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NEUTRON PHYSICS DIVISION

Annual Progress Report

Period Ending May 31, 1973

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NEUTRON PHYSICS DIVISION
ANNUAL PROGRESS REPORT
For Period Ending May 31, 1973

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R. W. Peelle, Associate Director

AUGUST 1973

OAK RIDGE NATIONAL LABORATORY
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Introduction

F. C. Maienschein

Essentially all of the programmatic activities in the Neutron Physics Division are directed toward an understanding of the mechanisms whereby radiations are produced and transported through media. This is the case whether the goal is the protection of personnel and equipment in the vicinity of high-energy particle accelerators; the design of devices to detect high-energy radiations; the development of precise and safe techniques for the radiation treatment of cancer patients; the design of structures and equipment to withstand radiation damage from nuclear detonations; the uninterrupted operation of instrumentation aboard military vehicles moving within the atmosphere; the protection of personnel or equipment on spacecraft; or the efficient and safe operation of liquid-metal fast breeder reactors. In combination, these goals require that radiations of many types and of broad energy ranges be considered and that their interactions in a variety of materials be investigated.

In the past the largest fraction of the Division's efforts has been concentrated on the radiations and materials of concern to the designers of shields for reactors and for structures exposed to nuclear detonations. In both cases the radiations of interest are neutrons of relatively low energy (less than 14 MeV) and the secondary gamma rays the neutrons produce while traversing the shield materials. Our studies of these radiations and our attempts to apply the results to specific shield designs have led to the development of a "shield analysis procedure" that is highly sophisticated in comparison to the old empirical process in which shield parameters were derived from experiments bearing some similarity to the shield systems of interest. The transition began with the development of calculational methods that yield quantitatively meaningful solutions of the Boltzmann radiation transport equations for problems involving large thicknesses of materials. Basic nuclear-interaction data sets that are problem independent are used as input, and as the transport methods have been improved and verified, uncertainties in problem solutions have frequently been shown to be due to deficiences in the data sets. Thus, the identification of requirements for nuclear data sets has become a crucial part of the procedure.

The process of improving the data sets has recently received impetus with the introduction of "sensitivity" analyses that can isolate the effect of a specific change in a data set and thereby indicate its importance to the problem solution. Concomitantly the need for the data measurers, evaluators, and processors to interact with each other, as well as with the shield analysts, has become increasingly important. In fact, it is quite likely that the major contribution of the Neutron Physics Division has been to bring together these various groups in one organization and at one physical location, since experience has shown that proximity is essential to achieving the level of cooperation required.

The shield analysis procedure resulting from these efforts in reactor and weapons radiation shielding consists of steps, or elements, that are clearly differentiated and interact with each other as shown in Fig. 1. This same procedure applies wholly or in part to all other shielding programs within the Division (the detector studies and cancer radiotherapy studies being classified as shielding programs). It also applies to reactor core studies, which are expected to comprise a larger fraction of the Division's work in the future. Moreover, many of the transport methods and data sets resulting from this approach are exported for use by non-ORNL agencies, largely through the cooperative efforts of the Radiation Shielding Information Center, which is an integral part of the Division. It seems worthwhile, therefore, to describe the procedure and to point out the applications of its various elements to the different program areas. As this is done in the remainder of this introduction, parenthetical references are frequently made to sections of the annual report in which progress in the specific programs is presented.

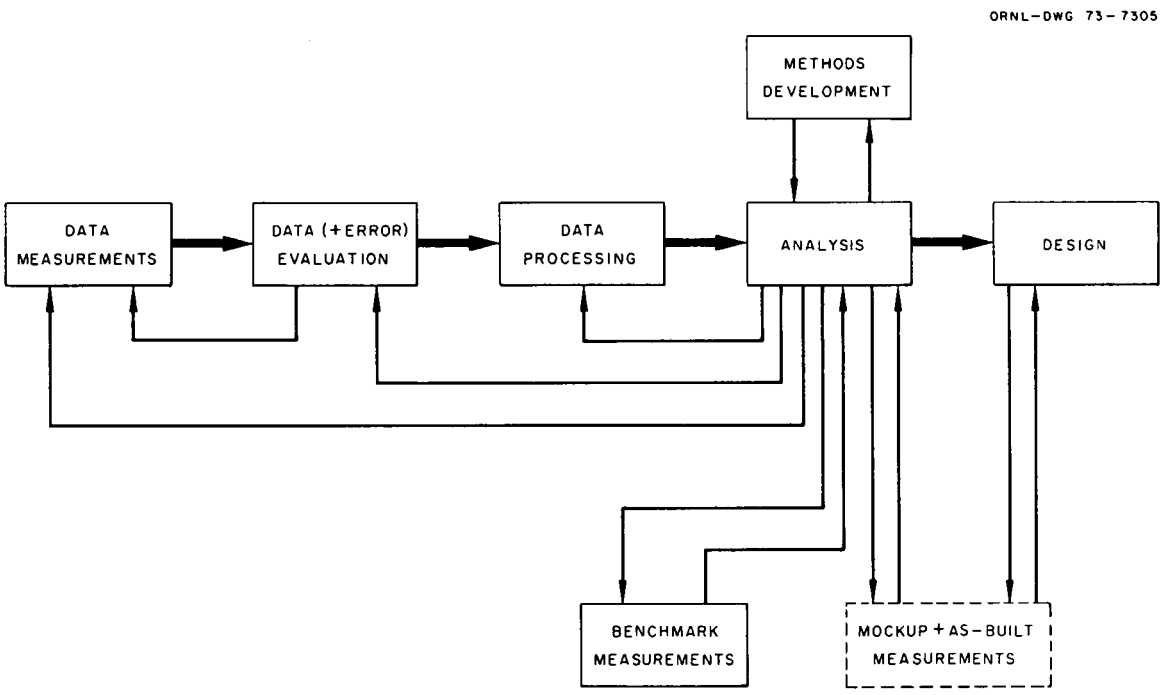

Fig. 1. Elements of radiation shielding (or reactor core) analysis.

RADIATION SHIELDING ANALYSIS

Elements of Radiation Shielding Analysis

The elements of radiation shielding analysis range from those that are strongly physics oriented to those emphasizing engineering goals and include the following:

1. **Data measurements.** Nuclear data needs which are emphasized most strongly for "low-energy" radiation shielding analysis are those for very accurate neutron total cross sections over a wide energy range and for gamma-ray production following neutron interactions. The bulk of all data available for neutron inelastic scattering above 4 MeV was obtained at the ORNL Van de Graaff facility. Analysis and reporting of these data are now being completed (Section 6) and they will soon be incorporated in the Evaluated Nuclear Data Files (ENDF/B) of the National Neutron Cross Section Center.

Extensive data on the energy spectra of the gamma rays produced by interactions of thermal neutrons are available from many laboratories, but comparable data for more energetic neutrons (to >1 MeV) have been so difficult to obtain that for many years recourse was taken in nuclear model calculations whose accuracies were difficult to assess. Recent experiments at the Oak Ridge Electron Linear Accelerator (ORELA) have completely changed this picture and data on gamma rays produced by high-energy neutrons are now being obtained rapidly and economically for all materials of interest (Section 3). These data will dominate the relevant sections of the ENDF/B data sets in future years.

For high-energy particle transport calculations, the data needs are so vast that the role of measurement is limited to checking the intranuclear-cascade model calculations that are used as the basic data generator. The greatest current interest in additional high-energy data generation is for the energy and angular characteristics of secondary particles from the interactions of heavy nuclei. High-energy particles inevitably generate low-energy secondaries, and the cross sections for these secondaries are obtained from the "low-energy" files assembled for reactor and weapons radiation shielding programs. Over ten years ago, an experimental program was initiated to check the predictions of the intranuclear-cascade model within energy regions that could practically be measured. This year the program winds up with the analysis of secondary neutron spectra produced by the interactions of medium-energy protons accelerated at the Oak

Ridge Isochronous Cyclotron (ORIC). Other groups have produced related measurements and the intranuclear-cascade model is validated in general – only for back angles does it deviate widely from experiment. Part of the measurements made in this program led to discovery of the giant quadrupole resonance by scientists in the ORNL Physics Division (Section 2).

2. **Data and error evaluation.** ORNL has contributed heavily to the evaluation of neutron cross sections for the Defense Nuclear Agency (DNA) (Section 3). DNA identifies a continuing responsibility for the elements important to its program and the designated individuals retain cognizance of new or altered measurements for these elements. This is probably the optimum arrangement for data evaluation.

Evaluation is best carried out by individuals or groups who have direct experience with data measurements and recourse to model calculations to fill in gaps where no measurements exist. The ORNL group is well equipped in both respects.

A major future task for data evaluators is the determination of best estimates of uncertainties in the data which must be available for sensitivity analysis. Furthermore, correlations among types of data (or elements of the covariance matrix) are required. These include correlations over energy (both short and long range), correlations among various partial cross sections, and correlations among or between isotopes. ORNL has taken the lead in proposing a format for adding uncertainties and correlations for selected isotopes in the upcoming fourth version of the ENDF/B national reference data file (ENDF/B-IV).

3. **Data processing.** Nuclear data, even after evaluation, must be processed into formats acceptable to multigroup transport codes. The many choices of group structures, weightings within the groups, and description of angular scattering make this a complex task. Considering other factors, such as the production of secondary gamma rays by neutrons and handling the violent variations of the neutron cross sections in the resonance region, increase the complexities. A massive code system, AMPX, has been developed for DNA at ORNL and many specialists devote full time to developing and maintaining this system (Section 4).

Processing codes are expensive to develop and operate and AMPX will be used to provide data sets for many other users. For scoping studies and noncritical use, it may be efficient to use "standard" or reference cross-section data sets. The Radiation Shielding Information Center (RSIC) distributes such sets to the shielding community as part of its distribution of information (Section 5). For detailed design calculations, especially for systems containing materials that exhibit much structure in the variation of neutron cross section with energy, such as iron, it is necessary to demonstrate with care that the cross-section set used is capable of handling the detail. Otherwise results may be grossly in error.

4. **Shield analysis.** The analysis of radiation shields may be differentiated from design. Typically, the design of any system depends upon many factors, of which shielding is only one, and a "design" group takes the overall responsibility. It will usually use rather crude methods to determine the effectiveness of many shield configurations. An "analysis" will follow for selected designs and this analysis may be performed by another group which specializes in this area. As at ORNL, the analysis group may be involved in analyzing many shield systems and therefore be able to develop and maintain methods and data-processing capabilities which exceed those that could be supported by a single program.

For shield systems whose high performance is crucial, powerful analytical techniques may be necessary in order to optimize the shield performance with respect to the parameter(s) of interest. This problem is best typified by the programs developed for reducing shield weights for Space Nuclear Auxiliary Power (SNAP) systems (Section 8).

5. **Shield design.** ORNL participation in the design process is generally limited. However, ORNL did provide assistance in the design of the shield of the FFTF (Fast Flux Test Facility) by WARD (Westinghouse Advanced Reactors Division). The design responsibility clearly remained with WARD but problems were recognized and solved using the coupled discrete-ordinates and Monte Carlo capability at ORNL which exceeds that available anywhere else (Section 8). Such cooperative efforts require the closest coordination between the analysis and design groups and a high degree of responsiveness in terms of reaction time on the part of the analysis group. The FFTF shield analysis probably represents a useful model of how such a cooperative effort should be carried out.

6. **Methods development.** Methods development has been concentrated upon discrete ordinates and Monte Carlo solutions of the transport equation. Much of the development and use of methods for "low-energy" transport, with nuclear data that have been tested for validity in integral experiments, was

pioneered at ORNL (Section 4). The methods are now being adopted widely for shielding analysis throughout the U.S. and the rest of the world, albeit with recurring complaints about the cost of computing time. Alternate approaches to shield design with large factors of conservatism can only lead to substantially greater overall system costs, however. Overall, there is little doubt that the ORNL-developed, one-dimensional discrete ordinates code ANISN is now the most widely used method of shield analysis in the world. The two-dimensional discrete ordinates code DOT is also very popular, as is the ORNL-developed Monte Carlo code MORSE. Analysis and design of shields requires the continuing development and improvement of such methods. A new version of DOT is planned as DOT-IV, and MORSE is being broadly improved.

For large and complex systems, coupling of the various codes has presented virtually the only viable approach to radiation transport analysis. Furthermore, coupled or chained calculations can be used efficiently to determine the effects of changes in only part of a system. For this case, the calculation is repeated only for the perturbed part, leaving the remainder of the calculation unchanged. Numerous developments are under way to facilitate the use of the existing coupling codes DOMINO and FACT.

Perturbation sensitivity analysis is now carried out with the one-dimensional code SWANLAKE, which is based on ANISN. Capabilities are needed for two-dimensional problems, for time-dependent systems, and for calculations with point cross sections. Concepts are now being investigated which may lead to each of these capabilities.

The techniques developed at ORNL for high-energy radiation transport calculations depend upon quite complex Monte Carlo methods which are less susceptible to export. The tendency therefore is to use more approximate methods elsewhere and to have them checked against calculations performed here for the purpose.

7. **Benchmark measurements.** Benchmark experiments are designed to test in a definitive manner selected important aspects of analysis methods or nuclear data. Sensitivity analysis is now being used to identify the most important areas.

The clearest examples of useful benchmark experiments at ORNL are those of neutron transmission through very thick samples. These measurements, carried out at the Tower Shielding Facility and ORELA (Sections 8 and 3), can test total cross sections over a broad energy range. In the tests to date, all total cross sections, with a single exception, failed to pass the tests and all (but one) must be remeasured to higher accuracy. Other neutron attenuation measurements through thick samples of sodium indicate no major cross-section problems. Similar measurements for iron allow a determination of the minimum number of groups that will account for the great detail in the neutron cross-section variation with energy. In recent benchmark measurements of neutron streaming through simulated pipes of sodium, the available analytical methods were verified (Section 8).

8. **Mockup and as-built measurements.** Our experience is that measurements with shield mockups are of quite limited value since they usually vary from the system of interest sufficiently so that uncertainties in translation dominate the results. Intuitive judgment indicates that measurements for systems "as built" should be of great value in checking methods even if the results are obtained too late to influence the design. For reactors in the U.S., however, only limited information has been obtained in this manner, primarily because of difficulties of access and the high cost of special low-power operation to facilitate the spectral measurements which are alone capable of testing methods in detail. The Europeans rely rather heavily upon as-built measurements and we are examining, together with HEDL (Hanford Engineering Development Laboratory), the possibilities of useful measurements for the FFTF at reasonable cost.

Interactions Among Elements of Radiation Shielding Analysis

As pointed out earlier, the information flow among the elements of radiation transport analysis indicated in Fig. 1 is tremendously facilitated by having the groups in the same organization and physical location. The old idea of the importance of maintaining a program of critical size applies with full force here and it is demonstrably cost effective.

The flow of information along the heavy arrows to the right in Fig. 1 presumably requires little comment. Data are measured, evaluations in conjunction with the results of other related measurements are

made, errors and correlations may be added, and the data are then processed and used in the analysis that eventually determines a shield design. The feedback from integral measurements has already been indicated. The feedback through sensitivity analysis deserves further comment, however.

1. **The role of sensitivity analysis.** Perturbation or variational theory can indicate within a useful degree of approximation what is the effect of changing a piece of nuclear data (or the exactness of an analysis method) upon a desired answer for a radiation shielding problem (Section 4). In this way, the importance of a particular cross section or a selected energy range for this cross section can be determined quantitatively. The advantages over intuitive selection of importance are tremendous. In the future, the complicated committee structure devised to request cross-section measurements should give way to sensitivity theory. The need for measurements and evaluations will be largely established in this manner. The needs will remain broadly problem-dependent of necessity.

In a similar manner, the degree of detail required in data processing (number of energy groups or coefficients of expansion in angle) can be determined to correspond to the desired accuracy in the answer for a given problem.

Furthermore, by incorporating the best estimates of all pertinent data uncertainties in an analysis, it is possible to determine the accuracy of the result. This is obviously a vital capability and it justifies the considerable effort which will be required to add uncertainty (or error) files to the national reference data set (ENDF/B). Preliminary studies show the crucial role of correlations of data in such calculations and the correlations must also be added to the reference set.

2. **The role of RSIC.** Obviously, great importance must be attached to the diffusion of shielding analysis methods to other organizations. The Radiation Shielding Information Center takes the leading role in this information transfer, not only with respect to information developed at ORNL but also that from other installations within the U.S. and other countries (Section 5). RSIC generally enters Fig. 1 at Data Evaluation and aids users in all blocks to the right.

The level of assistance from RSIC, especially with regard to computer-oriented problems, is very high and this helps account, for example, for the widespread use of ANISN noted earlier. The cost effectiveness of this high degree of assistance is difficult to quantify but consideration is being given to extending similar coverage to a few other selected areas. A problem of nonimbeddedness immediately arises. RSIC prospers as a shielding information analysis center because it is imbedded in a large group devoted to shielding problems. Extensions to other areas must succeed or fail depending upon the effectiveness in opening communication lines corresponding to those in Fig. 1.

Program Areas in Radiation Shielding Analysis

The varied mix of program areas identified below represents in a real sense an integration at the working level in radiation shielding analysis. Few, if any, of the programs could have afforded development of the methods and experimental facilities which are collectively supported. Equally crucial, the large total effort allows staff members to specialize in selected areas, such as the development of maximum-efficiency two-dimensional discrete ordinates codes or sensitivity analysis techniques for the benefit of all programs. Even programs which may seem unrelated have a substantial degree of overlap with others since, in fact, they were all developed on that basis.

Although the programs use largely common methods, their goals are diverse. In order to accommodate different requirements for the distribution of published results, this annual report is divided into two parts. Identifiable areas from both parts include the following:

1. **High-energy accelerator shielding and detector studies.** Work in this area started with the analysis of radiation shield problems in the construction of high-energy accelerators. Limited activity of this type continues, but interest has spread to include studies of the performance of instruments and the analysis of experiments at high-energy accelerators (Section 1). Clearly, the number of high-energy accelerators is relatively limited and the community of those interested in related radiation transport problems is small compared to reactor shielding, for example. This substantially facilitates the communication of results and methods.

2. **Space radiation shielding.** Space-related radiation-transport research is being phased out at ORNL and a major handbook has been prepared for use by the nonspecialist in shield analysis. However,

substantial interest remains in the effects upon man in space of heavy nuclei, and these effects depend substantially upon the nuclear interactions of the heavy nuclei. A model is being developed to allow the prediction of the interaction probabilities and of the spectra of nuclear reaction products (Section 1).

3. **Cancer radiotherapy**. The methods of transport developed for medium- and high-energy particles for the above areas are directly applicable in calculating the interactions of similar particles in radiotherapy. Potential advantages in treating cancer follow from more favorable patterns of energy deposition than is possible with the photons that are now used and/or from selective killing of cancer cells. The ORNL calculations (Section 1) provide more quantitative details for planning radiobiology experiments and clinical procedures than are available otherwise. Furthermore, they promise to compare for the first time on a uniform basis the major particle types: protons, neutrons, alphas, pions, heavy ions, and the conventional photons. The heavy-ion calculations share development of the model mentioned in connection with space radiation, thus indicating a typical example of the overlap of interests between programs. The pion studies are made jointly with the Health Physics Division at ORNL.

