22] have produced broad-group, pseudo-application-independent libraries for distribution with their system. This approach allows the analyst to perform a problem-dependent resonance treatment and temperature correction on these libraries (via the NITAWL or BONAMI modules of both the AMPX and SCALE systems) prior to their use in a radiation transport code. Of course the original collapse from an AMPX fine-group library uses a weighting spectrum W(E) that may or may not be optimal for the application at hand.

4.4. RESPONSE DATA

Normally, the radiation environment is first calculated in terms of particle flux and then translated via response functions to personnel exposure, heat generation, material damage, etc. The response function may be a single conversion factor that is multiplied by the total flux to obtain the total response. More often, the response is a function of energy and is multiplied by the group-wise neutron or gamma-ray flux and summed over groups to yield the total response. In either case, inaccuracies or uncertainties in the response data relate directly to uncertainties in the final answer.[23]

In reviewing response data, it is important to distinguish between microscopic quantities such as absorbed dose, energy deposition, and atom displacements, and macroscopic consequences such as human illness, metal fracture, and electronic component failure. In general, microscopic response functions are known reasonably well, perhaps in the range of 5 to 20%, while macroscopic responses may vary by orders of magnitude. Therefore, the two classes of data will be addressed separately.

Microscopic response data most applicable to spent fuel transport, storage, and handling are kerma and absorbed dose. These response functions are typically derived from basic ENDF data, and reflect a similar level of accuracy. Some additional uncertainty arises from the exclusion of minor but contributing reactions, or from over-simplification of the geometric models used to compute energy deposition or absorbed dose. However, the combined uncertainties of the nuclear data and the approximations used in constructing the response functions appear acceptably small and do not typically require special attention. Kerma responses are available from the International Commission on Radiation Units and Measurements (ICRU)[24] and from the MACKLIB-IV response library.[25] Dose response functions are available from a variety of sources, and are often included in multigroup cross-section libraries available from RSIC. The most commonly used flux-to-dose conversion factors used in recent years are those from ANSI/ANS 6.1.1-1977.[26] This ANSI standard provides polynomial coefficients for an analytic fit of the conversion factors as a function of energy. This format allows conversion factors to be easily generated for any selected group format. However, it should be noted that a recent ICRU study[27] recommends an increase in the neutron quality factor (and hence flux-to-dose conversion factors) of approximately a factor of 2.

By contrast, damage or failure-type data are considered highly uncertain. This appears to be due to either the lack of understanding of the complex mechanisms involved or the lack of empirical data. Also, the nature or severity of the consequence may depend on the surrounding environment and the pre/post-irradiation history of the particular material. Healing effects in the human body and annealing effects in many materials further complicate the accurate characterization of macroscopic responses.

Damage responses most applicable to storage and handling of spent fuel are human tissue damage, metal component damage (embrittlement, swelling, fracture), organic/synthetic material damage (embrittlement, softening), and optical component darkening (hot cell windows). Of these, human tissue damage warrants perhaps the least concern since Federal regulations require sufficiently conservative design limits (in terms of dose) to reasonably preclude the possibility of an observable response (cancer, leukemia, etc.). Therefore, the large uncertainties associated with these responses do not directly impact the shield designer.

Metal component damage also appears to be of little concern since the dominant damage mechanisms are primarily neutron-induced. A conservative design criterion used in light-water reactor systems is that load-bearing components must not exceed a neutron exposure of 10^{21} cm^{-2}. A neutron source of 2×10^{10} s^{-1} corresponds to about 30 typical PWR spent fuel assemblies (see Fig. 2.1) and assuming the entire source is concentrated in a 1-m-diam cylinder would give a yearly exposure to the cylinder (e.g., a cask) on the order of 2×10^{13} cm^{-2}, which would correspond to a lifetime of 50 million years.

Organic and synthetic materials will be present in casks and hot cells in the various seals, impact limiters, and insulators used. A summary of the radiation tolerance of many polymers and elastomers indicates that most of these materials experience an almost continuous degradation of physical properties over the exposure range of 10^6 to 10^{10} rads. This information has been mostly obtained from actual irradiation of material samples and is accurate for the specific test conditions. However, large uncertainties arise from extrapolating the test data to other materials and to other conditions such as temperature, humidity, and material stresses.

Radiation darkening of glass within the MRS hot cells will present some concern, especially regarding optical components in the visual surveillance equipment. Fortunately, the damage response is fairly well characterized, so long as the glass composition and impurities are accurately known.

4.5. SOURCES OF BUILDUP FACTOR DATA

Approximate methods for the calculation of the transport of primary photons are frequently employed, and these methods often require the use of buildup factors (see Sect. 3.4). Values of the buildup factor are determined from experiments and transport theory calculations that are based on assuming an infinite homogeneous shield. Buildup factor data are also available as coefficients and parameters for fitting functions which facilitate their use. One of the most used forms, the Taylor form, is a sum of exponentials which allows the buildup factor to be easily combined with the exponential transport kernel. The equations can be integrated analytically over source surfaces or volumes of simple shape.

The point kernel, or kernel integration, method is used almost exclusively for photons. It is very seldom used for neutrons because the neutron cross section generally is a rapidly changing function of energy and nuclide, and no simple tabulation of buildup factors would be possible. The method has been implemented in a large number of computer codes, most of them treating a general three-dimensional geometry and using buildup factor data in some form. The buildup factor data can be stored in a table. Interpolated values for use in a numerical integration or coefficients for a fitting function can be stored. The coefficients apply to the various shielding materials and source energies. The argument of the buildup factor is the number of mean free paths, x, between the source point and the "detector." The number of mean free paths (mfp) can be evaluated even though many materials may be traversed between the source and detector. However, as noted in Sect. 3.4, this situation can cause the computed dose to be in great error because the available buildup factor data are for particular homogeneous materials.

Two of the more popular forms for buildup factors are the Taylor representation:

$$B(x) = A_1 \exp(a_1 x) + A_2 \exp(-a_2 x) ,$$

where A_1, A_2, a_1, and a_2 are empirical constants and $A_2 = 1 - A_1$, and the Berger form:

$$B(x) = 1 + Cx[\exp(Dx)] ,$$

where C and D are empirical constants. A relatively new form, with remarkable ability to accurately reproduce transport theory results even for low energy and low atomic number (where other functions fail to fit accurately), is the geometric progression (G-P) form:

$$B(E,x) = \begin{cases} 1 + (b-1)(K^x - 1)/(K-1) & \text{for } K \neq 1 \\ 1 + (b-1)x & \text{for } K = 1 , \end{cases}$$

$$K(x) = cx^a + d^*[\tanh(x/X_k - 2) - \tanh(-2)]/[1 - \tanh(-2)] ,$$

where x is the source-detector distance in mfp, b is the value of the buildup factor at 1 mfp, and K is the multiplication per mfp. The second equation represents the dependence of K on x, while a, c, d, and X_k are fitting parameters which depend on source energy.

An American Nuclear Society Standards Working Group, ANS-6.4.3, is developing a set of evaluated gamma-ray isotropic point-source buildup factors and attenuation factors for a standard reference data base.[28] A largely unpublished set of buildup factors calculated with the moments method at the National Bureau of Standards is being evaluated by recalculating key values with Monte Carlo, integral transport, and discrete ordinates methods. This 1985 data base is being reduced using the 5-parameter G-P fitting function and is being incorporated into several point kernel codes.

4.6. CONCLUSIONS

The radiation transport analyst should bear in mind the pitfalls of using the same broad-group library for every project. Experience will help to indicate when caution should be employed. The availability of libraries that allow the derivation of problem-dependent sets gives the analyst the tools needed to do the job properly.

In Sect. 7 some assessment studies are described that employ many of the libraries discussed in this section. Results indicated that additional work is warranted to be able to develop ready-to-use cross-section libraries for spent fuel cask analyses.

Improved buildup factor data have recently become available and need to be utilized within existing point kernel codes.

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5. REVIEW OF CODES AND DATA

The previous sections have provided a review of the methods and techniques most often used for predicting radiation doses from shielded spent fuel or high-level radioactive waste. This review points out the important aspects of each component that make up a complete radiation dose evaluation: radiation source specification, selection and/or processing of appropriate radiation transport data, proper simulation of the radiation transport, and final dose (or response) evaluation. A variety of computer programs has been developed over the years to treat each of the separate aspects of a complete shielding analysis. The major source of information on available codes and data libraries associated with radiation shielding is the Radiation Shielding Information Center (RSIC) at Oak Ridge National Laboratory. Through a cooperative agreement with the DOE National Energy Software Center at Argonne National Laboratory and the OECD Nuclear Energy Agency Data Bank in Paris, France, the RSIC staff have been able to effectively serve the needs of the United States and worldwide scientific communities for software and information regarding radiation shielding.

The computer code collection (CCC numbers), peripheral shielding routines (PSR numbers), and data library collection (DLC numbers) distributed by RSIC are listed, briefly described, and categorized by function/keyword in ref. 1. This reference indicates that RSIC distributes approximately 63 discrete ordinates code packages, 95 Monte Carlo code packages, and 64 point kernel code packages. In addition to these packages, there are a few proprietary codes and not-for-U.S.-distribution foreign codes that provide additional tools for radiation shielding analyses. Fortunately, many of the above packages available from RSIC could be quickly eliminated for the present work because (1) the package was developed for special-purpose shielding applications (e.g., nuclear weapon detonation, space flight) or limited geometries, and (2) the package consists of a code or data that have been superseded by a more versatile or up-to-date program or data library. Beyond this, the criteria used to assess available packages were:

1. physics model(s) (see Sects. 2–4);
2. problem solving capability and flexibility (see Sects. 2–4);
3. geometric capabilities (see Sect. 3);
4. source and completeness of data (see Sects. 2 and 4);
5. validation and/or demonstrated accuracy pertinent to shielded spent fuel applications;
6. efficiency;
7. ease-of-use and documentation;
8. availability and compatibility; and
9. maintenance program.

The first five criteria noted above are of prime importance in determining the relative merits of a particular code or data library for accurately solving the shielding problems of concern in the transport, storage, and handling of spent fuel or high-level radioactive waste. The first criteria was used to assess the adequacy of the physics model employed, while the second criteria deals with the adequacy and versatility of the solution approach (for codes) or data generation methods (for data libraries). These two criteria, together with the geometries for which a code solution can be obtained and the completeness of available data, provide the basis for problem applicability as discussed in detail in Sects. 2–4. Validation and/or demonstrated accuracy for the required applications provide a further indication of the known or perceived value of a code or data package.

The last four criteria pertain more to the usability and software quality assurance features of the package. The relative importance of the calculational efficiency in a package will vary with the application. For safety analysis or licensing calculations, the efficiency of a code is much less important than its accuracy. However, for initial design or scoping work the reverse may be true. Ease-of-use and appropriate documentation are essential features if a code is to be readily used by "non-expert" users. Likewise, the availability and computer compatibility of the code, along with a viable centralized maintenance program, has bearing on the ease with which DOE contractors will be able to obtain, operate, and update the package along accepted quality assurance guidelines.

Reference 2 contains a section on considerations necessary in choosing a suitable discrete ordinates code for general applications. The considerations discussed fit within the assessment criteria used here and offer valuable insight into the complex issues and questions that should arise in determining the "best" code. Based on the authors' knowledge and available reference material, the attempt in the following sections is to provide an overview description of the premier codes selected using the stated criteria. Sections 5.1–5.3 discuss radiation source generation codes, radiation transport and dose evaluation codes, and cross-section data libraries, respectively, for the known DOE applications cited in Sect. 1. Appendices A–B contain abstracts for a select few of the codes and data libraries discussed in Sects. 5.2–5.3. Then Sect. 5.4 discusses a modular code system that illustrates one approach to performing nuclear fuel facility and package design analyses using standardized (i.e., fixed) analytic sequences. There is some overlap in the designated categories. For example, the ISOSHLD/RIBD-II code package provides both the gamma radiation source (from fission products only) and a gamma shielding analysis within a single calculation.

5.1 CODES FOR RADIATION SOURCE GENERATION

Table 5.1 provides a list of the codes which, on an initial overview, appeared suitable and/or commonly used for generating spent fuel radiation source terms. All the codes are available from the RSIC computer code collection. These codes were selected from the RSIC collection based on the assessment criteria stated above. The emphasis of the assessment was directed at the code's capability for generating accurate and complete radiation source terms from the calculated isotopics. An assessment of the codes with regard to the depletion and decay models is beyond the scope of this report.

The evaluation was performed using the documentation for each code package. Codes were eliminated for a variety of reasons. A tremendous plus for the U.S. codes was the accessibility of the developers and major users who could be utilized in any future efforts. Also, none of the foreign codes appear to offer any significant advantage over the available U.S. codes. This rationale is the one major reason for not recommending DCHAIN2, PEPIN, RASPA, and RICE-CCC. In addition, none of these codes have light element libraries, DCHAIN2 and PEPIN do not appear to have actinide libraries available, and RASPA data were oriented towards a unique reactor type (SNR 300 fast reactor).

The remaining codes of Table 5.1 warrant more careful attention. The most widely known code in the table is the original ORIGEN code which serves as a basis for several of the other codes: ORIGEN-JR, KORIGEN, ORIGEN2, and ORIGEN-S. Although ORIGEN is still widely used by industry, the four updated codes all provide significant improvements over the original version. These improvements are well documented in the respective references for each updated code. Thus, although the original ORIGEN code is still very widely used, the availability of greatly improved versions caused the code to be omitted as one of the premier codes. Of the four updated ORIGEN codes, the U.S. codes ORIGEN2 and ORIGEN-S appear best for DOE applications involving spent fuel isotopic characterization.

Table 5.1. Computer programs utilized for generation of radiation source terms

Code (RSIC CCC No.)/ developer	Language	Known computer implementation	Description and comments	Refs.
DCHAIN2 (CCC-370) Japan Atomic Energy Research Institute	FORTRAN IV	FACOM 230-75	Point calculation of nuclide transmutation via Bateman equations. Nuclear data library for 1170 fission products. Gamma source spectrum computed by FPGAM auxiliary code (CCC-386). Good documentation.	3
EPRI-CINDER (CCC-309) Los Alamos National Laboratory	FORTRAN IV	CDC-6600	Point depletion code for computing actinide and fission product atom densities. Solution via Bateman equations. Auxiliary codes required for generating radiation source spectra and strengths. Other code versions are CINDER2, CINDER3, CINDER7, and CINDER10. Data libraries and availability vary between versions.	4,5,6
FISPIN (CCC-413) United Kingdom Atomic Energy Authority	FORTRAN IV	ICL 2982	Point depletion code for evaluating fission product, actinide, and structural material inventories. Data libraries for each group of nuclides. Gamma energy spectrum (fixed groups) and total neutron source generated.	7
KORIGEN (CCC-457) Karlsruhe Nuclear Research Center, Federal Republic of Germany	FORTRAN IV assembler	IBM 3033	Point depletion code for actinides, fission products, and light elements. Solution by matrix exponential method. Substantial update of original ORIGEN code and data libraries. Good documentation. Photon spectra (fixed groups) and neutron source strength provided.	8
ORIGEN (CCC-217) Chemical Technology Division, Oak Ridge National Laboratory	FORTRAN IV	IBM 360/370 CDC 6600	Point isotope generation and depletion code. Solution by matrix exponential method. Actinide, fission product, and light element libraries available. Photon source spectra (fixed groups) and neutron source strength generated using outdated data and/or analytic functions.	9
ORIGEN-JR (CCC-399) Japan Atomic Energy Research Institute	FORTRAN IV	FACOM 230-75	Update of ORIGEN code with burnup-dependent cross sections allowed. Substantial improvement to generate neutron and gamma source strengths and spectra (fixed groups) for ANISN, DOT-II, and QAD-P5 shielding codes.	10

Table 5.1. (continued)

Code (RSIC CCC No.)/ developer	Language	Known computer implementation	Description and comments	Refs.
ORIGEN2 (CCC-371) Chemical Technology Division, ORNL	FORTRAN IV	IBM 360/370 CDC, VAX, PRIME, UNIVAC, IBM PC	Significant update of the ORIGEN code to remove deficiencies, improve input features, provide new and better data libraries (actinide, fission product, and light elements). Photon source spectra (fixed groups) and neutron source strength improved over ORIGEN code. Well documented and widely used.	11,12,13
ORIGEN-S (CCC-466) (CCC-475) Nuclear Engineering Applications Department at ORNL	FORTRAN IV FORTRAN 77	IBM 360/370 CDC CRAY-XMP	Significantly updated version of the ORIGEN code developed for the SCALE system. Decay data and photon data same as for ORIGEN2. Radiation source (n and γ) strength and spectra provided in user-specified or default multigroup energy structure. Well documented.	14,15
PEPIN (CCC-285) Centre d'Etudes Nucleaires de Saclay, France	FORTRAN IV	IBM 360/370	Point code that solves appropriate differential equations to obtain fission product concentrations, activities, photon spectra, and decay heat. Poorly documented in English.	16
RASPA (CCC-352) INTERATOM, Federal Republic of Germany	FORTRAN IV	CDC CYBER 172 CDC 6600	Point code for calculation of buildup and decay of fission products and actinides. Data tailored to SNR 300 reactor. Gamma source spectra generated for any multigroup format.	17
RIBD-II (CCC-79) Pacific Northwest Laboratories	FORTRAN IV	IBM 360/370 UNIVAC 1108	A subroutine within the ISOSHLD II and III point kernel codes. Performs a reactor point depletion analysis to produce gamma source spectra for fission products. Fission product data libraries available for generic thermal and fast reactors.	18
RICE-CCC (CCC-348) Central Electricity Generating Board, United Kingdom	FORTRAN IV	IBM 370/65 UNIVAC	Point depletion code for evaluating fission product and actinide inventories. Data libraries available. Photon energy spectrum generated. Neutron source strength from spontaneous fission only.	19,20,21

The ORIGEN-JR code provides neutron and gamma source spectra (fixed-group format) for input to shielding codes, but the basic rudiments (and shortcomings) of the ORIGEN code and data libraries are the same. In contrast, KORIGEN has updates similar to those of ORIGEN2 and is widely used in the Federal Republic of Germany. The main differences between ORIGEN2 and KORIGEN appear to be in the nuclear data that are used. KORIGEN was not investigated further because it was a foreign code with no distinct advantage over ORIGEN2 and one distinctive liability—no available actinide cross-section library for BWR reactors.

The ORIGEN2 code is the most popular of the updated versions of the ORIGEN codes. The library data and radiation source-term evaluation offer a significant improvement to the ORIGEN code. ORIGEN2 provides the gamma spectra in an 18-energy-group format which matches the group format of the 22n-21γ FCXSEC cross-section library[22] for all but the last few high-energy groups (typically unimportant for spent fuel). However, only the neutron source strength is provided by ORIGEN2. Thus, the analyst must generate a neutron spectrum in the required group structure when using ORIGEN2. Also, if using a gamma cross-section library with a different group structure other than that for which the source is provided, the analyst must adjust or interpolate the ORIGEN2 gamma source spectrum.

The ORIGEN-S code provides complete neutron and gamma source spectra in any multienergy-group format. Thus, the shielding analyst is provided with the flexibility to select a multigroup cross-section library without needing to interpolate from one fixed group to another. ORIGEN-S outputs the gamma source spectrum from each isotopic group (light element, fission product, and actinide), the total gamma spectrum, the separate spectrum for (α,n) and spontaneous fission neutrons, and the total neutron spectrum.

The CINDER series of codes represent the major alternative to the ORIGEN codes in the United States. As with the ORIGEN-type codes, there are several updated versions of the CINDER code[23] which have been developed and are currently in use at Los Alamos National Laboratory (LANL). Of these, EPRI-CINDER is the only one publicly available from RSIC. For the CINDER codes, LANL uses an auxiliary code called SPEC5 (not available from RSIC) to evaluate the spent fuel source spectra. The user may manually calculate or write coding to compute the combination of CINDER nuclide densities and SPEC5 spectra, account for significant bremsstrahlung from UO_2, and add gamma rays from spontaneous fission or (α,n) reactions as needed. The neutron spectrum may be produced by using the SOURCES code.[24] Another limitation of EPRI-CINDER is that light element libraries are not available. Thus, potential radiation sources arising from activation of light elements (e.g., ^{59}Co) must be evaluated in some alternate fashion.

Although older and far more limited than the ORIGEN- or CINDER-type codes, the RIBD-II code has been heavily used for spent fuel gamma sources because it is interfaced with the point kernel code ISOSHLD to provide an easy-to-use procedure for gamma-ray source generation and shielding analysis. The RIBD routine is limited to evaluating the gamma source spectra from fission products only and requires another routine called BREMRAD[25] to evaluate the bremsstrahlung source spectra. A summary of the ISOSHLD/RIBD system is included in Appendix A.

In a more complex and complete fashion, the SAS2 shielding sequence of SCALE (see ref. 26 and Sect. 5.4) uses ORIGEN-S to generate radiation source spectra for subsequent input to a radiation transport module.

The only code not mentioned in the above discussion is FISPIN. Like KORIGEN, the FISPIN code seems to be a high quality code and appropriate for the specified applications. But, as a foreign code, it offers no distinct advantage over the updated ORIGEN- or CINDER-type codes.

5.2 CODES FOR RADIATION DOSE EVALUATION

This section will separately provide a discussion of relevant codes that utilize the three basic techniques presented in Sect. 3. In contrast to Sect. 3, the approximate point-kernel codes will be discussed prior to the more accurate, but more complex, discrete ordinates and Monte Carlo codes.

5.2.1 Point Kernel Codes

As noted in Sect. 3, codes that utilize point-kernel techniques provide only approximate evaluations of the primary gamma-ray dose from a source. However, these codes are inexpensive, computationally fast, and far less cumbersome or complex relative to discrete ordinates or Monte Carlo codes. They are well suited for scoping studies, but their incompleteness (no neutrons or secondary gammas) and approximate nature could call into question their use for final design or safety analyses.

Table 5.2 provides a list of six of the more popular point-kernel codes. Of these, the QAD family of codes have surely enjoyed the greatest popularity and use. Originally developed at Los Alamos National Laboratory in the 1960s, it has been successfully updated by a variety of users. The latest and best version of QAD is QAD-CGGP which features the flexible, three-dimensional combinatorial geometry package (CG), the standard buildup factor data of ANS-6.4.3, and the geometric progression (GP) fitting function for the buildup factor data. These latter two features represent a substantial improvement over the basic buildup factor data and interpolation scheme currently used in most other codes. Only G33-GP (for single-scatter applications) has been updated to incorporate the new data and GP interpolation. The improvement is most evident for shield materials of low- or very high-Z number and/or low (<0.5 MeV) photons. The CG geometry feature of QAD-CG and QAD-CGGP is attractive because the geometry input description can be easily interchanged for use in combinatorial geometry versions of MORSE (see Sect. 5.2.2).

It is very difficult to determine which of the six codes in Table 5.2 is the best in terms of the assessment criteria, although the ANS-6.4.3 buildup data and GP interpolation appear to provide an advantage to QAD-CGGP and G33-GP (where a single-scatter code is needed). The ISOSHLD code, however, does have the nice feature of generating an irradiated fission product source using the RIBD routine. Also, an extremely user-friendly version of ISOSHLD (called MICROSHIELD) has been developed in a proprietary package (see ref. 32). The other codes in the table also have attractive, but less noticeable, features that distinguish them from QAD-CGGP or G33-GP in terms of the assessment criteria. It might be hypothesized that proprietary for-sale codes such as MICROSHIELD or PATH which see their users as valuable for-profit customers may have a more systematic approach to quality assurance criteria--maintenance, ease-of-use, and validation.

Note that the new buildup factor data and GP fitting functions could be rather easily added to any of the point-kernel codes mentioned in this section. Many, if not all, of these codes will probably be updated at some time once the advantage of the new data and fitting function is realized.

Other codes that use approximate procedures are also available for many specific applications that lie within the DOE interests. For example, the SKYSHINE codes[46,47] use a data base generated by discrete ordinates and Monte Carlo codes to estimate the transmission and reflection of gamma rays and neutrons by concrete and steel, and for the scattering of radiation in air. This code has been successfully used to provide efficient (low cost) and satisfactory dose results for long-range air transport applications (e.g., the determination of site dose from nuclear facilities).

Table 5.2. Computer programs based on point-kernel techniques utilized for radiation dose evaluation

Code (RSIC CCC No.)/ developer	Language	Known computer implementation	Description and comments	Refs.
G33-GP (CCC-494) S3 (CCC-322) Original code from Los Alamos National Laboratory	FORTRAN 77 FORTRAN IV	IBM 360/370 IBM PC Data General	Gamma-ray scattering code using point-kernel techniques. Based on a calculated single-scatter source, doses at detectors are evaluated with and without buildup. Direct beam responses (without the single-scatter) are also evaluated with and without buildup. Nontrivial geometric input specifications. Up-to-date buildup factor data in G33-GP. S3 is Westinghouse updated version of original G33.	27,28
ISOSHLD[a] (CCC-79) Pacific Northwest Laboratories	FORTRAN IV	IBM 360/370 UNIVAC IBM PC	Code uses direct point-kernel techniques to generate gamma doses for common geometric models. Source may be input directly or calculated via the RIBD routine (see Table 5.1). An extremely user-friendly, for-sale version called MICROSHIELD is available for the PC (see ref. 32).	29-32
MERCURE 4-V5 (CCC-142) CEA Centre d'Etudes Nucleaire de Saclay France	FORTRAN IV	IBM 360	Gamma-ray kernel integration code for straight line attenuation in three-dimensional geometries defined by planes and quadric surfaces. Stochastic integration of point sources as volume, simplified geometry input, and utilization of multigroup ANISN-formatted photon data are new features over MERCURE-3.	33
PATH GA Technologies, Inc.	FORTRAN	CDC, CRAY, IBM, UNIVAC, VAX	Proprietary point-kernel code available from GA. Buildup factor specification can vary with source and dose point. Claims to be "fully validated and suitable for nuclear licensing applications."	34,35
QAD[a] (CCC-48, 307, 346, 396, 401, 448, 493) Original code from Los Alamos National Laboratory	Version-dependent	IBM 360/370 CDC 6600, CDC CYBER, IBM PC UNIVAC, PRIME Data General	The QAD family of codes make up seven different code packages in the RSIC code collection. All use direct point kernel techniques and differ principally in the available geometry package, source integration method, buildup factor interpolation scheme, and ease-of-input. Latest buildup factor data and attractive geometry in new QAD-CGGP (CCC-493). Most widely used of point-kernel codes.	36-44
SCAP (CCC-418) Westinghouse Advanced Reactors Division	FORTRAN IV	CDC-7600	Single-scatter or albedo scatter point-kernel methods. Numerical integration of point source results over source volume. Anisotropic or isotropic point source representation allowed.	45

[a]Code summary provided in Appendix A.

5.2.2 Discrete Ordinates Codes

The discrete ordinates codes provide a numerical solution to the Boltzmann transport equation and, as such, are more appropriate for general applications than point-kernel or other appropriate codes. However, the added complexity of these codes requires greater computational resources and user involvement. Table 5.3 lists the premiere discrete ordinates transport codes and known auxiliary codes that facilitate accurate radiation dose evaluations. The table includes three one-dimensional (1-D) discrete ordinates codes (ANISN, ONEDANT, and XSDRNPM), two two-dimensional (2-D) discrete ordinates codes (DOT and TWODANT), and three auxiliary codes for use in evaluating doses at point detectors. Geometry requirements and/or level of desired computational effort typically dictate the selection of a 1-D or 2-D code. Often a shield configuration can be reasonably approximated in one dimension (plane, cylinder, or sphere), and the 1-D programs can combine the accuracy of discrete ordinates with the near speed of point-kernel techniques.

The 1-D ANISN code in Table 5.3 is probably the most widely used radiation shielding code (point-kernel or otherwise) both in the United States and abroad. The code has been updated and maintained since its development in the late 1960s. Using the numerical solution techniques of ANISN, the XSDRN code[59] evolved from its initial release in 1969 to the present version called XSDRNPM-S with the following added features: (1) solutions using double-precision flux arrays to circumvent potential convergence difficulties; (2) more user-friendly input (availability of parameter default values, automatic generation of appropriate angular quadrature, etc.); and (3) increased flexibility in the input/output and processing of multigroup cross-section data. Because of its basis in the well-established ANISN code, its increased flexibility and ease-of-use, and its presence in a well-maintained modular code system (SCALE),[60] XSDRNPM-S would be the code of choice recommended to new users.

The ONEDANT code is the third 1-D code noted in Table 5.3. The code is much newer than ANISN, XSDRNPM, and the older LANL code called ONETRAN.[61] For deep-penetration problems (common to spent fuel shielding applications), ONEDANT appears to be more restrictive because it uses only the standard diamond-difference flux extrapolation technique with negative fluxes set-to-zero-and-corrected. ANISN and XSDRNPM-S include options for theta-weighted diamond-difference models. Although the various flux models give nearly the same solution in the limit of very small-mesh intervals, the theta-weighted method generally retains a better accuracy for larger-mesh intervals than does the standard diamond difference technique. Thus, a user interested in using mesh sizes larger than required by standard diamond differencing would find ANISN and XSDRNPM to be more attractive. References 2, 52, and 62 present good discussions of various flux models. One advantage of ONEDANT is that it does provide a diffusion acceleration technique not available in ANISN or XSDRNPM. Although this feature speeds up the convergence process, the potential increased efficiency is of marginal value for 1-D problems.

For problems requiring 2-D discrete ordinates shielding analyses, the DOT code has become the international standard. The latest version, DOT 4.3, represents a significant advancement in computing efficiency and speed; however, most problems of reasonable size still require substantial computer resources. The DOT codes have been developed primarily for radiation shielding analysis while TWOTRAN and TWODANT have been developed in a reactor/core physics environment. This difference in emphasis explains why DOT is typically selected where shielding calculations are of prime import. Like ONEDANT, the TWOTRAN and TWODANT codes allow only the standard diamond-difference flux option. Incorporation of a variety of flux model options reflects the DOT emphasis on allowing accurate solution of complex shielding problems. Also, the DOT manual provides an excellent explanation of the basic theory and numerical techniques employed in the code.