4. **Weapons radiation shielding.** Most if not all systems of the military services are potentially subject to radiations from nuclear weapons. Determination of the degradation of weapons systems requires accurate calculations of the transport of these radiations through the atmosphere and system itself. A continuing and well-integrated program of research funded by the Defense Nuclear Agency has led to a capability of predicting steady-state and time-dependent neutron and gamma-ray transmission through air (Section 4). An important problem, which was recently resolved, followed from the data for gamma-ray production from fast-neutron interactions in nitrogen. This program has supported the development of several generally useful analysis methods, with special emphasis upon time dependence. DNA-supported data-processing and evaluation efforts have already been indicated.

5. **SNAP reactor shielding.** The national program to use nuclear reactors as auxiliary power sources in space has been discontinued. In the several years of work on the shielding analysis of such systems, a number of widely useful methods were developed, including the multigroup Monte Carlo code MORSE. In a real sense, the SNAP systems represented the highest premium upon exact shield design and analysis. Therefore, the optimization codes ASOP and SHAPE (Section 8) were developed based on the discrete ordinates code ANISN. A small amount of shielding analysis is expected to continue in support of auxiliary power supplies using heat from radioisotopes.

6. **LMFBR shielding.** Analysis in support of the design of shielding for the FFTF is nearing completion (Section 8). The use of advanced analysis methods apparently saved $>\$10^7$ above the cost of the analysis, although such estimates are difficult to verify. A major remaining task is the analysis of the final system as built. Results of this analysis can be used for comparison with measurements for the completed reactor.

Attention is shifting to the Liquid Metal Fast Breeder Reactor (LMFBR) demonstration plant. The approach to analysis of shielding problems will be modeled after that used for the FFTF, although it is reasonable to expect that streaming problems will be recognized earlier in the design process. As for the FFTF, perhaps the major problem is that of spent fuel storage within the vessel. This fuel has the effect of converting low-energy neutrons to fission neutrons and thus increasing the streaming along the vessel wall to the reactor top head by many orders of magnitude.

REACTOR CORE ANALYSIS

Elements of Reactor Core Analysis

The elements of measurement and analysis shown in Fig. 1 apply equally well for shielding and reactor core studies. In fact, the shield analysis methods developed at ORNL have proven to be so readily adaptable to nonshielding problems that they are frequently used, largely by others, for reactor core design problems. Work in this area in the Division is performed as part of the LMFBR program and thus is less broadly distributed than the shielding work in the Division. Its various elements can be identified as follows:

1. **Data measurements.** After the coming fiscal year, ORELA and the Fast Neutron Generator (FNG) at Argonne National Laboratory are expected to be the only accelerator facilities heavily dedicated to obtaining nuclear data in support of U.S. reactor programs. ORELA is best suited for cross-section measurements below about 1 MeV and FNG for higher energy measurements. The past program of

measurements at ORELA has been concentrated upon the fissile materials, as well as upon secondary gamma-ray production and neutron inelastic scattering, as has already been mentioned in the discussion of shielding.

The impact of the ORELA program is shown by the new version of the national reference data set (ENDF/B-IV) now being assembled. For the important fissile nuclei, the capture and fission cross sections below ~100 keV are predominantly based upon ORELA results (Section 6). For capture in ^{238}U, ORELA results differ from other recent results and an "average" value will be used in ENDF/B-IV. The differences are about equal to the uncertainties assigned to the capture cross sections. A major continuing activity will be directed toward reducing the ^{238}U capture uncertainties since they are judged to have an important effect upon the breeding ratio of an LMFBR. The judgement of the importance for the performance of LMFBR's of various cross sections, including ^{238}U capture, was made several years ago on the basis of rather approximate calculations. It now appears that sensitivity analysis has an important role in working backward from desired accuracies in reactor performance to allowable data uncertainties (see item 4 below).

2. **Data and error evaluation.** Active participation in CSEWG (Cross Section Evaluation Working Group) continues by Neutron Physics Division staff members. In addition to the activities relating to shielding, they have provided major input and consultation for the evaluations for fissile and fertile isotopes. As has already been indicated, these activities will be broadened to encourage the provision of estimates of uncertainties and correlations for at least the data determined by sensitivity analysis to be of most importance for LMFBR design.

3. **Data processing.** It is tentatively planned to incorporate within ORNL's AMPX data-processing system LASL's new code MINX, which combines neutron cross sections into multigroup sets. This will give at ORNL a capability for applying in the resonance region the standard f-factor treatment of neutron cross sections.

4. **Reactor core analysis.** A program is under way which provides supporting calculations for the reactivity surveillance procedures for the FFTF (Section 7). In particular, during reactor startup the neutron detectors which monitor the reactivity status are outside the core and thus have a very low efficiency while operating in a harsh background of noise and gamma radiation. Discrete-ordinates calculations in one and two dimensions have been made to guide the design of experimental tests of the planned detectors. Later, interpretation routines will be provided to guide the reactor operators in the use of signals from the subcriticality monitor during reactor startup.

The only other current core analysis program is designed to apply the methods of sensitivity theory developed for shielding analysis to the question of which nuclear data are most important for LMFBR design. With the input of errors and correlations from data-evaluation efforts, data uncertainties will be determined as required to achieve specified uncertainties in core performance (in terms of breeding ratio, void coefficients, etc.). Data correlations have been shown to influence crucially the results that are obtained. The earlier U.S. calculations contained crude but plausible assumptions about data correlations. Calculations to date have been limited to simple benchmark systems.

5. **Methods development.** As already indicated, ORNL-developed analysis methods have been used elsewhere for reactor core analysis. Examples include LMFBR core design and analysis of irradiation experiments in the EBR-II using DOT.

Future additional development will include the three-dimensional diffusion-theory code VENTURE, which is an outgrowth of CITATION. Every effort will be made to make this code useful for design problems.

1. Theoretical Studies of Medium- and High-Energy Radiation Transport

1.0 INTRODUCTION

R. G. Alsmiller, Jr.

Theoretical studies of medium- and high-energy radiation transport are pursued on a continuing basis. For several years the work has been directed at the shielding of high-energy accelerators and manned space vehicles. In the past year a substantial part of the effort has continued to be directed at accelerator and space applications, but a large part of the effort has also been directed at studying the use of a variety of radiations – negatively charged pions, neutrons, protons, and heavy ions – in cancer radiotherapy. The calculational techniques that have been developed primarily for shielding purposes are applicable to many accelerator and space problems that are only peripherally related to shielding, such as the design of high-energy particle detectors, and work in these nonshielding areas in the past year has been conducted as part of both the AEC- and the NASA-supported programs.

Radiotherapy is an important aid in the treatment of cancer and is used on about one-half of all cancer patients. Very approximate estimates indicate that about 60,000 lives per year might be saved if new and improved radiotherapeutic techniques were available. At the present time, both in the U.S. and in the world, there is considerable interest in attempting to obtain these needed improvements by using a variety of particles, other than the conventionally used photons, for radiotherapy. The calculational techniques developed at ORNL as part of the medium- and high-energy transport programs make it possible to obtain much of the information needed by experimenters to design and understand the preclinical and clinical trials that will be conducted with the various particles. A program was therefore initiated at ORNL in the past year with NSF/RANN support to carry out the required calculations and supply the needed data.

Accelerator Program

Shielding continues to be a major activity of the accelerator program, and during the past year shielding calculations have been carried out to aid in the design of a 200-GeV proton beam dump for the National Accelerator Laboratory and to aid in the design of a 400-MeV electron beam dump for the accelerator being constructed at the Laboratory of Nuclear Sciences at the Massachusetts Institute of Technology.

Another major activity of the program has been the carrying out of calculations to aid numerous investigators in designing high-energy-particle detectors. The calculational techniques developed to study the nucleon-meson cascades induced by high-energy particles in shields have been shown to give good agreement with experimental data obtained with various kinds of high-energy-particle detectors. This agreement gives confidence in the calculations and enables us to obtain at a relatively small cost data which are needed to improve the detector design and which would be very expensive to obtain experimentally.

To obtain a reliable estimate of the dose equivalent received by personnel who work in the vicinity of accelerators is both difficult and important. One method that has been proposed to obtain this required dosimetry information is to measure the neutrons that leave the human body when it is exposed to an incident neutron fluence and to attempt to relate the measurements to the dose equivalent produced in the body. During the past year, extensive calculations were carried out at the request of the health physics group at the National Accelerator Laboratory to test the feasibility of this method of dosimetry, and it was found that, in general, dosimeters based on this principle are not reliable. These calculations are also of

interest because they indicate the type of interaction that occurs between the medium- and high-energy shielding programs and the low-energy shielding program in the division. The cross-section data used in the dosimetry calculations were developed as part of the present program, but the two-dimensional discrete ordinates computer code DOT that was used was developed as part of the low-energy program (see Section 4). Only because of the large amount of work that had been done in the low-energy program to develop the code DOT could the medium-energy dosimetry calculation needed by the health physics group at NAL be carried out in a straightforward manner.

Space Program

In the past several years, the National Aeronautics and Space Administration has sponsored considerable research on the transport methods and physical data needed to design the shielding required to protect astronauts against radiation in space. As part of the ORNL program, a handbook titled "Shielding of Manned Space Vehicles Against Protons and Alpha Particles" (ORNL-RSIC-35) has been published which summarizes the available information on the shielding of manned space vehicles against protons and alpha particles. The discussion and results presented in the handbook are primarily intended for nonexperts, and no extensive background in space-radiation or charged-particle transport theory is presupposed. A large amount of numerical data is presented to aid mission planners who must decide with little effort whether a radiation hazard is likely to exist on a given mission. If a radiation hazard is thought to exist, then the more detailed shielding methods and computer codes discussed in the handbook must be used to obtain adequate information.

The areas of most uncertainty in the shielding of manned space vehicles which are to travel outside of the earth's magnetosphere are those associated with the high-energy heavy ($A > 4$) galactic cosmic rays. Theoretical studies of the transport of these particles through shields are very inadequate at the present time because there is very inadequate information on the nuclear-reaction products produced when these high-energy heavy particles collide with nuclei of the shield. In an effort to improve this situation, work has been carried out during the past year to formulate a nuclear-reaction model which will provide the needed nuclear-reaction-product information. A model, which relies heavily on previous nuclear-reaction work carried out as part of the shielding program, has been formulated, and results obtained with this model have been compared with the very small amount of experimental data that exist. The degree of agreement between the calculated results and the experimental data is promising, but improvements in the model must be made before the model can be considered in any sense adequate.

Cancer Radiotherapy Program

One of the major goals of the program is to make by means of calculations an objective comparative study of the various types of radiation – negatively charged pions, neutrons, protons, and heavy ions – which have been proposed for use in cancer radiotherapy. The ultimate therapeutic value of the various types of radiation must be determined, of course, by patient irradiation. Only by calculation, however, is it feasible to make a comparison of all of the radiation types under the same conditions and for the same biological endpoints. Also, the detailed nature of the calculations will make it possible to compare many quantities (e.g., LET spectra) which cannot be readily obtained experimentally.

To make the comparisons as meaningful as possible, it will be necessary to compare not only physical quantities, such as absorbed dose, but also important biological quantities, such as cell-survival probabilities, and therefore a significant portion of the program during the past year has been devoted to incorporating the available cell-survival model into the computer codes that are used to carry out the transport calculations.

Definitive calculations on the use of heavy ions in cancer radiotherapy cannot be carried out at the present time because the nuclear-reaction products produced when high-energy heavy ions collide with tissue nuclei are not adequately known. The information needed here is the same as the information discussed under the space program which is needed for shielding against galactic cosmic rays. Therefore, the nuclear-reaction model being developed to provide this information will be utilized in both the space and the cancer programs.

The other major objective of the program is to use the calculational capabilities existing at ORNL to supply design data to those investigators engaged in preclinical and clinical trials using the various radiations. Every effort is being made to supply data requested by users throughout the United States. As part of this collaboration with the various experimental groups, calculated results will be compared with experimental data in order to both understand the experimental data and ensure the validity of the calculations.

1.1 PHOTON DOSE RATES FROM THE INTERACTIONS OF 200-GeV PROTONS IN IRON AND IRON-LEAD BEAM STOPS[1]

T. A. Gabriel and R. T. Santoro

The calculated photon dose rates from the long-lived ($\tau_{1/2} > 1$ min) beta- and gamma-active nuclides produced when 200-GeV protons are incident on a semi-infinite cylindrical iron beam stop having a radius of 40.64 cm (16 in.) are compared with the calculated photon dose rates from long-lived beta- and gamma-active nuclides produced by 200-GeV protons in semi-infinite beam stops having a 30.48-cm (12-in.) radius iron core but surrounded by either 5.08 cm (2 in.) or 10.16 cm (4 in.) of lead. Data are also presented comparing the calculated photon dose rates from the long-lived beta- and gamma-active nuclides produced when 200-GeV protons are incident on semi-infinite cylindrical iron beam stops having radii of 10.16 cm (4 in.), 20.32 cm (8 in.), 30.48 cm (12 in.), and 40.64 cm (16 in.).

1. Abstract of ORNL-TM-3945 (October 1972); also of paper published in *Particle Accel.* **4**, 169 (1973).

1.2 SHIELDING AGAINST THE NEUTRONS PRODUCED WHEN 400-MeV ELECTRONS ARE INCIDENT ON A THICK COPPER TARGET[1]

R. G. Alsmiller, Jr., and J. Barish[2]

Neutron-transport calculations have been carried out using the method of discrete ordinates, and the dose equivalent as a function of radius in spherical shields of various compositions is presented. The incident-neutron spectra used are characteristic of the spectra emitted in the angular intervals of 0 to 30 deg, 30 to 60 deg, 60 to 120 deg, and 120 to 180 deg when 400-MeV electrons are incident on a thick copper target. Results are given for shields of soil, concrete, ilmenite, iron, and iron followed by soil.

1. Abstract of ORNL-TM-4060 (April 1973) and of paper submitted for journal publication.
2. Mathematics Division.

1.3 ENERGY DEPOSITION AND ENERGY-DEPOSITION FLUCTUATIONS IN AN IONIZATION SPECTROMETER AND A TOTAL-ABSORPTION NUCLEAR-CASCADE COUNTER[1]

T. A. Gabriel and K. C. Chandler[2]

Calculations have been carried out to determine the energy deposition and energy-deposition fluctuations produced by incident 28-GeV/*c* protons on an ionization spectrometer. In obtaining the pulse-height characteristics of the spectrometer, the nonlinearity of the light pulses is taken into account by the use of Birks' law and is shown to be of importance. A discussion of the experimental difficulties encountered in locating the position of the initial proton interaction within the spectrometer is also presented. Similar calculated results on the energy deposition and energy-deposition fluctuations are presented for 8-GeV/*c* negative pions incident on an NaI(Tl) total-absorption nuclear-cascade (TANC) counter. Also included for 8-GeV/*c* incident negative pions is the laterally integrated energy deposition as a function of depth in a tin absorber. In general, the calculational approach used is shown to yield good agreement with the experimental data.

1. Abstract of ORNL-TM-4118 (May 1973) and of paper submitted for journal publication.
2. Mathematics Division.

1.4 ENERGY DEPOSITION AND FLUCTUATION IN A LARGE ORGANIC SCINTILLATOR[1]

T. A. Gabriel and J. D. Amburgey[2]

A renewed interest in ionization spectrometers and total-absorption nuclear-cascade (TANC) counters, which can be used to determine the energy of incident hadrons, has occurred recently due to the planning and building of the new multi-GeV hadron accelerators around the world and to the continuing interest in the high-energy portion of the galactic and solar cosmic-ray hadron spectra. Since these devices must be calibrated before they can be of much use and since multi-GeV hadron beams are not yet readily available, a realistic calculational approach to the calibration problem is not only a necessity but it can yield valuable insight into further design and development.

In the work reported here, calculations have been carried out to obtain the energy deposition and fluctuation in a large (100 in. in diameter and 140 in. in length) cylindrical organic liquid scintillator when protons and charged pions in the low-GeV energy range are incident. The three-dimensional, high-energy nucleon-meson transport code HETC[3] is used to obtain a detailed description of the nucleon and meson cascade produced in the device. The electromagnetic cascade produced by the gamma rays from neutral-pion decay and the electrons and positrons from muon decay are taken into account using a modified version of the Monte Carlo code developed by Beck.[4] The nonlinear response of the organic scintillator is obtained using Birks' law.[5]

The integrated energy deposition and leakage produced by 3-GeV/c protons incident on the large scintillator are presented in Table 1.4.1. As can be seen, the major source of energy deposition is from primary and secondary proton ionization, charged-pion ionization, and from neutral pions. The major source of leakage is from neutrons. The remaining energy not accounted for is due to binding and escaped neutrino energy.

Table 1.4.1. Energy deposition and leakage in an organic scintillator (CH_2, ρ = 0.87 g/cm^3) by 3-GeV/c incident protons

	Energy deposition (MeV)
Primary ionization	136.72
Secondary proton ionization	874.89
π^+ and π^- secondary ionization	158.13
μ^+ and μ^- secondary ionization	7.72
Nuclear recoil and evaporated charged particles other than protons	68.35[a]
Excitation energy following evaporation	17.38[a]
Neutrons with energy <15 MeV	42.56
Electromagnetic from decay of π°	223.73
Electromagnetic from decay of $\mu^\pm$	22.17
Total	1551.65

Type	Leakage energy (MeV)		
	Front	Side	Back
Protons	0.33	14.00	88.31
Neutrons	4.86	94.70	111.50
$\pi^{\pm b}$	3.01	6.53	11.52
$\mu^{\pm b}$	0.06	0.53	0.73
Gamma rays	10.40	47.95	18.94
$e^{\pm b}$	1.55	8.71	3.47
Total	20.21	172.42	234.47

[a]Assumed to deposit energy at point of their origin.
[b]Includes rest mass energy.

Additional data concerning the fluctuations for several particle types at several energies will also be presented.

1. Paper presented at the American Nuclear Society Meeting, June 10–15, 1973, Chicago, Illinois; published in *Trans. Am. Nucl. Soc.* **16**, 362 (1973).
2. Mathematics Division.
3. K. C. Chandler and T. W. Armstrong, *Operating Instructions for the High-Energy Nucleon-Meson Transport Code HETC*, ORNL-4744 (1972).
4. Harold L. Beck, *A Monte Carlo Simulation of the Transport of High-Energy Electrons and Photons in Matter*, HASL-213, Health and Safety Laboratory, USAEC (1969).
5. J. B. Birks, *The Theory and Practice of Scintillation Counting*, The MacMillan Company, New York (1964).

1.5 THE CALCULATED RESPONSE OF ALBEDO-NEUTRON DOSIMETERS TO NEUTRONS WITH ENERGIES ≤400 MeV[1]

R. G. Alsmiller, Jr., and J. Barish[2]

The calculated response of several albedo-neutron dosimeters that use ^{6}LiF as the neutron sensing element is presented for neutron energies ≤400 MeV. For each of the dosimeter geometries considered, results are presented for both monoenergetic and continuous incident neutron spectra and for both normally and isotropically incident neutron fluences. Data are given to indicate the effect on the response of an air gap between the dosimeter and the tissue phantom.

In general, it is found that the relative response of the dosimeters considered, i.e., the ratio of the neutron-absorption reactions in the ^{6}LiF to the dose equivalent in the tissue phantom, is not at all constant as a function of incident neutron energy as it would be for an ideal dosimeter.

1. Abstract of ORNL-TM-3984 (December 1972) and of paper submitted for journal publication.
2. Mathematics Division.

1.6 REACTION CROSS SECTIONS FOR 30- TO 60-MeV PROTONS ON VARIOUS ELEMENTS: COMPARISON OF THEORETICAL RESULTS WITH EXPERIMENT[1,2]

Hugo W. Bertini

The theoretical reaction cross sections that were calculated using an intranuclear-cascade model were compared with recent experimental results for protons at 30, 40, 50, and 60 MeV on complex nuclei. Fifteen reactions were selected arbitrarily, and the agreement was found to be within 10% in all 15 cases.

1. Work partially funded by the National Aeronautics and Space Administration under Order No. H-38280A.
2. Abstract of paper published in *Phys. Rev.* **C5**, 2118 (1972).

1.7 CALCULATIONS OF SPALLATION-FISSION COMPETITION IN THE REACTIONS OF PROTONS WITH HEAVY ELEMENTS AT ENERGIES ≤3 GeV[1]

R. L. Hahn[2] and H. W. Bertini

The intranuclear-cascade codes recently discussed by Bertini were modified to include fission-spallation competition in the *heavy elements* during the evaporation phase of the reaction and to use an empirical, energy-independent relation for (Γ_n/Γ_f). Calculations of the reactions of protons with ^{238}U at several energies from 0.15 to 3.0 GeV, and with ^{235}U and ^{232}Th at 0.7 GeV, have been done to illustrate the

results that are obtainable with these codes. The calculations do not allow any adjustment of parameters. However, the range of applicability of the calculations, especially their extension to nuclei (with $Z \lesssim 91$) that are not very fissionable, was investigated by means of the parameter Z_f, below which fission was taken to be relatively unimportant. A Z_f value of 91 was found to give results that agreed best with experimental data. In general, comparison with a large collection of experimental spallation yields, total fission cross sections, and particle multiplicities indicated that the calculations are able to reproduce the trends, and often the details, exhibited by the data. In the case of neutron multiplicities, only the calculations without fission effects agreed with the data, indicating that it is the energy available for evaporation, and not the fission competition, that influences neutron emission.

1. Abstract of paper published in *Phys. Rev.* **C6**, 660 (1972).
2. Chemistry Division.

1.8 SHIELDING OF MANNED SPACE VEHICLES AGAINST PROTONS AND ALPHA PARTICLES[1,2]

R. G. Alsmiller, Jr., R. T. Santoro,
J. Barish,[3] and H. C. Claiborne

In this report the available information on the shielding of manned space vehicles against protons and alpha particles is summarized. The emphasis in the report is on shielding against Van Allen belt protons and against solar-flare protons and alpha particles, but information on shielding against galactic cosmic rays is also presented.

The report is primarily intended as a handbook for nonexperts in space shielding. For the most part, the approximation methods discussed are those that are standard in the space-shielding literature. However, a large amount of numerical data, not previously published, on the validity of the various approximation methods is presented, and these data may be of interest to those who are familiar with space shielding.

1. Work funded by the National Aeronautics and Space Administration under Orders H-38280A and H-79272A.
2. Abstract of ORNL-RSIC-35 (November 1972).
3. Mathematics Division.

1.9 SHIELDING OF MANNED SPACE VEHICLES AGAINST GALACTIC COSMIC-RAY PROTONS AND ALPHA PARTICLES[1,2]

R. T. Santoro, R. G. Alsmiller, Jr., and K. C. Chandler[3]

Calculated results are presented of the absorbed-dose rates and dose-equivalent rates as a function of depth in tissue when galactic cosmic-ray proton and alpha-particle spectra are isotropically incident on a spherical shell shield with a tissue sphere at its center. Aluminum shield thicknesses of 5 and 20 g cm^{-2} are considered. It is found that the dose rates from incident alpha particles are comparable to those from incident protons, and for both protons and alpha particles there is a very appreciable contribution to the dose rates from nuclear-reaction products.

1. Work funded by the National Aeronautics and Space Administration under Order H-38280A.
2. Abstract of ORNL-TM-4029 (February 1973) and of paper to be published in *Nuclear Science and Engineering.*
3. Mathematics Division.

1.10 DKDATA: SUBROUTINE FOR RETRIEVING RADIONUCLIDE GAMMA-RAY DECAY DATA FROM RSIC DATA SET DLC-19/DECAYGAM[1,2]

J. W. Wachter

DKDATA is a subroutine written in Fortran IV which returns to the calling program information concerning the gamma-ray decay characteristics of a nuclide of specified atomic number and mass. These

data are initially read from the Radiation Shielding Information Center Data Set DLC-19/DECAYGAM on first entry to the subroutine, and the pertinent data for all nuclides of interest are stored for use in subsequent calls.

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1. Work funded by the National Aeronautics and Space Administration under Orders H-38280A and H-79272A.
2. Abstract of ORNL-TM-4095 (February 1973).

1.11 SPAR, A FORTRAN PROGRAM FOR COMPUTING STOPPING POWERS AND RANGES FOR MUONS, CHARGED PIONS, PROTONS, AND HEAVY IONS[1,2]

T. W. Armstrong and K. C. Chandler[3]

SPAR is a FORTRAN IV program that computes the stopping powers and ranges for muons, pions, protons, and heavy ions in any nongaseous medium at energies from zero to several hundred GeV. The method of calculation and the input required are described, and computed stopping powers and ranges for various particles slowing down in water and in tissue are given.

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1. Work partially funded by the National Science Foundation, Order NSF/RANN AG-399, and by the National Aeronautics and Space Administration, Order H-38280A.
2. Abstract of ORNL-4869 (May 1973).
3. Mathematics Division.

1.12 CALCULATIONS OF NEUTRON FLUX SPECTRA INDUCED IN THE EARTH'S ATMOSPHERE BY GALACTIC COSMIC RAYS[1,2]

T. W. Armstrong, K. C. Chandler,[3] and J. Barish[3]

Calculations have been carried out to determine the neutron flux induced in the earth's atmosphere by galactic protons and alpha particles at solar minimum for a geomagnetic latitude of 42°N. Neutron flux spectra in the energy range from $\sim 10^{-8}$ to $\sim 10^{5}$ MeV at various depths in the atmosphere were calculated using Monte Carlo and discrete ordinates methods, and various comparisons with experimental data are presented. The magnitude and shape of the calculated neutron-leakage spectrum at the particular latitude considered support the theory that the cosmic-ray-albedo-neutron-decay (CRAND) mechanism is the source of the protons and electrons trapped in the Van Allen belts.

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1. Work partially funded by the National Aeronautics and Space Administration under Order H-38280A.
2. Abstract of ORNL-TM-3961 (October 1972) and of paper to be published in *Journal of Geophysical Research.*
3. Mathematics Division.

1.13 THE CALCULATION OF HEAVY-ION INTERACTIONS[1]

H. W. Bertini, T. A. Gabriel, R. T. Santoro, and N. M. Larson[2]

The interactions of energetic nucleons ($E \gtrsim 100$ MeV) with complex nuclei have been shown to be reasonably well represented by the method of intranuclear cascades followed by evaporation.[3] In this method the life histories of each incident nucleon and all nucleons that interact with it are followed until they escape from the nucleus or are captured. Every interaction is assumed to be a free-particle-type interaction with the individual nucleons of the nucleus. These interactions are modified to include the effects of the Fermi motion of the bound nucleons, the changing nucleon density and changing nuclear

potential with nuclear radius, and the exclusion principle. After the life histories of all of the particles involved in these collisions (for each incident particle) are followed, the remaining nucleus is made to lose its residual excitation energy by particle evaporation.[4]

This approach and the associated computer programs are being adapted to the calculation of heavy-ion interactions. The underlying assumption is that at sufficiently high interaction energies (MeV per nucleon $\gg$ binding energy per nucleon) the heavy-ion reaction can be represented in large part as the high-energy interaction of two Fermi gas clouds. As the clouds merge, cascades develop simultaneously in both, with nucleons being knocked out of both, until they separate. Each cloud (nucleus), now generally reduced in mass and in a highly excited state, moves away from the other, losing its excitation energy by the "boil off" of particles.

As a first step in these calculations, the simultaneous development of the cascade in each nucleus is approximated in the following manner: if the incident heavy ion consists of A_p nucleons ($p \equiv$ projectile), then $A_p - Z_p$ neutrons and Z_p protons are sent into a stationary target nucleus one at a time, and the cascades for each of these nucleons are allowed to develop in the target, independently of the other incident nucleons. The nucleons of the projectile that interact in the target are removed from the projectile, leaving holes therein. The nucleons of the projectile that miss or simply pass through the target are considered to form a residual projectile (with the holes), and hence this fragment is in an excited state. The direction of the fragment is altered slightly from the initial projectile direction to account for the fact that the vector momentum of the particles (due to the Fermi motion) removed from the projectile does not, in general, add to zero. It is assumed that prior to the reaction the vector momenta of the Fermi motion of all of the particles within the projectile add to zero. When particles are removed, the vector momentum of the remaining particles is not zero, and hence the residual projectile is allowed recoil in the direction of the

Table 1.13.1. Fragmentation cross sections for fragments produced in the angular interval 0–0.1 deg from 29.4-GeV (2.1-GeV/nucl.) ^{14}N on carbon

Fragment	Cross section (mb)		
	Theory[a]		Experiment[b]
	A	B	
$^{7}_{3}$Li	1.7 ± 1.2	1.6 ± 0.61	9.1 ± 1.3
$^{7}_{4}$Be	2.2 ± 1.3	1.6 ± 0.61	8.0 ± 1.0
$^{9}_{4}$Be	1.0 ± 1.0	0.23 ± 0.23	3.0 ± 0.3
$^{8}_{5}$B	0	0	5.1 ± 0.6
$^{10}_{5}$B	5.6 ± 2.2	5.8 ± 1.1	14.4 ± 2.9
$^{11}_{5}$B	3.7 ± 1.7	6.4 ± 1.2	10.7 ± 1.3
$^{12}_{5}$B	5.0 ± 1.8	2.3 ± 0.7	1.9 ± 0.4
$^{9}_{6}$C	0	0	0.14 ± 0.02
$^{10}_{6}$C	0	0.23 ± 0.23	0.96 ± 0.12
$^{11}_{6}$C	10.0 ± 4.0	4.1 ± 1.0	11.3 ± 1.1
$^{12}_{6}$C	51.0 ± 6.0	51.8 ± 3.4	46.0 ± 9.0
$^{13}_{6}$C	44.0 ± 5.0	16.1 ± 1.9	9.2 ± 1.8
$^{12}_{7}$N	4.2 ± 1.6	0.23 ± 0.23	0.63 ± 0.13
$^{13}_{7}$N	42.0 ± 5.0	15.6 ± 1.9	7.7 ± 1.5

[a]Results in column A were obtained using "standard" nuclear configuration information. Results in column B were obtained using modified nuclear configuration information in which the diffuseness of the nuclear edge has been decreased.

[b]H. H. Heckman et al., *Phys. Rev. Lett.* 28, 926 (1972). Measurements were made at 0 deg.

resultant momentum. Both the residual target and projectile are in excited states and they are made to lose this excitation energy by particle evaporation.[4]

For this first step in the calculation, the cascade is allowed to take place in the target only, but this accounts for only half of the reaction; i.e., the weight of this event is $\frac{1}{2}$. The other half of the reaction is calculated by letting A_t ($t \equiv$ target) nucleons with appropriate energy strike the projectile (which is now assumed to be stationary) and by letting the cascade develop in the projectile. This calculation is carried out in the same manner described above, but at the end of the interacting process the results are transformed back to the laboratory frame. Each forward and corresponding "backward" calculation is repeated, using Monte Carlo techniques, until a sufficient number of samples representing the heavy-ion interactions has been taken.

A somewhat similar approach was tried for alpha particles on complex nuclei, where the alpha particle was assumed to consist of four nucleons impinging on a target.[5] The "backward" calculation was not included. The agreement of the calculated results with experimental data was fair.

It is acknowledged that there are many deficiencies in this approach; the most notable is probably the need to include the reduction in nuclear density as the cascade proceeds. However, the calculation of heavy-ion reactions is an extremely complicated problem that has heretofore defied formulation. The method being tried is our first attempt at penetrating the bulwarks of these reactions where existing programs need only be modified and not developed. Comparisons of the predicted results with experimental data are being made, but the supply of available data is extremely meager.

In Table 1.13.1 a comparison is made between two sets of calculated results and the experimental data of Heckman et al.[6] for 29.4-GeV nitrogen nuclei incident on carbon. The comparison is made for the angular interval of 0–4 mrad and for a velocity interval of 1–2% of the incident projectile velocity. The calculated results in the column labeled A were obtained using the nuclear configuration that has been accepted as the "standard" in the nucleon-cascade code.[3] The nuclear configuration defines the nuclear dimensions, nucleon-density distributions, and the Fermi energies for the projectile and target nuclei. The calculated results in the column labeled B were obtained using a modified nuclear configuration that decreases the diffuseness of the edge of the nucleus. The agreement between the calculated and experimental data is encouraging.

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1. Work partially funded by the National Aeronautics and Space Administration, Order H-38280A, and by the National Science Foundation, Order NSF/RANN AG-399.

2. Mathematics Division.

3. Hugo W. Bertini, *Phys. Rev.* **C6**, 631 (1972); *Phys. Rev.* **188**, 1711 (1969); and *Phys. Rev.* **131**, 1801 (1963), with erratum *Phys. Rev.* **138**, AB2 (1965).

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6. H. H. Heckman et al., *Phys. Rev. Lett.* **28**, 926 (1972).

1.14 PION DOSE CALCULATIONS[1]

T. W. Armstrong

The application of the Monte Carlo code HETC for performing pion-dose calculations is discussed, and several comparisons of calculated and measured depth-dose distributions induced by neutrons, protons, and negatively charged pions are presented. The use of the code to predict cell survival is also discussed.

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1. Abstract of ORNL-TM-3985 (October 1972) and of paper presented as a seminar on "Physics Input for Radiotherapy" at Los Alamos Scientific Laboratory, August 7, 1972.

1.15 A COMPARISON OF THE ABSORBED DOSE FROM NEGATIVELY CHARGED PIONS, PROTONS, AND NEUTRONS[1]

R. G. Alsmiller, Jr., R. T. Santoro, and J. Barish[2]

It is reasonably well established that negatively charged pions have physical properties that make them very favorable for use in cancer radiotherapy. The actual extent to which negatively charged pions are more suitable than protons or neutrons, however, is not well established. To obtain a partial answer to this question, calculations have been carried out with the high-energy transport code HETC[3–6] for beams of negatively charged pions and protons incident on tissue and with the O5R[7] code for a beam of neutrons incident on tissue. In all cases, the tissue was taken to be a slab 30 cm thick.

For both pions and protons, the incident beam was assumed to have a circular cross section with a radius of 1 cm and the particles in the beam were assumed to be normally incident on the tissue. The energy distributions of the incident pions and protons were determined so that the absorbed dose integrated over all radii would be approximately a constant over the depth interval of 14 to 16 cm. The numerical procedure used to determine these energy distributions is discussed in Appendix C of ref. 6. The actual energy distributions used in obtaining the results presented here are shown in Fig. 1.15.1.

The energy of the incident neutrons was assumed to be 15 MeV and the neutrons were assumed to emanate from a point 100 cm in front of the tissue; i.e., a source-to-skin distance of 100 cm was assumed. It was further assumed that the neutrons are emitted isotropically from the point source and only those neutrons in a solid-angle element with polar angle θ_s are incident on the tissue; i.e., it was assumed that all other neutrons are removed by a collimator. The tangent of the angle θ_s was taken to be $(115)^{-1}$; i.e., the incident beam was taken to have a radius of 1 cm at a depth of 15 cm into the tissue slab.

The calculated absorbed doses integrated over the indicated radial intervals are shown in Fig. 1.15.2 as a function of depth in the tissue slab for incident pions, protons, and neutrons. For comparison purposes, the proton and neutron absorbed doses have been normalized to be equal to the pion absorbed dose at the surface in each radial interval. To obtain absolute results in units of rad cm^2 (incident particle)$^{-1}$, the values given in Fig. 1.15.2 must be multiplied by the appropriate factor given in Table 1.15.1.

For all radial intervals other than the 0- to 1-cm interval, the ratio of the maximum absorbed dose to the surface absorbed dose is larger for incident pions than for incident protons. In the 0- to 1-cm interval, this is not the case, but, in considering this, it must be remembered that the incident proton and pion beams were assumed to have a circular cross-sectional area with a 1-cm radius. The pion absorbed dose for the 0- to 1-cm radial interval decreases with depth up to 12 cm because the pions are being removed from the radial interval being considered by multiple Coulomb scattering. Protons are also being removed from this radial interval by multiple Coulomb scattering, but the effect is more apparent for pions than for protons. Beyond the region of peak absorbed dose, the absorbed dose from the incident-pion beam is considerably larger than the absorbed dose from the incident-proton beam for all radial intervals considered. The neutron absorbed dose is a monotonically decreasing function (except for statistical fluctuations due to the fact that the calculations were performed using Monte Carlo techniques) of increasing depth for all radial intervals considered. For the same surface absorbed dose, the neutron beam

Table 1.15.1. Normalization factors

(The absorbed dose values in Fig. 1.15.2 must be multiplied by the appropriate value of N to obtain absorbed dose in units of [rad cm^2 (incident particle)$^{-1}$].)