Table 5.3. Computer programs based on discrete ordinates techniques utilized for radiation dose evaluation

Code (RSIC CCC No.)/ developer	Language	Known computer implementation	Description and comments	Refs.
ANISN[a] (CCC-82,253-255,314,514) Oak Ridge National Laboratory	FORTRAN IV FORTRAN 77	IBM/360/370 IBM PC CDC 7600	General 1-D discrete ordinates coupled neutron-gamma radiation transport code. Most popular version is ANISN-ORNL (CCC-254). Flux or activities at a detector site can be evaluated. The Westinghouse version, ANISN-W (CCC-255), and a recent version from EG&G (CCC-514) are available for an IBM PC.	48,49
DOT[a] (CCC-89,209,252,276, 319,320,429) Oak Ridge National Laboratory	FORTRAN IV	IBM 360/370 CDC UNIVAC CRAY	General 2-D discrete ordinates coupled neutron-gamma radiation transport code. Latest and best version is DOT 4.3 (CCC-429) although DOT 3.5 (CCC-276) still heavily used. Earlier versions are obsolete. DOMINO II (PSR-162) couples DOT IV to the Monte Carlo MORSE-CG code (CCC-203). Fluxes and activities calculated. Excellent documentation of theory and techniques.	50-52
FALSTF (CCC-351) Oak Ridge National Laboratory	FORTRAN IV Assembler	IBM 360/370 CDC	Calculates doses exterior to a shield based on DOT 3.5 calculated fluxes in cylindrical geometry. Doses evaluated as sum of last flight contributions from shield regions. Eliminates potential ray effects in air or void outside cylinder. Only available for DOT 3.5.	53
ONEDANT[b] (CCC-428) Los Alamos National Laboratory	FORTRAN IV FORTRAN IV/Assembler FORTRAN 77	CDC 7600, UNIVAC IBM 370 VAX, CRAY	General 1-D discrete ordinates coupled neutron-gamma radiation transport code. Modular program developed to be very user-friendly. Fluxes and/or activities provided at detector points.	54
SPACETRAN (CCC-120) Oak Ridge National Laboratory	FORTRAN IV	IBM 360/370	Evaluates dose for detectors at various distances from the surface of a cylinder. Integrates ANISN leakage or DOT 3.5 flux data. Eliminates potential ray effects in air or void outside a cylinder. Not accurate for detector points near the cylindrical surface.	55
TWODANT[b] (CCC-456) Los Alamos National Laboratory	FORTRAN IV FORTRAN IV/Assembler FORTRAN 77	CDC 7600 IBM 370 VAX, CRAY	General 2-D discrete ordinates coupled neutron-gamma radiation transport code. TWODANT is basically the ONEDANT package with the one-dimensional SOLVER module replaced with a two-dimensional SOLVER module.	56

Table 5.3. (continued)

Code (RSIC CCC No.)/ developer	Language	Known computer implementation	Description and comments	Refs.
XSDOSE[a] (CCC-466) Oak Ridge National Laboratory	FORTRAN IV FORTRAN 77	IBM 370 CDC CRAY	Used in conjunction with XSDRNPM (or ANISN) to compute the neutron/photon flux and the resulting dose rate at various points outside a finite cylinder, sphere, rectangular slab, or circular disc. Uses direct line-of-sight integration of surface angular flux over the surface. Eliminates potential ray effects from discrete ordinates outside shield. Extremely easy to use.	57
XSDRNPM[a] (CCC-466) Oak Ridge National Laboratory	FORTRAN IV FORTRAN 77	IBM 370 CDC CRAY	1-D discrete ordinates coupled neutron/gamma-ray transport code based on ANISN. Extends ANISN capabilities to provide user-friendly features, automatic quadrature generation, and flexibility in weighting cross sections. Easily coupled to XSDOSE for doses exterior to shield.	58

[a]Code summary provided in Appendix A.
[b]Combined ONEDANT/TWODANT summary provided in Appendix A.

Although not included in Table 5.3, there are currently three 3-D discrete ordinates codes. These codes are only practical on vector operation computers such as the CRAY. The Japanese have produced ENSEMBLE[63] for 3-D reactor shielding problems. THREETRAN[64] has been developed at LANL, and DOT IV has been extended at ORNL to produce TORT.[65] The TORT code has undergone extensive verification testing and limited validation.[66] There could be some need of these 3-D codes in applications where flux or dose mappings around building internals or hot cells is required.

Table 5.3 includes three auxiliary codes that were developed to provide an easy means of accurately evaluating the flux or dose at a point exterior to a shield. For problems where doses are required exterior to a shield in a low scattering medium (air, void, etc.), extension of the discrete ordinates spatial mesh out into the exterior medium is often unattractive because

1. a penalty is paid for the extra spatial mesh (typically a fine spatial mesh and angular quadrature are needed for curvilinear geometries);
2. for 1-D problems there is no good way of accounting for the finite dimensions of the shield from which the radiation leaks; and
3. ray effects in multidimensional problems are very difficult to alleviate and can yield unreliable results.

To alleviate these problems, FALSTF, SPACETRAN, and XSDOSE have been written for use with the ANISN, DOT, and XSDRNPM codes. Although available for DOT 3.5, public versions of FALSTF and SPACETRAN are not available for any of the DOT IV codes. The SPACETRAN code is computationally more efficient than FALSTF but is inaccurate close to the shield and can be unreliable if an inappropriate spatial mesh or angular quadrature is used. The XSDOSE code has the best numerical techniques of all these codes, but is currently limited to use with the 1-D ANISN or XSDRNPM codes. The techniques utilized in XSDOSE eliminate the difficulties inherent in the 1-D SPACETRAN method.

5.2.3 Monte Carlo Codes

Table 5.4 lists the four premiere Monte Carlo codes that are generally available in the United States for performing radiation shielding analyses. Historically, a number of general-purpose Monte Carlo codes were developed in the late 1960s and early 1970s. The SAM-CE code was perhaps the leader in the creation of an attractive, easy-to-use geometry package (combinatorial geometry or CG), handling of point cross-section data, and implementation of various biasing techniques. However, because of its easy-to-use features, accessible ANISN-formatted cross-section data, and ready availability, the MORSE code emerged in the late 1970s as the most widely used Monte Carlo code for radiation shielding. The latest versions of MORSE (CGA and SGC/S) utilize multigroup cross sections, a wide variety of source and particle biasing features, and a CG package with nested array features.[68,75] The version of SAM-CE in RSIC is old and incomplete with regard to some routines that the developers provide for a fee. Like SAM-CE, updates of other codes provided to RSIC in the early 1970s are probably available from private companies or consultants (e.g., ref. 76).

Although the MORSE codes may still be the most widely used Monte Carlo shielding codes, the MCNP code developed at LANL is rapidly gaining in popularity. Once regarded as a highly specialized code that was difficult to use, the MCNP developers have made a concerted effort to retain the sophisticated attributes of the code and still provide an easy-to-use and readily acceptable tool. The main areas of sophistication concern the use of point energy cross-section data and development of "automatic" biasing schemes. The automatic biasing schemes are an attempt to reduce the required user expertise in analyzing a problem. The only potential disadvantage with MCNP is its inability to perform adjoint analyses (see Sect. 3.1).

Table 5.4. *Computer programs based on Monte Carlo techniques utilized for radiation dose evaluation*

Code (RSIC CCC No.)/ developer	Language	Known computer implementation	Description and comments	Refs.
MCNP[a] (CCC-200) Los Alamos National Laboratory	FORTRAN 77	CDC 7600 CRAY, VAX IBM 3033	General-purpose Monte Carlo code for coupled neutron/photon particle transport Capable of handling point energy and discretized cross-section data. New features for automatic generation of importance functions. Flexible geometry capabilities. Source and response estimator specification flexible and easy to use. Well-supported program with constant improvements and updated. Well documented.	67
MORSE[a] (CCC-127,203,258 261,277,368,394, 466,471,474) Oak Ridge National Laboratory	FORTRAN IV	FACOM M-200 IBM 360/370 CRAY, VAX UNIVAC CDC	General-purpose multigroup Monte Carlo code for coupled neutron/photon particle transport. Most widely used of Monte Carlo codes. Latest versions from ORNL in CCC-466 and CCC-474 have a popular, easy-to-use geometry package capable of generating multiple arrays within arrays. Flexibility in specifying source, response estimator, and biasing mode easy via wide variety of user-supplied routines.	68-71
SAM-CE (CCC-187) Mathematical Applications Group, Inc.	FORTRAN IV	CDC 6600 IBM 360/370	General-purpose code for coupled neutron/photon particle transport. Excellent geometry package available as proprietary option. Excellent treatment of physics using Monte Carlo techniques. Limited availability of cross sections in required format and limited user community.	72
TRIPOLI 2.2 (CCC-272) CEA Centre d'Etudes Nucleaires de Saclay, France	FORTRAN IV Assembler	IBM	General-purpose code for neutron or photon particle transport. Handles point energy or discretized cross-section data. Coupled neutron/photon problems cannot be treated. Secondary gamma sites generated and subsequent transport treated with MERCURE (CCC-142). Excellent biasing techniques available for deep penetration problems.	73,74

[a]Code summary provided in Appendix A.

The only foreign code in Table 5.4 is the French code TRIPOLI. This code provides perhaps the most sophisticated (but hard to use) biasing schemes of any Monte Carlo code. It also utilizes a point energy representation of the cross sections. The major drawback to the RSIC version of TRIPOLI is that it does not handle coupled neutron/photon problems. The ability to handle coupled problems is available to the developers and will be made available in a new version (TRIPOLI 3) that will probably be released in the near future. However, there is very little user experience in the United States with TRIPOLI, and it offers no distinct advantages over MCNP.

5.2.4 Summary

Sections 5.2.1–5.2.3 have highlighted acceptable codes for evaluating radiation doses from spent fuel. The sections note the areas where a code or codes appear to have a deficiency in the physics model, numerical technique, or available data. Nearly all of the codes meet acceptable standards based on the assessment criteria outlined earlier. However, the foreign codes would generally not be heavily used in the United States because of lack of a distinct technical advantage and lack of support by a U.S. installation or body of users. Based on this preliminary assessment, the point kernel code QAD-CGGP, the discrete ordinates codes XSDRNPM (or ANISN) and DOT 4.3, and the Monte Carlo code MCNP would be recommended fur further assessment and/or validation for spent fuel shielding applications.

The three types of solution techniques—point kernel, discrete ordinates, and Monte Carlo—are in some respects competitors. But an objective assessment would show them to provide a nice complement to one another. In considering the complete design evaluation of a cask fleet or repository/handling facility, each technique can prove useful as the accuracy requirements and/or need for modeling detail increase as the design is finalized.

The general advantages and disadvantages of each technique is provided in Sect. 3. A prudent user should understand the specific application requirements prior to selecting the technique to be used. Utilizing more than one code/technique on a problem is often necessary[77] and/or useful for a proper solution or for adequate confidence in the results. Reference 78 provides an interesting hot cell analysis where all these techniques were used to provide the final desired result.

5.3 CROSS-SECTION DATA LIBRARIES FOR SHIELDING ANALYSIS

Section 4 discusses three areas of shielding analysis data: cross-section data, response data, and buildup factor data. For dose evaluation, the ANSI Standard flux-to-dose conversion factors[79] have become the accepted norm for presenting calculated doses. Buildup factor data have typically been built into codes and there has been little, if any, standard for the source of the data. However, as noted in Sects. 4.5 and 5.2, a standard set of buildup data has been formulated and is beginning to be utilized by the point kernel codes.[80] There is little question that these referenced standard data sets provide the most attractive choice of dose conversion and buildup factor data. Likewise, for continuous energy Monte Carlo shielding codes, the available point cross-section libraries are the clear choice over discretized data. On the other hand, no one processed cross-section set has been accepted for general use by radiation transport codes that require multigroup cross sections. Section 4.1 provides a review of the prime sources of cross-section data and the difficulties of generating generic mutligroup sets for wide-ranging application areas.

This section provides a review of the various types of available cross-section libraries and discusses those currently used for spent fuel shielding analysis and those that have potential for future use. The primary differences between various types of cross-section sets will hopefully be clarified. Even more so than with radiation transport codes, the "best" multigroup data library will probably vary from application to application. Keeping in mind the general assessment criteria, this section notes libraries that have been widely used and those that need further assessment for spent fuel shielding applications. Appendix B has summaries of selected libraries.

5.3.1 Fine-Group Reference Libraries

As discussed in Sect. 4.1, multigroup cross-section libraries can be characterized by both the number of energy groups in the library and the degree to which the library is application-dependent. Fine-group libraries typically have 100 or more neutron energy and 30 or more gamma groups. The finer resolution on the neutrons is required to accurately incorporate information regarding their more rapid cross-section variation with energy. It is unlikely that multidimensional discrete ordinates or Monte Carlo calculations would be routinely used at the fine-group level, but the user could perform one-dimensional discrete ordinates calculations with such a set, determine typical spectra that would be more appropriate for given applications, and collapse the fine-group set to a more manageable broad-group level. Such a user could avoid the complete processing of cross sections and still have some flexibility. The fine-group libraries also serve as reference libraries because (1) they provide documentation on the original source of the data, and (2) they can be used in benchmark or reference calculations by which a daughter broad-group, production library is judged.

A relatively small number of application-dependent fine-group libraries in discrete ordinates format have been available for general use in radiation transport calculations. Some that are available from RSIC are listed in Table 5.5. Of these libraries, the EURLIB-III[81] and JSD-100/120[82] appear potentially the best for spent fuel applications (based on data source and intended applications). However, the most desirable situation for an analyst is one in which a problem-dependent library can be prepared for each application without getting into the cross-section processing business in a full-scale way. Such a situation is possible through the availability of fine-group, pseudo-application-independent libraries in

Table 5.5. Some fine-group libraries in discrete ordinates format developed for specific applications

Library[a]	Contributor	Energy groups	Processor	Source	Applications/ (No. elements)
DLC-27/ AMPX01	ORNL	104n,22g	AMPX	ENDF/ B-III, DNALIB	Concrete, Air/ (9)
DLC-28/ CTR	ORNL	52n,21g	SUPERTOG, POPOP4 (Collapse)	ENDF/ B-III, DNALIB, POPLIB	Fusion Neutronics/ (23)
DLC-35/ EURLIB-III	ESIS, IKE, EIR	100n,20g	AMPX	ENDF/ B-IV	Benchmarks/ (13)
DLC-37/ EPR	ORNL	100n,21g	AMPX	ENDF/ B-IV	Fusion Neutronics/ (46)
DLC-51/ JSD-100/ 120	JAERI	100n,20g	MACS	ENDF/ B-IV	Fission Reactors/ (46)

[a]The DLC (Data Library Collection) number represents the RSIC reference for the data library.

"flexible formats." A list of several libraries that utilize a "flexible" approach is given in Table 5.6. This new concept in multigroup cross-section library generation and distribution was put into practice in the late 1970s through the development of AMPX-generated libraries such as VITAMIN-C[83] and CSRL.[84]

Table 5.6. Some fine-group libraries in "flexible" formats developed for various general applications

Library[a]	Contributor	Energy groups	Processor (format)	Source	Applications/ (No. elements)
DLC-41/ VITAMIN-C	ORNL	171n,36g	MINX, AMPX/ (AMPX)	ENDF/ B-IV, LENDL	Fusion, Fast Reactor Core & Shielding/ (66)
DLC-42/ CLEAR	ORNL	126n,36g	MINX, AMPX/ (CCCC, AMPX)	ENDF/ B-IV, LENDL	Fast Reactor Core and Shielding/ (61)
DLC-43/ CSRL	ORNL	218n	AMPX/ (AMPX)	ENDF/ B-IV	Criticality Safety/ (65)
DLC-52/ EPRMASTER	ORNL	100n	AMPX/ (AMPX)	ENDF/ B-IV	Fusion Neutronics/ (46)
DLC-53/ VITAMIN-4C	ORNL	171n,36g	MINX, AMPX/ (CCCC, AMPX)	ENDF/ B-IV, LENDL	Fusion, Fast Reactor Core & Shielding/ (61)
DLC-113/ VITAMIN-E	ORNL	174n,38g	MINX, AMPX/ (AMPX)	ENDF/ B-V, LENDL	A Variety of Radiation Transport Applications/ (77)
DLC-95/ CSRL-V	ORNL	227n-44g	NJOY, AMPX (AMPX)	ENDF/ B-V, LENDL	Criticality Safety, Other Radiation Transport Applications (64)

[a]The DLC (Data Library Collection) number represents the RSIC reference for the data library.

The AMPX format is very comprehensive, retaining essentially all the reactions and transfer processes that are in the original ENDF/B data. Various modules of the AMPX system are available for performing various manipulations of the data. These include mode conversion (AIM), selective retrieval (AJAX), combining neutron and photon libraries (CHOX), self-shielding and temperature correction via the Bondarenko factor method (BONAMI), self-shielding and temperature correction via the Nordheim Integral Method (NITAWL), and energy group collapse (MALOCS). Thus, a user can begin with fine-group AMPX "master" library and perform resonance self-shielding, temperature correction, and group collapse to end up with a broad-group, problem-dependent "working" library for direct use in a radiation transport code. The user admittedly has to do considerable more work to apply such a system, but the effort is still substantially less involved than performing the original multigroup processing from ENDF/B point data.

There are fine-group shielding libraries in the CCCC[85] format such as DLC-53/VITAMIN-4C, but that particular format has not proven to be as useful as the AMPX format for coupled neutron/gamma libraries. The CCCC format has been updated with an extended version called MATXS[86] and libraries based on ENDF/B-V that have been generated at LANL using NJOY-II are available from RSIC. A computer code called PSR-206/TRANSX-CTR[86] is available for performing the conversion, self-shielding, collapsing, and discrete ordinates library production from data in MATXS format. However, currently no truly fine-group MATXS-formatted libraries are available from RSIC.

Of the libraries shown in Table 5.6, the VITAMIN-C and VITAMIN-E[87] libraries are the most widely used for shielding applications. DLC-113/VITAMIN-E is an ENDF/B-V version of the popular VITAMIN-C library. The CSRL library is comparable in quality to the VITAMIN-C library, but does not have any gamma data, and, thus is limited to neutron transport applications. A new ENDF/B-V version of CSRL has been developed[88] with a coupled 227n-44γ group structure. Any one of these libraries could be used as the starting point to generate a broad-group working library for a particular spent fuel shielding application.

5.3.2 Broad-Group Production Libraries

Broad-group libraries are developed for production use and, whether generated from a fine-group library or developed directly from evaluated data, are typically application-dependent libraries. Some of the older broad-group libraries generated directly into a discrete ordinates format are shown in Table 5.7. Typically these libraries were developed and used successfully for a given project and results obtained with the data were published. Other analysts, with radiation transport problems very similar in nature, were also able to use the libraries. However, the resonance treatment, temperature corrections, and spectral weighting functions are fixed for a particular application and may be entirely inappropriate for other applications where the shielding and source material or the source spectrum are different.

Of the available libraries provided in Table 5.7, only the first three appear feasible for use in spent fuel shielding analyses. The first library, CASK,[89] was developed for depleted uranium shipping casks with a water-filled cavity. The energy grouping was done based on typical spent fuel spectra. The data source for this library is quite old and the resonance correction for ^{238}U is inadequate if the subcritical multiplication source is important to the dose. However, CASK has been one of the most widely used (for all type applications) ANISN-formatted libraries. The second library, FEWG1,[90] was developed for radiation transport through concrete and air. The work was sponsored by the Defense Nuclear Agency (DNA), and the group structure was developed for applications with source spectra from nuclear weapons. However, the library may be useful for analysis of concrete casks and dose evaluation in and around concrete buildings where fuel handling takes place. The library also has an extensive selection of kerma response functions for various materials. The CLAW-IV library[91] was developed for

Table 5.7. Some broad-group libraries in discrete ordinates format developed for specific applications

Library	Contributor	Energy groups	Processor	Source	Applications/ (No. elements)
DLC-23/ CASK	ORNL	22n,18g	SUPERTOG, POPOP4 (Collapse)	ENDF/ B-II, POPLIB	Shipping Casks/ 29)
DLC-31/ FEWG1	ORNL/ DNA	37n,21g	AMPX	ENDF/ B-IV, DNALIB	Concrete, Air/ (43)
DLC-36/ CLAW-IV	LANL	30n,12g	NJOY	ENDF/ B-IV	General/ (48)
DLC-64/ UKCTRI	U. BIRM-INGHAM(UK)	46n	GALAXY	UKNDL	Fusion Neutronics/ (25)
DLC-73/ GARG	BARC (India)	27n	FIGARO	ENDF/ B-IV	Fast Reactor/ (16)
DLC-84/ MENSLIB	LANL	60n	DANA5, CROIX IC+E	ENDF/ B-IV	High-Energy Shielding (E to 60 MeV) (8)
DLC-92/ GICX40	JAERI	42n,21g	SUPERTOG, POPOP4	ENDF/ B-III	Fusion Neutronics/ (40)

shielding analyses related to weapons applications. Although a potential candidate for spent fuel shielding applications, it appears to have too few gamma groups in the energy range of importance to spent fuel applications.

Since the late 1970s, the more attractive procedure for developing a coupled broad-group library has been to process (resonance shielding and temperature correction) and collapse a fine-group, pseudo-application-independent library to create a production, application-dependent library. A collection of these libraries is shown in Table 5.8. The most applicable libraries for spent fuel shielding analyses are the BUGLE-80,[92] SAILOR,[93] and FCXSEC[22] libraries, all of which are ANISN-formatted. The BUGLE-80 and SAILOR libraries are nearly identical. The primary difference is the availability in SAILOR of mixed macroscopic cross sections for PWR and BWR reactor applications.

The BUGLE-80 library and its parent VITAMIN-C are listed in ANSI/ANS-6.1.2/1983 as suitable cross-section sets for nuclear radiation protection calculations for nuclear power plants. The standard lists the processing procedures and verification efforts required to be included in the standard. The group structure in the library is good for spent fuel radiation sources. However, testing of the BUGLE-80 library was done primarily for concrete shields and resonance processing was not done on nonconcrete nuclides. The weighting spectrum used in the collapse from VITAMIN-C was that of a concrete medium. Thus, the validity of the library for nonconcrete shielded applications needs further testing.

Table 5.8. Some broad-group application-dependent libraries developed from fine-group libraries in "flexible" format

Library	Contributor	Energy groups	Master library source	Applications/ (No. elements)
DLC-48/ PVC	ORNL	36g	DLC-41/VITAMIN-C	Photon Transport/ (38)
DLC-58/ HELLO	ORNL	47n,21g	DLC-41/VITAMIN-C, Intranuclear Cascade	High-Energy Damage (E to 60 MeV)/ (10)
DLC-75/ BUGLE-80	ORNL, ANS-6.1.2	47n,20g	DLC-41/VITAMIN-C	Standard for Concrete, LWR Shielding (66)
DLC-76/ SAILOR	SAI, ORNL	47n,20g	DLC-41/VITAMIN-C	BWR and PWR Radiation Transport Analyses/ (58)
DLC-85/ FCXSEC	ORNL	22n,21g	DLC-41/VITAMIN-C	Fuel Cycle Shielding Analyses/ (Many)
DLC-86/ FLUNG	ORNL	35n,21g	DLC-41/VITAMIN-C	Fusion Neutronics (41)
DLC-87/ HILO	ORNL	66n,21g	DLC-41/VITAMIN-C, Intranuclear Cascade	High-Energy Damage (E to 400 MeV)/ (17)

The FCXSEC library was for fuel cycle shielding analyses. A generic fusion-fission-1/E-Maxwellian spectrum was used to collapse from the VITAMIN-C group structure. Resonance self-shielding was performed for three background cross sections (composition dependent) 0.1, 1000, and 10^8 b/atom. Macroscopic cross sections are available with appropriate resonance processing for several mixtures routinely used in spent fuel shielding analyses.

As stated in the previous paragraphs, the ANISN format or, more generally, the discrete ordinates format, is a "working" format; that is, the radiation transport codes read these formats directly. No *further resonance or temperature correction is possible. A newer approach generates a broad-group* library with a selected weighting spectrum, but retains the "flexible" AMPX-like format that provides the neutron resonance information. The shielding libraries provided with the SCALE system were the first to use this approach. The libraries are provided in the AMPX "master" format, and the SCALE sequences use BONAMI and NITAWL modules to do the resonance and temperature correction (cheap, relative to the radiation transport analysis) for each particular problem and alter the format from a master to an AMPX "working" format. Libraries in SCALE with no resonance information (e.g., CASK 22n-18γ) follow the same procedure but no actual processing takes place; that is, BONAMI and NITAWL are merely used to change the master format to a working format. Installations that do criticality analyses have resonance processing codes available because resonance processing is of extreme importance in evaluating an accurate neutron multiplication factor

To date, there are very few libraries that follow the above approach. The 27n-18γ library in SCALE is the most prominent. The neutron data were collapsed from the CSRL library, and the gamma data were created directly using various AMPX modules. The library group structure and weighting function was selected to be appropriate for spent fuel shielding applications. The large number (13) of thermal neutron groups can increase the cost of a discrete ordinates shielding analysis unless the outer iterations are limited by code input.

The only other broad-group libraries available in the flexible format are the MATXS libraries from Los Alamos National Laboratory (see Table 5.9). However, the MATXS1 and MATXS5 libraries contain no resonance information and are simply MATXS-formatted versions of CLAW-IV. The only library of potential interest is the DLC-116/MATXS6 library. However, there appears to be too many neutron groups to be used for production work.

Table 5.9. Some libraries in "MATXS" format that are available from RSIC

Library	Contributor	Energy groups	Processor/ (format)	Source	Applications/ (No. elements)
DLC-114/ MATXS1	LANL	30n,12g	NJOY-II (MATXS)	ENDF/ B-IV, LANL	MATXS Equiv. of DLC-36/ CLAW-IV/ (64)
DLC-115/ MATXS5	LANL	30n,12g	NJOY-II (MATXS)	ENDF/ B-V, LANL	ENDF/B-V Equivalent of MATSX1/ (87)
DLC-116/ MATXS6	LANL	80n,24g	NJOY-II (MATXS)	ENDF/ B-V	Fast Reactor, Shielding, Fusion/ (91)
DLC-117/ MATXS7	LANL	69n	NJOY-II (MATXS)	ENDF/ B-V	EPRI-CPM Group Structure,PWR Studies/ (80)

5.3.3 Point Cross-Section Libraries

As noted in Sect. 4.1.3, point Monte Carlo cross-section libraries are typically processed for use with a particular code. The MCNP code package (CCC-200) provides cross-section sets based on ENDF/B-IV. Both true point cross sections and point data averaged into discrete groups are provided. A separate data package (DLC-105) is provided for the ENDF/B-V based cross-section sets for MCNP because of restrictions on distributing ENDF/B-V data outside the United States. For shielding applications, the point cross-section libraries and continuous-energy treatment allowed in some Monte Carlo codes is a superior physics approach than that offered by multigroup libraries.

5.4 THE SCALE COMPUTATIONAL SYSTEM

As evidenced from the previous sections of this report, the number of different techniques, codes, and data libraries can confuse even a routine user as to the appropriate procedure for obtaining an accurate dose evaluation. This situation combined with the expertise required to use (and not abuse) many of the available analytic tools forces many users to employ the tools they have had the most experience with (or the easiest-to-use tool), whether it is the best tool for a particular problem or not. This section provides a summary of a modular code system called SCALE that was developed in an effort to ease many of the burdensome input and code interface requirements necessary to perform a complete shielding analysis for a specific category of applications.[94] To date, it is the only analytic system of its kind for doing a complete spent fuel shielding analysis.

The SCALE system was developed to be an easy-to-use analytic tool for performing criticality, shielding, and heat transfer analysis of nuclear fuel facilities and packages. As a modular code system, SCALE is designed to provide common data interface files, input format, and data processing procedures for system analysis. The development concept was: (1) use well-established computer codes and data libraries, (2) have an easy-to-use input format designed for the occasional user and/or novice, (3) combine and automate analyses requiring multiple computer codes or calculations into standard analytic sequences, and (4) be well documented and publicly available. A host of validated data bases, (e.g., material compositions, thermal properties, cross sections) were also incorporated to allow easy input (via keywords) and data accessibility. The analytical sequences are automated to perform the necessary data processing (e.g., problem-dependent resonance self-shielding and temperature correction of cross sections), generate the input to well-established computer programs (functional modules), initiate module execution in proper sequence, and perform any needed post-processing of the analytic results. Thus, the user is able to select an analytic sequence characterized by the type of analysis (criticality, shielding, or heat transfer) to be performed and the geometric complexity of the system being analyzed. The user then prepares a single set of input for the control module corresponding to this analytical sequence. The control module input is in terms of easily visualized engineering parameters specified in a simplified, free-form format. The control modules use this information to derive additional parameters and prepare the input for each of the functional modules in the analytical sequence. Back-to-back execution of individual modules is allowed.

The shielding analysis capabilities developed for the SCALE system center around many of the well-established codes and libraries noted in Sects. 5.1–5.3. Radiation transport is performed by the one-dimensional (1-D) discrete ordinates code XSDRNPM and the multidimensional Monte Carlo code MORSE-SGC which uses the MARS combinatorial geometry package for easy modeling of complex geometries. (Multidimensional discrete ordinates codes were omitted because of geometric restrictions and difficulty with incorporating them in an automated sequence.) These radiation transport codes along with other SCALE modules for cross-section processing (BONAMI, NITAWL), spent fuel source generation (ORIGEN-S), and dose evaluation (XSDOSE) are incorporated into four **Shielding Analysis Sequences**: SAS1, SAS2, SAS3, and SAS4.

The first shielding control module to be released was SAS3. The sequence provides automated data processing, but basically relies on the user's expertise with MORSE (or Monte Carlo techniques) to ensure reliable dose results. The next analytic sequence, SAS2, automates all the steps of a complete shielding analysis: (1) a depletion and decay analysis for a specified assembly geometry and irradiation history, (2) generation of gamma and neutron source strength and spectra, and (3) a one-dimensional radial shielding calculation (XSDRNPM-S) and dose evaluation (XSDOSE) for a transport/storage cask. SAS1 and SAS4 are two new sequences that have been extensively tested and used at ORNL since 1985. SAS1 is basically a user-friendly tool for cross-section preparation and subsequent 1-D shielding analysis using XSDRNPM-S and XSDOSE. SAS4 provides an easy-to-use, automated procedure to obtain radiation doses exterior to a transport/storage cask via a three-dimensional Monte Carlo analysis.

The SAS4 module of SCALE is designed to eliminate user interaction in selecting Monte Carlo biasing parameters for deep-penetration shielding problems. The module has been heavily tested for spent fuel cask applications. All the required biasing parameters are derived from results of an adjoint XSDRNPM-S calculation and automatically input to MORSE so that the user is rid of this difficult input task. A simplified input option is also allowed for the geometry model of Figs. 5.1–5.2. Of significance is the fact that homogeneous and heterogeneous spent fuel models are easily specified. This type of application-specific simplification makes the use of the complex, general-purpose radiation transport codes easy to use in an appropriate manner.

The general flow diagram of one of the simplest modules, SAS1, is shown in Fig. 5.3. The first portion of the sequence prepares cross sections (optionally cell weighted) via the BONAMI, NITAWL, and optional XSDRNPM calls. This portion of the sequence is common to all the sequences. The last portion of the sequence allows repeated XSDRNPM/XSDOSE calculations. The radiation source for SAS1, SAS2 (radiation transport), and SAS4 are obtained via interface files output from ORIGEN-S. The SAS2 case can be halted after the depletion portion of the analysis is done to provide source spectra and concentrations at discharge. Different decay times for the spent fuel source can be considered by generating a new ORIGEN-S output file from the discharge concentrations on the old file. Thus, dose rates for a variety of cooling times and different cask designs or models can be easily obtained using the various shielding sequences.

There are a number of improvements that could be made to the SCALE system. However, taken together, the shielding sequences provided in SCALE offer an excellent example of a user-oriented computational tool that can be used for source generation, preliminary shield design, final safety analyses, and review calculations.

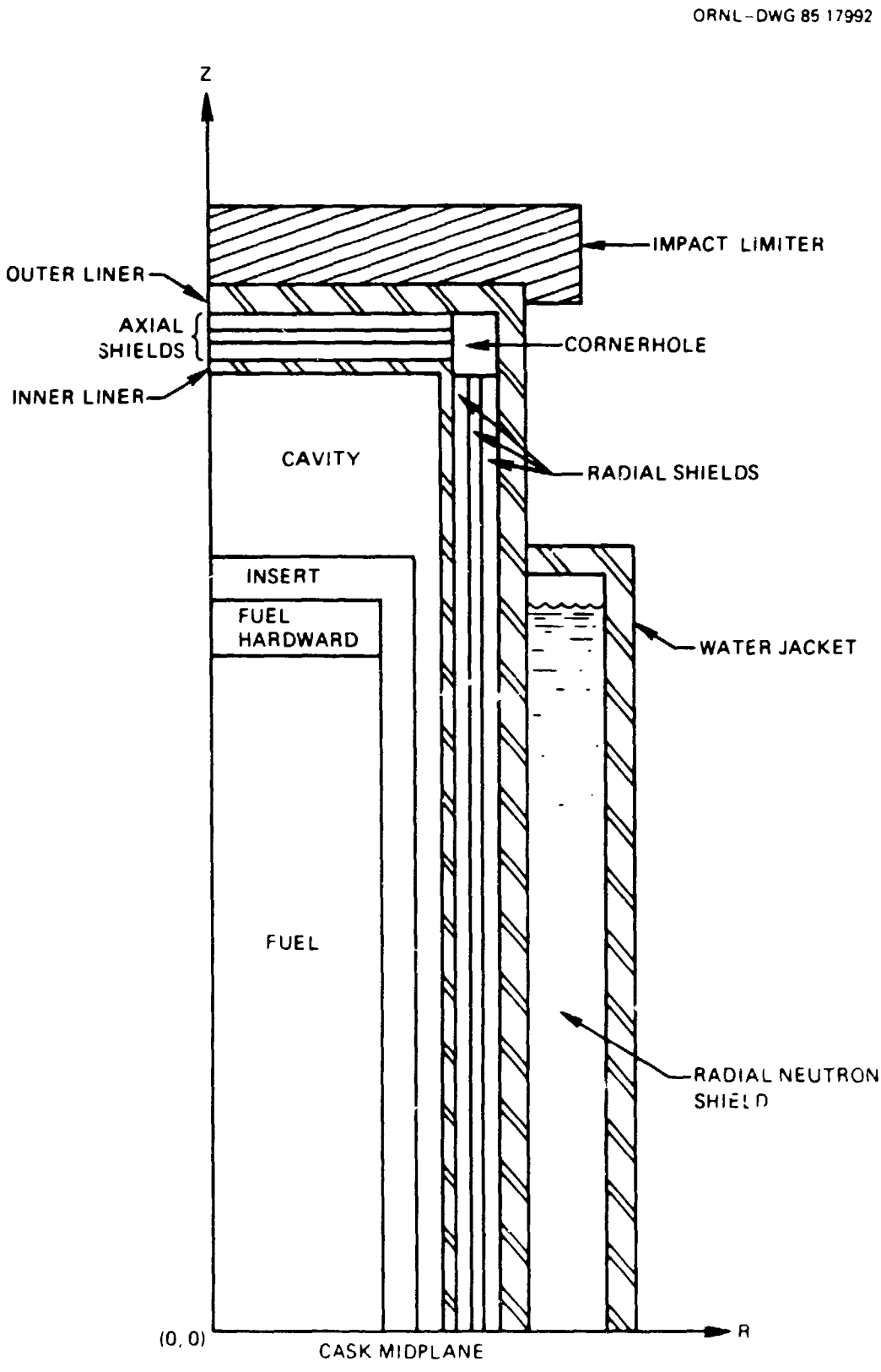

Fig. 5.1. SAS4 shipping cask model for homogeneous source (fuel) regions (IGO = 0)

ORNL-DWG 85-17996

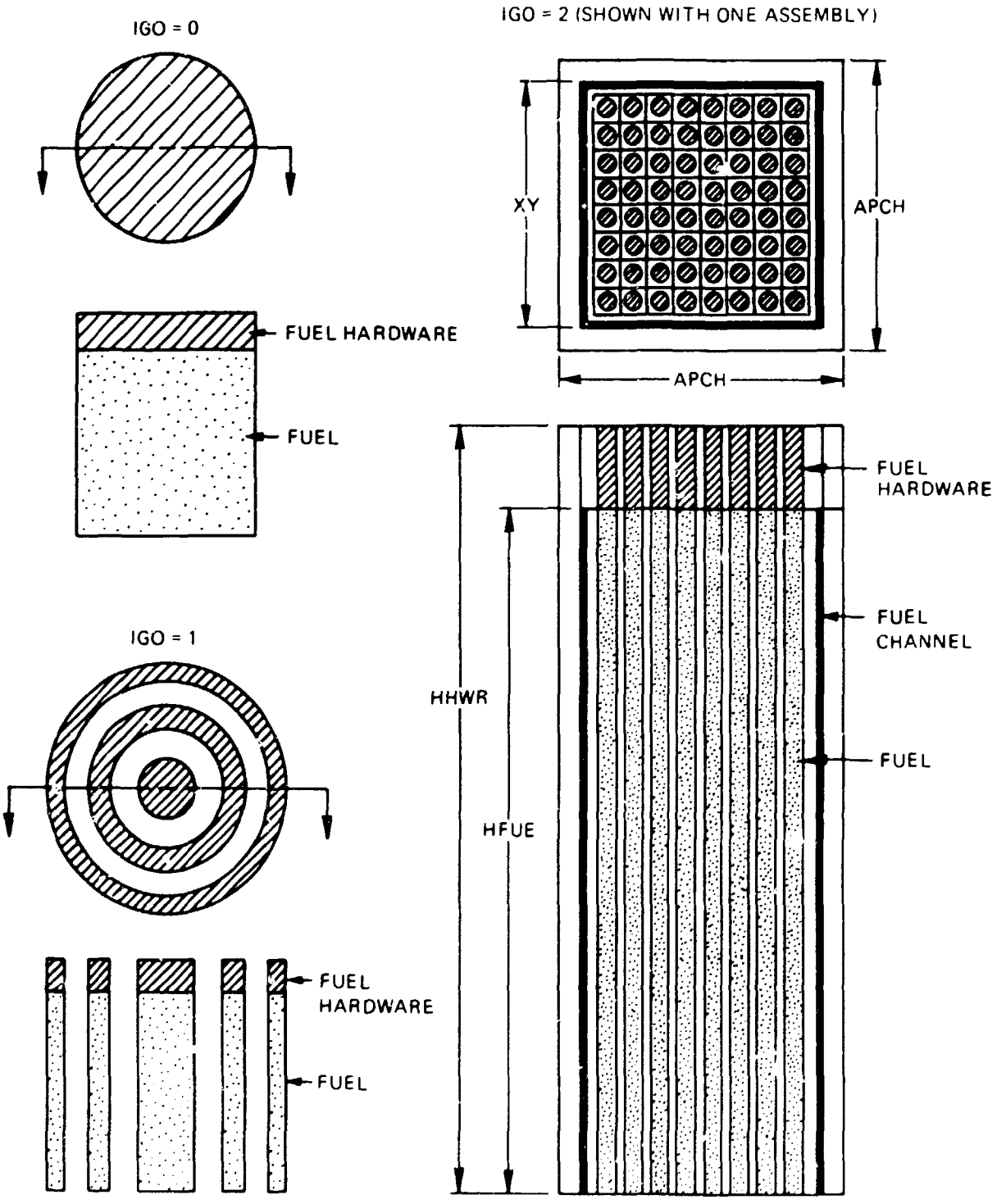

Fig. 5.2. Geometry options of SAS4 source region for simplified geometry input.

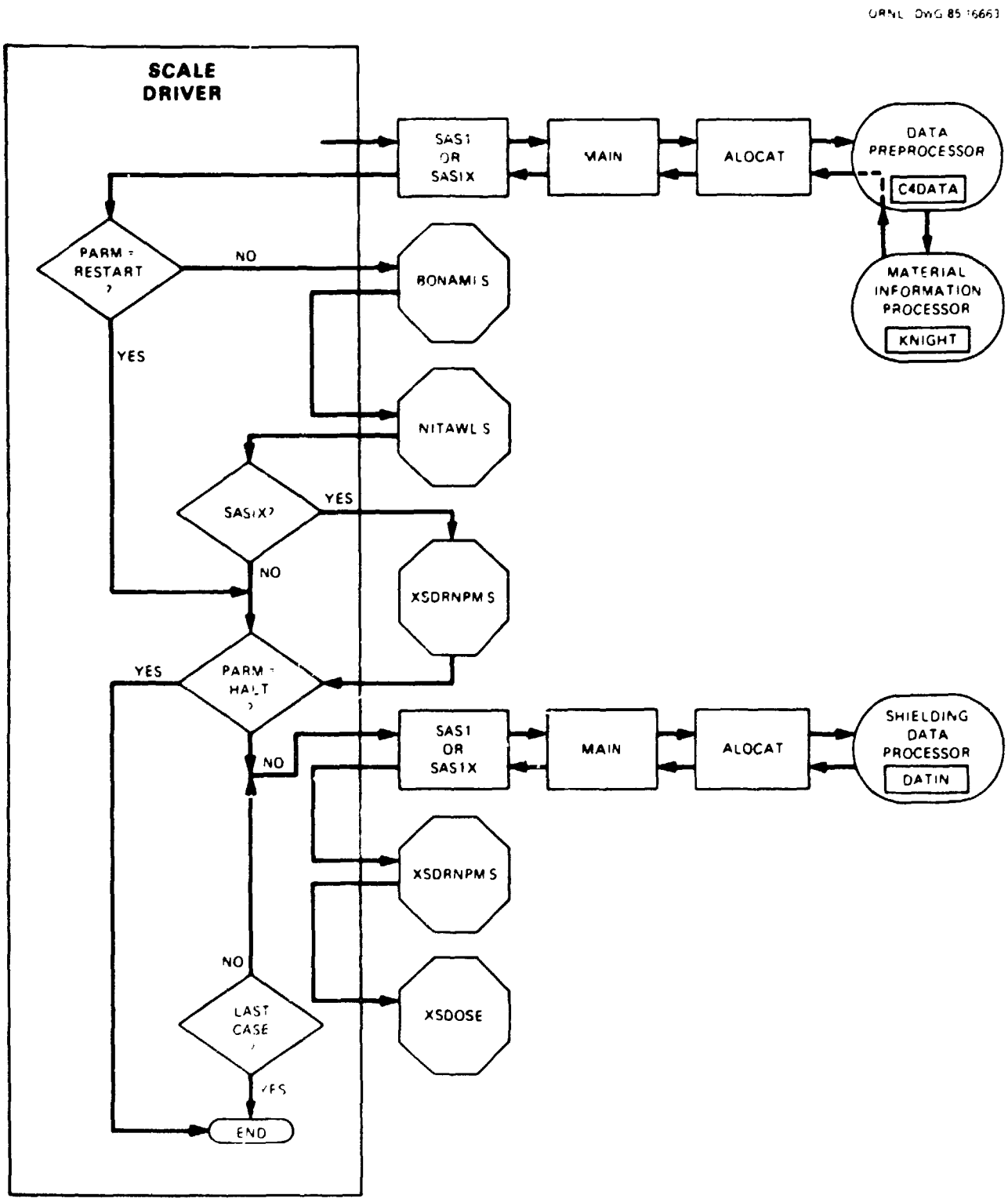

Fig. 5.3. General SAS1 flow diagram.

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6. SOFTWARE ASSESSMENT PROCEDURES

There is a continuing search for means to test the various calculational methods used for radiation transport analyses. Uncertainties in calculated results arise from several areas including the properties of the source, the cross sections of materials involved in the calculation, modeling limitations, calculational method approximations, and statistical uncertainty of Monte Carlo results. At least three methods have been employed to assess or verify calculations: calculational benchmarks, experimental benchmarks, and measurements at operating facilities.[1,2]

6.1 COMPARISON WITH EXPERIMENT

The best scheme to assess the technical validity of a code is to compare analytic results from various codes and/or data libraries against experimental results designed for the application. In essence, this provides a validation of the software for the intended application. Comparisons with experiment can also reveal where further fundamental measurements or development are required. Experiments are often of two types—integral and benchmark.

Integral experiments are so named because they measure integral, or macroscopic, properties of a system. Also, they normally test discrete analytic elements such as differential nuclear data or computer algorithms in an integral manner similar to the way these elements are used in the actual design analysis. Integral experiments typically serve one of two purposes: (1) data or methods verification, characterized by idealized geometries which isolate and enhance specific differential elements, or (2) design verification, characterized by geometries which are prototypic of the actual system design. Both types of experiments provide quality assurance by assessing the adequacy of either the analytic tools or the final system design.

Benchmark experiments represent an elite class of integral experiments and must satisfy certain criteria in addition to the functional intent of the experiment. To be considered as a benchmark, the experiment must have well-defined sources and detector responses, accurately described geometry and material compositions, known sources of uncertainty, and complete documentation. These stringent demands often require significant effort beyond the normal execution and reporting of an experiment, which unfortunately has limited the availability of qualified benchmark problems. However, many pseudo-benchmark experiments have been performed which provide useful and reliable data but lack the formal packaging of a bonafide benchmark.

Limited verification of nuclear data is possible via an accepted collection of data-testing benchmark experiments identified by the Shielding Data Testing and Application Subcommittee of the Cross-Section Evaluation Working Group (CSEWG). They presently support 12 benchmark problems[3] (see Table 6.1) and have cognizance of a similar number of candidates. Because of the degree of accuracy with which gamma-ray interaction data can be measured, none of the CSEWG shielding benchmark experiments address these data, but rather deal only with neutron transport and secondary gamma-ray production data. Although extremely valuable, these benchmarks only provide tests of total cross-section data and are limited in the number of materials considered.

Few integral-type experiments exist for spent fuel shielding applications. Some do exist for cask-type geometries,[4–8] but they vary greatly in quality and, for all but one (ref. 5), the source is actual spent fuel. The use of spent fuel for the radiation source adds greatly to the uncertainty of any related analysis because typically the actual source spectra or pertinent isotopics are not measured, but must be calculated via ORIGEN-type analyses. These experiments also vary widely in their documentation in that an accurate analysis of the experimental model would be difficult based on the information publicly reported. However, these experiments may be a valuable source of information for assessing the total software package (data and code) employed by an analyst. To date, only the analyses associated

Table 6.1. Integral experiments recommended by CSEWG

	Shielding Data Testing (SDT) Series
SDT1.	Iron Broomstick Experiment—an experimental check of neutron total cross sections, R. E. Maerker (ORNL-3867, ENDF-166, revised)
SDT2.	Oxygen Broomstick Experiment—an experimental check of neutron total cross sections, R. E. Maerker (ORNL-3868, ENDF-167, revised)
SDT3.	Nitrogen Broomstick Experiment—an experimental check of neutron total cross sections, R. E. Maerker (ORNL-3869, ENDF-168, revised)
SDT4.	Sodium Broomstick Experiment—an experimental check of neutron total cross sections, R. E. Maerker (ORNL-3870, ENDF-169 revised)
SDT5.	Stainless Steel Broomstick Experiment—an experimental check of neutron total cross sections, R. E. Maerker (ORNL-3871, ENDF-170, revised)
SDT9.	Neutron Attenuation Measurements in a Mockup of the FFTF Radial Shield, P Rose, H. Alter, R. Paschall, A. W. Thiele (AI-AEC-13048, ENDF-181)
SDT10.	Calculational Models for LLL Pulsed Spheres, E. F. Plechaty, R. J. Howerton (UCID-16372—^{6}Li, ^{7}Li, Be, C, N, O, Mg, Al, Tl, Fe, Pb, ^{235}U, ^{238}U, ^{239}Pu
SDT11.	The ORNL Benchmark Experiment for Neutron Transport Through Iron and Stainless Steel, Part 1, R. E. Maerker (ORNL/TM-4222, ENDF-188)
SDT12.	The ORNL Benchmark Experiment for Neutron Transport Through Sodium, R. E. Maerker (ORNL/TM-4223, ENDF-189)
	Shielding Benchmark (SB) Series
SB2.	Experiment on Secondary Gamma Ray Production Cross Sections Arising from Thermal-Neutron Capture in Each of 14 Different Elements Plus Stainless Steel, R. E. Maerker (ORNL/TM-5203, ENDF-227)
SB3.	Experiment on Secondary Gamma-Ray Production Cross Sections Averaged Over a Fast-Neutron Spectrum for Each of 13 Different Elements Plus Stainless Steel, R. E. Maerker (ORNL/TM-5204, ENDF-228).
SB5.	Calculation of Neutron and Gamma-Ray Energy Spectra for Fusion Reactor Shield Design: Comparison with Experiment, R. T. Santoro, R. G. Alsmiller, Jr., J. M. Barnes, and G. T. Chapman, *Nucl. Sci. Eng.* **78**, 259 (1981).

with each experimental program have been done. Reference 9 provides ORIGEN2/QAD/DOT analyses of a storage cask loaded with BWR assemblies.[8] The FCXSEC library was employed. The calculated results vary considerably in comparison to the measured results and are as much as a factor of 2 to 4 lower or higher in different areas of the cask. This type of discrepancy is not very appealing if one wishes to optimize a shield design and accurate computational predictions are desired.

In contrast, many high-quality integral experiments have been performed to test computational methods applicable to reactor shielding problems, especially for advanced reactors such as the Fast Flux Test Facility,[10] the Clinch River Breeder Reactor, and the Gas-Cooled Fast Breeder Reactor.[11] These experiments contributed greatly to the development of the DOT discrete ordinates code and the MORSE Monte Carlo code. Besides validating the basic algorithms of these codes, the experiments were valuable in providing guidelines for the proper selection of the various input parameters. This included the order and directional biasing of angular quadratures, the number of energy groups, the resolution of the spatial mesh, and the degree of detail required in the geometry models.

While validation for the codes' algorithms can be confidently extended to the use of these codes for spent fuel and high-level waste shielding applications, the guidelines and operating experience gained by analyzing reactor-oriented experiments do not entirely apply to spent fuel shielding applications. In particular, the increased importance of gamma-ray transport introduces several new areas of concern. In the past, little attention has been given to the selection and number of gamma-ray energy groups and the energy weighting functions used to create multigroup cross sections. Also, gamma-ray interactions tend to be more angular dependent than neutron interactions, which requires higher-order polynomial expansions of the cross sections. Additionally, evaluation of doses in low scattering medium will certainly present problems of ray effects in multidimensional discrete ordinates calculations. Hence, integral testing of existing methods appear desirable for problems that are more specific to spent fuel shielding applications.

6.2 COMPARATIVE ANALYSIS

As noted above, there is a distinct lack of high-quality shielding experiments available to assess the software packages. Given the lack of experimental data available to verify the physics, an alternative is to compare the analytic results obtained from analyses of a variety of independently developed codes and data libraries. Although the comparison does not allow a conclusion as to the "correct" answer, it allows analysts to (1) study the effect and/or uncertainty of using various methods, codes, and data for a particular analysis, (2) study the theory or software techniques (see Sects. 2–4) to determine the source of difficulty with deviant results obtained for an application, and (3) investigate the variance in calculated results caused by difficulties in input and/or approximations/assumptions used by experienced independent users.

Comparative exercises such as these have been carried out in the nuclear data[12] and shielding[13–14] areas to investigate a variety of applications. Principal sponsors of these efforts have been the International Atomic Energy Agency and the Organization for Economic Cooperation and Development (OECD). Currently, the OECD Nuclear Energy Agency Committee on Reactor Physics is sponsoring a working group for intercomparison of computational methods for spent fuel transport casks. The effort is just getting started, but some of the initial work performed to date by the U.S. delegation (ORNL) is provided in Sect. 7. After some agreement is obtained for various "calculational benchmark" problems, the working group plans to move on to analysis of some existing experimental data.

In a comparative analysis, quality calculations performed with a point Monte Carlo code using evaluated data are often taken as the standard against which other techniques, codes, and data are studied. Of course, variation between the point Monte Carlo results must be resolved first.

Of course an ideal calculational benchmark is one that specifies a particular radiation transport problem for which an analytical answer is known. It allows a developer to test a new method to judge how well it does against known solutions. The American Nuclear Society Shielding Standards Committee (ANS-6) and the RSIC published a compilation of several such benchmarks (ORNL-RSIC-25).

Another effort of some import is the method assessment efforts undertaken in developing an ANSI standard such as those of refs. 15–16. Another working group, ANS 6.6.2, is beginning an effort to develop a recommended standard for calculation and measurement of direct and scattered neutron radiation emitted from high-level nuclear waste. The result of such a standards activity typically provides valuable insight into the proper procedure for evaluating a code or data set for use in a selected application.

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7. CALCULATIONAL ASSESSMENT ACTIVITIES

Section 6 describes the best calculational assessment scheme as one that compares analytic results against experimental results. However, the scope of this report did not allow for a thorough calculational assessment of the various techniques, codes, and data libraries discussed in Sects. 2–5 via the limited experimental data that are available. Instead, this section compares a selection of calculational results performed recently at ORNL in support of a variety of projects involving the analysis of spent fuel casks. These comparative results serve to illustrate the analytic differences that result from the use of the various calculational tools. Where possible, an explanation for the differences is provided and a discussion presented regarding their impact on scoping, design, and licensing analyses for various spent fuel shielding calculations. The information in this section will also help to provide a basis for justifying some of the recommendations presented in Sect. 8.

7.1 METHODS ASSESSMENT

7.1.1 Radiation Source Spectra

As noted in Sect. 2.3, many analysts obtain a total spent fuel neutron source and then generate a groupwise energy spectrum using an analytic fission spectrum function. In contrast, some codes supply groupwise neutron spectra based on analytic techniques derived from experimentally measured spontaneous fission and (α,n) spectra (see Sect. 2.2). To evaluate the potential impact of the two procedures, two identical 1-D discrete ordinates analyses were performed using (1) a fission spectrum for the neutrons and (2) a neutron spectrum generated by ORIGEN-S and based on measured isotopic spectral data (see Sect. 2.2). The total source strength for both calculations was identical and corresponded to PWR fuel depleted to 35 GWD/MTU and cooled for 10 years. Radial neutron dose rates for the truck cask shown in Fig. 7.1 were obtained using the SAS1 module of SCALE (see Sect. 5.4). The results indicate that, for this cask model, the neutron source with a fission spectrum yields a dose rate 7% lower than the dose corresponding to the neutron spectrum generated via the procedure of Sect. 2.2. Although this is a minor difference, the effect may become slightly more pronounced for problems where the (α,n) contribution is greater.

Also, mentioned in Sect. 2.3 is the importance of ensuring that gamma sources are binned into energy groups in a way that conserves the total energy—not the number of photons. The effect obviously depends on the discrete line source and the particular multigroup energy format that is used. The effect is illustrated here using the comparative benchmark cask problem developed by an OECD international working group on shielding analysis methods. The cask consists of a cast iron body as depicted in Fig. 7.2. Because nuclides emit photons at discrete energy levels, the working group specified a discrete line photon source as provided in Table 7.1. The resulting particle-conserving and energy-conserving source spectra for the photon group structure of the CASK and SCALE 27n-18g library are shown in Table 7.2. The resulting doses on the side wall of the cask are about 9–10% lower for the energy-conserving source.

7.1.2 Geometric Model

Sections 3.2–3.4 discuss the geometric modeling limitations of the various radiation transport techniques, and Sect. 3.5 notes the potential importance of the geometry capabilities provided by a code. This section will show an example of comparative results from using (1) 1-D and 2-D discrete ordinates codes and (2) a homogeneous and heterogeneous model of the spent fuel.

It may sometimes be difficult to determine the appropriateness of using 1-D codes for a problem. A good example of when they are and are not appropriate can be easily illustrated with a spent fuel cask geometry. The cast iron cask of Fig. 7.2 was used. Identical neutron and gamma sources were employed and the SCALE 27n-18g cross-section set was utilized.

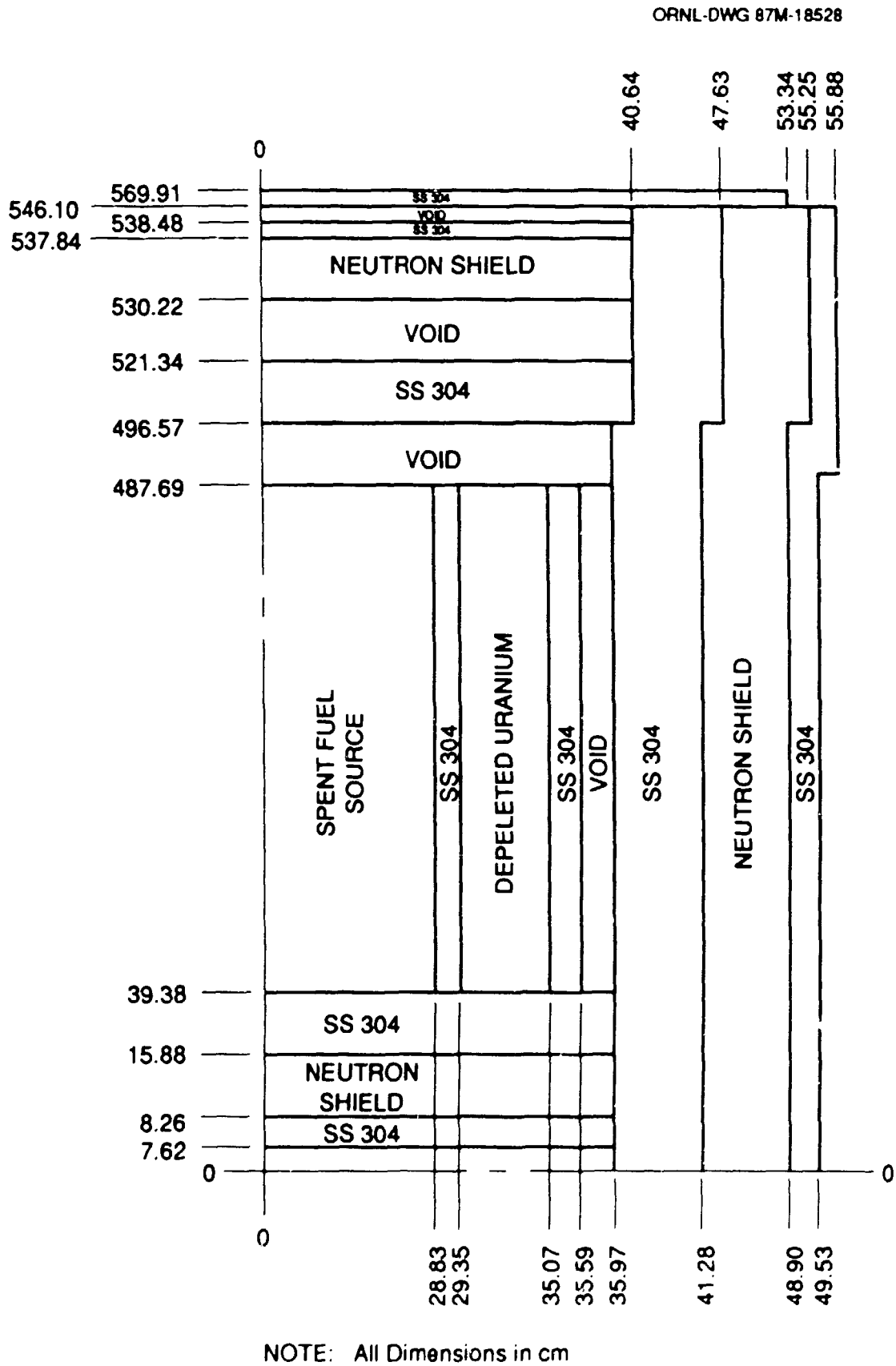

Fig. 7.1. Depleted uranium/stainless steel shielded truck cask model.

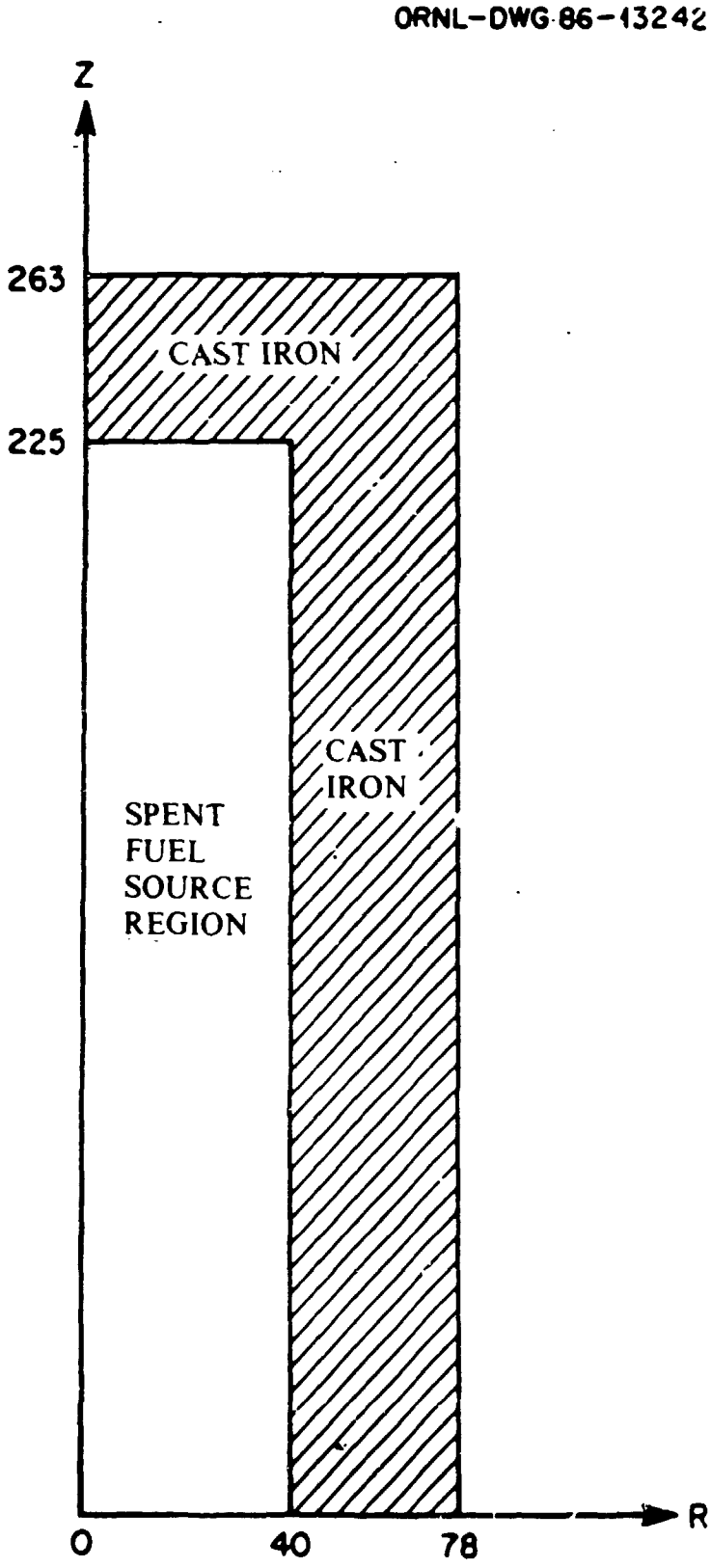

Fig. 7.2. Geometry of cast-iron cask specified by OECD working group.

Table 7.1. Discrete line gamma source for OECD cask problem

Energy (MeV)	Source strength (photons/s)
0.6	2.53+16[a]
0.7	2.32+16
1.0	6.95+14
1.3	5.50+14
1.7	6.15+12
2.1	2.70+14
2.4	2.54+12
2.8	1.32+12

[a]Read as 2.53×10^{16}.