Radial interval	N for pions	N for protons	N for neutrons
0–1.0 cm	1	1.81	0.113
0–2.5 cm	1	1.78	0.114
0–5.0 cm	1	1.70	0.117
0–∞	1	1.48	0.134

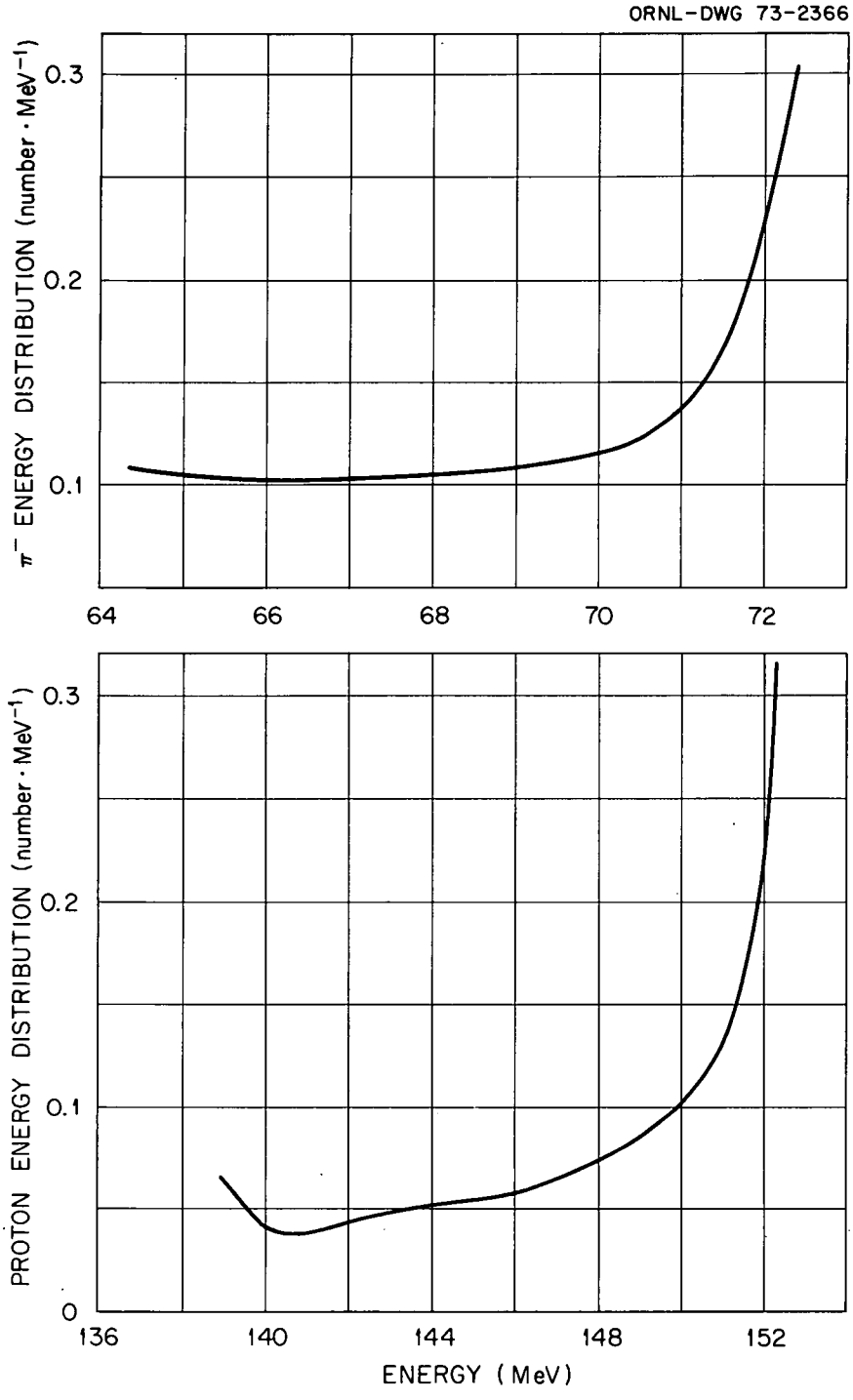

Fig. 1.15.1. Energy distribution of incident negatively charged pions and protons that will produce an absorbed dose that is approximately constant in the 14- to 16-cm depth interval in a 30-cm-thick tissue slab. Both distributions are normalized to unity.

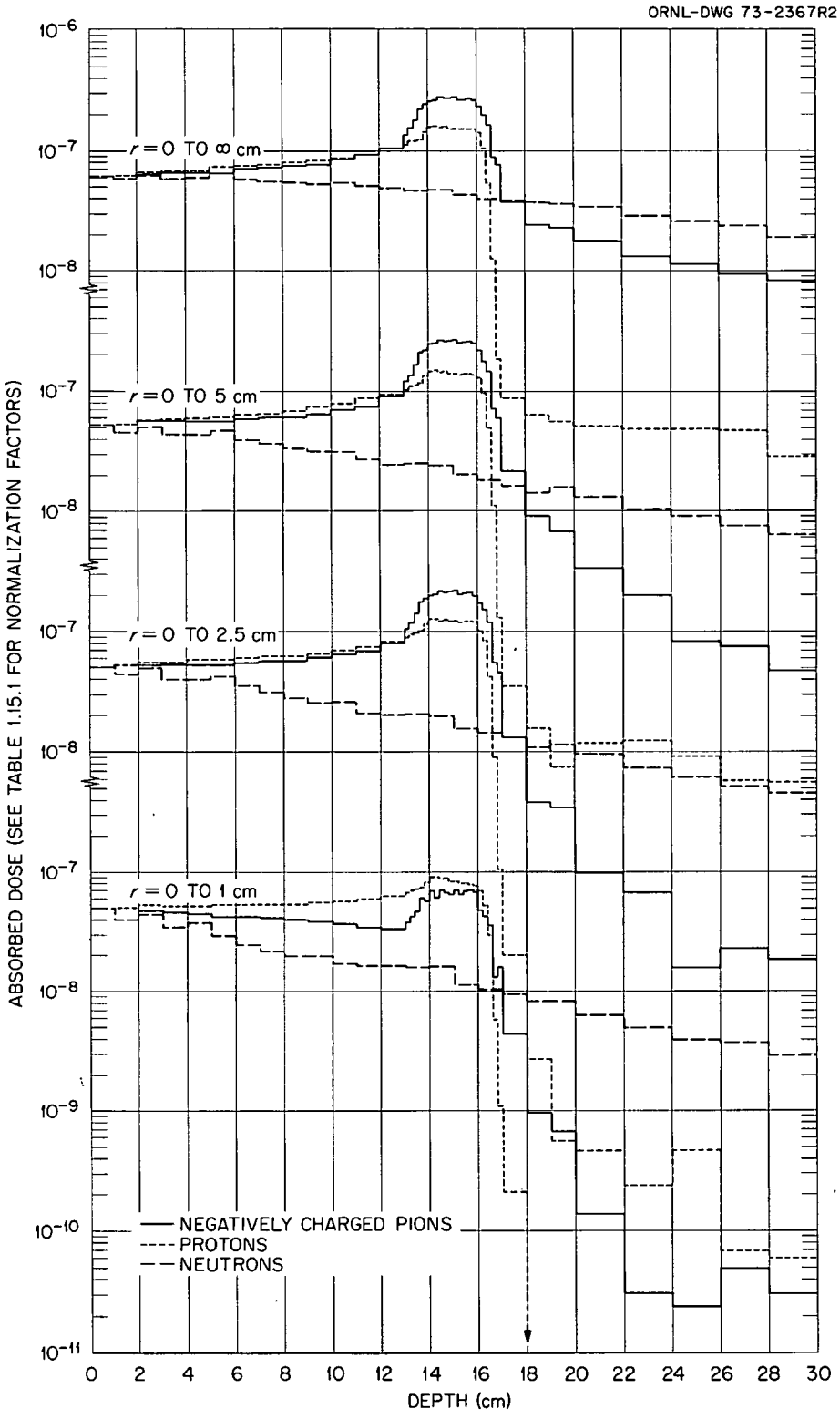

Fig. 1.15.2. Absorbed dose integrated over the indicated radial intervals vs depth in tissue for incident negatively charged pions, protons, and neutrons. (The beam parameters and geometry are described in the text.)

gives a higher exit dose in all radial intervals than does either the pion or proton beam. The results in Fig. 1.15.2 are, of course, dependent on the beam parameters used. In particular, the angle θ_s for neutrons is much smaller than that which usually will be used for patient treatment, and therefore the neutron results given in Fig. 1.15.2 are not realistic. Work is in progress to obtain results similar to those shown in Fig. 1.15.2 for a larger "tumor," and in this case the neutron-beam parameter will be more realistic.

The absorbed dose may not be an accurate measure of the biological damage and therefore may not provide a satisfactory basis for assessing the relative merits of the various particles for use in cancer radiotherapy. In obtaining the results presented in Fig. 1.15.2, the type, energy, and angular distribution of all of the particles that are produced in nuclear interactions have been obtained as a function of depth and radius. This is the information that is needed to calculate cell-survival probabilities as a function of position in tissue for the various types of incident particles. Work is in progress to obtain cell-survival-probability calculations for the cases considered in Fig. 1.15.2, and thus a comparison similar to that shown in Fig. 1.15.2 but based on cell survival will be available shortly.

The high-energy transport code HETC in its published form is not capable of treating incident alpha particles. However, the code has recently been modified, using an approximate model to predict particle production from alpha-particle-nucleus collisions,[8] and may now be used for incident alpha particles.[9] Calculations with this modified code are being carried out to obtain absorbed-dose and cell-survival-probability data for the case of an alpha-particle beam incident on a tissue slab. The beam parameters being used are similar to those used for incident pions and protons to obtain the results shown in Fig. 1.15.2; i.e., the alpha particles will be normally incident on the tissue and the beam will have a circular cross-sectional area with a radius of 1 cm. The energy distribution of the incident alpha particles will be such that the absorbed dose integrated over all radii is approximately constant over the 14- to 16-cm depth interval in the tissue slab.

Calculations of the absorbed dose and cell-survival probabilities for the case of ^{60}Co gamma rays incident on a tissue slab are also being carried out. The results in this case will be obtained with the photon transport code OGRE.[10] The geometry being used for incident ^{60}Co gamma rays is the same as that used for neutrons to obtain the results shown in Fig. 1.15.2 except that the source-to-skin distance is taken to be 80 cm and the tangent of the polar angle defining the solid angle in which the photons are incident is taken to be $(95)^{-1}$.

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1. Work funded by the National Science Foundation under Order NSF/RANN AG-399.

2. Mathematics Division.

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4. T. W. Armstrong and B. L. Bishop, "Calculation of the Absorbed Dose and Dose Equivalent Induced by Medium-Energy Neutrons and Protons and Comparison with Experiment," *Radiat. Res.* **47**, 581 (1971).

5. T. W. Armstrong and K. C. Chandler, "Monte Carlo Calculations of the Dose Induced by Charged Pions and Comparison with Experiment," *Radiat. Res.* **52**, 247 (1972).

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1.16 CALCULATION OF SPATIALLY DEPENDENT CELL-SURVIVAL PROBABILITIES[1]

T. W. Armstrong and K. C. Chandler[2]

A computer program that reads the particle transport data generated and stored on magnetic tape by the code HETC and computes spatially dependent (r and z) cell-survival probabilities, RBE, and OER using the model of Katz et al.[3] has been written and is operable. The program is applicable for incident pions, protons, and neutrons.

Cell-survival calculations have been made for the case of a negatively charged pion beam of circular cross section 2.5 cm in radius normally incident on an infinite slab of tissue 30 cm thick. The momentum distribution of the incident pions was specified to obtain a uniform π^--capture distribution in the depth interval from 12.5 to 17.5 cm. Results for single-port entry, where the beam is incident on one side of the slab, and double-port entry, where an equal number of pions is incident on both sides, have been computed.

Figure 1.16.1 shows, for two-port entry, the depth dependence of the absorbed dose and the OER, aerobic RBE, and cell survival for T-1 human kidney cells. These results were computed using the latest model parameters (which differ somewhat from the published values[3] for T-1 cells) provided by R. Katz. The incident pion fluence (8.6×10^8 pions/cm^2 from each side) was chosen to obtain 30% aerobic cell survival in the peak dose region. The RBE and OER are computed at the 10% survival level.

At present, experimental data on the spatial dependence of cell survival are not available to test the validity of the calculations. Experimental data on the spatial dependence of the cell survival of T-1 kidney

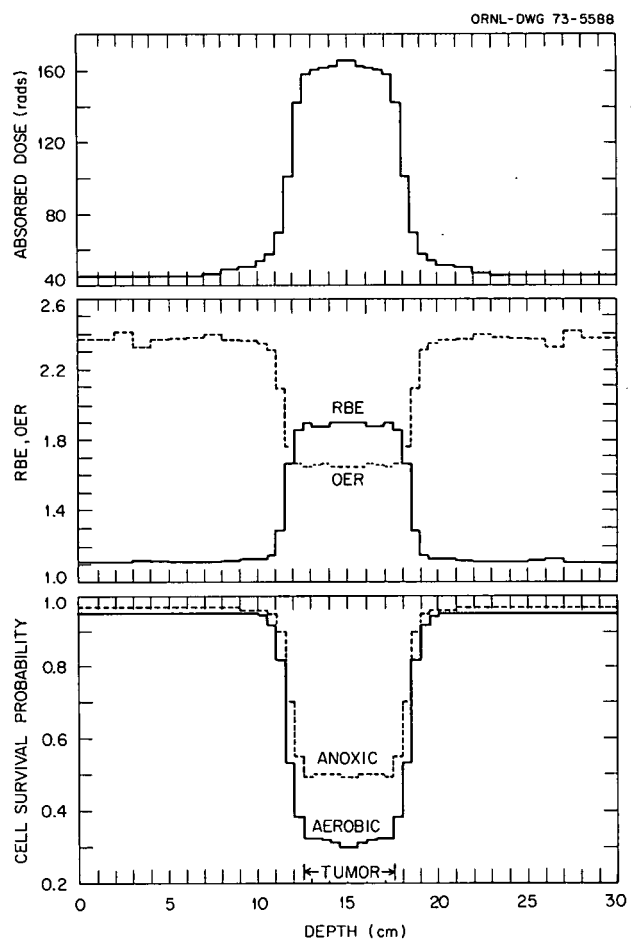

Fig. 1.16.1. Depth dependence within a 2.5-cm radius about the beam axis of the absorbed dose and OER, aerobic RBE, and cell survival under anoxic and aerobic conditions for T-1 human kidney cells produced by two opposing pion beams designed to give a uniform π^--capture density between depths of 12.5 and 17.5 cm.

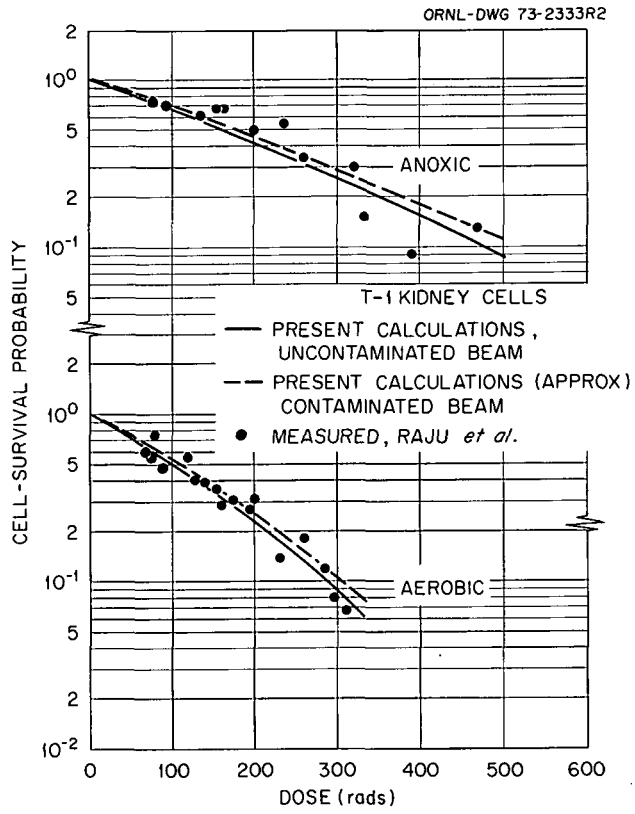

Fig. 1.16.2. Comparison of calculated and measured[8] cell survival probabilities for negatively charged pions.

cells for incident pions[4] and incident neutrons[5] are expected in the near future. These data should provide a definitive test of the calculations, and comparisons will be made as the data become available. In the interim, we have compared calculated and measured cell-survival probabilities for two cases which do not involve any spatial dependence. Barendsen and Broerse[6] have made measurements of the survival of T-1 kidney cells exposed to 14-MeV neutrons. We have used HETC to compute the energy spectra of secondary charged particles produced by 14-MeV neutron bombardment of tissue nuclei. These spectra and the Katz et al. model were used to calculate the cell-survival probability, and excellent agreement[7] with the experimental data was obtained. Also, Raju et al.[8] have placed T-1 cells in the stopping region of a pion beam and measured the cell survival. We have calculated the cell survival in the peak dose region (0- to 2.5-cm radius, 12.5- to 17.5-cm depth interval) for the beam considered in the calculations, and a comparison with the Raju et al. data is shown in Fig. 1.16.2. Since the beam used in the experiment was contaminated (65% pions, 10% muons, and 25% electrons), the calculated cell survival for a pure pion beam has been modified in an approximate manner to include the effects of the incident muons and electrons (for the same contamination fractions as in the experiment), and calculated cell survival for the contaminated beam is also shown in Fig. 1.16.2.

The program for calculating cell-survival probabilities seems to be working properly, and the program will now be used to compute the radial and depth dependence of cell survival, RBE, and OER for incident proton and neutron beams, as well as for other pion beams.

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1. Work funded by the National Science Foundation under Order NSF/RANN AG-399.
2. Mathematics Division.
3. R. Katz, B. Ackerson, M. Homayoonfar, and S. C. Sharma, "Inactivation of Cells by Heavy Ion Bombardment," *Radiat. Res.* **47**, 402 (1971).

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5. Paul Todd, Pennsylvania State University, private communication, 1972.

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1.17 CALCULATION OF THE DOSE INDUCED IN TISSUE BY NEGATIVELY CHARGED PION BEAMS[1,2]

T. W. Armstrong, R. G. Alsmiller, Jr., and K. C. Chandler[3]

Calculations have been carried out using the Monte Carlo radiation transport code HETC to determine the spatial distribution of the absorbed dose produced in tissue by monoenergetic negatively charged pion beams. The depth dependence of the absorbed dose has been computed for narrow (zero width) negative-pion beams incident normally on one side of a slab of tissue 60 cm thick. Beam energies of 53, 82, and 108 MeV (corresponding to ranges in tissue of approximately 10, 20, and 30 cm) were used. For the beam having a range of 20 cm, the absorbed dose as a function of the lateral distance from the beam axis has also been computed. The use of the results from monoenergetic beams to synthesize the incident-energy distribution needed to produce desired depth-dose distributions is discussed, and, as an example, the energy spectrum of the incident beam required to produce a uniform absorbed dose over the depth interval from 20 to 30 cm is computed.

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1. Work partially funded by Los Alamos Scientific Laboratory, Order CMI-7364-1, and by National Science Foundation, Order NSF/RANN AG-399.

2. Abstract of ORNL-TM-4078 (March 1973) and of paper submitted for journal publication.

3. Mathematics Division.

1.18 THE EFFECT OF BONE IN THE USE OF NEGATIVELY CHARGED PIONS IN CANCER RADIOTHERAPY[1]

R. T. Santoro, R. G. Alsmiller, Jr., and K. C. Chandler[2]

When negatively charged pions are used to irradiate a tumor, the pions may or may not pass through bone before coming to rest and being captured in the vicinity of the tumor. Since the composition of bone is considerably different from that of tissue, it is necessary to know how the presence of bone along the pion path should be taken into account in treatment planning.

To answer this question, calculations have been carried out with the high-energy transport code HETC[3] for cases with bone both present and absent. The model used is that of a zero-width beam of monoenergetic (53 MeV) negatively charged pions normally incident on a slab of thickness 30 g cm^{-2}. In the first case, the slab was composed entirely of tissue, while in the second case the slab was composed of tissue except that a 1.08-cm (= 2 g cm^{-2}) thick slab of bone was inserted at a depth of 1 g cm^{-2}; i.e., the bone began at a depth of 1 g cm^{-2} and ended at a depth of 3 g cm^{-2}. The case considered here for tissue only is one of the cases discussed in detail in ref. 3, and the method of calculation is the same as that described in ref. 3. The composition of bone was taken from ref. 4.

The absorbed dose integrated over the indicated radial intervals is shown in Fig. 1.18.1 as a function of depth in the slab. Note that the absorbed doses in the figure are expressed in ergs cm^{-1} (incident pion)$^{-1}$ to avoid any ambiguity about density, and the depth is expressed in g cm^{-2}. For all depths and all radial intervals considered, the differences between the solid and dashed histograms are within the statistical accuracy of the calculations. Thus, insofar as absorbed dose is concerned, the presence of bone near the surface of the tissue and well removed from the region where the pions are stopping and being captured may to a good approximation be taken into account by measuring depths in g cm^{-2}.