Table 7.2. Particle- and energy-conserving multigroup gamma source spectrum corresponding to discrete line gamma source of Table 7.1

IG	Upper energy limit (eV)	Particle-conserving source spectrum	Energy-conserving source spectrum
1	1.00+7	0.	0.
2	8.00+6	0.	0.
3	6.50+6	0.	0.
4	5.00+6	0.	0.
5	4.00+6	0.	0.
6	3.00+6	1.32+12	1.344+12
7	2.50+6	2.73+14	2.547+14
8	2.00+6	6.15+12	5.713+12
9	1.66+6	0.	0.
10	1.33+6	1.25+15	9.120+14
11	1.00+6	0.	3.861+14
12	8.00+5	4.85+16	3.404+16
13	6.00+5	0.	1.518+16
14	4.00+5	0.	0.
15	3.00+5	0.	0.
16	2.00+5	0.	0.
17	1.00+5	0.	0.
18	5.00+4	0.	0.
Total		5.00+16	5.078+16

Table 7.3 shows dose results from the SAS1 module of SCALE (uses XSDRNPM-S/XSDOSE combination) and from DOT-IV for points radially outward from the cask along the axial midplane. The table shows that a 1-D radial analysis of a typical cask compares well with a 2-D analysis for doses along the axial midplane. The 1-D assumption of an infinite cask height appears valid since little if any radiation leaking from the ends of the cask can contribute to the dose at the given points. A comparison of the neutron doses of Table 7.3 shows the surface doses to agree, but at 2 m out, the 1-D results are 10% higher than the 2-D results. This is expected because the XSDOSE evaluation from the cask finite axial surface must use an angular flux from the 1-D XSDRNPM model which of necessity assumes an axially infinite cask surface (i.e., an angular flux distribution is invariant along the axial cask surface). The 2-D analysis predicts the flux change over the axial finite surface, and, thus, the dose at ≥ 1 m from the cask is lower due to a lower (and more realistic) contribution from the ends of the cask. This trend is not seen with the gamma dose which differs by about 11% both on the surface and at 2 m out. The difference at the surface is probably caused by use of a finer (better) mesh in the 1-D analysis than that used for the 2-D analysis. Most likely, the relative difference remains nearly constant because of a highly forward-peaked photon angular flux which allows little, if any, contribution from the portion of the axial surface removed from the midplane. The apparent conclusion is that 1-D radial analyses are fine for evaluating slightly conservative doses along the midplane. A code like XSDOSE can also evaluate doses off the midplane, but these will be even more conservative in comparison to 2-D doses. Remember, also, that 1-D codes cannot treat any type of axial source distribution in the radiation transport calculation.

Table 7.3. DOT IV and SAS1 radial doses along axial midplane for OECD cast iron cask

Code	Dose type	Dose (mrem/h)[a] Surface	1 meter	2 meters
DOT IV	Neutron	61.5	18.3	9.5
	Gamma	37.7	14.8	8.8
SAS1[b]	Neutron	62.0	19.2	10.7
	Gamma	42.1	16.1	9.8

[a]Doses in mrem/h using ANSI standard flux-to-dose conversion factors.

[b]Employs XSDRNPM/XSDOSE codes.

A far different situation exists for the evaluation of dose rates at the top and bottom of a cask. In this case, a 1-D assumption is poor because a relatively large proportion of the axially directed source particles eventually leak out the sides of the cask. It is possible to attempt a simulation of this radial leakage by specifying a "buckling" parameter in the 1-D input. This parameter is derived from the problem geometry and has its basis in diffusion theory. The results of Table 7.4 indicate the variation in the calculated axial dose as the radial buckling is changed in 1-D analyses of the cask/storage canister geometry shown in Fig. 7.3. In comparison to 2-D calculations, the 1-D (SAS1) results drastically overpredict the dose when no buckling is used and slightly underpredict the dose when reasonable buckling values are employed. This effect is particularly dramatic for neutrons, which indicates a larger relative amount of leakage out the radial surfaces. So, although 1-D calculations can be useful for radial analyses of casks, caution is called for before they are used in axial analyses. This comparison should provide excellent motivation for using multidimensional analysis tools for problems where geometry effects are of potential importance. Indeed, problems involving hot cell analyses or multiple casks in and around buildings may have 3-D effects that should be considered for best results.

Table 7.4. Calculated axial dose rates at canister surface for open cask/closed storage canister configuration

Analysis method	Neutron dose[a] (mrem/h)	Gamma dose (mrem/h)
MORSE-SGC/S[b]		
R = 0/20 cm	296.44(0.077)	
R = 20/34 cm	254.15(0.057)	
R = 34/42 cm	201.82(0.059)	
R = 42/47.63 cm	189.89(0.066)	
R = 0/34 cm	-	91.58(0.173)
SAS1 using XSDRNPM-S/XSDOSE[c]		
No buckling	1257.1	110.10
Cask radius-equivalent buckling	171.8	81.05
Canister radius-equivalent buckling	92.5	67.97

[a]Numbers in parentheses denote fractional standard deviations. All doses evaluated using ANSI standard flux-to-dose conversion factors.

[b]Inner/outer radii of circular detector area given. R = 34 cm is extent of lead shield.

[c]Dose rates at radial centerline of canister, R = 0.

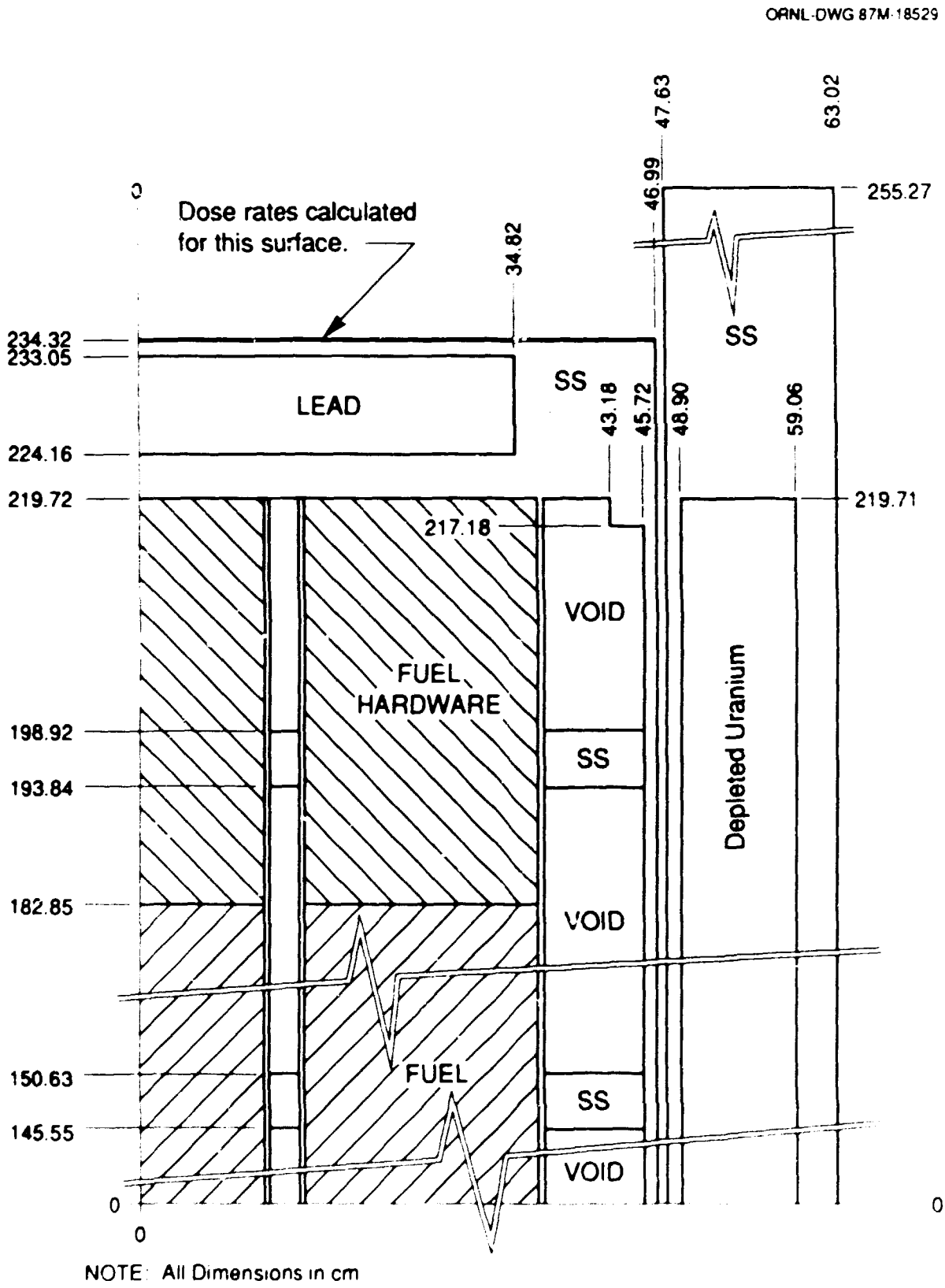

Fig. 7.3. R-Z plane view of the cask/dry canister configuration.

Besides the geometry considerations involving the shield (e.g., the cask body), an analyst must consider the geometry used for the source. Discrete ordinates codes are usually restricted to a homogenized model of the source. Use of different homogenization schemes alters the dose results as evidenced by Table 7.5. Using a homogenized source region equal to the fuel assembly area is a popular approach, but it is often nonconservative in comparison to an approach that homogenizes the source over the entire cask cavity. The latter option nearly always produces a larger gamma dose since the fuel is actually spread out over a larger effective area and fuel self-shielding is decreased. Table 7.6 indicates the effect of using a heterogeneous model of the fuel assemblies in a cask (Fig. 7.4) vs a reasonable homogeneous model (Fig. 7.5). The Monte Carlo analyses were performed using two different initial random numbers and indicate that, at least for neutron dose, there is no advantage in using a heterogeneous model.

Table 7.5. Radial surface dose rates for cask model of Fig. 7.1 for different source homogenization

Source homogenization	Neutron dose[a] (mrem/h)	Total gamma dose[a] (mrem/h)
Source area equivalent to fuel assembly area	27.3	98.57
Source area equivalent to cask cavity area	28.45	89.95

[a]All doses evaluated using ANSI standard flux-to-dose conversion factors.

Of course with the use of multidimensional codes comes the higher computational cost. Thus, the simpler 1-D tools have a distinct advantage (if used properly) for scoping analysis and even final design or licensing analysis where conservatism can be allowed.

7.1.3 Consideration of Fission Neutrons

As the effective multiplication factor (k_{eff}) of a system increases towards a value of 1.0, the importance of the neutrons emitted from fission reactions becomes increasingly important to a shielding analyst. For a dry system where k_{eff} is very low, an analyst can typically consider fission neutrons by modifying the fixed spent fuel neutron source by the factor $1/(1-k_{eff})$. However, for a wet system (occurring in various accident scenarios or when a cask is removed from a pool and prior to purging), where k_{eff} approaches 1.0, this multiplication factor tends to greatly overestimate the neutron dose. This effect is seen in the dose results of Table 7.7 for the OECD cast iron problem of Fig. 7.2. This table indicates that use of a correct fission source is necessary for accurate neutron dose results if k_{eff} is large [probably >0.7, although more analyses are required to determine where the $1/(1-k_{eff})$ approximation breaks down].

Table 7.6. Dose rates for depleted-uranium cask models of Figs. 7.4-7.5

Dose type, Detector location	Two homogeneous fuel zones (Fig. 7.5)			Heterogeneous fuel (Fig. 7.4)	
	DOT-IV	MORSE-SGC/S for two different initial random numbers		MORSE-SGC/S for two different initial random numbers	
Neutron Axial Detectors					
Surface-averaged	-	365.05(.057)[a]	366.18(.049)	342.27(.039)	362.92(.041)
91.44 cm	63.70	63.01(.046)	65.46(.042)	59.09(.032)	60.14(.034)
182.88 cm	19.78	19.73(.044)	20.54(.041)	18.55(.032)	18.96(.033)
Corner	30.17	34.23(.136)	32.08(.105)	27.73(.115)	33.11(.140)
Number of histories	-	90x120[c]	90x120	100x200	100x200
Running time	-	7.4	7.6	47.5	48.6
Neutron Radial Detectors					
Surface-averaged	-	891.31(.020)	859.66(.023)	881.98(.034)	858.68(.024)
91.44 cm	252.00	256.81(.027)	254.01(.027)	264.56(.066)	235.28(.062)
182.88 cm	125.30	126.71(.022)	125.45(.022)	130.13(.056)	119.96(.051)
Corner	30.17	30.15(.117)	26.19(.076)	38.52(.233)	53.28(.366)
Number of hist.	-	80x100	80x100	50x100	50x100
Running time	-	12.2	12.0	42.4	40.7
Total running time[b]		97.2	19.6	19.6	89.9
Gamma Axial Surface Detectors					
Cask surface		1544.40(.064)[a]	1786.90(.078)	1456.88(.063)	1359.28(.041)
100 cm from surface		142.82(.070)	156.43(.077)	125.37(.057)	122.49(.041)
200 cm from surface		97.17(.071)	109.79(.092)	89.79(.067)	85.52(.049)
300 cm from surface		67.99(.082)	72.79(.090)	62.63(.080)	55.40(.048)

[a]Fractional standard deviation.

[b]In IBM-3033 minutes. For the MORSE-SGC/S calculations, the running time includes that of the XSDRNPM-S adjoint calculations; for the DOT-IV calculation, the running time includes that of the FALSTF calculations.

[c]Interpreted as 90 batches of 120 histories per batch.

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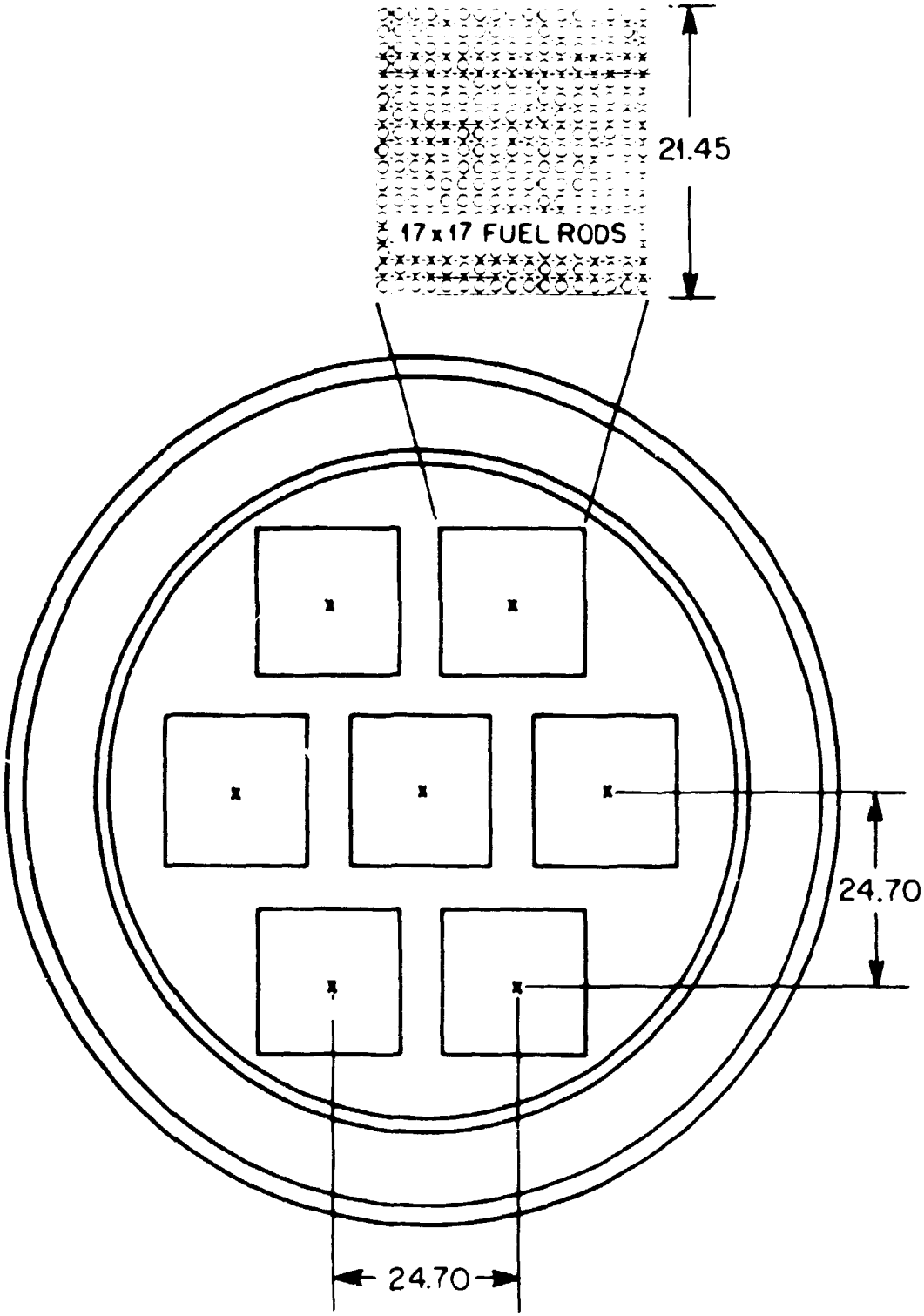

Fig. 7.4. Arrangement of 7 PWR assemblies in depleted uranium cask.

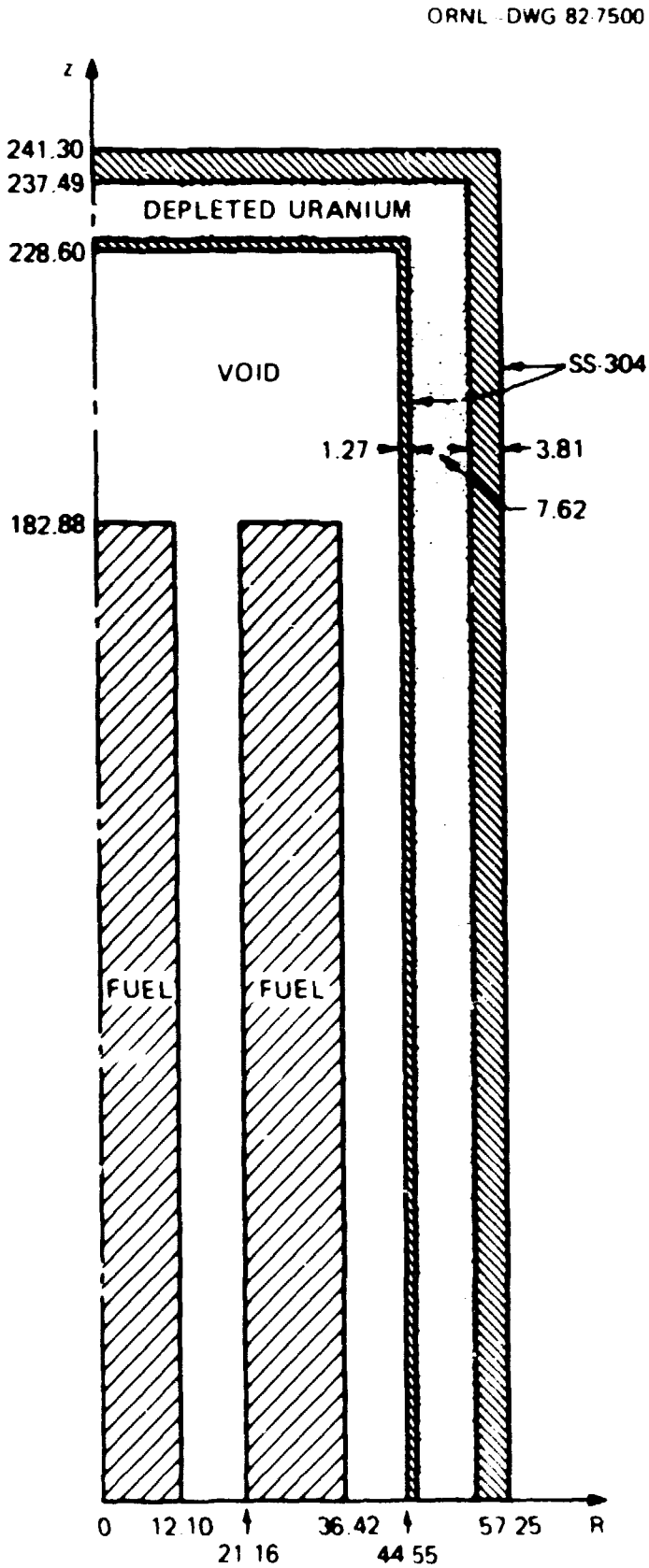

Fig. 7.5. Upper half of depleted-uranium cask (all dimensions in cm).

Table 7.7. Neutron dose rates (mrem/h) for OECD cast iron cask for wet and dry configurations[a]

	Dose with fission source calculated as part of shielding analysis		Fixed source dose multiplied by $1/(1-k_{eff})$[c]
	CASK library[b]	SCALE library[b]	SCALE library
Water-filled cavity	25.88 (k_{eff}=0.855)	51.61 (k_{eff}=0.939)	89.18
Dry cavity	72.67 (k_{eff}=0.180)	77.72 (k_{eff}=0.200)	77.21

[a]All shielding analyses performed with SAS1 module of SCALE and ANSI standard flux-to-dose conversion factors.

[b]k_{eff} values shown are those obtained by the 1-D SAS1 calculation during the shielding analysis.

[c]k_{eff} obtained from KENO V.a analysis of the wet and dry cask models
k_{eff} = 0.197 for the dry cask
k_{eff} = 0.940 for the wet cask

Although most radiation transport codes can consider the fission neutron source, care must be taken in selecting an appropriate cross-section library. The 22n-18g CASK library yields neutron doses one-half that of the 27n-18g SCALE library. This difference can be traced back to inappropriate resonance cross sections for ^{238}U in the CASK library. Thus, the fixed ^{238}U resonance cross sections in CASK make that library inappropriate for systems where neutrons from subcritical multiplication are important.

7.2 CODE AND DATA ASSESSMENT

7.2.1 Point Kernel Codes

This section reviews a brief comparison[1] of two versions of the QAD series of codes—QAD-CG and QAD-CGGP, both discussed in Sect. 5.2.1 and Appendix A.

As indicated in Sect. 5.2, the two QAD versions were very similar to each other with differences occurring in three areas: (1) the range of basic cross-section data (i.e., mass attenuation coefficients); (2) interpolation methods for the mass attenuation values; and (3) the buildup factor method utilized. The basic cross-section values were similar for QAD-CG and QAD-CGGP, but QAD-CGGP cross sections contain a wider range of energies (0.01 to 30 MeV for QAD-CGGP vs 0.05 to 10 MeV for QAD-CG). QAD-CG uses a linear interpolation method to evaluate the point cross-section values at the mean energy for each energy range. QAD-CGGP uses a log-log interpolation to calculate the point cross-section values. The remaining difference between QAD-CG and QAD-CGGP is in the calculation of buildup factors. QAD-CG uses the standard exponential buildup factor method, whereas QAD-CGGP uses the new geometric progression (GP) buildup method. QAD-CGGP has the option of using either buildup factor method; thus, a comparison between the two methods can be easily performed.

Table 7.8 gives the doses for a variation of the truck cask (no neutron shield, less depleted uranium) model of Fig. 7.1 at the surface of the cask along the axial centerline and at points 1, 2, and 10 m from the surface. Doses are given for QAD-CG, QAD-CGGP with standard buildup factors, QAD-CGGP with the GP buildup factors and for the SAS1 1-D radiation transport module at each detector point. The QAD-CGGP results with both types of buildup factors are virtually identical, indicating that the different methods for obtaining buildup factors have no effect in this case. The QAD-CG and QAD-CGGP results are, however, quite different. This difference is almost exclusively due to the two different cross-section interpolation schemes used by the two codes. The cross sections were compared and for the primary materials differences of much less than 1% were seen. The effect of varying the interpolation method from linear to log-log was seen to be around 2% in the Fe, which is sufficient to cause the variations seen in the results. The ratios of the SAS1 results to both QAD-CG and QAD-CGGP are given in Table 7.8. The QAD-CG values seem to give results much closer to SAS1 than the QAD-CGGP results, but this agreement could be fortuitous since this geometry is a mixture of materials and QAD, in general, does not perform accurately for such a case.

Table 7.8. Comparison of QAD-CG and QAD-CGGP doses (rem/h) with SAS1 (1-D transport) for truck cask of Fig. 7.1

Dose[a] location	QAD-CG	QAD-CGGP[b] (old buildup factor)	QAD-CGGP[c] (GP buildup factor)	SAS1	SAS1/ QAD-CG	SAS1/ QAD-CGGP
Surface	5.025-1[d]	6.240-1	6.245-1	5.107-1	1.016	0.818
1 meter	1.644-1	2.040-1	2.041-1	1.485-1	0.903	0.728
2 meters	9.782-2	1.213-1	1.215-1	8.480-2	0.867	0.698
10 meters	8.550-3	1.051-2	1.051-2	9.379-3	1.097	0.892

[a]All doses are at a specified distance from the outer cask surface at the axial centerline.

[b]QAD-CGGP cases ran with standard exponential buildup factors.

[c]QAD-CGGP cases ran with geometric progression buildup factors.

[d]Read 5.025-1 as 5.025×10^{-1}

The above conclusion is strengthened by the results shown in Table 7.9 for the OECD cask model of Fig. 7.2. Here the QAD-CGGP results are consistently higher than the QAD-CG values as before, but the QAD-CGGP results are in much better agreement with the SAS1 results at the cask surface than the QAD-CG values. In this case, the geometry is very simple and contains only one material and hence, the QAD results should be very good. The QAD-CG results at points off the surface once again are in better agreement with the SAS1 results, but this is simply due to conservatism in the QAD calculations at points external to a cylindrical source. This can be shown by observing the behaviors of the two ratios at the external dosimeter points. The QAD-CG results are consistently 8 to 10% higher than the QAD-CGGP results all the way out to 100 m. Thus, the QAD-CG ratios away from the surface are closer to unity simply because the QAD-CG ratio at the surface was much higher than for the QAD-CGGP case.

Table 7.9. Comparison of QAD-CG and QAD-CGGP doses with SAS1 (1-D transport) for OECD benchmark case

Dose location[a]	Doses (mrem/h)				
	QAD-CG	QAD-CGGP[b] (GP BF)	SAS1	SAS1/ QAD-CG	SAS1/ QAD-CGGP
Surface	45.57	50.22	52.20	1.145	1.039
2 m	12.57	13.84	12.29	0.978	0.888
10 m	1.7	1.9	1.4	0.845	0.770
50 m	8.545-2[c]	9.461-2	6.869-2	0.804	0.726
100 m	2.168-2	2.402-2	1.733-2	0.799	0.722

[a]All doses are at specified distance from the outer cask surface at the axial centerline.

[b]QAD-CGGP cases were run with the Geometric Progression (GP) buildup factors (BF) in all cases.

[c]Read as 8.545×10^{-2}.

The unexpected conclusion from this brief comparison is that the QAD versions can provide significantly different results not only from variation in the data and interpolation used for the buildup factors, but also from the interpolation of the point attenuation (photon cross section) values. Further investigation with other point kernel codes and/or shielding materials would be valuable. A comparison of QAD-CG and QAD-CGGP results together with results for various Monte Carlo and discrete ordinates codes is shown in the next section for the simpler OECD cask model.

7.2.2 Radiation Transport Codes

A limited comparison of results from several transport codes was done to assess the agreement between various codes for the OECD cast iron cask model of Fig. 7.2. Analyses were performed using the SAS1 (XSDRNPM/XSDOSE), and SAS4 (MORSE-SGC) modules of SCALE, DOT IV, and MCNP. In addition, QAD-CG and QAD-CGGP analyses were done to provide a further comparison between point kernel and radiation transport codes.

The source specifications (^{235}U fission neutron spectrum and energy-conserving spectrum of Table 7.2) and multigroup cross-section library (SCALE 27n-18g) was identical for the SAS1, SAS4, and DOT IV analyses. Doses from DOT IV were actually evaluated using an in-house version of the FALSTF code. The MCNP calculations used the discrete line gamma source data of Table 7.1 and the ENDF/B-IV point cross-section data available with the MCNP Version 3. The attenuation and buildup factor data sets are those provided with the QAD versions which were used.

The dose results obtained from the analyses are shown in Table 7.10. Based on a knowledge of the techniques, geometry model, and data used by the codes for these analyses, the following comments and observations can be made from the tabulated results.

1. The relatively good agreement between 1-D and 2-D codes for sidewall cask doses has been previously noted in Sect. 7.1.1.

Table 7.10. Comparison of dose rates (mrem/h) from various radiation transport codes for the OECD cast iron cask model of Fig. 7.2[a]

	Sidewall			Bottom		
	Neutron dose	Primary gamma dose	Secondary gamma dose	Neutron dose	Primary gamma dose	Secondary gamma dose
Surface						
QAD-CG	-	33.1	-	-	-	-
QAD-CGGP	-	35.8	-	-	-	-
SAS1	62.0	41.7	0.41	-	-	-
DOT IV	61.5	37.4	0.41	-	-	-
DOT IV-avg	57.4	36.3	0.38	-	-	-
SAS4-avg	58.0(.02)[b]	37.0(.04)	0.35(.07)	46.5(.06)	42.3(.12)	-
MCNP-avg	64.1(.02)	34.1(.07)	0.46(.08)	39.8(.13)	50.9(.30)	0.18(.34)
1 Meter						
QAD-CG	-	-	-	-	-	-
QAD-CGGP	-	-	-	-	-	-
SAS1	19.2	14.4	0.13			
DOT IV	18.3	15.5	0.13	7.4	12.1	0.05
SAS4	18.8(.02)	20.0(.20)	0.11(.25)	7.3(.05)	10.9(.10)	-
MCNP	20.8(.02)	13.5(.10)	0.14(.06)	7.5(.06)	11.8(.15)	0.05(.14)
SAS4-avg	13.0(.02)	10.1(.04)	0.08(.08)	3.8(.08)	3.7(.10)	-
2 Meters						
QAD-CG	-	9.1	-	-	-	-
QAD-CGGP	-	9.9	-	-	-	-
SAS1	10.7	9.7	0.08	-	-	-
DOT IV	9.5	8.7	0.07	2.3	4.3	0.02
SAS4	10.0(.02)	11.9(.30)	0.04(.08)	2.3(.05)	3.8(.08)	-
MCNP	11.1(.02)	7.7(.07)	0.08(.05)	2.4(.06)	4.4(.14)	0.02(.15)
SAS4-avg	7.3(.02)	6.2(.04)	0.04(.07)	1.7(.07)	2.3(.09)	-
10 Meters						
QAD-CG	-	1.3	-	-	-	-
QAD-CGGP	-	1.4 -	-	-	-	
SAS1	0.95	1.17	0.007	-	-	-
DOT IV	0.78	0.95	0.006	0.10	0.22	0.001
SAS4	0.80(.18)	1.03(.131)	0.005(.19)	0.10(.05)	0.20(.07)	-
MCNP	0.91(.02)	0.85(.06)	0.006(.04)	0.11(.06)	0.23(.14)	0.001(.17)

[a]"avg" indicates dose is averaged over cavity height for the sidewall doses and over cavity diameter for axial doses. Otherwise, point detectors are used and located at the axial midplane for the sidewall doses and at the radial center for the axial doses.

[b]Number in parentheses indicates value of one fractional standard deviation.

2. The QAD-CG and QAD-CGGP sidewall surface results are, respectively, 11.8% and 4.3% lower than the 2-D results of DOT IV but increase to, respectively, 37% and 47% higher than DOT IV at the 10-m mark. This general trend is also true in comparing QAD with the other radiation transport codes. Thus, for this problem, comparison of the QAD methodology to radiation transport techniques produces slightly lower results at the shield surface and increasingly higher results as the distance from the shield increases. The QAD results show a relative increase at greater distances because the buildup factors are based on infinite mediums.

3. Note that the QAD and SAS1 results of Table 7.10 are about 25 to 30% lower than those reported in Table 7.9 for the same model! The difference is due to the energy group structure used for the gamma source. The results of Table 7.9 were obtained using the energy spectrum developed for the 20-gamma groups of the BUGLE library, but the results of Table 7.10 were calculated with the 18-gamma-group spectrum of the 27n-18g SCALE library. The predominant line energy (contributing 85 to 90% of the dose) is at 2.1 MeV. The energy group intervals encompassing this line energy are 2 to 3 MeV for the BUGLE library and 2 to 2.5 MeV for the 27n-18g library. Thus, for this group, the source energy utilized by QAD (i.e., average group energy) was 2.5 MeV for the BUGLE spectrum and 2.25 MeV for the 27n-18g library. A QAD case using the explicit line energies yields a dose of 29.37 mrem/h at the surface. Thus, it appears that for some problems (those with important discrete line sources), the calculated groupwise spectrum needs to tightly bound the important line energies.

4. For neutrons, the results agree to within 17% for the sidewall point detector and agree even better for the axial point detector. The DOT IV results are the lowest while the MCNP results are the highest. However, the excellent agreement between DOT IV and SAS4 indicate that some (or all) of the disparity between DOT and MCNP may be due to differences in the cross-section data (see Sect. 7.2.3). The low fractional standard deviations achieved by SAS4 and MCNP provide for good confidence in the results. These same trends appear to hold generally for the secondary gamma doses.

5. For photons, the doses are higher for DOT IV than for MCNP by a maximum of 12% (at 10 m). As with the neutron results, the MCNP-DOT discrepancy appears to be a cross-section data difference (see Sect. 7.2.4). The relatively high fractional standard deviations reported with the SAS4 point detector results makes it difficult to obtain more than a general comparison of the results.

6. The surface-averaged results provided by SAS4 allow the peak-to-average value to be evaluated and indicate a flattening of the flux as the distance from the shield increases. Note that the peak-to-average value is very high for the cask bottom, thus indicating the need for an adequate multidimensional code if accurate dose profiles are to be obtained.

7. The high fractional standard deviation (fsd) reported for several of the SAS4 gamma doses needs to be assessed to determine if MCNP gave better fsds because of better methods or because more Monte Carlo histories were run. Incorporation of the Klein-Nishina next-event estimator (already available in MORSE-CG and MORSE-CGA) is expected to improve the fsd from MORSE-SGC.

8. Due to the basic Monte Carlo methodology, neither SAS4 nor MCNP can generate accurate point detector results near a scattering medium (see Sect. 3.3). This is the reason why only surface-averaged results are provided on the cask surface.

7.2.3 Cross-Section Data

As noted in the previous section, it was suspected that much of the difference between the multigroup code results and those of MCNP was due in large part to different cross-section data. This section presents the results of a study performed to assess the variability of different multigroup cross-section libraries and compare them with results from the ENDF/B-IV-based MCNP point library.[2] Based on the excellent agreement for the sidewall surface doses between SAS1 and DOT IV, the SAS1 module was employed as a relatively cheap, but accurate, tool to use in comparing various cross-section sets. The analyses were performed on the OECD cast iron cask model of Fig. 7.2. The code parameter data and radiation sources were identical for all the analyses.

Four broad-group libraries distributed by RSIC and routinel, used for spent fuel shielding analyses were selected as the basis for this study: the 47n-20g BUGLE-80 library, the 22n-21g FCXSEC library, the 27n-18g coupled library from SCALE, and the 22n-18g CASK library. The BUGLE-80 and FCXSEC libraries are collapsed from the 171n-36g VITAMIN-C library. The neutron data for the SCALE library is from the 218n-group CSRL-IV library. Using the group structure of the selected broad-group libraries, several variations of the base libraries were investigated by recreating the library (with slight changes as noted in Table 7.11) from the fine-group libraries. Variations in the fine-group data (ENDF/B-IV vs ENDF/B-V), resonance self-shielding techniques (problem-dependent vs problem-independent processing), and collapsing spectrum were all investigated.

Table 7.11 provides information on the subtle differences between the libraries, and Table 7.12 shows the dose rate results from the comparative study. The broad-group (libraries 1–4) calculations were performed with $S_{16}P_3$ specifications, but the fine-group (libraries 5–7) calculations were run as S_8P_3. All the libraries except 1a, 2a, and 4 contain Bondarenko factors or resonance parameters that allow a problem-dependent resonance treatment via BONAMI or NITAWL. As seen in Table 7.12, there is a fairly widespread in dose rates as a function of the input library. A large amount of comparative-type information can be gleaned from a study of Table 7.12. Some of the major findings of interest are noted below.

1. The spectrum used to collapse the gamma-ray data is important (compare results from libraries 1c and 1d, or libraries 3b and 3c). The gamma-ray dose using a concrete or flat spectrum appears to be about 50% higher than when an iron spectrum (from fine-group analysis of the problem) is used. The different weighting actually causes cross-section changes of only a few percent, but these changes are magnified by nearly an order of magnitude in the final dose because of the deep penetration nature of the problem.

2. There is a surprising discrepancy between the gamma dose results of the "fine"-group libraries 5 and 6. This discrepancy is perhaps caused by (a) the sensitivity of the dose to small differences in the gamma-ray cross sections and b) the fact that these calculations are not truly "fine"-group calculations. The CSRL-V library has four energy groups in the important energy ranges while the VITAMIN-E library has only two energy groups. Thus, it appears that a finer group structure than has been customary is required to have a true "fine"-group gamma-ray library for this problem. Note that these "fine" group results lie on either side of the MCNP result of 34.1 ± 7% reported in Table 7.10.

3. Nearly a 40% variation in the secondary gamma doses can be seen (e.g., compare results from libraries 4 and 1d) for Model II where the polyethylene causes the secondary gammas to become important relative to the neutrons.

4. Proper problem-dependent resonance self-shielding of the neutron data appears to be important. Libraries 1a and 2a have a limited amount of self-shielding performed in a problem-independent fashion. Comparison with results from libraries 1b and 2c, respectively, for which complete, problem-dependent resonance self-shielding was done (via BONAMI), indicates that an inadequate resonance treatment of the shield material can significantly lower the dose.

Table 7.11. Cross-section libraries used to obtain results of Table 7.12

Cross-section library	Description
1a	47n-20g group collapsed from 171n-36g VITAMIN-C library with concrete spectrum - ENDF/B-IV data. Concrete materials only have been processed by BONAMI. This is the BUGLE-80 library.
1b	47n-20g group collapsed from 171n-36g VITAMIN-C library with concrete spectrum - ENDF/B-IV data. All resonance materials have Bondarenko factors.
1c	47n-20g group collapsed from 174n-38g VITAMIN-E library with concrete spectrum - ENDF/B-V (Fe, Mod 3) data. All resonance materials have Bondarenko factors.
1d	47n-20g group collapsed from 174n-38g VITAMIN-E library with iron cask spectrum - ENDF/B-V (Fe, Mod 3) data. All resonance materials have Bondarenko factors.
1e	47n-20g group collapsed from 174n-38g VITAMIN-E library with iron cask spectrum - ENDF/B-V (Fe, Mod 3) data. Includes new iron data recently measured at ORNL (see Ref. 11). All resonance materials have Bondarenko data.
2a	22n-21g group collapsed from 171n-36g VITAMIN-C library with fusion/fission-1/E-Maxwellian weighting for neutrons, flat weighting for photons - ENDF/B-IV data (converted from RSIC ANISN Library). All materials have been resonance processed via BONAMI and σ_0 values of 0.1, 1000, and 10^8 are provided. This is the FCXSEC library.
2b	22n-21g group collapsed from 171n-36g VITAMIN-C library with concrete spectrum - ENDF/B-IV data. All resonance materials have Bondarenko factors.
2c	22n-21g group collapsed from 171n-36g VITAMIN-C library with fusion-fission-1/E-Maxwellian weighting for neutrons and flat weighting for photons. All resonance materials have Bondarenko factors.
3a	27n-18g group collapsed from 218n ENDF/B-IV library. Gamma data created in 18 group format. Fission-1/E-Maxwellian weighting for neutrons and flat weighting for photons.
3b	27n-18g group collapsed from 227n-44g CSRL-V libraries with fission-1/E-Maxwellian weight function for neutron groups, flat weight for photons - ENDF/B-V (Fe, Mod 1) data. All resonance materials contain resonance parameters.
3c	27n-18g group collapsed from 227n-44g CSRL-V libraries with iron cask spectrum - ENDF/B-V (Fe, Mod 1) data. All resonance materials contain resonance parameters.
3d	34n-18g group collapsed from 227n-44g CSRL-V libraries with iron cask spectrum - ENDF/B-V (Fe, Mod 1) data. All resonance materials contain resonance parameters.
4	22n-18g group CASK library, assorted data sources. Neutron cross sections collapsed from 104 group structure using weighting spectrum for uranium/water mixture.
5	227n-44g CSRL-V libraries processed through AMPX-II from ENDF/B-V data. Bondarenko factors provided for unresolved resonance region.
6	174n-38g VITAMIN-E library processed through MINX (neutron) and AMPX (gammas) from ENDF/B-V data.
7	218n CSRL-IV library processed with AMPX from ENDF/B-IV data with a fission-1/E-Maxwellian weighting function.

Table 7.12. Radial surface doses (mrem/h) from the OECD cask model using a 1-D discrete ordinates code and various cross-section libraries

Cross-section library[c]	Model I,[a] fixed-source results			Model II,[b] fixed-source results		
	Neutron[d]	Primary gamma	Secondary gamma	Neutron	Primary gamma	Secondary gamma
1a (47n-20g BUGLE-80)	3.680+1	5.220+1	0.468	4.345	2.147+2	4.419
1b (47n-20g)	5.434+1	5.220+1	0.447	5.574	2.147+2	5.132
1c (47n-20g)	5.050+1	5.143+1	0.440	5.088	2.119+2	5.254
1d (47n-20g)	5.127+1	3.407+1	0.429	5.200	1.515+2	5.312
1e (47n-20g)	5.187+1	3.407+1	0.429	5.340	1.515+2	5.322
2a (22n-21g, FCXSEC)	1.401+2	-	0.430	15.12	-	5.201
2b (22n-21g)	5.781+1	4.184+1	0.425	4.982	1.857+2	3.901
2c (22n-21g)	1.501+2	4.448+1	0.377	16.28	1.981+2	4.166
3a (27n-18g, SCALE)	6.200+1	4.171+1	0.410	5.963	1.840+2	4.604
3b (27n-18g)	5.035+1	4.108+1	0.407	4.640	1.816+2	4.345
3c (27n-18g)	5.180+1	2.667+1	0.412	5.482	1.295+2	4.023
3d (34n-18g)	5.177+1	2.666+1	0.412	5.480	1.295+2	4.021
4 (22n-18g, CASK)	5.957+1	4.163+1	0.421	5.639	1.837+2	3.669
5 (227n-44g, CSRL-V)	5.020+1	2.795+1	-	-	-	
6 (174n-38g, VITAMIN-E)	5.479+1	3.980+1	-	-	-	
7 (218n, CSRL-IV, 1/E weighting for Fe)	3.675+1					

[a] Dry cask model with 38 cm of iron shielding.
[b] Dry cask model with 32 cm of iron shielding and 6 cm polyethylene.
[c] Read as 3.680×10^{1}.
[d] See Table 7.11 for explanation.

5. Comparing the results from libraries 1b and 1c indicates that there is about an 8% difference between the ENDF/B-IV and ENDF/B-V cross-section data for materials in this problem.

6. The spectrum used to collapse the neutron data can also be important for this shield material. The data collapsed with the fusion-fission-1/E-Maxwellian spectrum (libraries 2a and 2c) cause a large (and inaccurate) rise in the doses. Further detailed investigation found the problem to arise from an unfortunate (for iron, at least) selection of broad-group energy intervals combined with a weighting spectrum that switched from 1/E to fission at an inappropriate location in energy (0.1 MeV). The 0.55–1.1 MeV group of library 2 bracketed the large iron inelastic scattering threshold at 0.87 MeV. This broad group scheme combined with the fission weighting to produce signficant differences in the collapsed cross sections in this important energy range. This is also a major factor in explaining the high dose results obtained with library 3a in comparison to results from its parent fine-group calculation. Also, neither library 3a nor library 7 (processed using resonance parameters) have any effective resonance shielding for the iron in this problem because ENDF/B-IV did not provide resonance parameters above 60 keV.

7. The results using libraries 3b, 3c, and 3d are all in very good agreement with each other as well as with the fine-group value obtained with library 5. These three cases are all based on the 227n-44g CSRL-V library, with libraries 3c and 3d collapsed using the same weight function, but with seven high-energy groups added to the 3d library. The agreement of results from library 3b with the other two is interesting since it was collapsed with a very similar spectrum as for libraries 2a and 2c discussed above. However, for this case, the selection of the breakpoint for switching from a 1/E to a fission spectrum was a better choice (0.9 MeV) for an iron shield and a group boundary was provided at 0.9 MeV.

8. None of the fine multigroup libraries (5–7) agree particularly well with the neutron dose (64.1 ± 2%) using the MCNP point cross sections (see Table 7.10). Some of the broad-group results agree with the MCNP value much better than the fine-group results, but it is suspected that the agreement is fortuitous in light of several of the comments noted above. Based upon comparison of results from libraries 1b and 1c and libraries 1c and 6, it appears that a fine-group ENDF/B-IV VITAMIN-C result would be within about 10% of an MCNP result which uses ENDF/B-IV point data.

Although limited to spent fuel shielded by cast iron, this study does point out the fallacy of using "off-the-shelf" cross-section libraries without regard to particular aspects of the radiation source, geometry, and material compositions. The broad-group libraries 1a, 2a, 3d, and 4 of Table 7.11 are readily available from RSIC and are routinely used for spent fuel cask analyses. However, the calculated dose rates present in Table 7.12 indicate that these libraries provide (1) neutron dose results that vary by a factor of almost four (1a versus 2a), and (2) gamma dose results that disagree from 30% to 50% with results from parent fine-group calculations. Calculations using fine-group libraries, one point data library, and variations of libraries 1a, 2a, 3d, and 4 indicate the radiation doses differ because of inadequate resonance self-shielding, use of improper weighting spectra, and/or a poor selection of energy group boundaries for the particular problem being analyzed. Another finding of this study was that there exists some unexpected discrepancies among results generated with fine-group and point data libraries. Further study in this area is needed.

In an effort to demonstrate that the phenomena in Table 7.12 are not just true for a cast iron cask, libraries 1b, 2b, and 3a of Table 7.11 were used in a SAS1 analysis of the depleted uranium/stainless steel truck cask in Fig. 7.1. The resulting doses shown in Table 7.13 indicate similar trends as found for the cast iron cask.

Table 7.13. Radial surface does from the truck cask of Fig. 7.1 using a 1-D discrete ordinates code and various section libraries

Cross-section library (see Table 7.11)	Doses (mrem/h)	
	Neutron	Total gamma
1b (47n-20g)	33.54	102.30
2b (22n-21g)	31.03	98.57
3a (27n-18g)	40.06	102.10

The MCNP user is also not totally free of data worries. The ENDF/B-IV discretized neutron data library available with MCNP was also used to analyze the cast iron cask. The resulting dose rate of 38.0 mrem/h is nearly half that of the dose rate obtained with the point data and indicates the discrete data's inability to properly account for the iron cross-section resonances (compare with results of library 1a). Thus, the discrete data yields answers faster and cheaper, but they are, most likely, inappropriate for final analyses (as stated in the MCNP manual).

7.3 REFERENCES

1. B. L. Broadhead and C. V. Parks, "Point Kernel Versus Radiation Transport for Iron Deep Penetration Problems," *Trans. Am. Nucl. Soc.* 55, 295 (June 1987).

2. C. V. Parks et al., "Intercomparison of Cross-Section Libraries Used for Spent Fuel Cask Shielding Analyses," *Proceedings of Theory and Practices in Radiation Protection and Shielding*, ISBN: 0.89448-132-0, Vol. 2, p. 559, 1987.

8. CONCLUSIONS AND RECOMMENDATIONS

Shielding analyses associated with the storage, transport, and handling of spent fuel represents a broad class of applications that have recently become of major importance in both the government and private sector. However, the review provided by this report concludes that the validity and/or accuracy of analytic results can be clouded by uncertainty in the calculated radiation source spectra, the wide variety of radiation transport and point kernel methods and codes, and the sensitivity of the final doses to processed cross-section data. Specific conclusions and recommendations are listed below. The first six recommendations follow directly from the six conclusions that are provided.

8.1 CONCLUSIONS

8.1.1 Radiation Source Generation Codes

The radiation source strength and spectra supplied to a shielding analysis code has a direct and important impact on the calculated dose. Currently, the ORIGEN-type codes are the most widely used codes for calculating the spent fuel or high-level waste (HLW) isotopics that are used to produce the source strength and spectra. The ORIGEN-S code currently has the most complete and convenient means of providing photon and neutron source spectra for input to multi-energy-group codes.

8.1.2 Radiation Transport Codes

The current generation of radiation shielding codes is adequate to meet the analysis needs of the DOE Waste Management Program. However, the diversity of applications (cask fleet, interim storage facility, repository) and calculational needs (benchmark analyses, production analyses, scoping analyses) require that codes be selected from each of the major techniques used for radiation transport modeling. If validated in a consistent manner, such a set of codes would complement each other in (1) scoping and preliminary design (point kernel and one-dimensional discrete ordinates codes), (2) final design (discrete ordinates codes), and (3) investigation of modeling bias (continuous energy or point Monte Carlo codes).

8.1.3 Data Libraries

Standard gamma-ray buildup factor data (for point kernel codes) and flux-to-dose conversion factors are provided, respectively, by ANS-6.4.3 and ANSI/ANS-6.1.1. Point cross sections from the latest evaluated nuclear data file (ENDF/B-V) provide an adequate data library for continuous energy Monte Carlo codes. However, existing multi-energy-group cross-section libraries (produced from ENDF/B files) have provided a wide variability in calculated results for a shielded spent fuel application (see Sect. 7.2.3).

8.1.4 User Expertise

Accurate evaluation of neutron and gamma-ray doses from shielded spent fuel or HLW is a difficult task that requires a large amount of user expertise to correctly identify appropriate modeling assumptions, provide adequate input data (source specification, code input data, and cross-section data), and interpret/verify the final results. A validated, high-quality code in the hands of an inexperienced user is often less reliable than an approximate, poor-quality code in the hands of an experienced radiation shielding analyst. However, for given generic applications, it should be possible to enhance existing software interfaces and input to ease the excessive and often redundant dependence on user expertise in a production environment.

8.1.5 Code and Data Validation

The major U.S. shielding analysis software reviewed in this report are well-established tools that have evolved over a 20- to 25-year period. However, as discussed in Sect. 6, high-quality integral experiments adequate for code and data validation have often been limited to very simple systems or in support of specialized shielding needs (i.e., specific reactor designs). Although dose measurements from casks loaded with spent fuel have been made, no concerted effort has been undertaken to use the available measured data for validating any particular codes and/or data library. However, each of the codes has probably been evaluated through the use of the limited integral experiment data at some time or another. These comparison efforts have typically been performed by various users and often were never formally documented.

8.1.6 Quality Assurance/Maintenance Program

The major U.S. shielding codes and data libraries are public domain software. Most of the codes exist in many different versions which are either updates provided by the original developer or enhancements by major users. Little, if any, software development was performed under a formal QA program.

The services of the Radiation Shielding Information Center (RSIC) as a central site for the existing documentation and software has been invaluable for publicizing new software and keeping many useful codes and data libraries from being lost to the user community. Although the viable code versions are normally available from RSIC, many of the code packages and data libraries no longer have a principal technical contact who has a mandated (funded) responsibility for software maintenance (including documentation changes) with a QA plan that would allow complete compliance with current interpretations of ANSI/ASME NQA-1 or NUREG-0856. Historically, software developers have often passed QA and maintenance responsibility onto the users, particularly as funding support for the code development was reduced or deleted by the sponsoring organization.

8.2 RECOMMENDATIONS

8.2.1 Provide Interface with Isotope Generation Code

The isotope generation code selected for use by the DOE Waste Management Program needs to allow for neutron and photon strength and spectra to be easily provided to radiation transport codes. Besides user specification of a multienergy-group format, the code should also allow convenient input of photon line data and/or continuous energy spectra to codes such as QAD and MCNP which do not require multienergy grouping.

8.2.2 Select Radiation Transport Codes

Based on this assessment, it is recommended that the point kernel code QAD-CGGP, the discrete ordinates codes ANISN (one-dimensional analysis) and DOT 4.3 (two-dimensional analysis), and the Monte Carlo code MCNP be selected for further assessment work and/or validation relative to use in general spent fuel and/or HLW applications. If the need for an integrated code system is established (see Sect. 8.2.4), there should be strong consideration given to using XSDRNPM and MORSE-SGC rather than ANISN and MCNP. The reasoning is that XSDRNPM and MORSE-SGC would be more amenable (because of data handling methods and MORSE/QAD common geometry features) to incorporation into a unified, consistent system. The need for codes that use different solution methodologies and limitations is discussed in the conclusions and based on the background information of Sects. 3, 5, and 7. These codes were selected because they best satisfy (in the authors' judgment) the overall assessment criteria provided in Sect. 5.

8.2.3 Establish Multigroup Cross-Section Library(ies)

The analysis results shown in Sect. 7.2.3 indicate that further work is needed in order to establish a multigroup library (or libraries) that are adequate for the various applications required by the DOE Waste Management Program. As indicated by the background information of Sect. 4, it may be necessary to provide several different libraries in order to accurately predict the radiation transport through different shielding mediums. Using existing and/or enhanced ENDF/B-V libraries, the selected multigroup transport codes should be employed to compare with existing experimental dose measurements to provide a basis for adoption of adequate multigroup cross-section libraries.

8.2.4 Integrate the Software System

A unified, easy-to-use system needs to be developed that includes standard data libraries, consistent input and automated data processing (e.g., resonance self-shielding, temperature correction, etc.) where possible, and common interface files. The system would contain the selected point kernel, discrete ordinates, and Monte Carlo codes to allow maximum flexibility for accurate and efficient scoping, design, and safety evaluations. The system will also contain needed auxiliary codes for necessary data processing and dose evaluation.

8.2.5 Software Validation

A software validation program needs to be initiated. The initial objectives of the program should be to (1) determine the accuracy of the selected codes and data libraries in comparison to the existing measured data (see Sect. 6.1) applicable to shielded spent fuel, and (2) identify and/or design integral or benchmark experiments that are needed to supplement the existing experimental data in order to show compliance with licensing and/or quality assurance requirements.

8.2.6 Establish Centralized Expertise

Deficiencies in the quality assurance and maintenance programs available for the selected software has been noted in the conclusions. It is recommended that the DOE Waste Management Program establish a "shielding support center" to meet the needs of the various projects within the program. The functions of the support center would include

1. serving as the technical contact for the DOE various waste management projects to answer questions or provide guidance regarding software capabilities, appropriate use (input, modeling assumptions, etc.) of the software, accuracy of results, and the numerical and/or theoretical models employed in the software;
2. maintaining and documenting the validated codes and data libraries under quality assurance guidelines that meet the requirements of ANSI/ASME NQA-1 and NUREG-0856; and
3. serving as the technical interface between the projects and developers for providing/obtaining enhancements that may be required to meet specific project needs.

To provide consultation in a complete, efficient, and readily available fashion requires that the center be established at an institute with recognized capabilities in software development and analysis for shielding applications.

8.2.7 Identify Applications

To assist software developers and shielding analysts involved in the above recommendations, it would be beneficial for the DOE waste management projects to better identify the applications where accurate shielding analyses are required to reduce project cost and/or comply with NRC regulations. This activity will allow shielding analysis experts involved in the development and validation exercises to concentrate their efforts on the most important application areas. This identification process could also enable an estimate to be made of the cost/benefit of improved calculational accuracy on design concepts.

Appendix A

SUMMARIES OF SELECT CODES USEFUL FOR RADIATION DOSE EVALUATIONS

ISOSHLD/RIBD

CODE IDENTIFICATION

ISOSHLD (II and III)/RIBD-II developed by:
Battelle Memorial Institute
Computer Science Corporation
General Electric Company
Pacific Northwest Laboratory
Richland, Washington

SUMMARY

ISOSHLD calculates the decay gamma-ray dose at the exterior of a shielded radiation source. ISOSHLD II has the added capability of solving shielding problems for which bremsstrahlung may contribute totally or partially to the source of radiation. ISOSHLD III contains a revised photon probability library for use with ISOSHLD, but does not calculate bremsstrahlung. It was assembled in 1967 from the most current data. The source zone may be one of a number of common geometric shapes. The source strength is also calculated if it originates from fission products produced under known irradiation conditions. RIBD-II performs a reactor point depletion reactor fuel analysis, producing photon source spectra, including bremsstrahlung (in ISOSHLD II) at specified cooling times.

MAIN PREDICTED VARIABLE

Dose rate at the exterior of a shielded radiation source.

OTHER PREDICTED VARIABLES

Energy flux at a dose point.
Group energy production photon rates.
Photon decay spectra in ISOSHLD I or III.
Photon decay and bremsstrahlung spectra in ISOSHLD II.

EQUATION SOLVED

Point kernel integration of the photon dose rate is performed numerically, or analytically when possible, for all points within the isotropic source S_o.

$$D_{tot} = \int_E \int_V \frac{K(E)S_o(E,V)B(E,b_1)e^{-b_1}}{4\pi\ \rho^2(V)}\ dVdE\ ,$$

where

$$b_1 = \sum_{i=1}^{N} \mu_i t_i \quad ;$$

D = photon dose rate at detector, R/h;
S_0 = emission rate of gamma rays, photon/s;
t_i = slant distance through the i^{th} shield, cm;
ρ = distance from source to dose point, cm;
B = buildup factor;
μ_i = linear absorption coefficient of the i^{th} shield, cm^{-1};
N = number of shields;
K = conversion of gamma-ray flux to dose rate.

FEATURES AND LIMITATIONS

5 source cooling times
500 radioactive isotopes
5 shield regions including source regions
25 energy groups
20 materials in each shield region
11 source geometries available
Bremsstrahlung and decay photon source spectra for only fission products is produced.
The actinide transmutation products are not computed (at least as documented).
Method does not include photon nor neutron spectra produced in spontaneous fission and (α,n) reactions of actinides.

ANALYTICAL METHOD - NUMERICAL ALGORITHM

The standard point attenuation kernel is numerically integrated over the volume for 25 source energy groups. Buildup is considered a characteristic of the last shield region (or a specific different region) but dependent on the total number of mean free paths from the dose point. Buildup factors are obtained by interpolation on effective atomic number from a table of point isotopic buildup factor data. Mixed mass attenuation coefficients are obtained from a library of basic data using code input material density specifications.

The source strength may be specified as (1) the emission from a selection of fission products irradiated under specific conditions, (2) the curies of particular fission and/or activation products, or (3) the number of photons per second of energy E specified by input. If the source originates in a combination of fission products and their daughters, these are calculated by a fission product inventory procedure which runs through transmutation calculations for each product or daughter (subroutine RIBD) ISOSHLD II also calculates shielded dose rates from bremsstrahlung sources. A routine BREMRAD (RSIC CCC-31) assesses the bremsstrahlung source spectra from the β decay properties of the isotopes of interest. Bremsstrahlung photons per group for 25 energy groups (9 groups below 0.1 MeV have been added) are obtained by interpolation from tables of resolved spectra. This spectral mesh, for internal and external bremsstrahlung, is tabulated as a function of the following parameters: β-emitting and stopping nuclides with atomic numbers of 10, 30, 50, 70, 90; ratio of photon energy to β end point energy for 25 intervals from 0.00375 to 1.0; β end point energies at the intervals 0.1 .2, 0.5, 1, 2, and 4 MeV.

Buildup factors for photon energies less than 0.1 MeV are interpolated from a table which contains data for 5 values of initial photon energy in the range 0.01 to 0.2 MeV, seven values of shield thickness in the range 4 to 20 mfp and 6 atomic numbers in the range 13 to 92. The entire shielding problem is solved for most types of isotope shielding applications without reference to a shielding handbook for basic data.

CURRENT USES:

Isotope shielding analysis and total decay heat rates at specified cooling times are computed.

PROGRAM INTERFACE:

The RIBD-II code is the routine RIBD called by ISOSHLD codes.
RIBD-II is also interfaced with the RACER, RIBD-IRT, and COMRADX4 codes.

LANGUAGE:

FORTRAN IV

INPUT DATA LIBRARY:

- RIBD isotope library used by subroutine RIBD to calculate fission product inventory. It contains 450 fission products and daughters. Fission product libraries have been produced for both a generic thermal reactor and a generic fast reactor. Cross sections for actinide, transmutation product interactions are probably omitted (RSIC ISOSHLD package includes no documentation on these data).
- A gamma photon abundance library which contains these 450 fission products plus 48 activation products, the energy yield and abundance of all principal gamma rays emitted by each isotope during decay is used to calculate the number of photons of various energies produced by an array of radioactive isotopes.
- Mixed mass attenuation coefficients. This library enables ISOSHLD to perform the attenuation calculation at the specified photon energies if only photon generation rates and photon energies are known.
- Buildup factor library contains the buildup factor coefficients for 16 photon energies and a maximum of eight materials.

The data are included in separate card image files for ISOSHLD II and III.
The BREMRAD code package can be used to calculate the bremsstrahlung spectrum mesh for ISOSHLD II.

FORM OF OUTPUT:

Print or list format without any graphic output.

COMPUTERS AND OPERATING SYSTEM USED:

Originally designed for UNIVAC 1107 and modified for IBM 360/370 (ISOSHLD II) and UNIVAC 1108 (ISOSHLD III). A version of ISOSHLD is also available for the IBM PC.

CORE AND DISK REQUIREMENTS:

220K bytes core size and four data sets of about 1000 to 2000 card images each.

TYPICAL RUNNING TIME:

Dose from cylindrical volume source - 20 integration increments in each direction, fission product inventory calculations with 5 decay times, 25 energy groups, 4 shield layers, 5 materials homogenized into each shield layer and the source volume: 6 minutes UNIVAC 1107 (most other source geometries require less computation time).

DOCUMENTATION:

1. R. L. Engle, J. Greenborg, and M. M. Hendrickson, *ISOSHLD - A Computer Code for General Purpose Isotope Shielding Analysis*, BNWL-236, Brookhaven National Laboratory, 1966, and Supplement of 1967.
2. G. L. Simmons, J. J. Regimbal, J. Greenborg, E. L. Kelly, Jr., and H. H. Van Tuyl, *ISOSHLD-II: Code Revision to Include Calculations of Dose Rate from Shielded Bremsstrahlung Sources*, BNWL-236 Sup. 1, Brookhaven National Laboratory, 1967.
3. C. A. Mansius, *A Revised Photon Probability Library for Use with ISOSHLD III*, BNWL-236 Sup. 2, Brookhaven National Laboratory, 1969.
4. R. O. Gumprecht, *Mathematical Basis of Computer Code RIBD*, DUN-4136, Douglas-United Nuclear, 1968.
5. J. L. Rash, *Use of Computer Code RIBD for Fission Product Analysis*, GE-HAPO RL-NRD-610, General Electric Company, 1965.
6. "BREMRAD: External and Internal Bremsstrahlung Calculation Code," CCC-31, available from Radiation Shielding Information Center at Oak Ridge National Laboratory.
7. J. Greenborg, "ISOSHLD: Evolution, Experience, and Benchmarking," *Proceedings of the Topical Conference on Theory and Practices in Radiation Protection and Shielding*, April 22-24, 1987, Knoxville, Tennessee, ISBN: 0-89448-132-0, Vol. 1, April 1987.

PROGRAM AVAILABILITY

The ISOSHLD/RIBD codes and libraries are packaged by RSIC as CCC-79. Requests for ISOSHLD codes and libraries can be mailed to:

Radiation Shielding Information Center
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 37831

or telephoned to:

615/574-6176 or to FTS 624-6176.

A for-sale version of ISOSHLD designed to be user friendly (menu-driven) is available from

Grove Engineering, Inc.
P. O. Box 720
Washington Grove, MD 20880
(301) 258-2727

QAD-CGGP

CODE IDENTIFICATION:

QAD-CGGP
The original QAD was developed at Los Alamos National Laboratory, Los Alamos, NM.
This version based on CCC-307/QAD-CG contributed by Bechtel Power Corporation, Gaithersburg, MD. Update by:
Japan Atomic Energy Research Institute
Tokyo Institute of Technology
Original Japanese version updated to provide double precision combinatorial geometry of CCC-203/MORSE-CG by Oak Ridge National Laboratory.