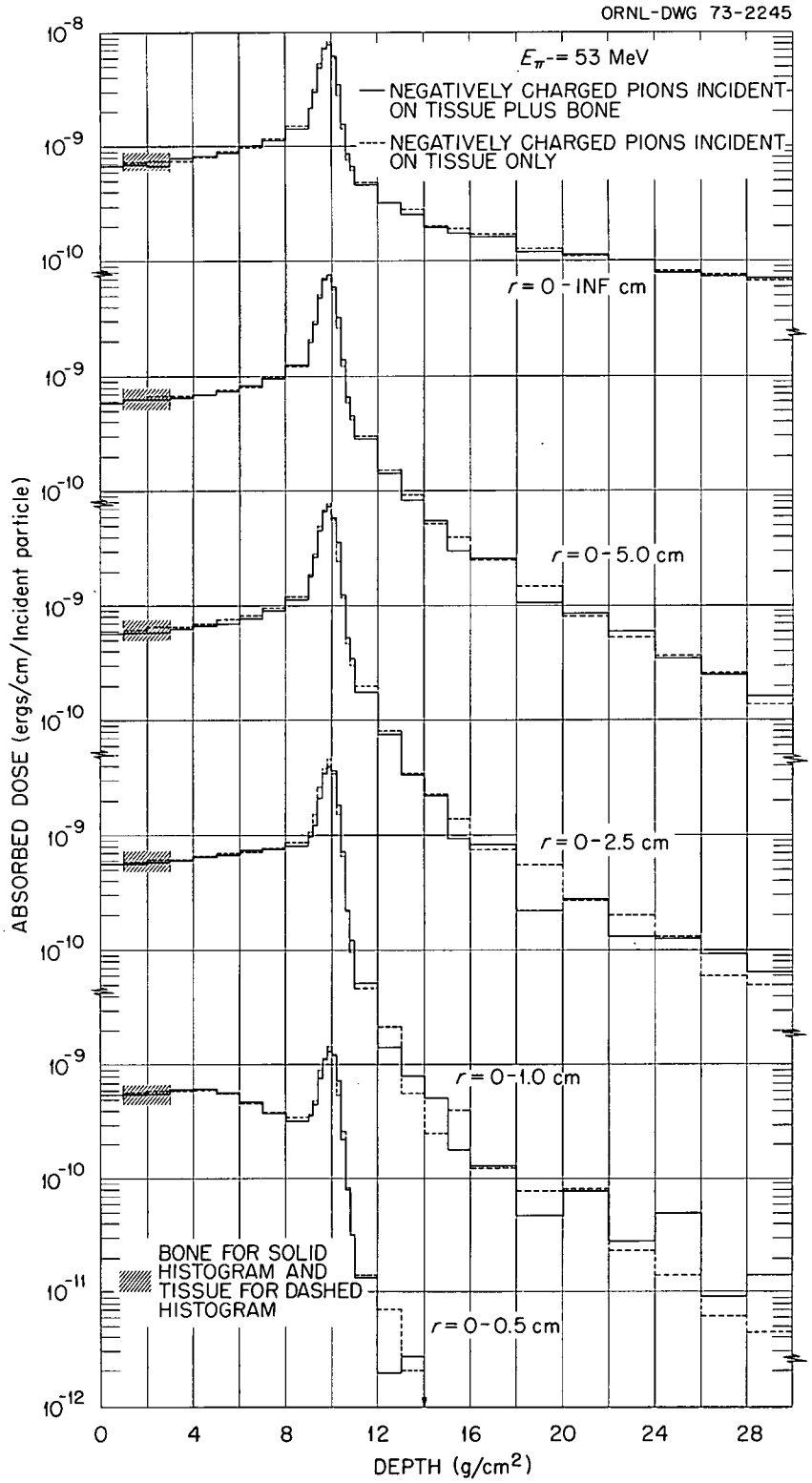

Fig. 1.18.1. Absorbed dose integrated over the indicated radial intervals vs depth in g cm^{-2}. (The tissue-bone configuration is described in the text.)

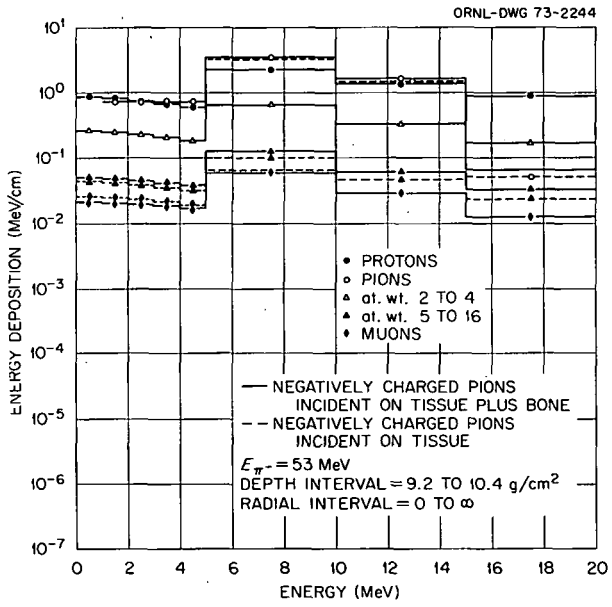

Fig. 1.18.2. Energy deposition per unit distance vs energy in the indicated depth and radial interval by various types of charged particles.

The absorbed dose may not be an accurate measure of the biological damage and therefore may not be a satisfactory basis for treatment planning with negatively charged pions. Work is in progress to compare cell-survival probabilities and LET spectra as a function of depth and radius for the two cases considered in Fig. 1.18.1, but results are not yet available. In the interim, some conclusions may be drawn from the energy-deposition spectra of the various types of charged particles.[5] In Fig. 1.18.2 the energy depositions per unit depth, i.e., the energy depositions per unit volume integrated over all radii, by various charged particles in the depth interval of 9.2 to 10.4 g cm^{-2}, i.e., in the vicinity of the maximum absorbed dose, are compared for the two cases considered in Fig. 1.18.1. When the dashed line does not appear, it is covered by the solid line. The differences between the corresponding spectra when bone is both present and absent are quite small. This is also the case in several other depths and radial intervals that have been considered and are not shown. On the basis of this information, it seems likely that the presence of bone near the surface of the tissue and well removed from the region where the pions are stopping and being captured may, when biological damage is considered, be to a good approximation taken into account by measuring depths in g cm^{-2}, but this conclusion must remain tentative until the cell-survival-probability calculations are available.

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1. Work funded by the National Science Foundation under Order NSF/RANN AG-399.
2. Mathematics Division.
3. T. W. Armstrong, R. G. Alsmiller, Jr., and K. C. Chandler, *Calculation of the Dose Induced in Tissue by Negatively Charged Pion Beams*, ORNL-TM-4078 (1973); submitted for journal publication.
4. J. F. Janni, *Calculations of Energy Loss, Range, Pathlength, Straggling, Multiple Scattering, and the Probability of Inelastic Nuclear Collisions for 0.1 to 1000-MeV Protons*, AFWL-TR-65-150, Air Force Weapons Laboratory, 1966.
5. See Appendix B of ref. 3 for a discussion of the manner in which energy-deposition spectra may be used in conjunction with weighting factors to assess biological damage.

2. Medium-Energy Nucleon Spectroscopy

2.0 INTRODUCTION AND SUMMARY

R. W. Peelle

Medium-energy nucleon spectra have been observed by our group both in the laboratory and near the top of the atmosphere. The first abstract in this section covers the final report of a neutron spectroscopy program using a balloon-borne scintillation spectrometer. This program was undertaken because of its practical as well as physics interest, because of the similarity of the needed techniques to those of our earth-bound spectrometry program, and because the high-energy shielding group can estimate neutron spectra in the atmosphere as an offshoot of their other work. Typical data are compared with those from experiments in Fig. 2.0.1. The work did not lead as we had hoped to extended studies aboard a satellite.

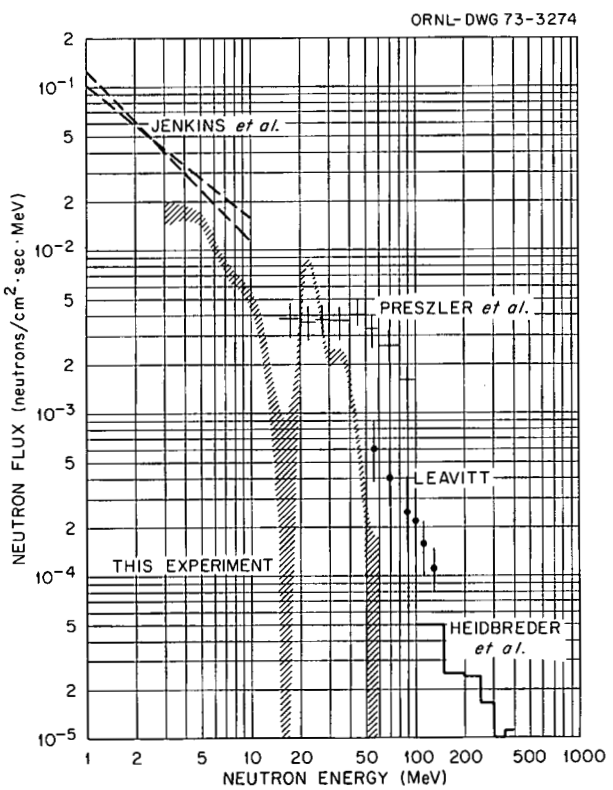

Fig. 2.0.1. Neutron spectrum measured by Zobel et al. at 9-g/cm^2 residual atmosphere at latitude 40 deg north, compared with the results of other experiments. The experimental conditions for these measurements varied, but altitude, latitude, and solar-cycle variations would have been expected to offset each other sufficiently to allow a direct comparison. The peaked structure near 20 MeV could have been induced by a difficulty in the discrimination between neutron- and photon-induced pulses in the liquid scintillator, but the overall magnitude below 30 MeV was almost unambiguously given by the data. In the experiment of Zobel et al., the spectrometer was held a considerable distance (100 ft) from the massive gondola supported by the balloon. This refinement was not possible in all the experiments.

Our program for measurements of differential cross sections for reactions of medium-energy protons is ending after a dozen years. The National Aeronautics and Space Administration supported the work to assure itself a strong technical base for handling the effects of nuclear reactions in the spacecraft shields that protect astronauts against the natural radiations in space. The work in earlier years included studies at the Harvard (160-MeV) and Chicago (450-MeV) proton synchrocyclotrons, but in recent years work has concentrated at the Oak Ridge isochronous machines, mostly using protons in the range from 30 to 65 MeV. The experiments have been distinguished by very broad coverage of the spectra of secondary particles as a function of angle and energy, as well as by a strong effort to include cross sections for both the outgoing neutrons and the charged particles. The group recognized at the outset that the primary charged particles produce the zero-order radiation damage to space crews and that actual shield analysis and probably even cross-section estimation for emission of the secondary radiations would be performed calculationally because the huge volume of data involved could not be obtained empirically. The role of our experiments was to validate if possible some form of intranuclear cascade (INC) or other calculational model which could be used to estimate the doubly differential cross sections from reactions in spacecraft shields. (Section 1 covers current theoretical efforts for space shielding.)

With considerable oversimplification, one can summarize here the overall conclusions reached so far in this program:[1]

1. For shield design purposes the intranuclear cascade model, particularly the local Bertini version, is appropriate and is still the only reasonable way to estimate broad-ranged secondary neutron and proton doubly differential cross sections over the studied range of incident energies. Proton, deuteron, and presumably neutron emission in the continuum region generally seem to be characterized by smoothly varying cross sections which are not dependent upon details of nuclear structure, and so do not change much going from one nuclide to its neighbor (except in the evaporation region where there are changes induced by Q-value variations). This observation, along with the model's quantitative success, supports use of the INC model. Cross sections at backward angles are badly underestimated but are not apt to have importance for shielding studies as much as for theoretical understanding and perhaps for practical importance around high-energy accelerators such as meson factories. Certainly for thin shields, the average effect of differences between INC theory and experiment can be of no importance wherever the reaction products yield only first-order corrections to the result. The 10% to 40% differences in angle-integrated emission spectra observed for incident energies of 30 to 60 MeV are more apt to be important in the assessment of a damage function such as that for fast neutrons >12 MeV in tissue.

2. For the incident energy region from 30 to 60 MeV which our group has investigated most exhaustively, the coupling of the Bertini INC with the Dostrovski-type evaporation analysis does not accurately reproduce either the ratio of protons to alpha particles or the approximately correct spectral balance of high- and low-energy charged particles, particularly for medium-weight targets. (Studies are not now sufficiently complete to allow final assessment of this question for neutrons.) We believe that the source of the difficulty can be broken down among three identified effects. First, the inverse cross sections in the Dostrovski evaporation system are inadequate and by their nature provide an underestimate of alpha-particle production. Second, there is evidence in the preequilibrium model studies of Kalbach-Cline that even the low-energy portion of the emitted alpha-particle spectrum may predominantly originate in preequilibrium rather than equilibrium reactions. In oxygen and carbon, where (n,α) reactions analogous to the (p,α) reactions in our experiments are important in the estimation of tissue damage from incident neutrons, these two difficulties combine with the tendency of these nuclides to fragment as alpha particles. Finally, at least for the incident energy region below 100 MeV for targets as heavy as Al, the angle-integrated nucleon spectra fall ~30% below observations for the higher-energy portion of the spectra where evaporation processes can't influence results. Because of this, the model provides too great an average excitation energy to the equilibrium portion of the reaction process, with the consequence that too many model particles are boiled off. In the incident energy region most extensively studied, the underestimate of the cascade contribution may originate at least in part from neglect in the model of preequilibrium emission of energetic nucleons in the decay of deep-lying hole states generated by primary knockout reactions. In the INC models the excitation energy associated with these hole states is assumed to go entirely into excitation energy available for boiloff reactions, while preliminary studies with the Kalbach-Cline exciton model indicate that preequilibrium nucleon emission should be important.

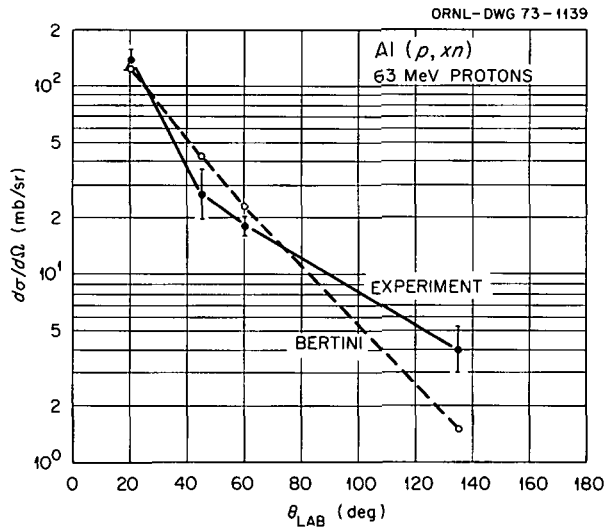

Fig. 2.0.2. Differential cross section for emission of neutrons over ~10 MeV in reactions of 63-MeV protons with Al. The experimental points are the preliminary ORNL values of Wachter et al., while the calculated ones are from the intranuclear cascade model of Bertini.

3. Where nuclear collective effects are important the INC model is not expected to reproduce the detailed features of the energy spectra, but sum rules are interpreted to suggest that overall intensity estimates are not degraded by this difficulty because the INC model conceptually includes all the single-particle transitions. The possibility has not yet been excluded that a strongly forward-peaked differential cross section from a collective effect, like excitation of the isobaric analogue of the ground state of the target in a (p,n) reaction, could produce a significant error in penetration analysis of a thick shield. In practice this underestimate would be offset by the tendency of the INC model to overpredict, at least for incident energies below 100 MeV, the importance of simple quasifree scattering.

4. The exciton model of preequilibrium reactions is able to cope semiquantitatively with the angle-integrated spectra of the several types of emitted charged particles, including d, t, ^{3}He, and alpha. No other model has been worked out which even begins to explain the high-energy components of the observed spectra of complex particles.

Since the most-employed INC model was and is developed and used within the closely allied space shielding theoretical group, good feedback of data and ideas has always been possible between experimental and theoretical groups concerning the properties of the INC model and the effects of possible modifications in it. In our experimental work there has been considerable overlap between the techniques and equipment used in these studies and in the neutron and gamma-ray spectroscopy associated with neutron interactions in the lower energy region. Such economies of scale are of course to be expected in a large active laboratory.

Papers 2.2, 2.3, and 2.4, which deal with these studies, reflect the final reporting of the experiments observing charged particles and interim reporting of the analogous results for neutrons using flight-time spectroscopy. Figure 2.0.2 shows typical results for neutron emission. Paper 2.5 represents a delayed final publication of work done much earlier in a systematic exploration of reaction mechanisms in the energy range accessible to the tandem Van de Graaff.

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1. This summary excludes advances of experimental and data-analysis techniques that have been made available to aid work in other fields. The work of Burrus et al. on spectrum unscrambling sponsored under this program has proved to be particularly important.

2.1 MEASUREMENT OF THE NEUTRON ENERGY SPECTRUM AT 9 g/cm^3 RESIDUAL ATMOSPHERE[1,2]

W. Zobel, T. A. Love, J. T. DeLorenzo,[3] C. O. McNew,[3]
R. H. Baldry,[3] and H. W. Parker[4]

An experiment to measure the neutron energy spectrum at an altitude corresponding to 9-g/cm^3 residual atmosphere was performed near solar maximum. The nondirectional spectrometer employed was flown at geomagnetic latitude 40° N from Palestine, Texas, on June 17, 1969. The experimental arrangement is described, the data reduction scheme is discussed, and the results are presented for the neutron spectrum in the energy range from 3 to 60 MeV. The spectrum is compared with those from other experiments and from calculations. The intensity is greater than the calculations of Lingenfelter after application of an altitude correction, but is lower than the measurement of Preszler, Simnett, and White and the calculations of Armstrong, Chandler, and Barish.

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1. Work funded by USAEC Activity 05 03 02; flight costs and participation by NASA personnel provided by NASA-MSFC (Space Science Laboratory), Huntsville, Alabama.

2. Abstract of ORNL-TM-3877 (June 1973); a preliminary version of this abstract was published in last year's annual report.

3. Instrumentation and Controls Division.

4. Marshall Space Flight Center, Huntsville, Alabama.

2.2 COMPLETE HYDROGEN AND HELIUM PARTICLE SPECTRA FROM 30- TO 60-MeV PROTON BOMBARDMENT OF NUCLEI WITH A = 12 TO 209 AND COMPARISON WITH THE INTRANUCLEAR CASCADE MODEL[1,2]

F. E. Bertrand[3] and R. W. Peelle

Differential cross sections for the production of proton, deuteron, triton, helium-3, and alpha particles from as many as ten targets (A = 12 to 209) were measured using 29-, 32-, and 62-MeV incident protons. The particles were detected, with ≈0.2-MeV (FWHM) energy resolution for protons, over a secondary energy range of ≈2-6 to 62 MeV in a total absorption telescope composed of three solid-state detectors. Representative results are shown for cross sections differential in energy and angle, as well as for angle- and energy-integrated cross sections. For incident 60-MeV protons the integral magnitude of the non-evaporation charged-particle production is found to be $\sim 10^2\ A^{1/3}$ mb. Fewer protons but more complex particles were measured for carbon and oxygen targets than expected from an $A^{1/3}$ dependence for either component alone. The continuum cross sections for $Z = 1$ particles at a given angle (mb-sr^{-1}-MeV^{-1}) are nearly independent of incident energy when measured with incident protons in the 30- to 60-MeV energy range. Nonevaporation production of complex particles ($A \geqslant 2$) is 25 to 40% of that for protons.