SUMMARY:

QAD is a point kernel code designed to calculate fast neutron and gamma-ray penetration of various shield configurations. Estimates are provided of the uncollided gamma-ray flux, dose rate, and energy deposition at specified detector points. The fast neutron dose is also provided via a modified Albert-Welton kernel. The point kernel method is a very fast and reliable radiation calculational method when it is applied to a system to which its theoretical limitations apply.

MAIN PREDICTED VARIABLE:

Gamma-ray dose at a point outside a shield.

OTHER PREDICTED VARIABLES:

Energy deposition
Neutron doses

EQUATION SOLVED:

Point kernel integration of the photon dose rate is performed numerically, or analytically when possible, for all points within the isotropic source S_o,

$$D_{tot} = \int_E \int_V \frac{K(E)S_o(E,V)B(E,b_1)e^{-b_i}}{4\pi\ \rho^2(V)}\ dVdE\ ,$$

where

$b_i = \sum_{i=1}^{N} \mu_i t_i$;

D = photon dose rate at detector, R/h;
S_o = emission rate of gamma rays, photon/s;
t_i = slant distance through the i^{th} shield, cm;
ρ = distance from source to dose point, cm;
B = buildup factor;
μ_i = linear absorption coefficient of the i^{th} shield, cm^{-1};
N = number of shields;
K = conversion of gamma-ray flux to dose rate.

FEATURES AND LIMITATIONS:

1. QAD-CGGP contains the same double-precision combinatorial geometry routines from CCC-203/MORSE-CG. Thus, the CG input is interchangeable and any geometry model set up for QAD-CGGP can be used by MORSE-CG, MORSE-CGA, or MORSE-SGC. Geometric models are created with CG by considering unions, differences, and/or intersections of simple 3-D bodies such as spheres, cylinders, boxes, etc.
2. QAD-CGGP has new buildup factor data endorsed by the ANS-6.4.3 standards working group along with a new geometric progression (GP) fitting function that allows interpolation of the buildup factor data far more accurately than previous schemes. Significant improvements are seen for low- or very high-Z materials and low (<0.5 MeV) energies. Buildup factor data available for 22 materials for absorption and air exposure responses.
3. The neutron results from all QAD versions are highly unreliable.
4. Code is restricted to 100 x 100 x 100 x, y, z intervals for the source mesh and 30 gamma groups. Number of detectors is restricted by the machine memory available.

ANALYTIC METHOD - NUMERICAL ALGORITHM:

In the gamma-ray calculation, the point kernel method involves representing the gamma-ray source by a number of point isotropic sources and computing the line-of-sight distance from each of these source points to the detector point. From the distance through the shielding regions and the characteristics of the shielding materials, the geometric attenuation and material attenuation are calculated. The energy transferred along the line of sight is then calculated based on this attenuation and the appropriate buildup factor is applied to account for the scattered radiation. A modified Albert-Welton kernel or kernels obtained from the moments method solution of the Boltzmann equation are used in evaluating neutron penetration.

LANGUAGE:

FORTRAN 77

INPUT DATA:

The data are input in fixed format as indicated in the user manual. All material attenuation and buildup data is available in the data library which is read during execution.

OUTPUT:

Uncollided flux, dose rate, flux and dose buildup, and energy deposition at specified detector points. Print or list output with no available graphics.

TYPICAL RUNNING TIME:

The sample problem took 30 CPU seconds on the IBM 3033, including compiling and linking. Execution required more than an hour on the IBM PC and 18 seconds on the CRAY XMP.

COMPUTER HARDWARE REQUIREMENTS:

The code has been run at ORNL on the IBM 3033, the CRAY XMP, the Data General Eclipse MV/4000, and the IBM PC; it requires 1244K bytes of storage on an IBM 3033 to compile and 308K bytes to execute the sample problem. An 8087 co-processor is required for the IBM PC version.

COMPUTER SOFTWARE REQUIREMENTS:

The code was tested using FORTRAN 77 compilers running under IBM's MVS operating system and Data General's AOS/VS operating system. The IBM PC version was compiled by the IBM Professional compiler (Version 1.00) and runs under PC DOS. Under the CRAY CTSS operating system, the CFT111E compiler was used which referenced CFTLIB in the loading. All references to REAL*4 and REAL*8 were removed in the CRAY version.

PROGRAM AVAILABILITY:

QAD-CGGP is packaged by RSIC as CCC-493 and available by sending requests to

Radiation Shielding Information Center
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 37831

or telephoned to:

615/574-6176 or to FTS 624-6176.

Information on other versions of QAD are available from RSIC upon request.

ANISN

CODE IDENTIFICATION:

ANISN was originally developed at Oak Ridge National Laboratory as a successor to the DTF-II code developed at Atomics International.

CONTRIBUTORS:

Updated and various versions (compatible hardware and minor software changes) have been contributed by:

Oak Ridge National Laboratory, Oak Ridge, Tennessee Wehrwissenschaftliche Dienststelle, Federal Republic of Germany University of California, Berkeley, California Nuclear Assurance Corporation, Atlanta, Georgia Electrowatt Engineering Services, Ltd., London, England Goodyear Aerospace Corp., Litchfield Park, Arizona Goodyear Atomic Corp., Piketon, Ohio	ANISN-ORNL, CCC-254
Westinghouse Astronuclear Laboratory, Pittsburgh, Pennsylvania NASA Marshall Space Flight Center, Huntsville, Alabama Kent State University, Kent, Ohio	ANISN-W, CCC-255
EG&G Idaho, Inc., Idaho Falls, Idaho	ANISN/PC, CCC-514

SUMMARY:

ANISN is a one-dimensional discrete ordinates coupled neutron gamma-ray radiation transport code for slab. sphere, or cylindrical geometries. It is one of the most widely used transport codes and has been applied to a variety of fixed-source, multiplying system, and criticality problems. Criticality search may be performed on any one of several parameters. In addition to providing spatial, energy, and angular dependent fluxes, ANISN also provides energy group and spatial averaged cross sections.

MAIN PREDICTED VARIABLE:

Fluxes as a function of spatial mesh, energy, group, and angular interval.

OTHER PREDICTED VARIABLES:

Group and spatial-averaged cross sections.

Responses and activities, including those for materials not actually appearing in the system (e.g., detector materials).

k_{eff} for criticality calculations.

EQUATION SOLVED:

The one-dimensional discrete spatial, energy and angular-dependent Boltzmann transport equation, in either the forward or adjoint mode (see Sect. 3.1).

FEATURES AND LIMITATIONS:

ANISN was designed to solve deep-penetration problems in which angle-dependent spectra are calculated in detail. The principal feature that makes it suitable for such problems is the use of a programming technique with optional data storage configurations which allows execution of small, intermediate, and extremely large problems. The problem size is limited only by machine size. ANISN also includes a technique for handling general anisotropic scattering, point-wise convergence criteria, and alternate step-function difference equations

that effectively remove the oscillating flux distributions sometimes found in discrete ordinates solutions. External force fields and nonlinear effects cannot be treated.

BOUNDARY CONDITIONS:

Vacuum, periodic, white, or albedo boundary conditions allowed for each of the two "outside" boundaries.

ANALYTIC METHOD - NUMERICAL ALGORITHM:

The transport equation is discretized into a set of coupled difference equations which are then solved by iteration, starting from an initial flux guess, until an input convergence criterion is reached. The diffusion term is written in spherical, infinite slab, or infinite cylindrical coordinates. The inscattering integral is approximated by a summation. Anisotropic scattering is included in a Legendre polynomial expansion of the multigroup cross-section data.

CONVERGENCE CRITERIA:

The angular integrated mesh-point flux is tested, for each group, after each integration against an input convergence parameter. The maximum flux difference determines if another iteration is required. A less-stringent option tests the spatially integrated flux. For criticality or upscatter problems the k_{eff} or upscatter ratio is tested at the end of each outer iteration against another input convergence parameter.

PROGRAM INTERFACE AND AUXILIARY ROUTINES:

The angular flux tape generated by ANISN can be saved for input to the XSDOSE code to evaluate doses at points exterior to the ANISN system boundary. Also, a number of auxiliary routines are avilable with most of the RSIC code packages to plot output data, generate discrete ordinates quadrature coefficient data, and perform other minor tasks.

LANGUAGE:

FORTRAN IV
FORTRAN 77

INPUT DATA LIBRARY:

Cross-section data must be in the ANISN format (from the AXMIX code) or GIP format from the GIP code. All input is in free-form FIDO format. AXMIX and GIP available from RSIC as peripheral shielding routines PSR-075.

OUTPUT:

All spatial mesh, group, and angular dependent fluxes are available as printed output or they may be stored on tape or disk. Angular intergrated fluxes and responses are also listed as well as the convergence and balance table information. Graphical output can be obtained by post-processing the stored data sets via the DOGS system available from RSIC as PSR-155..

COMPUTER REQUIREMENTS:

ANISN-ORNL is operable on the IBM 360/370, UNIVAC-1108, CDC 6600/7600, TR440, SIEMENS 7541, PRIME, or DEC-10, DEC-20 computers. ANISN-W is operable on the CDC-6600 and IBM PC.

The ANISN/PC version requires the 8087 co-processor, a 10-mb fixed disk, and about 640K memory. Compilation requires the IBM PC Professional FORTRAN compiler.

Memory must be about 50,000 words for a reasonable problem. Sequential scratch storage is required.

TYPICAL RUNNING TIME:

Problem dependent—however, most applications have execution times on the order of a few minutes on IBM mainframe computers.

DOCUMENTATION:

1. W. W. Engle, Jr., *ANISN, A One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering,* K-1693, Union Carbide Corp., Nuclear Division, Oak Ridge Gaseous Diffusion Plant, March 1967.
2. W. W. Engle, M. A. Boling, and B. W. Colston, *DTF-II, A One-Dimensional, Multigroup Neutron Transport Program,* NAA-SR-10951, Atomics International, March 1966.
3. R. K. Disney et al., *ANISN-W, A One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering,* WANL-TME-2778, Westinghouse Astronuclear, February 1977.
4. D. T. Ingersoll and C. O. Slater, *DOGS — A Collection of Graphics for Support of Discrete Ordinates Codes,* ORNL/TM-7188, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., March 1980.
5. D. Kent Parsons, *ANISN/PC Manual,* EGG-2500, EG&G Idaho, Inc., April 1987.

PROGRAM AVAILABILITY:

ANISN-ORNL is available as CCC-254 from RSIC. ANISN-W is available as CCC-255 and ANISN/PC is available as CCC-514. Requests for the code packages can be made in writing to:

Radiation Shielding Information Center
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 37831

or telephoned to:

615/574-6176 or to FTS 624-6176.

DOT IV

CODE IDENTIFICATION:

DOT IV developed by:
Oak Ridge National Laboratory, Oak Ridge, TN

The latest version is DOT 4.3.

SUMMARY:

DOT is a two-dimensional discrete ordinates coupled neutron gamma-ray radiation transport code. Fixed sources and sources resulting from particle interaction with the medium are allowed. The principal application is to the deep-penetration transport of neutrons and photons. Criticality (k-type and search) problems can also be solved. Since many physical systems associated with radiation can be approximated fairly accurately with a two-dimensional analysis--cylindrical reactors or spent-fuel casks, for example--DOT provides a rigorous analytic solution method. A particular advantage with the code is the ability to obtain flux (or response) contour plots in the system geometry as an aid for analyzing streaming paths or other geometric anomolies. Typical calculations require considerable computer resources in both running time and memory.

MAIN PREDICTED VARIABLES:

Spatial, energy, and angular dependent flux

OTHER PREDICTED VARIABLES:

Spatial and energy-dependent scalar fluxes
Spatial responses
k_{eff} for criticality calculations
Fission source rates

EQUATION SOLVED:

The two-dimensional discrete spatial, energy, and angular-dependent Boltzmann transport equation in either the forward or adjoint mode (see Sect. 3.1).

BOUNDARY CONDITIONS:

Vacuum, periodic, white, or albedo conditions allowed on all boundaries. An incoming angular surface source can also be specified on a boundary.

FEATURES AND LIMITATIONS:

1. Intrinsic to the multidimensional discrete ordinates method is the problem of ray effects caused by localized sources being transported through void or low-scattering media.
2. External force fields or nonlinear effects cannot be treated.
3. Flexible dimensioning is used throughout, so that no restrictions are imposed on individual problem parameters.
4. Certain options, especially diffusion theory, are not compatible with variable mesh and quadrature problems.
5. Output data sets can be used to provide an accurate restart of a previous problem or to deliver information to other codes.

ANALYTIC METHOD - NUMERICAL ALGORITHM:

The transport equation is discretized into a set of coupled difference equations which are then solved by iteration, starting from an initial flux guess, until an input convergence criterion is reached. The diffusion term is written in spherical, infinite slab, or infinite cylindrical coordinates. The inscattering integral is approximated by a summation. Anisotropic scattering is included in a Legendre polynomial expansion of the multigroup cross-section data.

Several techniques are available to remove the effects of negative fluxes caused by the finite difference approximation, and of negative scattering sources due to truncation of the cross-section expansion. The space mesh can be described such that the number of first-dimension (i) intervals varies with the second dimension (j). The number of discrete directions can vary across the space mesh and with energy. Direction sets can be biased, with discrete directions concentrated such as to give fine detail to streaming phenomena.

CONVERGENCE CRITERIA:

The angular integrated mesh-point flux is tested, for each group, after each iteration against an input convergence parameter. The maximum flux difference determines if another iteration is required. A less stringent option tests the spatially integrated flux. For criticality or upscatter problems the k_{eff} or upscatter ratio is tested at the end of each outer iteration against another input convergence parameter.

PROGRAM INTERFACE AND AUXILIARY ROUTINES:

A host of auxiliary programs has been developed for use with DOT IV, most of which are available within the Discrete Ordinates System (DOS):

DOS -	a driver program which coordinates problem execution (IBM only)
BNDRYS -	selects boundary fluxes for subsequent use as inner boundary sources
GIP -	prepares cross-section input from card or tape input
GRTUNCL -	prepares first-collision source due to a point source in RZ geometry (on or off axis)
RTFLUM -	edits flux files and converts between various file formats
DOMINO II (PSR-162) -	couples DOT IV to the multigroup Monte Carlo MORSE-CG (CCC-203) or MORSE-CGA (CCC-474) codes
DOGS (PSR-155) -	provides graphical display of DOT IV output

INPUT DATA LIBRARY:

Cross-section data must be in the ANISN format (from the AXMIX code) or GIP format from the GIP code. All input is in free-form FIDO format. AXMIX and GIP are available from RSIC as PSR-075.

OUTPUT:

The spatial and energy-dependent scalar fluxes and responses are printed out at boundaries as specified by input parameter. The angular flux moments may be retained on tape or disk and used to compute scalar fluxes at other boundaries through the use of the restart option. Spatial and group-dependent results are also available in plotted form as flux contours in the system geometry.

LANGUAGE:

FORTRAN IV

TYPICAL RUNNING TIME:

Running time is roughly proportional to:

Flux work units (FWU) = number of space mesh cells times number of directions times number of energy groups times number of iterations per group.

Depending on the options chosen, a rate of one million FWU per minute on the IBM 370/3033 computer is typical. Thus, a very large problem with 5,000 space cells, 48 directions, 50 energy groups, 10 iterations per group, and P_3 scattering would require roughly 1 to 1.5 h of CPU time. Execution on CDC or CRAY computers is usually faster.

COMPUTER HARDWARE REQUIREMENTS:

DOT 4.3 is operable on the IBM 3033, CDC, UNIVAC, or CRAY computers. DOT 4 was designed to be applicable to most sophisticated computers which support direct (random) access disk storage or the equivalent. It has special provisions for efficient use of a large slow memory from which data are moved to fast memory in strings. Certain directly addressed arrays of low usage can also be kept in slow memory, and slow memory is also used as a buffer between fast memory and certain disk files.

Memory must be approximately 50,000 words for small problems. The requirement expands with problem size. External data storage must be provided for nine scratch files, of which five must be direct (random) access. User-supplied input and output data files must be supplied on sequential-access devices (i.e., tapes or the equivalent).

DOCUMENTATION:

1. W. A. Rhoades and R. L. Childs, *An Updated Version of the DOT 4 One- and Two-Dimensional Neutron/Photon Transport Code*, ORNL-5851, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab. (April 1982). Extensive bibliography on DOT IV development work in this document.
2. W. A. Rhoades and M. B. Emmett, *DOS: The Discrete Ordinates System*, ORNL/TM-8362, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., September 1982.

PROGRAM AVAILABILITY:

DOT 4.3 is packaged by RSIC as CCC-429. The package can be requested by writing to:

Radiation Shielding Information Center
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 37831

or telephoned to:

615/574-6176 or to FTS 624-6176.

ONEDANT and TWODANT

CODE IDENTIFICATION:

ONEDANT and TWODANT developed by:
Los Alamos National Laboratory, Los Alamos, New Mexico
Conversion to IBM system by:
Argonne National Laboratory, Argonne, Illinois

SUMMARY:

ONEDANT solves the one-dimensional multigroup transport equation in plane, cylindrical, spherical, and two-angle plane geometries. TWODANT solves the two-dimensional, time-independent, multigroup discrete ordinates form of the Boltzmann transport equation in (x,y), (r,z), (r,θ) geometries. Both regular and adjoint inhomogeneous (fixed source) and homogeneous (k-effective) problems subject to vacuum, reflective, periodic, or white boundary conditions are solved. General anisotropic scattering is allowed and anisotropic inhomogeneous sources are permitted. ONEDANT and TWODANT are modularly structured in a form that separates the input and the output (edit function) from the main calculational (or solver) section. The TWODANT code is simply the ONEDANT package with the one-dimensional SOLVER module replaced with a two-dimensional version.

MAIN PREDICTED VARIABLES:

Spatial, energy, and angular dependent flux

OTHER PREDICTED VARIABLES:

Spatial and energy-dependent scalar fluxes
Spatial responses
k_{eff} for criticality calculations
Fission source rates

EQUATION SOLVED:

ONEDANT and TWODANT numerically solve, respectively, the one- and two-dimensional, multigroup form of neutral particle, steady-state form of the Boltzmann transport equation in either the forward or adjoint modes (see Sect. 3.1).

FEATURES AND LIMITATIONS:

1. Intrinsic to the multidimensional discrete ordinates method is the problem of ray effects caused by localized sources being transported through void or low-scattering media.
2. External force fields or nonlinear effects cannot be treated.
3. As modular systems, ONEDANT and TWODANT are quite flexible with regard to input and edit options. The INPUT and EDIT modules are common to both codes and interface with the separate SOLVER modules of both ONEDANT and TWODANT.
4. The code is variably dimensioned with a flexible, sophisticated data management and transfer capability. The code is designed for a three-level hierarchy of data storage. A small, fast core central memory (SCM), a fast access peripheral large core memory (LCM), and random-access peripheral storage. (For computing systems based on a two-level hierarchy of data storage, a large fast core and random access peripheral storage--a portion of fast core is designated as a simulated LCM to mimic the three-level hierarchy). Random access storage is used only if LCM (or simulated LCM) storage requirements are exceeded. Normally, an SCM of about 25,000 words of storage and an LCM (or simulated LCM) of a few hundred thousand words or less storage are sufficient to eliminate the need for using random access storage.

ANALYTICAL METHOD - NUMERICAL ALGORITHM:

The discrete-ordinates approximation is used for treating the angular variation of the particle distribution. The diamond-difference scheme is used for phase-space discretization. The TWODANT code solves the adjoint transport equation, by transposing (in energy) the matrices of scattering cross sections (conversion of a downscatter problem to an upscattering problem) and inverting the group order of the problem. Negative fluxes are eliminated by a local set to zero and correct algorithm. A diffusion synthetic acceleration method is used to speed the convergence of the iterations involved in the transport equation solution. The diffusion solver uses the multigrid method.

CONVERGENCE CRITERIA:

The ONEDANT and TWODANT solver modules employ the diffusion synthetic method to accelerate the iterative procedure used in solving the transport equation. Both inner iterations (concerned with the convergence of the pointwise scalar fluxes in each group for a given source distribution) and outer iterations (concerned with the convergence of the eigenvalue, the fission source distribution and the energy-group upscatter source if any or all are present) are monitored.

LANGUAGE:

FORTRAN IV CDC 7600 UNIVAC
FORTRAN IV - Assembler IBM 370/195 and IBM 3033
FORTRAN 77 VAX and CRAY

INPUT DATA LIBRARY:

The general procedure for generating the macroscopic cross sections appropriate to each zone in the problem is to begin with a basic library containing multigroup cross-section data for isotopes. Either of the standard interface files ISOTXS or GRUPXS can be used for providing the basic, multigroup cross section for isotopes. ISOTXS is an isotope-ordered binary file while GRUPXS is a group-ordered binary file.

FORM OF OUTPUT:

Print or list format without any graphic output. The EDIT module performs edit operations using multigroup, pointwise scalar fluxes generated in a previous execution of the SOLVER module or, perhaps, in some other neutronics code.

OPERATING SYSTEM:

CDC 7000, UNIVAC, IBM 370/195, IBM 3033, VAX, CRAY

CORE AND DISK REQUIREMENTS:

Input/output units and up to 14 interface units are required. The number of interface units needed is problem-dependent. Typically, 10 such units are used. For CDC-7600 computers, a 50,000-word small core (SCM) and large core (LCM) memory are required. For computers with only a single fast core, the fast core size must be sufficiently large to permit partitioning into an SCM and simulated LCM. Random-access auxiliary storage may occasionally be required if LCM (or simulated LCM) storage is insufficient for the problem being executed.

RUNNING TIME:

Running time is directly related to problem size and to central processor and data transfer speed. On the CRAY 1, a four-group, adjoint calculation of the eigenvalue of an R-Z model of the Fast Test Reactor (FTR) took 15 s. The calculation used transport-corrected P_0 cross sections, an S_4 angular quadrature, and a 31 by 68 spatial mesh.

DOCUMENTATION:

1. R. D. O'Dell, "Standard Interface Files and Procedures for Reactor Physics Codes, Version IV," LA-6941-MS, Los Alamos Scientific Laboratory, September 1977.
2. R. D. O'Dell, F. W. Brinkley, and D. R. Marr, "User's Manual for ONEDANT: A Code Package for One-Dimensional, Diffusion-Accelerated, Neutral-Particle Transport," LA-9184-M, Los Alamos National Laboratory, February 1982.
3. R. E. Alcouffe et al., *User's Guide for TWODANT: A Code Package for Two-Dimensional, Diffusion-Accelerated, Neutral-Particle Transport*, LA-10049-M, Rev. 1, Los Alamos National Laboratory, October 1984.
4. R. E. Alcouffe, "Diffusion Synthetic Acceleration Methods for the Diamond-Difference Discrete-Ordinates Equations," *Nucl. Sci. Eng.* **64**, 344 (1977).
5. R. E. Alcouffe, "The Multigrid Method for Solving the Two-Dimensional Multigroup Diffusion Equation," Proc. Am. Nucl. Soc. Top. Meeting on Advances in Reactor Computation: Salt Lake City, Utah, March 28-31, 1983, Vol. 1, pp. 340-351.

XSDOSE

CODE IDENTIFICATION:

XSDOSE - Oak Ridge National Laboratory, Oak Ridge, Tennessee

SUMMARY:

XSDOSE computes the n/γ flux and the resulting dose at various points outside a finite cylinder or sphere. It may also be used to compute the flux and/or dose at various points due to a finite rectangular surface source or a circular disc. It assumes the outgoing angular flux distribution on the rectangle, cylinder, sphere, or disc is independent of position and that the surrounding media is a void. The numerical technique is suitable for points on, close to, or far from the source. XSDOSE is typically used in conjunction with a fixed source XSDRNPM (or ANISN) calculation for an infinite slab, cylinder, or sphere.

MAIN PREDICTED VARIABLE:

Neutron and photon dose at various points on or outside a sphere, cylinder, slab, or disc.

OTHER PREDICTED VARIABLE:

Neutron and photon scalar flux at various points on or outside a sphere, cylinder, slab, or disc.

EQUATIONS SOLVED:

To determine the scalar flux at a point some distance from the source, XSDOSE numerically integrates what appears to be the angular flux at that point:

$$\phi_D = \int \psi(\Omega, r_D) d\Omega \ .$$

BOUNDARY CONDITIONS:

It assumes that the outgoing angular flux distribution on the rectangle, cylinder, sphere, or disc is independent of position and that the surrounding media is a void.

ANALYTICAL METHOD:

XSDOSE is typically used in conjunction with a 1-D transport calculation (usually a fixed-source XSDRNPM calculation for an infinite slab, cylinder, or sphere). It reads the angular flux produced by the 1-D calculation (XSDRNPM or ANISN) and performs the required numerical integration over a finite surface to obtain the actual scalar flux at those points specified by the user. By integrating the source only over the desired surface, one can properly account for the finite dimensions of the system without the use of an isotopic buckling connection. Using a direct line of straight integration of the angular flux over the surface precludes the possibility of ray effects and other anomolies typical of discrete ordinates methods in curvilinear geometries when the angular quadrature or spatial mesh is too coarse.

FEATURES AND LIMITATIONS:

1. Unlike earlier point-kernel codes that divided the desired surface into many near-rectangular finite elements, the numerical integration technique used in XSDOSE integrates the angular flux along circular line contours described on the surface in a fashion consistent with the angular quadrature used in the discrete ordinates calculation. When the user is free to input the number of contours used in the numerical integration, the scheme used is very insensitive to the number of intervals used and/or the relative location of the detector point to the surface.

2. The surface source is restricted to a sphere, a circular disc, a finite cylinder, or a finite rectangle.

3. Free-form input format.

RELATED PROGRAMS:

XSDRNPM is a one-dimensional discrete ordinates code which may be used to determine the neutron photon flux distribution within (and on the surface of) the given structure. It produces the angular flux file for XSDOSE. Alternately, the ANISN code may be used for that purpoee. Interface and input automated in SCALE shielding sequences SAS1 and SAS2.

LANGUAGE:

FORTRAN IV and FORTRAN 77 versions are available.

FUTURE DEVELOPMENT:

Extension of the code to interface with 2-D discrete ordinates codes would be useful.

INPUT DATA LIBRARY:

The code does not need cross-section data. Only the flux-to-dose conversion factors must be specified. (Straker-Morrison or ANSI Standard flux to dose conversion factors for gamma rays and neutrons.)

XSDOSE is designated to read any number of multigroup response functions off an AMPX master library or an AMPX working library in order to compute the flux and other energy-dependent response functions at various points of interest. This library may be a neutron cross-section library, a gamma cross-section library, or a fully coupled n-γ library.

FORM OF OUTPUT:

Print or list format with no graphic output.

OPERATING SYSTEM:

XSDOSE is operational on all IBM computers. Few, if any, changes would be required for UNIVAC, CDC, or CRAY machines.

CORE REQUIREMENTS:

The present release is for an IBM machine with a minimum of 50K bytes of storage.

TYPICAL RUNNING TIME:

On the IBM 360/91 and IBM 3033, it requires 1 second of CPU time for each detector point specified by the user.

DOCUMENTATION:

1. J. A. Bucholz, "XSDOSE: A Module for Calculating Fluxes and Dose Rates at Points Outside a Shield," as contained in Section F4 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200 (ORNL/NUREG/CSD-2), Vols. I, II, and III, April 1982.

2. N. M. Greene and L. M. Petrie, "XSDRNPM: A One-Dimensional Discrete Ordinates Transport Analysis Code," as contained in Section F3 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200 (ORNL/NUREG/CSD-2), Vols. I, II, and III, April 1982.

3. W. W. Engle, Jr., *ANISN: A One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering*, K-1693, March 1967.

PROGRAM AVAILABILITY:

XSDOSE is available from RSIC as part of the SCALE computer code package (CCC-466). The FORTRAN 77 version is packaged as CCC-475. Requests can be made by writing to

Radiation Shielding Information Center
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 37831

or telephoned to:

615/574-6176 or to FTS 624-6176.

XSDRNPM

CODE IDENTIFICATION:

XSDRNPM developed by:
Oak Ridge National Laboratory, Oak Ridge, Tennessee

SUMMARY:

This is a highly evolved one-dimensional discrete ordinates transport program which has a wide variety of features. Based on the ANISN program, XSDRNPM-S is capable of performing neutron or coupled neutron-gamma calculations with the scattering anisotropy represented to any arbitrary order. The primary emphasis in the solution algorithm is on the accurate calculation of detailed spectral variations. However, with sufficient angular quadrature and spatial mesh specifications, highly precise solutions to one-dimensional transport problems are obtained. The code is used for fixed source problems, evaluation of k-effective, and spatial or spectral weighting of cross sections. Also, a criticality search can be performed on any one of several parameters.

MAIN PREDICTED VARIABLES:

Spatial, angular, and energy-dependent fluxes.
Region and system reaction rate distribution.

OTHER PREDICTED VARIABLES:

Responses and activities, including those for materials not actually in the system (e.g., detector materials).
Spatial and energy averaged multigroup parameters.
Transport cross section for each nuclide.
k-effective for criticality calculations.

EQUATION SOLVED:

The one-dimensional discrete spatial, energy and angular-dependent Boltzmann transport equation, in either the forward or adjoint mode (see Sect. 3.1) Based on the calculated flux, spatial or energy-averaged cross sections are evaluated in a manner that conserves reaction rates.

FEATURES AND LIMITATIONS:

Same basic features and limitations of ANISN code. However, XSDRNPM has been designed to be easier to use, provide for double-precision flux arrays, and have flexible cross-section handling capabilities. Angular quadrature sets are generated automatically. Flexible cross-section weighting and formatting capabilities.

BOUNDARY CONDITIONS:

Vacuum, periodic, white, or albedo boundary conditions allowed for each of the two "outside" boundaries.

ANALYTIC METHOD - NUMERICAL ALGORITHM:

The transport equation is discretized into a set of coupled difference equations which are then solved by iteration, starting from an initial flux guess, until an input convergence criterion is reached. The diffusion term is written in spherical, infinite slab, or infinite cylindrical coordinates. The inscattering integral is approximated by a summation. Anisotropic scattering is included in a Legendre polynomial expansion of the multigroup cross-section data.

The finite-differencing in XSDRNPM-S is done with the weighted diamond-difference model with weighting parameters chosen on the basis of experience with the DOT IV code. Angular quadrature sets are calculated automatically for each of the one-dimensional slab, sphere, or cylinder geometries. Scattering expansion is treated to whatever order is provided in the cross-section sets.

CONVERGENCE CRITERIA:

Convergence in XSDRNPM-S is determined by tests on several quantities. The point values of the scalar fluxes must vary by less than a prescribed amount between outer iterations. Also, the ratio of source terms and scattering rates (up and down in energy) between outer iterations must converge. Provision is made for banding thermal groups and thereby accelerating upscatter convergence.

PROGRAM INTERFACE AND AUXILIARY ROUTINES:

XSDRNPM is interfaced to other modules of the AMPX and SCALE system via standard interface files that expedite use. It is used routinely in several shielding analysis modules of SCALE.

LANGUAGE:

FORTRAN IV and FORTRAN 77 versions are available.

INPUT DATA LIBRARY:

XSDRNPM accepts cross-section libraries in the AMPX working library format. All input is in the free-form FIDO format.

OUTPUT:

All spatial mesh, group, and angular dependent fluxes are available as printed output or they may be stored on tape or disk. Angular intergrated fluxes and responses are also listed as well as the convergence and balance table information. Graphical output can be obtained by post-processing the stored data sets via the DOGS system.