The proton spectra have been compared with predictions from the intranuclear cascade model. Differential spectral predictions compare well with the measured spectra for angles in the range ~25 to 60 degrees, and relatively poor predictions for small and large angles are more favorable when reflection and refraction by the potential well are included. Evidence is given that predictions for backward angles are greatly improved by allowing proton scattering from nucleon pairs within the model nucleus, but the A-dependent underprediction at extreme forward angles is not understood at all. The calculated angle-integrated spectra reproduce the measured spectral shape but consistently predict ≈30% too few nonevaporation protons for targets with $A \geqslant 27$.

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1. Work supported by National Aeronautics and Space Administration under Order L-12, 186.

2. Abstract of paper accepted for publication in *The Physical Review.*

3. Physics Division.

2.3 CROSS SECTIONS FOR HYDROGEN AND HELIUM PARTICLES PRODUCED BY 61-, 39-, AND 29-MeV PROTONS ON CARBON AND OXYGEN[1,2]

F. E. Bertrand[3] and R. W. Peelle

Tabulated differential cross sections are presented for proton, deuteron, triton, helium-3, and alpha particles produced in reactions of 61-, 39-, and 29-MeV protons with carbon and oxygen. Observations with energy resolution as fine as 200 keV were made at 2, 5, and 19 angles, respectively, for carbon and at 1, 4, and 18 angles for oxygen. Spectra are given in bins 1 to 5 MeV wide for energies above a cutoff of 2 to 6 MeV which is dependent on particle type. For 61-MeV incident protons on carbon, angular distributions are given for energy-integrated cross sections for emission of each of the five observed particles and for excitation of prominently excited states. Similar data are given for the oxygen target, except that few angular distributions are given for excitation of specific states. Angle-integrated energy spectra in both center-of-mass and laboratory systems are presented for each of the five outgoing particles. Since plastic scattering foils were used, cross sections for *p-p* scattering were obtained which proved to be consistent with interpolated values from the literature. Data analysis procedures are described and experimental uncertainties are tabulated.

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1. Work supported by National Aeronautics and Space Administration under Order L-12, 186.
2. Abstract of ORNL-4799 (July 1973).
3. Physics Division.

2.4 DIFFERENTIAL CROSS SECTIONS FOR CHARGED-PARTICLE EMISSION IN REACTIONS OF 59-MeV ALPHA PARTICLES WITH ^{12}C, ^{16}O, AND ^{54}Fe: COMPARISON WITH THE EXCITON MODEL OF PREEQUILIBRIUM PARTICLE EMISSION[1,2]

F. E. Bertrand,[3] R. W. Peelle, and C. Kalbach-Cline[4]

Cross sections differential in energy and angle are presented for the *p, d, t,* and alpha particles from reactions of 59-MeV alpha particles on C, O, and ^{54}Fe, and the angle-integrated differential spectra are compared with the predictions of an extended exciton model of preequilibrium reactions. The experimental results were obtained with a semiconductor telescope spectrometer and cover the whole energy range above a few MeV. Except for oxygen, the results are given with uncertainties of 5% to 10%; for oxygen relative intensities are valid at a given angle, but the absolute uncertainty is about 50%. The high-energy segment of the spectrum is highly anisotropic for all emitted particles, but for low energies the evaporation mechanism may be important for proton and perhaps alpha-particle emission. The inelastic alpha spectra from ^{54}Fe are more similar in shape to previous observations of the ^{54}Fe(p,xp) spectra than to the presently reported ^{12}C$(\alpha, x\alpha)$ results. Comparisons are made between the data and the exciton model assuming an initial configuration of four particles. The model was extended to recognize that for reactions of incident alpha particles the intensity of emitted alpha particles may constitute a significant fraction of the preequilibrium emissions. The empirical internormalization factor for the relative intensity of various exit particles (mass number m) is found to be consistent with the $m!$ value deduced previously from results with incident protons.

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1. Work partially supported by the National Aeronautics and Space Administration under Order L-12,186 and partially by the National Science Foundation.
2. Abstract of paper to be submitted to *The Physical Review.*
3. Physics Division.
4. Nuclear Structure Research Laboratory, University of Rochester, Rochester, New York; now at SPNBE, CEN de Saclay, 91 Gif-sur-Yvette, France.

2.5 ELASTIC AND INELASTIC SCATTERING OF 12-MeV PROTONS FROM ^{92}Mo, ^{94}Mo, ^{96}Mo, AND ^{100}Mo: TABULATED DIFFERENTIAL CROSS SECTIONS[1]

J. K. Dickens, E. Eichler,[2] R. J. Silva,[2] and I. R. Williams[3]

Numerical values of differential cross sections for elastic and inelastic scattering of 12.0-MeV protons from ^{92}Mo, ^{94}Mo, ^{96}Mo, and ^{100}Mo are reported in tabular form. Cross sections were determined at 5-deg intervals between laboratory angles of 20 and 165 deg. Inelastic scattering data are reported for 23 excited states of ^{92}Mo, 14 excited states of ^{94}Mo, 2 excited states of ^{96}Mo, and 6 excited states of ^{100}Mo.

1. Abstract of ORNL-TM-3913 (September 1972).
2. Chemistry Division.
3. Knoxville College, Knoxville, Tennessee.

3. Weapons Radiation Cross-Section Studies

3.0 INTRODUCTION AND SUMMARY

F. G. Perey

The Division is engaged in essentially all the activities supported by the Defense Nuclear Agency for the express purpose of compiling a large body of cross-section data for use in weapons radiation transport calculations (see Section 4). Having established a Working Cross Section Library at ORNL's Radiation Shielding Information Center, DNA supports measurements of differential cross sections for all the elements included in the Library (see Section 5), as well as experimental tests of full sets of cross sections. In addition, the Agency supports a cross-section evaluation program in which all available experimental cross sections for a given element are evaluated and additional cross sections are calculated as required.

Our participation in the experimental phase of this program includes measurements of neutron-scattering and gamma-ray-production cross sections and experimental checks of evaluated sets of cross sections (total, neutron scattering, and gamma-ray production). It also includes experimental checks of the techniques employed for using the cross sections in the transport calculations. All this work is performed at the Oak Ridge Electron Linear Accelerator (ORELA), where a pulsed-neutron beam having energies up to 20 MeV is available as a source. In addition, we have the responsibility for evaluating, maintaining, and updating specific cross-section sets, which involves the development of nuclear models for cross-section calculations. These various phases of our program are summarized below, with reference to papers in which more detail can be found.

Cross-Section Measurements

For the differential cross-section measurements, a thin sample of the nuclide of interest is placed in the ORELA pulsed-neutron beam, and the neutrons or gamma rays emerging at various angles from the beam are detected with NE-213 and NaI spectrometers respectively. The energies of the neutrons incident on and interacting with the sample are determined by time-of-flight techniques, and the energies of the detected particles are determined by spectral unfolding techniques. The thinness of the sample essentially precludes interactions of the secondary particles within the sample or successive interactions of the incident neutrons, so that the data can be directly reduced to cross sections.

To date most of our cross-section measurements have centered on gamma-ray-production cross sections. Because of significant differences between our first gamma-ray measurements and comparable measurements at other facilities, we delayed large-scale acquisition runs until we could perform a number of tests to verify our experimental technique. Having since gained great confidence in our method, we have embarked on a vigorous data-acquisition program which through FY 1973 has resulted in measurements of gamma rays emitted at angles of 125 and 90 deg for seven different nuclei (C, N, O, Mg, Al, Si, and Ta) and at an angle of 125 deg for three additional nuclei (Ca, Fe, and Cu). Most of the data for these ten nuclei have been reduced to cross sections, with several papers and reports having been published this year (see papers 3.1–3.3).

In view of the wealth of gamma-ray-production data released, we cannot comment here on all the results; however, we do point out that our data for nitrogen are particularly significant. Correct predictions of gamma-ray production by neutron interactions with the nitrogen of the atmosphere are essential to predictions of the gamma-ray fields produced by nuclear detonations, and discrepancies between two widely used gamma-ray-production cross-section sets for nitrogen are of long standing. Our results have

apparently resolved these discrepancies (see paper 3.4), since they strongly support the cross sections included in the DNA library as MAT 4133, Mod. 2 (a set evaluated by P. G. Young and D. G. Foster, Jr., of Los Alamos Scientific Laboratory). The validity of the cross sections will be investigated further when experimental data for nitrogen are obtained that can be compared with the results of transport calculations based on the evaluated cross sections (see next discussion).

Experimental Checks of Cross-Section Sets and Calculational Techniques

The experiments that check the validity of cross-section sets and calculational techniques vary with the particular type of test desired. For checks of total neutron-interaction cross sections, a relatively thick sample of the material of interest is placed in the pulsed-neutron beam and the neutrons transmitted uncollided through the sample are detected by an NE-211 plastic scintillator on the opposite side. With transmission in the sample taken into account, the total cross-section set for the element can be compared directly with the experimental results. This technique was used in FY 1973 to test the total cross sections for neutron energies from 0.2 to 20 MeV on nearly all elements for which DNA supports cross-section evaluations. The results for C, O, Al, Si, Ca, Fe, and SiO_2 have been reported (see paper 3.5), and with the exception of oxygen, all the total cross-section sets for these materials were found to be seriously deficient in some energy regions, particularly below 1 MeV. Thus further tests of revised sets for these elements may be necessary. Additional measurements for magnesium and copper have not yet been reduced.

The technique developed for testing neutron-scattering cross-section sets employs an NE-213 neutron detector placed along the axis of a ring-shaped sample that is coincident with the beam axis. The sample is preceded in the beam by a shadow shield whose diameter is such that the shield does not intercept neutrons directed toward the ring sample but does protect the detector from all neutrons except those scattered from the sample. The data are converted to time-dependent neutron spectra by unfolding the pulse-height spectra for particular time bins. The measurements are designed to maximize the count rate in order to provide adequate statistics for unfolding. They are also designed to minimize the time-of-flight between the point of scattering and the detector so that the time dependence of the unfolded spectra is closely correlated with the incident neutron energy, which is determined by the time of flight from the linac target to the ring sample. In some of the measurements structure is introduced in the data by filtering the linac beam through a thickness of the same material as the scattering sample itself.

During this year neutron-scattering measurements were made and reported for a carbon-ring sample at three scattering angles and for an iron-ring sample at one scattering angle, the latter with and without a filter in the beam (see paper 3.6). Other measurements were for samples of nitrogen and oxygen (water); however, the data reduction was not completed. (The calculations with which these results are compared are performed by another group; see paper 4.14.)

In general, tests of sets of gamma-ray-production cross sections have not yet been performed, although a few measurements have been made using a NaI detector and the same experimental arrangement used to check neutron-scattering cross sections. Preparations for such measurements were made during FY 1973, however, and these included an extensive study of the NE-213 detector as a gamma-ray detector. A response matrix obtained for the detector was cross calibrated with the response matrix for an NaI detector. This was done by performing measurements on radioactive sources using both the NE-213 and the NaI detector and unfolding the data from both detectors using as a window function the resolution function of the NE-213 detector. Having satisfied ourselves that the NE-213 detector can be operated reliably as a gamma-ray spectrometer with radioactive sources, we are studying its reliability for simultaneously detecting neutrons and gamma rays. If this capability is verified, checks of neutron-scattering cross-section sets and gamma-ray-production cross-section sets can be performed in the same experiment. Preliminary measurements have already been made for samples of oxygen (water), nitrogen, carbon, and iron.

Since these tests of various cross-section sets are effected by comparison with the results of transport calculations, the experiments also serve as cross checks of the calculational techniques. Other experiments, only one of which was performed this year, are designed to test specific facets of a calculational method. During FY 1973 an experiment of this type consisted of measurements of neutrons scattered from a 6-in.-long cylindrical sample of carbon. The results were used to test the transfer matrices for anisotropic

inelastic neutron scattering generated by AMPX, a modular computer code system that produces coupled neutron and gamma-ray cross sections for transport calculations (see paper 4.5).

Cross-Section Evaluations

Of the DNA-sponsored cross-section evaluations under way, ORNL now has the responsibility for silicon, calcium, iron, and lead, with magnesium to be added shortly. The evaluations cover all neutron-induced reactions in these elements from thermal energy to 20 MeV. Each evaluation is performed by analyzing all available experimental data on the element, with nuclear models used as tools in assisting the evaluation. For those energy regions in which no data are available, the cross sections are generated through the use of nuclear models alone. Thus a phase of this work is the study of nuclear models and the development of computer codes to implement any calculations required for specific aspects of the evaluations. Promising nuclear theories or concepts are investigated on a low-priority basis to ascertain their potential usefulness in evaluation work. In addition, the analyses of integral experiments aimed at validating the evaluated cross sections are studied to determine whether further revision of the cross-section sets are required.

Since we did not assume responsibility for silicon until late in the fiscal year, the work on this element has not yet progressed to the point that an evaluation is ready for release. However, evaluations have been released for the other three elements (see paper 3.7), and updated evaluations for calcium and iron are nearing completion. Since this is an ongoing program to provide cross sections in the specific detail needed for weapons radiation transport calculations, there is considerable interaction between the evaluators and those persons performing the calculations, as well as between the evaluators and those persons performing cross-section measurements.

LSA

3.1 SECONDARY GAMMA-RAY-PRODUCTION CROSS SECTIONS FOR SEVERAL MATERIALS[1,2]

G. L. Morgan, T. A. Love, J. K. Dickens, and F. G. Perey

Absolute gamma-ray-production cross sections have been measured as a function of the energy of both the incident neutron and the emitted gamma ray for tantalum, iron, silicon, and carbon. ORELA was used to produce a pulsed-neutron beam that impinged on a thin sample of the material at the 47-m flight-path station. Time-of-flight techniques were employed to determine the incident neutron energy, which covered a range up to 20 MeV. Gamma rays emitted from the samples at angles of 90 and/or 125 deg from the incident beam were detected with a 12.7 by 12.7 cm NaI crystal. The gamma-ray energies, varying between 0.7 and 10.6 MeV, were determined by unfolding the pulse-height spectrum of the detector. Detailed tables of the cross sections were transmitted to the National Neutron Cross Section Center. Figures 3.1.1 and 3.1.2 illustrate the type of data obtained for tantalum.

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1. Work supported by Defense Nuclear Agency under Subtask PC101.

2. Abstract of paper presented at American Nuclear Society National Topical Meeting on New Developments in Reactor Physics and Shielding, Kiamesha Lake, N.Y., September 12–15, 1972.

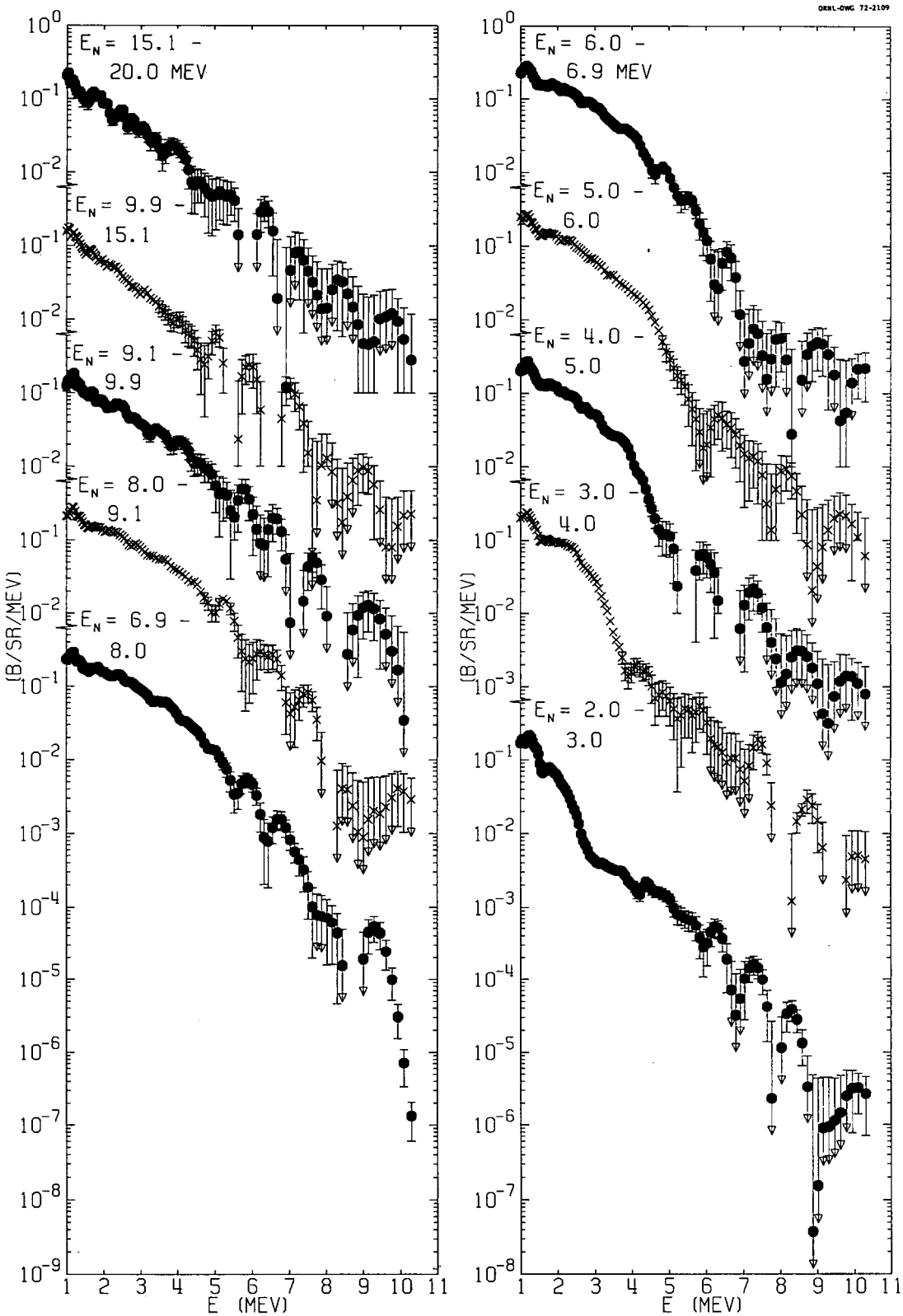

Fig. 3.1.1. Gamma-ray-production cross sections for tantalum for incident energies of 2 to 20 MeV and a gamma-ray emission angle of 125 deg. E = gamma-ray energy; E_n = neutron energy.