Cross-section output options to interface files are extensive. In addition to group collapsing, spatial weighting can be performed by cell, zone, region, or "inner cell" prescriptions. Either inscatter or outscatter formulations with an option of five current specifications may be used to obtain transport cross sections. Cross-section libraries can be output in ANISN (BCD or Binary), CCCC ISOTXS, or AMPX working formats.

COMPUTER:

IBM 360/370, IBM 3033, CDC 7600, CRAY. One direct access device is required.

TYPICAL RUNNING TIME:

Depends on angular quadrature set selected, mesh spacing, and number of energy groups. A typical calculation is on the order of a few minutes.

DOCUMENTATION:

1. N. M. Greene and L. M. Petrie, "XSDRNPM-S: A One-Dimensional Discrete-Ordinates Code for Transport Analysis," Vol. 2, Sect. F3 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, Vols. 1-3*, NUREG/CR-0200, U.S. Nuclear Regulatory Commission (originally issued July 1980, reissued January 1982, Revision 1 issued July 1982, Revision 2 issued June 1983, Revision 3 issued December 1984).

2. D. T. Ingersoll and C. O. Slater, *DOGS — A Collection of Graphics for Support of Discrete Ordinates Codes*, ORNL/TM-7188, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., March 1980.

PROGRAM AVAILABILITY:

XSDRNPM is available from RSIC as a part of the SCALE system (CCC-466). The FORTRAN 77 version is available as CCC-475. Requests should be made to RSIC by writing:

Radiation Shielding Information Center
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 37831

or telephoned to:

615/574-6176 or to FTS 624-6176.

MCNP

CODE IDENTIFICATION:

MCNP - developed at Los Alamos National Laboratory, Los Alamos, NM

SUMMARY:

MCNP is a continuous energy general-purpose coupled neutron gamma-ray radiation transport Monte Carlo code. The cross-section treatment reproduces the basic data to within 0.5% in most cases. Most problem types can be calculated from code input instructions alone, but the capability exists for user-supplied source and estimation routines. Many standard variance reduction options are available, and a relative new feature is the automatic generation of importance functions for splitting and Russian roulette parameters.

MAIN PREDICTED VARIABLE:

General phase-space-dependent flux and current.

OTHER PREDICTED VARIABLES:

Any response as defined by input data response functions.
k_{eff} for criticality calculations.

EQUATION SOLVED:

The forward time-dependent integral Boltzmann transport equation (see Sect. 3.1).

BOUNDARY CONDITIONS:

General - vacuum, specular reflections, periodic, albedo data, etc.

ANALYTIC METHOD - NUMERICAL ALGORITHM:

The Monte Carlo method is a machine-generated stochastic experiment in which the simulated particles (neutrons or photons) are followed from birth to death (absorption or leakage) using randomly selected variables from the natural or biased distributions of position, energy, direction, flight paths, collision mechanics, etc. Selection of biased variables requires adjustment of the mathematically simulated particle "weight," which remains unity for natural or unbiased calculations. The MCNP geometry is constructed from surfaces of first and second algebraic order (a torus capability also exists) which may be used directly or combined into spatial volumes which are then joined combinatorially. Although MCNP has many options for economizing both computer memory and computation time, state-of-the-art methods and capabilities exist at every level of the code.

CONVERGENCE CRITERIA:

Inherent in the Monte Carlo method is the statistical uncertainty of any calculated quantity due to the random nature of variable selection. For shielding calculations an uncertainty of 10% standard deviation is generally acceptable. The uncertainty is approximately inversely proportional to the square of the calculation time (i.e., to halve the uncertainty requires a factor of 4 increase in running time).

PROGRAM INTERFACE:

The RSIC distributed version of MCNP has no coupling capability with other codes.

LANGUAGE:

FORTRAN 77

INPUT DATA LIBRARY:

Cross-section data for the MCNP code must be processed by a special module of the NJOY code, the basic data being from the latest available ENDF evaluations. In addition to the true point data, a "discrete" set of data containing several hundred energy intervals is available, but may be inadequate if neutron resonances are important.

OUTPUT:

Standard output listing of results can become voluminous depending on the number of output options used. Various graphical and other post-calculation forms of output are also available.

RESTRICTIONS OR LIMITATIONS:

There are no code-related restrictions on problem size.

OPERATING SYSTEM:

CRAY, CDC, IBM, VAX - a FORTRAN 77 compiler is necessary.

CORE AND DISK REQUIREMENTS:

Most calculations can be run with 500-1000K words, depending on the cross-section data.

TYPICAL RUNING TIME:

Running time varies from a few minutes to several hours, usually depending on the geometric complexity of the problem, the degree of differentiality of results, and the statistical uncertainty requirements. Use of the point data or discrete data will also alter the running time.

DOCUMENTATION:

1. Los Alamos Monte Carlo Group, *MCNP—A General Monte Carlo Code for Neutron and Photon Transport, Version 3A.* LA-7396-M, Los Alamos Natl. Lab., September 1986.
2. Thomas E. Booth, *A Sample Problem for Variance Reduction in MCNP,* LA-10363-MS, Los Alamos Natl. Lab., October 1985.
3. B. L. Kirk and J. T. West, *Systems Guide to MCNP (Monte Carlo Neutron and Photon Transport Code).* ORNL/TM-9123, Martin Marietta Energy Systems, Inc., Oak Ridge Natl. Lab., June 1984.
4. S. N. Cramer, *Applications Guide to the RSIC-Distributed Version of the MCNP Code,* ORNL/TM-9641, Martin Marietta Energy Systems, Inc., Oak Ridge Natl. Lab., September 1985.

PROGRAM AVAILABILITY:

MCNP is packaged by RSIC as CCC-200. Requests can be made by writing RSIC at

Radiation Shielding Information Center
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 37831

or telephoned to:

615/574-6176 or to FTS 624-6176.

MORSE-CGA

CODE IDENTIFICATION:

MORSE-CGA (Combinatorial Geometry Array) developed at
Oak Ridge National Laboratory,
Oak Ridge, TN

SUMMARY:

MORSE-CGA is a general-purpose coupled neutron-gamma-ray radiation transport Monte Carlo code which utilized ANISN code format multigroup cross sections. Any system for which cross sections exist can be calculated in the forward or adjoint mode. Most realistic usages of the code will require some amount of user-written programming. MORSE-CGA is a new version of MORSE-CG revised to add a new array geometry module called MARS (RSIC PSR-117).

MAIN PREDICTED VARIABLE:

General phase-space-dependent flux and current.

OTHER PREDICTED VARIABLES:

Any response as defined by input data response functions.
k_{eff} for criticality calculations

EQUATION SOLVED:

The general time-dependent multigroup integral Boltzmann transport equations in the forward or adjoint mode (see Sect. 3.1).

BOUNDARY CONDITIONS:

General - vacuum, specular reflection, periodic, albedo data, etc.

FEATURES AND LIMITATIONS:

Use of multigroup libraries common to discrete ordinates codes enables easy coupling with discrete ordinates codes. It also allows comparison on a common basis (i.e., DOT-MORSE comparisons with identical cross-section sets).

ANALYTIC METHOD-NUMERICAL ALGORITHM:

The Monte Carlo method is a machine-generated stochastic experiment in which the simulated particles (neutrons or photons) are followed from birth to death (absorption or leakage) using randomly selected variables from natural or biased distribution of position, energy, direction, flight paths, collision mechanics, etc. Selection of biased variables requires adjustment of the mathematically simulated particle "weight," which remains unity for natural, or unbiased, calculations. MORSE allows use of most of the standard biasing or various reduction techniques either by input option or user-written routine. The physical geometry must be described by combinations of any of the elementary geometric bodies (combinatorial geometry) whose surfaces are described by first or second degree algebraic equations. The MARS "array of arrays" feature allows any repeating segment of the geometry to be specified only one time and then moved about via input translation and rotation instructions. The angular scattering treatment is created by discretizing a Legendre polynomial expansion such that the $N+1$ mathematical moments of the discrete distribution are the same as those from the truncated polynomial. Isotropic or anisotropic scattering up to a P_{16} expansion of the angular distribution is allowed.

Monte Carlo methods are used to solve the forward and the adjoint transport equations. Quantities of interest are then obtained by summing the contributions over all collisions, and frequently over most of phase space.

The MORSE code is organized into functional modules with simplified interfaces such that new modules may be incorporated with reasonable ease. The modules are (1) random walk, (2) cross section, (3) geometry, (4) analysis, and (5) diagnostic.

While the basic MORSE code assumes the analysis module is user-written, a general analysis package, SAMBO, is included. SAMBO handles some of the drudgery associated with the analysis of random walks and minimizes the amount of user-written coding. An arbitrary number of detectors, energy-dependent response functions, energy bins, time bins, and angle bins are allowed. Analysis is divided for each detector as follows: uncollided and total response, fluence versus energy, time-dependent response, fluence versus time and energy, and fluence versus angle and energy. Each of these quantities is listed as output. The diagnostic module provides an easy means of printing out, in useful form, the information in the various labeled commons and any part of blank COMMON. The module is very useful to debug a problem and to gain further insight into the physics of the random walk.

CONVERGENCE CRITERIA:

Inherent in the Monte Carlo method is the statistical uncertainty of any calculated quantity due to the random nature of variable selection. For shielding calculations an uncertainty of 10% standard deviation is generally acceptable. The uncertainty is inversely proportioned to the square of the calculation time; i.e, to halve the uncertainty requires a factor of four increase in running time.

PROGRAM INTERFACING AND AUXILIARY ROUTINES:

A host of auxiliary codes has been developed for use with MORSE. As noted above, MORSE-CGA interfaces in a modular fashion with the MARS (Mars Array System) geometry package. In addition, there are three other useful codes: BREESE-II (PSR-143), DOMINO-II (PSR-162), and PICTURE. BREESE is used to produce albedo data for MORSE, DOMINO couples MORSE to the DOT discrete ordinates code, and PICTURE allows easy checks of the geometric model via printer plots of 2-D slices through the geometry.

LANGUAGE:

FORTRAN-IV and FORTRAN 77 versions are available.

INPUT DATA LIBRARY:

Cross-section data must be in the ANISN code format multigroup structure. Computer memory requirements will be reduced if this data is processed external to the MORSE code execution by the XCHEKR module.

OUTPUT:

Standard output listing of results can become voluminous depending on the number of output options used. A history file (collision tape) permits post-processing of information independent of the main calculation. Collision density and geometry plots are available in several forms. The JUNEBUG-II module can be used to provide 3-D plots of the geometry.

RESTRICTIONS OR LIMITATIONS:

Due to variable dimensioning, there are no limitations except the maximum computer memory available.

OPERATING SYSTEM:

The RSIC code packages include those for IBM, CRAY, CDC, UNIVAC, and VAX computers.

CORE AND DISK REQUIREMENTS:

Most calculations can be run with 500 to 1000K words, depending on the cross-section data.

TYPICAL RUNNING TIME:

Running times vary from a few minutes to several hours, usually depending on the geometric complexity of the problem, the degree of differentiality of results, and the statistical uncertainty requirements.

DOCUMENTATION:

1. E. A. Straker, P. N. Stevens, D. C. Irving, and V. R. Cain, *The MORSE Code—A Multigroup Neutron and Gamma-Ray Monte Carlo Transport Code*, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., 1970.
2. M. B. Emmett, *The MORSE Monte Carlo Radiation Transport Code System*, ORNL-4972, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., February 1975.
3. M. B. Emmett, *The MORSE Monte Carlo Radiation Transport Code System*, ORNL-4972R1, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., February 1983.
4. M. B. Emmett, *The MORSE Monte Carlo Radiation Transport Code System*, ORNL-4972R2, Martin Marietta Energy Systems, Inc., Oak Ridge Natl. Lab., July 1984.
5. M. B. Emmett, *MORSE-CGA—A Monte Carlo Radiation Transport Code with Array Geometry Capability*, ORNL-6174, Martin Marietta Energy Systems, Inc., Oak Ridge Natl. Lab., April 1985.
6. J. T. West and M. B. Emmett, "MARS. A Multiple Array System Using Combinatorial Geometry," Vol. 3, Sect. M9 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, Vols. 1-3*, NUREG/CR-0200, U.S. Nuclear Regulatory Commission (originally issued July 1980, reissued January 1982, Revision 1 issued July 1982, Revision 2 issued June 1983, Revision 3 issued December 1984).
7. M. B. Emmett, *DOMINO-II, A General Purpose Code for Coupling DOT IV Discrete Ordinates and Monte Carlo Radiation Transport Calculations*, ORNL/TM-7771, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., May 1981.
8. V. R. Cain and M. B. Emmett, *BREESE-II: Auxiliary Routines for Implementing the Albedo Option in the MORSE Monte Carlo Code*, ORNL/TM-6807, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., July 1979.
9. M. B. Emmett, L. M. Petrie, and J. T. West, "JUNEBUG-II - A Three-Dimensional Geometry Plotting Code," Vol. 2, Sect. F12 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, Vols. 1-3*, NUREG/CR-0200, U.S. Nuclear Regulatory Commission (originally issued July 1980, reissued January 1982, Revision 1 issued July 1982, Revision 2 issued June 1983, Revision 3 issued December 1984).

10. Margaret B. Emmett, "PICTURE: A Printer Plot Package for Making 2-D Pictures of MARS Geometries," Vol. 3, Sect. M13 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, Vols. 1-3*, NUREG/CR-0200, U.S. Nuclear Regulatory Commission (originally issued July 1980, reissued January 1982, Revision 1 issued July 1982, Revision 2 issued June 1983, Revision 3 issued December 1984).

11. S. N. Cramer, *Applications Guide to the MORSE Monte Carlo Code*, ORNL/TM-9355, Martin Marietta Energy Systems, Inc., Oak Ridge Natl. Lab., August 1985.

PROGRAM AVAILABILITY:

MORSE-CGA is packaged by RSIC as CCC-474. Requests for the package can be made in writing to:

Radiation Shielding Information Center
Oak Ridge National Laboratory
P. O. Box X
Oak Ridge, TN 37831

or telephoned to:

615/574-6176 or to FTS 624-6176.

MORSE-SGC

CODE IDENTIFICATION:

MORSE-SGC (Supergroup Combinatorial Geometry) developed by:
Oak Ridge National Laboratory.
Oak Ridge, TN

SUMMARY:

MORSE-SGC is a supergroup version of the MORSE-CG multigroup Monte Carlo code. The supergroup feature allows use of the code in a restricted core memory computer environment, at the expense of increased running time and I/O. Cross-section data are moved into and out of core memory a "supergroup" at a time instead of having all cross sections in core at all times. MORSE-SGC uses the MARS geometry package and as such has identical geometry capabilities as in MORSE-CGA.

MAIN PREDICTED VARIABLE:

General phase-space-dependent flux and current.

OTHER PREDICTED VARIABLES:

Any response as defined by input data response functions.
k_{eff} for criticality calculations.

EQUATION SOLVED:

The general time-dependent multigroup integral Boltzmann transport equation (forward or adjoint).

BOUNDARY CONDITIONS:

General - vacuum, specular reflection, periodic, albedo data, etc.

FEATURES AND LIMITATIONS:

Use of multigroup libraries common to discrete ordinates codes enables easy coupling with discrete ordinates codes. It also allows comparison on a common basis (i.e., DOT-MORSE comparisons with identical cross-section sets).

ANALYTIC METHOD-NUMERICAL ALGORITHM:

The Monte Carlo method is a machine-generated stochastic experiment in which the simulated particles (neutrons or photons) are followed from birth to death (absorption or leakage) using randomly selected variables from natural or biased distribution of position, energy, direction, flight paths, collision mechanics, etc. Selection of biased variables requires adjustment of the mathematically simulated particle "weight," which remains unity for natural, or unbiased, calculations. MORSE allows use of most of the standard biasing or various reduction techniques either by input option or user-written routine. The physical geometry must be described by combinations of any of the elementary geometric bodies (combinatorial geometry) whose surfaces are described by first or second degree algebraic equations. The MARS "array of arrays" feature allows any repeating segment of the geometry to be specified only one time and then moved about via input translation and rotation instructions. The angular scattering treatment is created by discretizing a Legendre polynomial expansion such that the $N+1$ mathematical moments of the discrete distribution are the same as those from the truncated polynomial. Isotropic or anisotropic scattering up to a P_{16} expansion of the angular distribution is allowed.

Monte Carlo methods are used to solve the forward and the adjoint transport equations. Quantities of interest are then obtained by summing the contributions over all collisions, and frequently over most of phase space.

The MORSE code is organized into functional modules with simplified interfaces such that new modules may be incorporated with reasonable ease. The modules are (1) random walk, (2) cross section, (3) geometry, (4) analysis, and (5) diagnostic.

While the basic MORSE code assumes the analysis module is user-written, a general analysis package, SAMBO, is included. SAMBO handles some of the drudgery associated with the analysis of random walks and minimizes the amount of user-written coding. An arbitrary number of detectors, energy-dependent response functions, energy bins, time bins, and angle bins are allowed. Analysis is divided for each detector as follows: uncollided and total response, fluence versus energy, time-dependent response, fluence versus time and energy, and fluence versus angle and energy. Each of these quantities is listed as output. The diagnostic module provides an easy means of printing out, in useful form, the information in the various labeled commons and any part of blank COMMON. The module is very useful to debug a problem and to gain further insight into the physics of the random walk.

CONVERGENCE CRITERIA:

Inherent in the Monte Carlo method is the statistical uncertainty of any calculated quantity due to the random nature of variable selection. For shielding calculations an uncertainty of 10% standard deviation is generally acceptable. The uncertainty is inversely proportional to the square of the calculation time, i.e., to halve the uncertainty requires a factor of four increase in running time.

PROGRAM INTERFACE AND AUXILIARY ROUTINES:

MORSE-SGC is a module of the SCALE system and as such interfaces with several shielding analysis modules. Interfacing with the PICTURE module of SCALE also allows 2-D printer plots of slices through the MARS geometry model.

LANGUAGE:

FORTRAN IV and FORTRAN 77 versions are available.

INPUT DATA LIBRARY:

Cross-section data must be in the AMPX-code working library multigroup format. The data is processed in any of several modules external to MORSE-SGC.

OUTPUT:

Standard output listing of results can become voluminous depending on the number of output options used. Geometry plots are available in several forms. JUNEBUG-II provides 3-D plots of MARS geometry models.

RESTRICTIONS OR LIMITATIONS:

Due to variable dimensioning, there are no limitations except the maximum computer memory available.

OPERATION SYSTEM:

IBM

CORE AND DISK REQUIREMENTS:

Due to the supergrouping feature, calculations can be run on small computers, even PCs, at the expense of running time and I/O.

TYPICAL RUNNING TIME:

Running times vary from a few minutes to several hours, usually depending on the geometric complexity of the problem, the degree of differentiality of results, the statistical uncertainty requirements, and the number of supergroups.

DOCUMENTATION:

1. J. T. West, T. J. Hoffman, and M. B. Emmett, "MARS, A Multiple Array System Using Combinatorial Geometry," Vol. 3, Sect. M9 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, Vols. 1-3*, NUREG/CR-0200, U.S. Nuclear Regulatory Commission (originally issued July 1980, reissued January 1982, Revision 1 issued July 1982, Revision 2 issued June 1983, Revision 3 issued December 1984).
2. S. K. Fraley, *Users Guide to MORSE-SGC*, ORNL/CSD-7, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., March 1976.
3. E. A. Straker, P. N. Stevens, D. C. Irving, and V. R. Cain, *The MORSE Code - A Multigroup Neutron and Gamma-Ray Monte Carlo Transport Code*, ORNL-4585, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., 1970.
4. M. B. Emmett, *The MORSE Monte Carlo Radiation Transport Code System*, ORNL-4972, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., February 1975.
5. J. T. West and M. B. Emmett, "MARS, A Multiple Array System Using Combinatorial Geometry," Vol. 3, Sect. M9 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, Vols. 1-3*, NUREG/CR-0200, U.S. Nuclear Regulatory Commission (originally issued July 1980, reissued January 1982, Revision 1 issued July 1982, Revision 2 issued June 1983, Revision 3 issued December 1984).
6. M. B. Emmett, L. M. Petrie, and J. T. West, "JUNEBUG-II - A Three-Dimensional Geometry Plotting Code," Vol. 2, Sect. F12 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, Vols. 1-3*, NUREG/CR-0200, U.S. Nuclear Regulatory Commission (originally issued July 1980, reissued January 1982, Revision 1 issued July 1982, Revision 2 issued June 1983, Revision 3 issued December 1984).
7. Margaret B. Emmett, "PICTURE: A Printer Plot Package for Making 2-D Pictures of MARS Geometries," Vol. 3, Sect. M13 of *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, Vols. 1-3*, NUREG/CR-0200, U.S. Nuclear Regulatory Commission (originally issued July 1980, reissued January 1982, Revision 1 issued July 1982, Revision 2 issued June 1983, Revision 3 issued December 1984).

Appendix B

SUMMARIES FOR CROSS-SECTION DATA LIBRARIES OF POTENTIAL USE IN SPENT FUEL SHIELDING APPLICATIONS

VITAMIN-C

DATA LIBRARY IDENTIFICATION:

VITAMIN-C: 171n,36g Cross Sections in AMPX Interface Formats for Fusion and LMFBR Neutronics. Available from RSIC as DLC-41/VITAMIN-C

CONTRIBUTOR:

Oak Ridge National Laboratory, Oak Ridge, Tennessee.

SUMMARY:

Background

The United States Energy Research and Development Administration (ERDA) Division of Controlled Thermonuclear Research (DCTR) began in 1974 to sponsor the Radiation Shielding Information Center (RSIC) at Oak Ridge National Laboratory (ORNL) to provide nuclear data and other information to meet the needs of ERDA-DCTR contractors. The VITAMIN-C project was the first special activity of RSIC in its role as the Nuclear Data Center for ERDA-DCTR and involves the generation, packaging, distribution, validation, and maintenance of a general-purpose multigroup cross-section library for neutronics and other radiation transport studies. A single 171 neutron, 36 gamma-ray group cross-section library useful for both CTR and LMFBR neutronics analysis was defined through collaborative input from the user community, which also participated in a validation exercise on the transportability of the system. The master library was generated using the PSR-105/MINX neutron processor and the photon processors from the PSR-63/AMPX system. A preliminary release was made to stimulate implementation and testing at several installations to improve the quality of the library which was ultimately distributed as DLC-41/VITAMIN-C.

Scope

The MINX computer code generates multigroup neutron cross sections and self-shielding factors from evaluated cross-section files in ENDF format. Group constants were generated in the AMPX format by the IBM version of MINX. The Bondarenko method (narrow resonance approximation) is employed to create group-dependent resonance self-shielding factors to account for temperature and dilution effects. The evaluated data upon which VITAMIN-C is based are primarily ENDF/B-IV, but a few from the LENDL and ENDF/B-III libraries were also used. The photon interaction data are based on DLC-7/HPICE, designated the ENDF/B-IV photon data. The data are provided in the form of AMPX master libraries for neutron, photon production, and photon interaction data. AMPX master neutron, photon production, and photon interaction libraries are included for the following elements or isotopes:

H-1, Li-6, Li-7, Be-9, B-10, C-12, N-7, O-16, F, Na, Mg, Al-27, Si, P-31, S-32, Cl, K, Ca, Ti, V, Cr, Mn-55, Fe, Co-59, Ni, Cu, Zr, Nb-93, Mo, Sn, Ba, Eu-151, Eu-153, Ta-181, W-182, W-183, W-184, W-186, Pb, U-235, U-238, Pu-239, and Pu-240.

For the following elements or isotopes, only neutron data are available because no photon production data were available on ENDF/B-IV: H-2, H-3, He-3, He-4, B-11, Ag-107, Ag-109, Cd, Sm-149, Gd, Th-232, Pa-233, U-233, U-234, U-236, Np-237, Pu-238, Pu-241, Pu-242, Am-241, Am-243, Cm-244, and Zirc-2.

Photon interaction data are provided for essentially all elements.

DLC-41/VITAMIN-C was reorganized by removing the AMPX modules from the package. The sample problems are designed to be executed using PSR-117/MARS (or PSR-63/AMPX-II). The change was made to try to minimize the updating required when a change is made to a retrieval code needed by a particular DLC. No retrieval codes are now provided with the package.

Applications

VITAMIN-C was designed as a program for the development, generation, validation, and distribution of a general-purpose Processed Multigroup Cross Section Library (PMCSL) for use in controlled thermonuclear research (CTR) neutronics studies. However, the group structure and general flexibility of VITAMIN-C are such that it has served as the basis for the derivation of broad group libraries for a wide variety of applications. It is likely to be suitable for nearly all radiation transport applications where thermal upscatter is not important.

The major drawback is that the user must make operational the cross-section manipulation routines from the AMPX system. This feature is sometimes a problem for users with non-IBM systems, although versions of most routines have been made operational on CDC and UNIVAC systems and are available in RSIC package PSR-112/MAME.

RETRIEVAL CODE:

No retrieval codes are provided with the package but the user must have operational the PSR-63/AMPX-II, PSR-117/MARS, or, for non-IBM applications, PSR-112/MAME.

TYPICAL RUNNING TIME:

Running times will vary, but the most significant time involves card image to unformatted conversion of the neutron master libraries, which is typically 1 min per nuclide on an IBM-360/91.

DOCUMENTATION:

1. R. W. Roussin, C. R. Weisbin, J. E. White, N. M. Greene, R. Q. Wright, and J. B. Wright, *The CTR Processed Multigroup Cross-Section Library for Neutronics Studies*, ORNL-RSIC-37, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., July 1980.
2. R. W. Roussin and D. B. Simpson, "Sample Problems for DLC-41/VITAMIN-C," presented at the RSIC Workshop on Multigroup Cross-Section Handling Codes, March 1978.

CSRL

DATA LIBRARY IDENTIFICATION:

CSRL: A 218n Criticality Safety Reference Library for Cross-Sections in AMPX Master Library Format for Criticality Safety Studies. Available from RSIC as DLC-43/CSRL

CONTRIBUTOR:

Nuclear Engineering Applications Department at Oak Ridge National Laboratory, Oak Ridge, TN

SUMMARY:

Background

The XLACS module of the AMPX modular code system was used to generate a P3, 218 neutron group cross-section library from the latest ENDF/B-IV data for fuel, structural, and neutron-absorbing materials. The library is a data base for the generation of fine- or broad-group cross sections for cask calculations and other criticality safety neutronics analyses using Monte Carlo codes such as KENO or MORSE, or using one- or two-dimensional discrete ordinates codes such as ANISN or DOT, respectively. The data form the fine-group master library from which the ENDF/B-IV-based libraries for the CCC-466/SCALE-3 system are derived.

The objective in the selection of the energy group boundaries for the library was to fit the important cross-section structure of materials likely to appear in criticality safety problems.

Scope

The CSRL data are provided in the form of a 218 neutron group AMPX master library with the following elements or isotopes:

H-1, H-2, He-4, Li-6, Li-7, Be-9, B-10, B-11, C, N-14, O-16, F, Na-23, Mg, Al-27, Si, P-31, S-32, Cl, K, Ca, Ti, V, Cr, Mn-55, Fe, Co-59, Ni, Cu, Zr, Zirc-2, Nb-93, Mo, Ag-107, Ag-109, Cd, Sn, Ba-138, Gd, Dy-164, Lu-175, Lu-176, Hf, Ta-181, W-182, W-183, W-184, W-186, Re-185, Au-197, Pb, Th-232, U-233, U-234, U-235, U-236, U-238, Np-237, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Am-241, and Cm-244.

Applications

The energy group boundaries for the library fit the important cross-section structure of materials likely to appear in criticality safety problems. Emphasis was placed on the resonance and thermal energy ranges. The 218-energy-group structure includes 140 epithermal groups above, and 78 thermal groups below, 3.05 eV.

Since no photon production data are provided, the data are not directly applicable for most shielding problems.

RETRIEVAL CODE:

No retrieval codes are provided with the package but the user must have operational the PSR-63/AMPX-II, PSR-117/MARS, or, for non-IBM applications, PSR-112/MAME.

TYPICAL RUNNING TIME:

Running times will vary, but the most significant time involves card image to unformatted conversion of the neutron master libraries, which is typically 1m per nuclide on an IBM-360/91.

DOCUMENTATION:

1. W. E. Ford, III, C. C. Webster and R. M. Westfall, *A 218-Group Neutron Cross-Section Library in the AMPX Master Interface Format for Criticality Safety Studies,* ORNL/CSD/TM-4, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., July 1976.

2. W. E. Ford, III, R. M. Westfall, R. W. Roussin, B. R. Diggs, and J. B. Wright, "Sample Problems for a 218-Group Neutron Cross-Section Library in the AMPX Master Interface Format," Informal Notes from March 14-16, 1978, RSIC Seminar-Workshop on Multigroup Cross Sections.

VITAMIN-E

DATA LIBRARY IDENTIFICATION:

VITAMIN-E: 174n,38g Cross Sections in AMPX Interface Formats for General Neutronics Applications. Available from RSIC as DLC-113/VITAMIN-E

CONTRIBUTOR:

Oak Ridge National Laboratory, Oak Ridge, Tennessee.

SUMMARY:

Background

The successful application of DLC-41/VITAMIN-C, based on ENDF/B-IV, to a variety of radiation transport problems led to the development of specifications for an ENDF/B-V based cross-section library, denoted VITAMIN-E. A variety of small funding sources were pooled to produce a general application-independent library from which application-dependent cross-section libraries can be derived. These sources include the Department of Energy's Breeder and fusion programs, the Defense Nuclear Agency, and the Nuclear Regulatory Commission.

Scope

The energy structure of VITAMIN-E contains 174 neutron and 38 photon groups and includes the 171 neutron and 36 photon groups of VITAMIN-C as a subset. The group structure has fine detail in the energy region where cross section minima occur for important shielding materials. The ENDF/B-V special-purpose dosimetry, activation, and gas production files have also been processed into the VITAMIN-E group structure. The 174 neutron group data were processed with MINXI5; the 174 neutron, 38 photon group data were processed with LAPHNGAS (AMPX III); and the 38 gamma-ray group data with SMUG (AMPX III) from DLC-99/HUGO.

The MINXI5 computer code generates multigroup neutron cross sections and self-shielding factors from evaluated cross-section files in ENDF-V format. The Bondarenko method (narrow resonance approximation) is employed to create group-dependent resonance self-shielding factors to account for temperature and dilution effects. The evaluated data upon which VITAMIN-E is based are primarily ENDF/B-V, but a few data sets were generated from LENDL and other special evaluations.

The data are provided in the form of AMPX master libraries for neutron, photon production, and photon interaction data. AMPX master neutron, photon production, and photon interaction libraries are included for the following elements or isotopes:

H-1, Li-6, Li-7, Be-9, B-10, B-11, C-12, N-14, O-16, F-19, Na, Mg, Al-27, Si, P-31, S-32, Cl, Ar, K, Ca, Ti, V, Cr, Mn-55, Fe, Co-59, Ni, Cu, Ga, Zr, Nb-93, Mo, Cd, Sn, Ba, Gd, Ta-181, W-182, W-183, W-184, W-186, Pb, Th-232, U-235, U-238, Pu-239, Pu-240, Pu-241, Pu-242, Am-241, Am-242, Am-243, Cm-242, Cm-243, and Cm-244.

For the following elements or isotopes, only neutron data are available because no photon production data were available on ENDF/B-V:

H-3, He-4, Y-89, Cs-137, Hf-174, Hf-176-180, Re-185, Re-187, Pa-233, U-233, U-234, U-236, Np-237, Pu-238, and Am-242.

Photon interaction data are provided for elements with Z = 1 to 100.