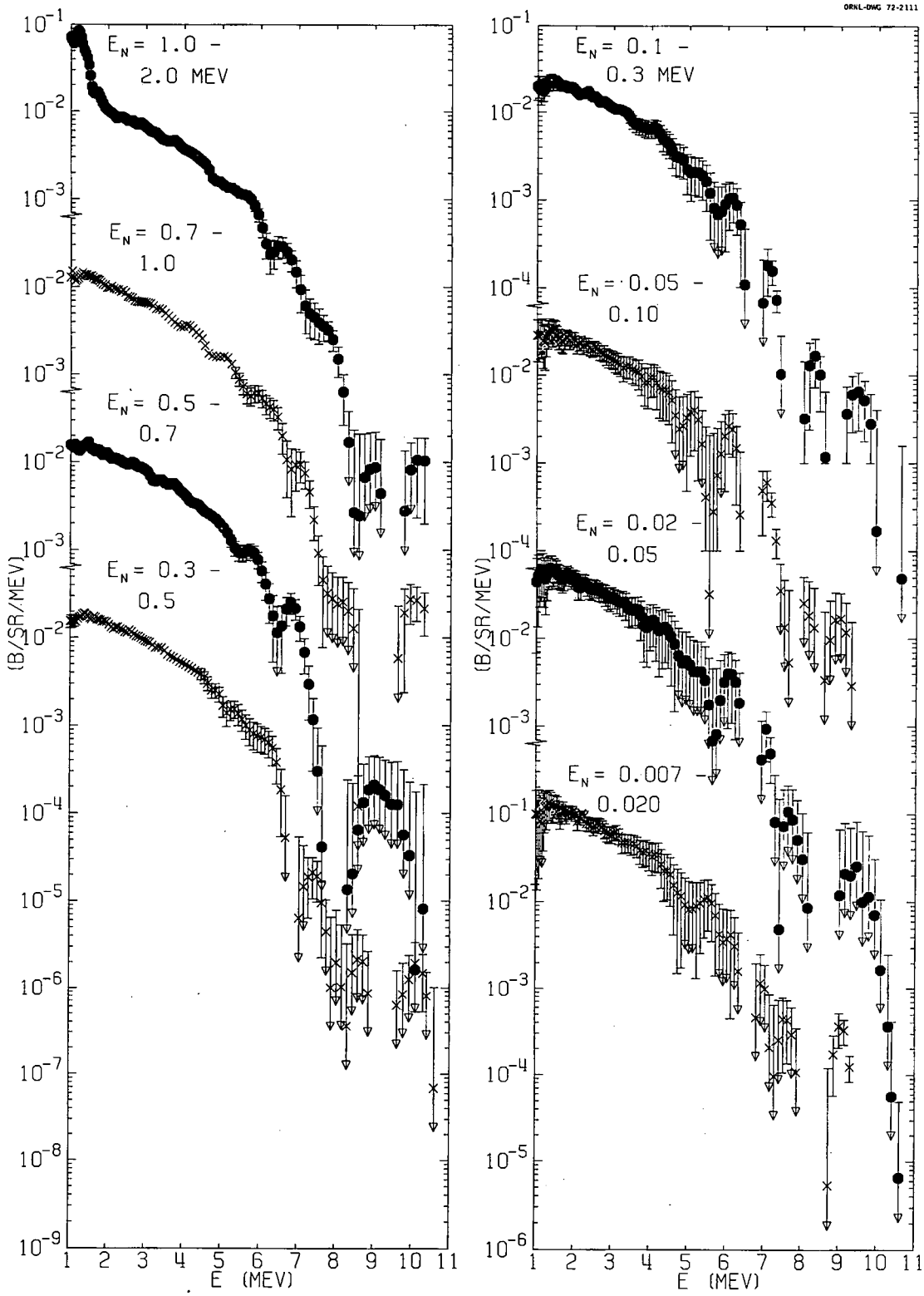

Fig. 3.1.2. Gamma-ray-production cross sections for tantalum for incident energies of 0.02 to 2 MeV and a gamma-ray emission angle of 125 deg. E = gamma-ray energy; E_n = neutron energy.

3.2 Cu($n,x\gamma$) REACTIONS[1,2]

J. K. Dickens, G. L. Morgan, and
G. G. Slaughter[3]

Gamma-ray production due to neutron interactions with copper is being studied using three different experimental arrangements. Production cross sections from natural copper for $1.0 \leqslant E_n \leqslant 20$ MeV suitable for shielding calculations are being measured at the 50-m station of the Oak Ridge Linear Accelerator (ORELA) using a NaI detector system.[4] Spectra were also obtained for small enriched isotopic samples of ^{63}Cu and ^{65}Cu using a Ge(Li) detector and 4.9-MeV neutrons produced using a Van de Graaff.[5] In addition, spectra were obtained from natural copper at the 10-m station of the ORELA for $0.5 \leqslant E_n \leqslant 10$ MeV using a Ge(Li) detector system.[6] The two sets of Ge(Li) data are being studied to obtain spectroscopic information.

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1. Work partially supported by the Defense Nuclear Agency under Subtask PC101.

2. Abstract of paper presented at Seattle Meeting of American Physical Society, November 2–4, 1972.

3. Physics Division.

4. J. K. Dickens, G. L. Morgan, and F. G. Perey, "Neutron-Induced Gamma-Ray Production in Iron for the Energy Range $0.8 \leqslant E_n \leqslant 20$ MeV," ORNL-TM-3850 (August 1972).

5. J. K. Dickens and F. G. Perey, "The ^{14}N($n,x\gamma$) Reaction for $5.8 \leqslant E_n \leqslant 8.6$ MeV," *Nucl. Sci. Eng.* **36**, 280 (1969).

6. O. A. Wasson and G. G. Slaughter, "Valency Neutron Capture in ^{92}Mo(n,γ)^{93}Mo"; submitted to *Physical Review C* for publication.

3.3 GAMMA-RAY PRODUCTION DUE TO NEUTRON INTERACTIONS WITH VARIOUS ELEMENTS FOR INCIDENT NEUTRON ENERGIES UP TO 20 MeV: TABULATED DIFFERENTIAL CROSS SECTIONS[1]

J. K. Dickens, T. A. Love, and G. L. Morgan

Numerical values of differential cross sections for gamma rays produced by neutron interactions with samples of Cu, Al, Ca, W, and N have been obtained for neutron energies between approximately 1 MeV and 20 MeV and for gamma-ray energies between 0.7 and 10.5 MeV. Measurements were made for all samples at a gamma-ray emission angle of 125 deg and for some samples at an angle of 90 deg. The gamma rays were detected with a NaI spectrometer and the data were reduced to differential gamma-ray-production group cross sections ($d^2\sigma/d\omega dE$). The energy intervals used for both the neutrons and the gamma rays varied with the sample. Pertinent parameters for the various samples are summarized below, with a reference to the report in which the data are presented.

For copper,[2] the neutron energy range was 1 to 20 MeV, with the energy intervals varying from 0.5-MeV widths for the 1- to 5-MeV range to 3-MeV widths for the 14- to 20-MeV range. The gamma-ray energy intervals varied from 20-keV widths for $E_\gamma \leqslant 1$ MeV to 160-keV widths for $E_\gamma \sim 9$ MeV. Measurements were made at $\theta_\gamma = 125$ deg only.

For aluminum,[3] the neutron energy range was 0.85 to 20 MeV, with the energy intervals varying from 0.2-MeV widths for the 0.85- to 1.5-MeV range to 3-MeV widths for the 14- to 20-MeV range. The gamma-ray energy intervals varied from 20-keV widths for $E_\gamma \leqslant 1$ MeV to 160-keV widths for $E_\gamma \sim 9$ MeV. Measurements were made for both $\theta_\gamma = 125$ deg and $\theta_\gamma = 90$ deg.

For calcium,[4] the neutron energy range was 0.7 to 20 MeV, with the energy intervals varying from 0.5-MeV widths for $E_n \leqslant 9$ MeV to 3-MeV widths for $E_n \geqslant 14$ MeV. The gamma-ray energy intervals varied from 20-keV widths for $E_\gamma \leqslant 1$ MeV to 160-keV widths for $E_\gamma \approx 9$ MeV. Measurements were made at $\theta_\gamma = 125$ deg only.

For tungsten,[5] the neutron energy range was 1 to 20 MeV, with the energy intervals varying from 0.5-MeV widths for the 1- to 8-MeV range to 3-MeV widths for the 14- to 20-MeV range. The gamma-ray energy intervals varied from 20-keV widths for $E_\gamma \leqslant 1$ MeV to 160-keV widths for $E_\gamma \sim 9$ MeV. Measurements were made for $\theta_\gamma = 125$ deg only.

For nitrogen,[6] the neutron energy range was 2 to 20 MeV, with the energy intervals varying from 1-MeV widths for the 2- to 10-MeV range to 3-MeV widths for the 14- to 20-MeV range. The gamma-ray energy intervals varied from 20-keV widths for $E_\gamma \leqslant 1$ MeV to 250-keV widths for $E_\gamma \sim 9$ MeV. Measurements were made for both $\theta_\gamma = 125$ deg and $\theta_\gamma = 90$ deg.

1. Work supported by Defense Nuclear Agency under Subtask PC101.
2. J. K. Dickens, T. A. Love, and G. L. Morgan, *Gamma-Ray Production Due to Neutron Interactions with Copper for Incident Neutron Energies Between 1.0 and 20 MeV: Tabulated Differential Cross Sections,* ORNL-4846 (February 1973).
3. J. K. Dickens, T. A. Love, and G. L. Morgan, *Gamma-Ray Production Due to Neutron Interactions with Aluminum for Incident Neutron Energies Between 0.85 and 20 MeV: Tabulated Differential Cross Sections,* ORNL-TM-4232 (June 1973).
4. J. K. Dickens, T. A. Love, and G. L. Morgan, *Gamma-Ray Production Due to Neutron Interactions with Calcium for Incident Neutron Energies Between 0.7 and 20 MeV: Tabulated Differential Cross Sections,* ORNL-TM-4252 (July 1973).
5. J. K. Dickens, T. A. Love, and G. L. Morgan, *Gamma-Ray Production Due to Neutron Interactions with Tungsten for Incident Neutron Energies Between 1.0 and 20 MeV: Tabulated Differential Cross Sections,* ORNL-4847 (January 1973).
6. J. K. Dickens, T. A. Love, and G. L. Morgan, *Gamma-Ray Production Due to Neutron Interactions with Nitrogen for Incident Neutron Energies Between 2.0 and 20 MeV: Tabulated Differential Cross Sections,* ORNL-4864 (April 1973).

3.4 IS THERE STILL A NITROGEN CROSS-SECTION DISCREPANCY?[1,2]

F. G. Perey and J. K. Dickens

For several years there have been great uncertainties as to which nitrogen neutron cross-section set should be used for transport calculations of 14-MeV neutrons in air. Various discrepancies were found between microscopic cross-section measurements, and difficulties were experienced in calculating correctly the results of integral experiments. Most neutron air-transport calculations have been performed using either the nitrogen cross-section set of Straker (1969) or of Young and Foster (1970). These two cross-section sets differ by about a factor of 2 in gamma-ray-production cross sections around 14 MeV. We have reviewed the status of these evaluated cross-section sets on the basis of recent work and conclude that the Young-Foster evaluation, MAT 4133 Mod 2, is more consistent with all the available information and should be preferred over the Straker set.

1. Work supported by Defense Nuclear Agency under Subtask PE075.
2. Abstract of ORNL-TM-4216 (May 1973).

3.5 A TEST OF NEUTRON TOTAL CROSS-SECTION EVALUATIONS FROM 0.2 TO 20 MeV FOR C, O, Al, Si, Ca, Fe, AND SiO_2[1,2]

F. G. Perey, T. A. Love, and W. E. Kinney

Neutron transmission measurements from 0.2 to 20.0 MeV have been made for the shielding materials carbon, oxygen, aluminum, silicon, calcium, and iron and the compound silicon dioxide. The measurements were performed at the ORELA Shield Test Station with a resolution of about 0.12 nsec/m on sample thicknesses varying from 0.65 to 0.9 atom/barn. The transmission measurements were compared with the predictions based on the Defense Nuclear Agency evaluated cross-section library. Since the total cross-section files for these elements are also the ones present in the ENDF/B-III library, we are also checking its total cross-section files for all of the elements with the exception of oxygen. There are serious discrepancies between our data and the predictions based on the evaluated files. These discrepancies are often large in the energy region from 0.2 to 0.6 MeV.

1. Work supported by Defense Nuclear Agency under Subtask PE075.
2. Abstract of ORNL-4823 (December 1972).

3.6 INTEGRAL NEUTRON SCATTERING MEASUREMENTS ON CARBON AND IRON FROM 1 TO 20 MeV[1]

G. L. Morgan, T. A. Love, and F. G. Perey

A series of experiments is under way in which the spectra of neutrons scattered from thick samples of a material are measured as a function of the scattering angle and the incident and exit neutron energies over the range from 1 to 20 MeV. A linac (ORELA) is used as the neutron source and a ring-shaped sample coincident with the neutron beam is positioned at the 47-m flight path. An NE-213 detector positioned along the beam center line is protected by a shadow bar so that only the neutrons scattered from the samples are detected. The energies of the incident neutrons are determined by time-of-flight techniques and the energies of the scattered neutrons are obtained from pulse-height unfolding techniques. The neutron beam has a smooth energy dependence, and when structure in the beam is needed the sample is preceded by a filter of the same material as the sample. The results are presented in forms suitable for comparison with transport calculations based on evaluated neutron cross-section files.

The application of this technique to 1-mfp thick samples of carbon and iron has been reported.[2,3] For carbon, the measurements were made for three scattering angles (60, 90, and 135 deg) and for iron they were made for one scattering angle (90 deg). The iron measurements were made with and without an iron filter (also about 1 mfp thick) preceding the sample in the beam.

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1. Work supported by Defense Nuclear Agency under Subtask PE075.

2. G. L. Morgan, T. A. Love, and F. G. Perey, *Integral Neutron Scattering Measurements on Carbon from 1 to 20 MeV,* ORNL-TM-4157 (April 1973).

3. G. L. Morgan, T. A. Love, and F. G. Perey, *Integral Neutron Scattering Measurements on Iron from 1 to 20 MeV,* ORNL-TM-4193 (June 1973).

3.7 CALCULATIONS OF NEUTRON AND GAMMA-RAY-PRODUCTION CROSS SECTIONS FOR CALCIUM AND LEAD[1,2]

C. Y. Fu and F. G. Perey

Extensive calculations of neutron and gamma-ray-production cross sections for calcium and lead have been made in conjunction with the cross-section evaluations for these materials.[3,4] Calculated results, if strongly favored by experimental data or if the latter were nonexistent, were adopted as the evaluated cross sections. Also, the calculations were used as a reliable way of interpolating, extrapolating, and normalizing the data. In this paper we outline the techniques used for the calculations and discuss several interesting results. The gamma-ray-production reactions considered were (n,n'), (n,p), (n,α), $(n,n'p)$, and $(n,n'\alpha)$ for ^{40}Ca and (n,n'), $(n,2n)$, and $(n,3n)$ for the individual lead isotopes ^{206}Pb, ^{207}Pb, and ^{208}Pb.

Techniques for these calculations are similar to those reported by Kinney and Perey,[5] and by Penny and Kinney;[6] i.e., the neutron shape elastic-scattering cross sections were calculated by the local optical model with energy-dependent parameters, the compound elastic- and inelastic-scattering and the reaction cross sections by the Hauser-Feshbach theory with width fluctuation corrections, and the direct-reaction inelastic-scattering cross sections, where the decay scheme of the residual nucleus was experimentally known, were directly obtained from the calculated neutron cross sections. To allow calculation of gamma-ray-production cross sections for arbitrarily high excitation energies, we have written a gamma-ray cascade routine to approximate the unknown branching ratios and continuum transitions by certain selection rules (see next paragraph). We have also written a statistical-model code to calculate the cross sections of tertiary reactions and multiple particle emission. All the calculations using different theories were made consistent by using the same set of optical-model potentials and parameters.

The selection rules adopted for the gamma-ray cascade routine are outlined below. Gamma-ray branching ratios, if not known experimentally in the discrete-level region, were filled by E1 selection rules. Levels that could not be deexcited by E1 selection rules were allowed to decay by other transitions with the smallest possible angular momentum in the order of M1, E2, M2, and so on. Transitions from a continuum bin to a discrete level were assumed to be dipole with weighting by the spin distribution in the

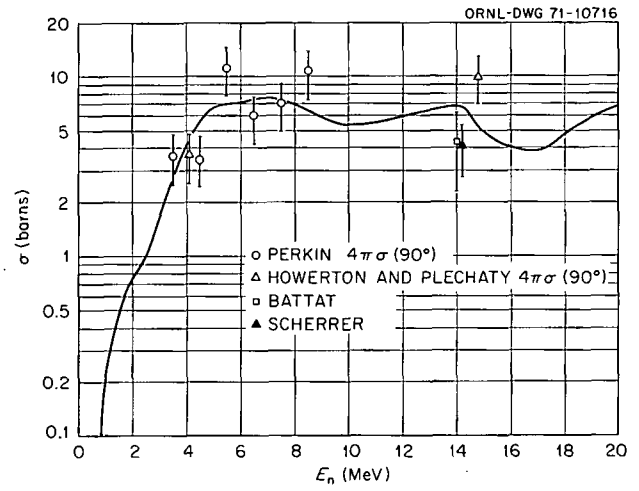

Fig. 3.7.1. Comparison of calculation with experiment for the total gamma-ray-production cross sections of lead.

continuum bin. We note that this cascade model does not involve any adjustable parameters, and that it worked reasonably well in all cases considered here.

As an illustration, the total gamma-ray-production cross sections for natural lead (53% ^{208}Pb, 23% ^{207}Pb, and 24% ^{206}Pb) from inelastic threshold to 20 MeV are shown in Fig. 3.7.1. The experimental data shown were taken from Perkin,[7] Howerton and Plechaty,[8] Battat,[9] and Scherrer.[10] Perkin[7] measured the production cross sections for $E_\gamma > 1.5$ MeV. The calculated percentage contributions to the total production cross sections for $E_\gamma < 1.5$ MeV were applied to Perkin's data to obtain the data shown in the figure. The calculated curve displays variations not indicated by the sparse data points. The break near 2.6 MeV marks the onset of inelastic scattering in ^{208}Pb. The peaks near 7 and 14 MeV correspond to the $(n,2n)$ and $(n,3n)$ thresholds respectively.

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1. Work supported by Defense Nuclear Agency under Subtask PC102.

2. Paper presented at American Nuclear Society International Meeting, November 12–17, 1972, *Trans. Amer. Nucl. Soc.* **15**(2), 961 (1972).

3. C. Y. Fu and F. G. Perey, *An Evaluation of Neutron and Gamma-Ray-Production Cross Sections for Lead,* ORNL-4765 (1972).

4. ENDF/B-III Material 1152 (calcium) evaluated by F. G. Perey, C. Y. Fu and W. E. Kinney of Oak Ridge National Laboratory; an updated version as DNA Material 4152 is available from the Radiation Shielding Information Center.

5. W. E. Kinney and F. G. Perey, "Calculated ^{56}Fe Neutron Elastic and Inelastic Scattering and Gamma-Ray-Production Cross Sections from 1.0 to 7.6 MeV," *Nucl. Sci. Eng.* **40**, 396 (1970).

6. S. K. Penny and W. E. Kinney, *A Re-evaluation of Natural Iron Neutron and Gamma-Ray-Production Cross Sections – ENDF/B Material 1124,* ORNL-4617 (1971).

7. J. L. Perkin, "Gamma Ray Spectra from Fast Neutron Interactions," *Nucl. Phys.* **60**, 561 (1964).

8. R. J. Howerton and E. F. Plechaty, "A Formalism for Calculation of Neutron Induced Gamma-Ray Production Cross Sections and Spectra," *Nucl. Sci. Eng.* **32**, 178 (1968).

9. M. E. Battat, R. W. Davis, and A. H. Frentrop, *Gamma Rays from 14-MeV Neutron Bombardment of C, O, Al, Fe, and Pb,* LA-1507 (1953).