Applications

The early phases of this cross-section library were focused on materials for fast reactor applications and were applied to benchmark testing of ENDF/B-V. More recently, requests have been made for additional materials to be added to the basic library for fusion, defense, and LWR applications. The library performs well for a variety of radiation transport problems where thermal upscatter is not important.

The user must make operational the cross-section manipulation routines from the AMPX system. This procedure is sometimes a problem for users with non-IBM systems, although versions of most routines are have been made operational on CDC and UNIVAC systems and are available in RSIC package PSR-112/MAME.

RETRIEVAL CODE:

No retrieval program is provided. The PSR-117/MARS or PSR-63/AMPX code packages are suggested for full implementation of the capabilities of VITAMIN-E. JCL and sample input are provided to execute a ZPR-6/7 and a CTR standard blanket sample problem using MARS.

TYPICAL RUNNING TIME:

The first part of the ZPR 6/7 infinite medium problem required 55,097 I/O's and 8.3 cpu min on the IBM 3033. This includes the 21,000 I/O's and 6.6 cpu min required to convert the formatted library to binary. The XSDRNPM run required only 37 cpu s and 6065 I/O's, and the GIP/ANISN run took 10,060 I/O's and 38 cpu s. The first part of the CTR standard blanket run required 58,066 I/O's and 10.15 cpu min. The XSDRNPM problem ran for 1.3 cpu min using 5147 I/O's, but the GIP/ANISN run required 1.16 cpu min and 9160 I/O's.

DOCUMENTATION:

1. R. W. Roussin et al., *Vitamin-E: A Coupled 174 Neutron, 38 Gamma-Ray Multigroup Cross-Section Library for Deriving Application Dependent Working Libraries for Radiation Transport Calculations,* Draft ORNL-RSIC Report, August 1984.

CSRL-V

DATA LIBRARY IDENTIFICATION:

CSRL-V: Processed ENDF/B-V 227-Neutron-Group and Pointwise Cross-Section Libraries for Criticality Safety, Reactor, and Shielding Studies.

DATA RETRIEVAL PROGRAMS:

No retrieval program is included in the package; however, the following code systems, which are distributed by RSIC, are available for retrieval of CSRL-V 227-Neutron-Group data:

PSR-63/AMPX-II: Modular Code System for Generating Coupled Multigroup Neutron-Gamma-Ray Cross-Section Libraries from Data in ENDF Format.

CCC-466/SCALE-3: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation.

CONTRIBUTOR:

Oak Ridge National Laboratory, Oak Ridge, Tennessee,

HISTORICAL BACKGROUND AND INFORMATION:

CSRL-V (Criticality Safety Reference Library based on ENDF/B-V) was prepared in support of the Office of Nuclear Material Safety and Safeguards, Office of Nuclear Regulatory Research, U.S. Nuclear Regulatory Commission, Washington, D.C. 20555

APPLICATION OF THE DATA:

The CSRL-V 227-Neutron-Group Library is a pseudo-problem-independent library in the sense that each processed cross-section data set for a material contains a broad range of multigroup data that closely parallel data in the ENDF/B library. CSRL-V data are intended for subsequent generation of problem-dependent fine- or broad-group cross sections for a broad range of applications, including shipping cask calculations, general criticality safety analyses, and reactor core and shielding analyses.

With CSRL-V data as input, the AMPX system can be used to generate problem-dependent cross sections for use with transport codes such as ANISN, DOT-IV, MORSE, VENTURE, KENO-IV, and XSDRNPM. Likewise, CSRL-V can be used as input to the SCALE system to generate problem-dependent cross sections for use within the criticality safety analyses system.

The CSRL-V Pointwise Library contains data for selected materials and reactions. The data can be plotted for comparison with multigroup data, used to generate weighting functions for the subsequent generation of weighted multigroup cross sections, and, in the case of the elastic scattering cross sections for resonance materials, used as input to the XLACS-II module of the AMPX system for the generation of multigroup data.

SOURCE AND SCOPE OF DATA:

The CSRL-V 227-Neutron-Group Library, which is also identified as the CSRL-V General Purpose Neutron (GPN) Library, is a P3 cross-section library in AMPX master format. The library was generated with the NPTXS, XLACS-II, TABU, and UNITAB modules of the AMPX system and the UNRESR and UXSR modules of the NJOY system.

A CSRL-V GPN data set includes one-dimensional multigroup cross-section data, transfer matrices for elastic and inelastic scattering reactions and for neutron producing reactions with arbitrary orders of scatter for fast and thermal data where required, resolved resonance parameters for subsequent processing via the Nordheim resonance process, Bondarenko factors for unresolved resonance processes for a broad range of temperatures and potential scattering cross sections, fission spectrum data, weighting function data, and the multigroup energy structure. The CSRL-V group structure covers a range of 10-5 eV to 20 MeV, including 79 thermal groups below 3 eV.

The 130-material GPN library includes processed data for all materials in the ENDF/B-V General Purpose File, several data sets prepared from LENDL data, hydrogen with water- and polyethylene-bound thermal kernels, deuterium with D2O-bound thermal kernels, carbon with a graphite thermal kernel, and special 1/V, dose factor, and lumped fission product data sets.

DATA FORMAT AND COMPUTER:

EBCDIC characters; IBM 360/91, 3033, etc.

DOCUMENTATION:

W. E. Ford, III, B. R. Diggs, L. M. Petrie, C. C. Webster, and R. M. Westfall, *CSRL-V: Processed ENDF/B-V 227-Neutron-Group and Pointwise Cross-Section Libraries for Criticality Safety, Reactor and Shielding Studies*, ORNL/CSD/TM-160 (NUREG/CR-2306), June 1982.

CONTENTS OF THE LIBRARY:

The following materials are included in the CSRL-V GPN Library: 1/V, H-1, H-2, H-3, He-3, He-4, Li-6, Li-7, Be-9, B-10, B-11, C-12, graphite, N-14, N-15, O-16, O-17, F-19, Na-23, Mg, Al-27, Si, P-31, S-32, Cl, Ar, K, Ca, Sc-45, Ti, V, Cr, Mn-55, Fe, Co-59, Ni, Cu, Zn-64, Ga, Kr-78, Kr-80, Kr-82, Kr-83, Kr-84, Kr-86, Zr, Zr-90, Zr-91, Zr-92, Zr-94, Zr-96, ZIRC-2, Nb-93, Mo, Tc-99, Rh-103, Ag-107, Ag-109, Cd, Cd-113, Sn, Xe-124, Xe-126, Xe-128, Xe-129, Xe-130, Xe-131, Xe-132, Xe-134, Xe-135, Xe-136, Cs-133, Ba-138, Sm-149, Eu-151, Eu-152, Eu-153, Eu-154, Gd-152, Gd-154, Gd-155, Gd-156, Gd-157, Gd-158, Gd-160, Dy-164, Lu-175, Lu-176, Hf, Hf-174, Hf-176, Hf-179, Hf-180, Ta-181, Ta-182, W-182, W-183, W-184, W-186, Re-185, Re-187, Ir-191, Ir-193, Au-197, Pb, Th-232, Pa-233, U-233, U-234, U-235, U-236, U-238, Np-237, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Am-241, Am-242m, Am-243, Cm-243, Cm-244, Cm-245, Cm-246, dose factors, and lumped fission products.

The following materials are included in the pointwise library: Na-23, Cr, Mn-55, Fe, Co-59, Ni, Cu, Kr-78, Kr-80, Kr-82, Kr-83, Kr-84, Kr-86, Zr, Zr-90, Zr-91, Zr-92, Zr-94, Zr-96, Nb-93, Mo, Tc-99, Rh-103, Ag-107, Ag-109, Cd-113, Xe-124, Xe-126, Xe-128, Xe-129, Xe-130, Xe-131, Xe-132, Xe-134, Cs-133, Sm-149, Eu-151, Eu-152, Eu-153, Eu-154, Gd-152, Gd-154, Gd-155, Gd-156, Gd-157, Gd-158, Gd-160, Dy-164, Lu-175, Lu-176, Hf, Hf-174, Hf-176, Hf-177, Hf-178, Hf-179, Hf-180, Ta-181, Ta-182, W-182, W-183, W-184, W-186, Re-185, Re-187, Au-197, Th-232, Pa-233, U-233, U-234, U-235, U-236, U-238, Np-237, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Am-241, Am-242, Am-243, Cm-243, Cm-244, Cm-245, and Cm-246.

HOW TO OBTAIN THE LIBRARY:

CSRL-V can be obtained from the Radiation Shielding Information Center, located at the Oak Ridge National Laboratory, Post Office Box X, Building 6025, Oak Ridge, Tennessee 37831.

CASK

DATA LIBRARY IDENTIFICATION:

CASK: 22n,18g, P3, Cross Sections in ANISN Format for Shipping Cask Analysis. Available from RSIC as DLC-23/CASK and similar data in CCC-466/SCALE-3.

CONTRIBUTORS:

Oak Ridge National Laboratory, Oak Ridge, Tennessee.
Science Applications, Inc., Huntsville, Alabama.
Division of Material Licensing, U.S. Atomic Energy Commission, Washington, DC

SUMMARY:

Background

The cross-section data in CASK were compiled for the purpose of performing shielding calculations for spent fuel shipping casks. The data and results obtained from their use were described at the 1972 annual ANS meeting in Las Vegas.

Scope

This library of coupled neutron and photon cross sections was compiled for several elements that are commonly used for shielding calculations. The coupled, P3, cross sections are given in the ANISN format which permits their usage in the discrete ordinates codes and the multigroup Monte Carlo code, CCC-203/MORSE. The SCALE version is in AMPX Master Library format (no resonance data available on library).

The library contains data for:
H-1, He-3, Be, B-10, C, N, O, Na, Mg, Al, Si, K, Ca, Ti, Cr, Mn, Fe, Ni, Cu, Zr, Mo, Sm, Ta, W, Pb, U-235, U-238, Pu-239, Pu-240.

The source of evaluated data for the neutron cross sections was primarily the ENDF/B-II library, supplemented by other sources, when necessary. PSR-13/SUPERTOG was used to generate resonance-corrected fine-group cross sections for 104 energy groups from the evaluated data. Single-level Breit-Wigner or multilevel Breit-Wigner resonance parameters were used by SUPERTOG to generate point cross sections for the resonance nuclides. Approximately 100 points per resolved resonance were used to integrate the point cross sections for the fine groups. In the unresolved resonance region, 81 points per fine group were used for the integration. A 1/E spectral weighting function was used.

The multigroup neutron cross sections in a 22-energy-group structure were obtained from the 104 group cross sections by averaging the various elemental cross sections across a fine group flux calculated by ANISN for a uranium-water mixture using fine group cross sections.

The secondary gamma-ray production cross sections were calculated by PSR-11/POPOP4. Gamma-ray transport cross sections were calculated for an 18 group gamma-ray energy structure by the SMUG code. The multigroup neutron cross sections, the secondary gamma production cross sections, and the gamma-ray transport cross sections were coupled to form a 40-group set. This is the same 40-group structure as used by Straker for various shielding calculations, particularly in air.

Calculations of the neutron and gamma-ray fluence from several shielding problems have been performed, and some results of these calculations are discussed in the packaged documentation.

Applications

The data were designed for use in shielding analysis of PWR depleted uranium water-flooded shipping casks. The results of such an analysis can be found in the packaged documentation.

The data were collapsed from a fine-group structure using a weighting function representative of a water-uranium mixture. Thus, the application of these data for problems not similar to the shipping cask type should be done with caution.

RETRIEVAL CODE:

A simple retrieval program is provided for conversion from card image the unformatted form.

TYPICAL RUNNING TIME:

On an IBM 360/91 computer, it requires 23 s to read the CASK data from a card image tape and rewrite it on an unformatted file.

DOCUMENTATION:

Included in the RSIC documentation:

1. R. W. Roussin, "Discussion of CASK Update," Informal note, June 1981.
2. Robert W. Roussin, "Energy Absorption Cross Sections in Multigroup Libraries," Informal note, April 1974.
3. Robert W. Roussin, "Changes to the DLC-23 Cross Sections," Informal note, March 1974.
4. Robert W. Roussin, "Changes to the Gamma-Ray Production Cross Sections for Some Materials in DLC-23/CASK," Informal note, October 1973.
5. G. W. Morrison, E. A. Straker, and R. H. Odegaarden, "A Coupled Neutron and Gamma-Ray Multigroup Cross Section Library for Use in Shielding Calculations," *Trans. Am. Nucl. Soc.* **15**, 535 (1972).
6. G. W. Morrison, E. A. Straker, and R. H. Odegaarden, "The Use of the MORSE Monte Carlo Code to Solve Shielding and Criticality Problems of Spent Fuel Casks," *Trans. Am. Nucl. Soc.* **15**, 547 (1972).
7. R. W. Roussin and J. B. Wright, "Contents, Energy Group Structure, and Weight Function Used for DLC-23/CASK," Informal notes, March 1975 Rev.

Background information:

8. E. A. Straker and M. L. Gritzner, *Neutron and Secondary Gamma-Ray Transport In Infinite Homogeneous Air*, ORNL-4464, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., 1969.

FEWG1

DATA LIBRARY IDENTIFICATION:

FEWG1: Coupled 37n, 21g P3, Cross Sections in ANISN Format for Defense Nuclear Agency Radiation Transport Applications. Available from RSIC as DLC-31/FEWG1-85.

CONTRIBUTOR:

Oak Ridge National Laboratory, Oak Ridge, Tennessee.

SUMMARY:

Background

In the early 1970s, a state-of-the-art cross-section library was developed for the Defense Nuclear Agency (DNA) in a 37-neutron, 21-photon energy group structure that can be used for radiation transport. It was the culmination of a vigorous program to provide Defense Department contractors with multigroup cross sections adequate to solve radiation transport calculations to an acceptable degree of accuracy. The program involved the sponsorship of cross-section measurements, evaluation, and cross-section processing methods development as well as integral experiment measurement and analysis. The evaluated library produced was known as the DNA Working Cross-Section Library and was maintained at the Radiation Shielding Information Center in the interim between released versions of ENDF/B.

Scope

The FEWG1 library, often called the "Few Group" library, was processed with the AMPX system. Multigroup data are provided for 41 nuclides of particular interest to the defense community. The library is based on cross-section data from the DNA Working Cross Section Library and ENDF/B-IV and photon production is included for each element. The 37 neutron groups are tailored to allow for the major peaks and valleys in the total neutron cross sections of nitrogen, oxygen, silicon, and iron, and the 21 photon groups are tailored to allow accurate calculation of pair production, annihilation photon transport, hydrogen capture, and backscatter photon transport.

A set of response functions useful in radiation transport applications is also included as part of the library.

The materials included in the library are:

H, H-3, Li-6, Li-7, Be-9, B-10, B-11, C-12, N, O, F, Na, Mg, Al, Si, Cl, K, Ca, V, Cr, Mn, Fe, Ni, Cu, Mo, Ta-181, W-182, W-183, W-184, W-186, Pb, U-235, U-238, Pu-239, Pu-240, Ar, Ti, Gd, P-31, S-32, Ba.

Applications

The library can be used to solve typical calculations of interest to the DNA radiation transport community, particularly those for concrete and air. Since the library is now somewhat dated, it is primarily a reference set against which other newer sets can be compared.

RETRIEVAL CODE:

A simple conversion program is provided for conversion from card image to unformatted form

DATA FORMAT AND COMPUTER:

Card image, ANISN format; IBM 370/3033.

TYPICAL RUNNING TIME:

Conversion required 20 s on the IBM 3033.

DOCUMENTATION:

1. D. E. Bartine, J. R. Knight, J. V. Pace, III, and R. W. Roussin, *Production and Testing of the DNA Few-Group Coupled Neutron-Gamma Cross-Section Library*, ORNL/TM-4840, Union Carbide Corporation, Nuclear Division, Oak Ridge Natl. Lab., March 1977.

CLAW-IV

DATA LIBRARY IDENTIFICATION:

CLAW-IV: Coupled 30n, 12$_\gamma$ Cross Sections Based on ENDF/B-IV for Radiation Transport Calculations. Available from RSIC as DLC-36C/CLAW-IV.

CONTRIBUTOR:

Los Alamos Scientific Laboratory, Los Alamos, New Mexico.

SUMMARY:

Background

The multigroup cross section data that have been in use for many calculations at Los Alamos National Laboratory for a number of years were prepared in a 30-neutron, 12-photon energy group structure and were based in large part on LANL evaluated data. Coupled sets for a number of important materials were produced by LaBauve and Seamon using data from ENDF/B-III and IV and distributed via RSIC as DLC-36/CLAW. With the complete release of ENDF/B-IV, and the development of the NJOY processing system, an ENDF-based version of the 30n, 12g library was prepared.

Scope

The data in DLC-36C/CLAW-IV were prepared from ENDF/B-IV using the NJOY 118) processing system. The library includes prompt and steady-state coupled sets for neutrons and photons in FIDO format (similar to the ANISN format but not directly usable in codes that accept that format), prompt and steady-state fission spectra for the fissionable isotopes and a table of useful response functions including heating and gas production. Basic radiation transport data are provided in the 30n, 12g structure for the following materials:

H, H-2, H-3, He-3, He-4, Li-6, Li-6A, Li-7, Be-9, Be-9A, B-10, B-11, C-12, C-12A, N-14, O-16, F-19, Na-23, Mg, Al-27, Si, Cl, K, Ca, Ti, V, Cr, Mn-55, Fe, Co-59, Ni, Cu, Zirc-2, Nb-93, Mo, Rh-103, Ag-107, Ag-109, Cd, Ta-181, W, Re-185, Re-187, Au-197, Pb, Th-232, Pa-233, U-233, U-234, U-235, U-236, U-237, U-238, U-239, Np-237, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Am-241, Am-243, Cm-244, Cm-245, Cm-246, Cm-247, Cm-248, Cf-249, Cf-250, Cf-251, Cf-252, STANLS, CONCRT.

Applications

This version, DLC-36C/CLAW-IV, is intended as a replacement for earlier versions of CLAW and represents a marked improvement since there are many more materials and a much more complete set of response functions. It is expected to do a reasonable job for problems where self shielding is not important.

RETRIEVAL CODE:

None provided.

TYPICAL RUNNING TIME:

Not applicable.

DOCUMENTATION:

1. R. J. Barrett and R. E. MacFarlane, *Coupled Neutron and Photon Cross Sections for Transport Calculations*, LA-7808-MS, Los Alamos National Laboratory, April 1979.

BUGLE-80

DATA LIBRARY IDENTIFICATION:

BUGLE-80: Coupled 47n, 20g, P3, Cross Sections in ANISN Format for LWR Shielding Calculations by the ANS-6.1.2 Working Group on Multigroup Cross Sections. Available from RSIC as DLC-75/BUGLE-80.

CONTRIBUTORS:

Oak Ridge National Laboratory, Oak Ridge, Tennessee.
ANS-6.1.2 Working Group.

SUMMARY:

Background

The 47-neutron, 20-gama-ray group, P3, cross-section library was developed at Oak Ridge National Laboratory for LWR shielding applications. It replaces DLC-47/BUGLE, which was the first library prepared for use by the ANS 6.1.2 Working Group on Shielding Cross Sections for concrete shielding applications. Studies by members of ANS 6.1.2 and others led to the specification and development of BUGLE-80. Since it has a different group structure, BUGLE-80 was given a different DLC number to help minimize confusion with the earlier version.

Scope

BUGLE-80 was derived by performing self-shielding, combining of neutron, photon production, and photon interaction data, and group collapsing from DLC-41/ VITAMIN-C using modules form the PSR-63/AMPX-II system. Resonance self-shielding was performed only for concrete materials. The evaluated data that serve as a source of data for VITAMIN-C (and hence BUGLE-80) are primarily ENDF/B-IV, but a few evaluations from LENDL and ENDF/B-III were also used. This group structure has been tailored to represent the spectral phenomena of typical LWR shielding problems. The collapsing spectrum was typical of that in the concrete shield of a typical LWR.

Coupled neutron and photon data are included for the 19 elements used in the concrete slab and LWR model calculations used by ANS 6.1.2. The macroscopic cross sections for the core, coolant, carbon steel, stainless steel, and concrete are also provided. Coupled cross sections for an additional 24 elements or isotopes are also included, and all are listed below:

H-1, Li-6, Li-7, Be-9, B-10, C-12, N-7, O-16, F, Na, Mg, Al-27, Si, P-31, S-32, Cl, K, Ca, Ti, V, Cr, Mn-55, Fe, Co-59, Ni, Cu, Zr, Nb-93, Mo, Sn, Ba, Eu-151, Eu-153, Ta-181, W-182, W-183, W-184, W-186, Pb, U-235, U-238, Pu-239, Pu-240, LWR core, LWR coolant, LWR low carbon steel, LWR stainless steel, and concrete.

An additional 23 elements and isotopes are also included, but only neutron data are provided because the evaluated data from which they were derived had no photon production data. Those with neutron data only are as follows:

H-2, H-3, He-3, He-4, B-11, Ag-107, Ag-109, Cd, Sm-149, Gd, Th-232, Pa-233, U-233, U-234, U-236, Np-237, Pu-238, Pu-241, Pu-242, Am-241, Am-243, Cm-244, and Zirc-2.

Kerma factor data derived from DLC-60/MACKLIB-IV package are also included in the 47n, 20g structure (49 materials) for the following materials:
H-1, He-4, Li-6, Li-7, Be-9, B-10, B-11, C, N-14, O-16, F, Na-23, Mg, Al-27, Si, Cl, K, Ca, Ti, V, Cr, Mn-55, Fe, Co-59, Ni, Cu, Nb, Mo, Ta-181, W-182, W-183, W-184, W-186, Pb, Th-232, Pa-233, U-233, U-234, U-235, U-236, U-238, Np-237, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Am-241, Am-243.

Data sets that include delayed photons from fission product decay, based on CCC-371/ORIGEN calculations for 10^{13}s irradiation time, are provided for U-235, U-238, and Pu-239.

Applications

The BUGLE-80 package has all the components needed to repeat the benchmark calculations used by ANS 6.1.2 in developing the final version. This includes the input to the AMPX-II modules, the input to ANISN for the benckmark runs, and the scalar flux outputs from the ANISN calculations. The cross sections should be useful for shielding situations where resonance self shielding and temperature effects are not important. BUGLE-80 is likely to perform better for these types of problems than CASK, FEWG1, and BUGLE.

RETRIEVAL CODE:

A simple conversion program is provided for conversion from card image to unformatted form. In addition, a SOURCE program is included which can calculate a fission spectrum in arbitrary group structure.

TYPICAL RUNNING TIME:

Running time for the library conversion is less than 1 min on an IBM-360/91.

DOCUMENTATION:

1. R. W. Roussin, "BUGLE-80: A Coupled 47-Neutron, 20-Gamma-Ray Group Library for LWR Shielding Calculations," Informal Notes, June 1980.

FCXSEC

DATA LIBRARY IDENTIFICATION:

FCXSEC: 22n, 21g Cross Sections in ANISN Format for Nuclear Fuel Cycle Shielding Calculations. Available from RSIC as DLC-85/FCXSEC.

CONTRIBUTOR:

Oak Ridge National Laboratory, Oak Ridge, Tennessee.

SUMMARY:

Background

The library once used for ANISN calculations for nuclear fuel cycle activities in the Chemical Technology Division at ORNL was an in-house, coupled 27-neutron, 20-photon group, microscopic cross-section library. It had two deficiencies:

1. the source of the evaluated data and the methods for producing the library were unknown, and
2. some of the cross-section data for key materials were apparently unknown.

To correct these problems, the FCXSEC libraries were created to

1. be based on "accepted," currently available, pseudo-problem-independent, cross-section data;
2. include a wide variety of nuclides in a variety of specified materials and concentrations;
3. have neutron and gamma-ray energy structures compatible with broad cases of radiation transport calculations required in nuclear fuel cycle studies;
4. be available as fine-group and broad-group microscopic libraries in AMPX master format and broad-group microscopic and macroscopic libraries in ANISN format;
5. be tested for accuracy by checking for internal data consistency; and
6. be documented with respect to the sources of the evaluated cross-section data, the processing of the data, and the results of the first-order check of the cross sections.

Scope

The FCXSEC library was derived from DLC-41/VITAMIN-C by performing self shielding, combining of neutron, photon production, and photon interaction data, and group collapsing using modules of the AMPX system. Macroscopic data in ANISN format were produced using PSR-75/AXMIX. Microscopic cross sections are available with background cross sections of 0.1, 10^3, and 10^8 b/atom as well as the appropriate values corresponding to each mixture in which an element or isotope occurs.

Macroscopic cross sections are provided for water, stainless steel 304, spent U-fuel, air, spent Th-fuel, Gd-2O3, Limonite concrete, type 2a concrete, boron in water, lithium, plutonium oxide, europium, boron in boral, and tungsten.

Microscopic cross sections for the constituents of the above materials are also contained in the package.

In addition, FCXSEC includes the following isotopes with background cross sections at 0.1, 10^3, and 10^8 b/atom:

Be, C-12, Na, Al-27, Ti, V, Mn-55, Fe, Co-59, Cu, Zircalloy, Nb-93, Mo, Cd, Sn, Ta-181, and Pb.

Applications

The library can be used for shielding design of fuel cycle facilities and is particularly suited for use in situations where components of the facilities correspond to the specific materials for which cross sections are provided.

RETRIEVAL CODE:

A simple retrieval program is provided for conversion from card image to unformatted form.

TYPICAL RUNNING TIME:

On an IBM 3033 computer it requires less than 1m to to perform the conversion.

DOCUMENTATION:

1. W. E. Ford, III, C. C. Webster, B. R. Diggs, R. E. Pevey, and A. G. Croff, *FCXSEC: Multigroup Cross-Section Libraries for Nuclear Fuel Cycle Shielding Calculations*, ORNL/TM-7038 (ENDF-287), Union Carbide Corporation, Nuclear Division, Oak Ridge Natl. Lab., May 1980.

SCALE 27n-18g

DATA LIBRARY IDENTIFICATION:

SCALE: 27n,18g Cross-Section Library in AMPX Format.
Packaged in CCC-466/SCALE-3.

CONTRIBUTOR:

Computing and Telecommunications Division
Martin Marietta Energy Systems, Inc.
Oak Ridge, Tennessee

SUMMARY:

Background

This library is one of the two "shielding" libraries that is part of the SCALE system (the other is the 22n,18g CASK library). The 27-neutron groups (a subset of the 218n fine group library in SCALE) were selected using an extensive validation procedure of the criticality analyses of uranium and uranium-plutonium systems. The 18-photon-group structure is the same as for the CASK library.

Scope

The data were generated using AMPX-II from ENDF/B-IV and are retained in the AMPX format for further processing within the SCALE system. The XLACS-II module was used for neutron cross-section processing using P3 scattering. The Nordheim treatment is employed for the resonance region. Thermal upscatter is present for the 13 groups below 3.05 eV. Data for 73 isotopes or elements are provided.

The photon production processing was done using LAPHNGAS, and the photon interaction data were generated using SMUG from the DLC-7E/HPICE library (the ENDF/B-IV photon interaction library.

Applications

The library is designed to be used in the framework of the SCALE system. The data are suitable for the prediction of neutron and photon fluxes in U and Pu-U systems, against which the 27n structure was benchmarked. The resonance and thermal treatments are superior to the typical lack of treatment provided in other broad-group libraries. Note that the energy group structure is sparse in the high-energy (>6-MeV) region and might be deficient in predicting the transport of high-energy neutrons. However, for spent fuel applications, this group structure should present no problem.

RETRIEVAL CODE:

A wide variety of manipulations are possible using the modules in the SCALE system. The data are currently available only in that system.

TYPICAL RUNNING TIME:

The cross-section manipulation part of a typical SCALE run is a minimal portion of the total CPU time.

DOCUMENTATION:

1. J. A. Bucholz et al., *Standard Composition Libraries*, Sect. M8 in *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, Vols. 1-3*, NUREG/CR-0200, U.S. Nuclear Regulatory Commission (originally issued July 1980, reissued January 1982, Revision 1 issued July 1982, Revision 2 issued June 1983, Revision 3 issued December 1984).

MCNPDAT

DATA LIBRARY IDENTIFICATION:

MCNPDAT: MCNP Cross-Section Data Library Based on ENDF/B-V. Available from RSIC as DLC-105.

CONTRIBUTOR:

Los Alamos Radiation Transport Group (X-6), Los Alamos National Laboratory, Los Alamos, New Mexico.

SUMMARY:

Background

The MCNP general-purpose Monte Carlo code, available from RSIC as CCC-200, has a representative set of cross-section data as an integral part of the package. These data are in two forms, "point" and "discrete", and are in particular formats required by the MCNP code.

None of the data sets in MCNP are based on ENDF/B-V. Rather, the ENDF/B-V based cross-section data for MCNP are collected as DLC-105/MCNPDAT. This separation, somewhat unusual for a data library that can only be used in a particular code, allows the control of the ENDF/B-V based data without hampering the distribution of the MCNP code itself.

Scope

The pointwise data, denoted RMCCS1 and considered to be the "recommended" set of neutron, photon production, and photon interaction data to be used in normal applications, are based primarily on ENDF/B-V data. A few exceptions are provided that are based on evaluated data from Los Alamos National Laboratory and Lawrence Livermore National Laboratory. These are evaluated data that are improvements over data released as ENDF/B-V or that provide photon production data not included therein.

Cross sections are provided for isotopes or elements covering much of the range from hydrogen to curium as follows:

H-1, H-2, H-3, He-3, He-4, Li-6, Li-7, Be-9, B-10, B-11, C, C-12, N-14, O-16, F-19, Na, Mg, Al-27, Si, P-31, S-32, Cl, Ar, K, Ca, Ti, V, Cr, Mn-55, Fe, Co-59, Ni, Cu, Ga, Zr, Nb-93, Mo, Rh-117, Pd-119, Cd, Sn, Ba, Eu, Gd, Ta-181, W, Pt, Au-197, Pb, Bi-209, Th-232, U-233, U-234, U-235, U-236, U-237, U-238, U-239, U-240, Np-237, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Pu-243, Am-241, Am-242m, Am-243, Cm-242, and Cm-244.

The discrete counterpart of RMCCS1 is denoted DRMCCS1. It divides the energy range into discrete "groups" over which reaction cross sections are averaged. The particles, however, are tracked with specific (not group) energies, and the scattering processes are treated in the same fashion as for the RMCCS1 data.

Both forms were generated at LANL using processing techniques, including the NJOY system, that provide libraries in the formats required by MCNP.

Applications

The data are designed for use in the MCNP Monte Carlo radiation transport system, which can be used for three-dimensional radiation transport calculations for neutrons and secondary photons, or primary photons. The pointwise library, RMCCS1, provides a nearly continuous description of the cross sections over the energy range from thermal to 14 MeV. The DRMCCS1 form allows faster computational times, with some sacrifice in accuracy depending on the particular problem.

RETRIEVAL CODES:

PRPR: FORTRAN 77 preprocessor source.

MAKXSF: A program that can be used to translate the data libraries into binary format. The PRPR code will translate MAKXSF to run on a particular hardware system.

TYPICAL RUNNING TIME:

Not available.

DOCUMENTATION:

Included in the RSIC documentation:

1. R. W. Roussin and B. L. Kirk, "DLC-105/MCNPDAT: MCNP Cross Sections Based on ENDF/B-V", Informal notes, May 1984.

Background information:

2. Los Alamos Radiation Transport Group, *MCNP—A Monte Carlo Code for Neutron and Photon Transport, Version 2B*, LA-7396-M, April 13, 1981.
3. J. T. West, "Cookbook for Installing MCNP Version 3," April 1983.
4. B. L. Kirk, "Addendum to J. T. West's Cookbook," June 1983.

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