10. V. E. Scherrer, R. B. Theus, and W. R. Faust, "Gamma Rays from Interaction of 14-MeV Neutron with Various Materials," *Phys. Rev.* **91**, 1476 (1953).

4. Weapons Radiation Shielding

4.0 INTRODUCTION AND SUMMARY

C. E. Clifford and F. R. Mynatt

The overall objective of the Division's Weapons Radiation Shielding program continues to be the accurate prediction of the radiation intensities produced in the vicinity of nuclear weapons detonations. Supported by the Defense Nuclear Agency (DNA), the program in previous years has largely concentrated on developing the basic methods needed for calculating the transport of weapons radiations over large distances in the atmosphere and through large shield thicknesses. As a result, several transport computer codes in which we have a high degree of confidence for classes of problems are now available, and our current program consists in adapting these codes or their derivatives to the solution of more realistic and complex problems. At the same time, we are attempting to improve the accuracy and efficiency of all the codes. The May, 1973, status of the program is summarized below and is supplemented by abstracts and papers that follow.

Development of Transport Techniques

Essentially all the transport computer codes used by us are based on one of two methods: the discrete ordinates method or the Monte Carlo method. Of these, the discrete ordinates method has several advantages, one of which is economy, but its limitation to problems whose geometries can be described in two space dimensions precludes its application when complicated configurations must be treated in detail. An obvious approach is to divide large transport problems into regions reduced to their simplest possible geometries and to use the discrete ordinates and Monte Carlo methods in series to calculate the transport through successive regions. In our program such "coupling" of the methods became practical when we developed MORSE, which is a Monte Carlo code that can use multigroup cross sections in the same format as our one-dimensional discrete ordinates code ANISN and two-dimensional code DOT. Now coupled problems are becoming routine, and, as would be expected, techniques for automatically interfacing the various codes are being devised. Among these is a coupling code called DOMINO. This code, which has been under development for the last couple of years and was checked out and released this year, transforms the output from a DOT calculation performed in two-dimensional cylindrical geometry for use in a three-dimensional MORSE calculation. Its most characteristic features are listed in paper 4.1.

Several improvements have also been made in the individual transport codes. In particular, DOT has undergone successive revisions and an improved version identified as DOT-III has recently been completed (see paper 4.2). In addition, a new technique for maintaining and modifying various multigroup cross-section sets assembled for use in DOT, as well as in ANISN and MORSE, has been developed (paper 4.3).

Although calculations based on multigroup cross sections are in general preferred for routine analyses, especially since they yield neutron and secondary gamma-ray results simultaneously, it is necessary to solve some problems with transport codes using the basic point cross sections. Only with point cross sections can particle interactions be treated in the detail required for diagnostic analysis of some integral experiments, and the well-known O6R and OGRE Monte Carlo point-code systems are still being applied. In addition, ANISN has been modified to match the Monte Carlo codes in treatment of cross-section detail. A version of ANISN is now available that uses a superfine energy group structure (1000 or more energy groups) and thus allows the calculation of one-dimensional problems with full cross-section detail, short computer execution time, and the benefits of full spatial detail provided by a deterministic method (see paper 4.4).

Because of the increasing demand for coupled multigroup neutron and gamma-ray cross-section sets that are tailored for specific problems, the development of a FORTRAN modular code system that rapidly produces the cross sections from ENDF/B point data was undertaken in 1971. Called AMPX, the system's Phase I version consists of the basic modules for calculating neutron, gamma-ray, and secondary gamma-ray production multigroup cross sections. This version is now operational on IBM-360 and CDC-6600 machines (see paper 4.5), and a preliminary Phase-II version is operational on the IBM machines alone. Phase II processes fully the angular distributions of secondary gamma rays and inelastically scattered neutrons, computes spatially dependent weighting functions for group collapsing, prepares multigroup library tapes for a variety of transport codes, including the codes using superfine group structures, and provides an interface with the SWANLAKE sensitivity analysis code (see below).

The modules in AMPX for calculating secondary gamma-ray production cross sections are later versions of codes that have been used for several years to generate cross sections from the relatively scarce secondary data included in ENDF/B files so that they could be tested in transport calculations. Examples of such tests, which are still under way, are reported in papers 4.6 and 4.7.

Development of Sensitivity Techniques

In addition to the transport codes per se, techniques for performing "sensitivity" studies are assuming an increasing importance in the DNA shielding program. In such studies, the sensitivity of the results obtained from a transport calculation to uncertainties in the cross sections used in the calculation is determined. Given the cross-section uncertainties, levels of confidence can then be assigned to the calculated quantities.

A mathematical formulation of a general sensitivity theory that serves as the basis for our studies is described in paper 4.8. This year the sensitivity analysis computer code SWANLAKE became available (see paper 4.9) and has already been used for several calculations. SWANLAKE can calculate and plot the normalized rate of change of one-dimensional discrete ordinates (ANISN) results with respect to changes in any partial cross section as a function of energy. For specified cross-section errors, the total error in a given problem solution can be obtained from the SWANLAKE results.

SWANLAKE has been applied to calculations of the neutron and secondary gamma-ray tissue doses produced in infinite air by three hypothetical neutron sources and also to calculations of the doses measured in the HENRE experiment. The calculations for the three hypothetical neutron sources (a 14-MeV source, a ^{235}U fission spectrum source, and a source typical of that from a thermonuclear weapon respectively) have been the subject of two papers presented at the American Nuclear Society this year and reprinted here as papers 4.10 and 4.11. The calculations for the HENRE experiment, in which an accelerator emitting nominally 14-MeV neutrons was operated at various heights above the ground, indicated that a long-standing discrepancy between the calculated and measured gamma-ray doses cannot be attributed to errors of reasonable magnitude in the nitrogen and oxygen cross sections.

Analyses of Integral Experiments

The accuracy of the various transport methods and of the cross sections used in them is tested by using the methods and data to analyze specially designed (or specially selected) integral experiments. Currently the emphasis is on the cross sections since for many problems the adequacy of the transport methods has already been established and the validity of the cross sections has not. Also, with the availability of sensitivity analysis techniques, the importance of specific cross sections to the analysis of an experiment can be ascertained, thereby indicating which cross sections must be determined most precisely for problems involving the same material.

During the past year a report was completed on a first-round Monte Carlo analysis of the Gulf Radiation Technology "concrete experiment" (see paper 4.12). In the experiment a pulsed and collimated beam of photoneutrons produced by bremsstrahlung interactions in a beryllium block impinged on a concrete shield, and neutrons and secondary gamma rays were detected on the beam center line beyond the shield. The analysis, performed some time ago, used pre-ENDF/B-III cross sections and the combined O6R and OGRE4D point Monte Carlo systems. The calculated and measured neutron count rates and energy

spectra are in reasonable agreement, but a disagreement between the calculated and measured secondary gamma-ray results persists. Hopefully the discrepancy will be resolved following the second-round analysis now in progress.

Another analysis completed this year was for a series of "pulsed-sphere" experiments performed at Lawrence Livermore Laboratory (paper 4.13). In these experiments a pulsed deuteron beam striking a tritium-loaded titanium target produced an anisotropic source of 14-MeV neutrons at the centers of relatively large spherical samples, and neutrons escaping from the spheres were detected at various angles from the beam as a function of their times of arrival. The analysis was performed with the O6R Monte Carlo system using cross sections from the DNA Working Cross Section Library. The samples were Fe, N, O, H_2O, and Li. Except for water, significant disagreements between calculated and measured count rates were found in some energy regions for all samples.

In both of the above analyses, cross sections suspected of being in error were identified, but the analyses of two other series of experiments, one performed at ORNL (see paper 3.6) and another at Gulf Radiation Technology, are expected to more nearly pinpoint errors in differential cross sections. In these experiments, scattered neutrons and secondary gamma rays are detected at various angles from a pulsed white neutron beam incident on spherical or ring-shaped samples of the materials of interest. The energies of the incident neutrons are determined by time-of-flight techniques and the energies of the detected particles by pulse-height unfolding techniques. The analyses, still in progress, consist of both O6R and MORSE Monte Carlo calculations to be followed by sensitivity studies. The materials under study are C, N, Fe, and O, with preliminary results for carbon discussed in paper 4.14.

Calculations of Weapons Radiation Transport

The development of many of the techniques employed in the transport methods, as well as much of the impetus for improving specific cross sections, has resulted from attempts to apply the methods and cross sections to real weapons shielding problems. Of these, one of the most important and most difficult problems has been the determination of the neutron and secondary gamma-ray fields produced by the neutrons generated in an in-air detonation. Prior to 1970, ORNL released several massive sets of "transport data" that could be used to construct free-field radiation environments produced by neutron sources having a variety of emission spectra. The data sets, obtained with both the discrete ordinates and the Monte Carlo method, were based on cross sections of early vintage, however, and we are now attempting to obtain some estimates of the effect that the latest ENDF/B-III cross sections will have on the results. Our first investigation, reported in paper 4.15, shows that for sources emitting 14-MeV neutrons or a spectrum of neutrons typical of a thermonuclear weapon, the neutron intensities in an infinite homogeneous medium of air would be higher and the secondary gamma-ray intensities would be lower. This study includes comparisons for numerous time-dependent responses for several sources.

We have also performed two calculational studies of the penetration of weapons radiation into Minuteman missile silos – the second one completed this year (see paper 4.16). Although the primary goal of these calculations was the determination of radiation intensities at specific locations in concrete silos subjected to specific burst conditions, they also served as models for developing transport code coupling techniques. In addition, they served as tests of the transport methods in that the results obtained with different methods (but with the same cross sections) are directly comparable. The second silo study also prompted the development of special techniques for calculating the streaming of radiation through complex-geometry regions of the silo. The calculations in both studies were performed with various combinations of the ANISN, time-dependent ANISN (TDA), DOT, and MORSE codes for given weapons neutron emission spectra.

Since the two silo studies did not use the same cross-section sets for air, and since neither study used the ENDF/B-III cross sections for air or concrete, the effect that the new cross sections would have on the results of these calculations is also under investigation. Calculations that have been under way for most of the year but are not yet documented are useful for comparing all combinations of three different sets of cross sections for air and concrete and should establish uncertainty estimates for the silo calculations. Although performed entirely with ANISN, the calculations are coupled in that the transport through the atmosphere is calculated in spherical geometry and the output is transformed for use as input in the

calculation of the penetration through the silo lid in slab geometry. This is a new technique which if shown to compare favorably with the two-dimensional DOT silo calculations will result in substantial savings in future large-scale calculations of the silo type.

LSA

4.1 DOMINO, A GENERAL PURPOSE CODE FOR COUPLING DISCRETE ORDINATES AND MONTE CARLO RADIATION TRANSPORT CALCULATIONS[1,2]

M. B. Emmett,[3] C. E. Burgart,[4] and T. J. Hoffman[4]

A method of coupling two-dimensional discrete ordinates calculations with Monte Carlo calculations is incorporated in the DOMINO code. In particular, DOT, a two-dimensional discrete ordinates code, has been coupled with MORSE, a Monte Carlo code.

The discrete ordinates calculation is limited to an *r-z* geometry. Either the DOT boundary angular fluxes or the angular fluxes at internal surfaces may be input to DOMINO. Any amount of surface may be used in DOMINO; i.e., from all mesh intervals down to a portion of one interval. The radii, axes, and quadrature set must be read into DOMINO. Appropriate cumulative probability distributions are calculated from the angular fluxes and written on a DOMINO tape. Four different types of DOMINO tapes may be written for use in Monte Carlo codes – upward from a disk, downward from a disk, inward from a cylindrical surface, and outward from a cylindrical surface. The DOMINO tape contains all necessary coupling information for use by the Monte Carlo code. The MORSE calculation may utilize this data in four ways: (1) as a source for a forward MORSE case; (2) as a scoring function for an adjoint MORSE case; (3) as a source for an adjoint MORSE case; or (4) as a scoring function for a forward MORSE case.

A detailed discussion of the coupling operation as well as a sample problem are included in the appendices. Logical flow charts of the routines are also presented.

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1. Work partially supported by Defense Nuclear Agency under Subtask PE074-02 and partially by Space Nuclear Systems Division of the U.S. Atomic Energy Commission.

2. Abstract of ORNL-4853 (July 1973); also abstract of paper presented at National Topical Meeting on New Developments in Reactor Physics and Shielding, September 12–15, 1972, and published in CONF-720901, p. 499.

3. Mathematics Division.

4. Now at Science Applications, Inc.

4.2 THE DOT-III MULTIGROUP TWO-DIMENSIONAL DISCRETE ORDINATES CODE WITH ANISOTROPIC SCATTERING[1,2]

W. W. Engle, Jr., M. L. Gritzner,[3] F. R. Mynatt,
W. A. Rhoades, and R. J. Rogers[4]

The DOT-III computer program solves the energy- and angular-dependent Boltzmann equation with general anisotropic scattering for rectangular, polar, or cylindrical geometries. Principal applications are to neutron and/or gamma-ray transport problems in either the forward or the adjoint mode. Both homogeneous and external source problems can be solved and searches on multiplication factor, time absorption, nuclide concentration, and zone thickness are available. However, the code is particularly designed and suited to the solution of deep-penetration radiation-transport problems.

The discrete ordinates, or Carlson's S_n, method is utilized to solve the Boltzmann equation. A good account of the historical development and application of this method is included by Mynatt et al. in a description of the development and verification of two-dimensional transport theory for radiation shielding applications.[1] Briefly, the discrete ordinates method involves the solution of difference equations derived in a term-wise manner by integrating the analytic form of the Boltzmann equation over a five-dimensional finite cell defined in terms of location, direction, and energy phase space variables. Supplementary difference equations are required to obtain a solution to the flux. These equations relate the average flux

for a cell with each pair of associated cell face fluxes. The equations should provide a good approximation to the true variation and at the same time be easily and quickly solved on the computer. Two forms of the supplementary equations which have been utilized in earlier versions of DOT are "diamond difference" and "step function" equations.

The cross sections required by DOT-III are of the multigroup, P_n, expansion type generated by codes such as AMPX (see paper 4.5). The utilization of this type of multigroup cross-section data allows the solution of coupled neutron and secondary gamma-ray transport problems with anisotropic scattering.

Various versions of DOT and related computer programs have been developed over the years and several have been placed in RSIC. Some examples of various applications of the program are found in references 6 through 11.

The DOT-III program incorporates some of the earlier features of DOT but also includes significant improvements to these versions of DOT. The new features are designed to improve the calculational ability and simplify the utilization of the code. Some of these are as follows:

1. An analytic first-collision source can be calculated internally and used.
2. A weighted difference mode is available by option or when linear gives negative flux values.
3. Multiple zones of convergence can be specified.
4. The iterative space-dependent scaling has been improved (logic and speed).
5. Sources can be specified on an internal boundary.
6. The flux output for restarting a subsequent calculation is written as each group is processed, and incomplete output can be used to restart a problem.
7. The angular flux can be output along either radial or axial boundaries, internal or external, and used as source in a subsequent problem.
8. Flux and group organized cross section input can be copied to allow reuse.
9. For coupled neutron and gamma-ray runs, outer iterations can be limited to neutron groups.
10. Flux guesses can be synthesized from one-dimensional calculations.
11. Input flux guesses can be made using results from other calculations with different P_l, S_n, or number of groups.
12. Scattering expansion order can be specified for each group.
13. Short list *I/Ø* is utilized, improving speed significantly.
14. Timing routines give breakdown of time consumption in major sections of the program.
15. Angular flux output can be obtained from single outer iteration problems.
16. Free field FIDØ input simplifies data preparation.
17. Multiple problems can be run.
18. User assignment of logical units is checked for errors.
19. Diffusion theory is available.
20. The amount of printed output can be selected to suit the user's need.

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1. Work partially supported by Defense Nuclear Agency under Subtask PEO74 and partially by Space Nuclear Systems Division of the U.S. Atomic Energy Commission.

2. Abbreviated version of paper presented by R. W. Roussin at NEA Computer Programme Library Seminar Workshop, Ispra, Italy, October 16–18, 1972; a more detailed description of DOT is given in ORNL-TM-4280 (1973).

3. Now at Science Applications, Inc., Huntsville, Ala.

4. Mathematics Division.

5. F. R. Mynatt, F. J. Muckenthaler, and P. N. Stevens, *Development of Two-Dimensional Discrete Ordinates Transport Theory for Radiation for Shielding,* CTC-INF-952 (AD-692168) (August 1969).

6. F. R. Mynatt, *A User's Manual for DOT,* K-1694 (1967).

7. R. G. Soltesz, R. K. Disney, and G. Collier, *Users Manual for DOT IIW Discrete Ordinates Transport Computer Code,* WANL-TME-1982 (1969); see also WANL-TME-1982 (Revision A) (1970).

8. D. Lindstrom, *Technical Report and User's Manual DASH-FORTRAN-IV Void Tracing and* S_n*-Monte Carlo Bridging Code,* SRT-TRMO1-W393-4C (May 1970).

9. D. G. Lindstrom and J. H. Price, *Coupled Discrete Ordinates – Monte Carlo Technique and Applications to NERVA,* AGC-NRO 1373 (1969).

10. P. A. Read, W. E. Selph, and R. J. Cerbone, *Duct Code Manual,* GULF-RT-10654 (April 1971).

11. R. Protsik and E. G. Leff, *User's Manual for DOT2DB: A Two-Dimensional Multigroup Discrete Ordinates Transport/Diffusion Code with Anisotropic Scattering,* GEAP-13537 (September 1969).

4.3 THE ALC1 PROGRAM FOR CROSS-SECTION LIBRARY MANAGEMENT[1,2]

W. A. Rhoades

The ALC1 program moves nuclide-organized cross-section sets from cards, disk, or tape to tape, disk, or card data sets. Options provide facility for updating, deleting, merging, and listing data sets. The output is in a form suitable for the ANISN-related S_n codes. ALC1 has advantages of speed, convenience, and flexibility over other codes previously used for these functions.

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1. This work partially supported by Defense Nuclear Agency under Subtask PEO74.
2. Abstract of ORNL-TM-4015 (1973).

4.4 APPLICATION OF THE DISCRETE-ENERGY TECHNIQUE TO DISCRETE-ORDINATES CALCULATIONS OF NEUTRON TRANSPORT IN IRON[1,2]

J. Ching,[3] E. Oblow, and H. Goldstein[4]

An algebraic equivalence of the point-energy and multigroup forms of the Boltzmann transport equation has been proven that has allowed the development of a discrete-energy, discrete-ordinates method for the solution of radiation transport problems. The method was constructed by matching a modified version of a cross-section processing scheme devised for the moments method code BMT with the one-dimensional discrete-ordinates transport code ANISN. The combined system, identified as MOMANS, computes fluxes directly from point cross sections in a single operation. In the cross-section processing, the group averaging required for multigroup calculations is replaced by a technique that generates transfer cross sections with all the features of interest retained, thereby increasing the detail in the calculated results. Test calculations in which the discrete-energy method was compared with the multigroup method have shown that for the same energy grid (number of points = number of groups), the discrete-energy method is faster but less accurate than the multigroup method. However, the accuracy of the discrete-energy method increases rapidly with an increasing fineness in the energy grid; thus for problems requiring results in great detail with respect to energy, the discrete-energy method is not only the most feasible method but also the most economical. This has been demonstrated by the application of the method to the transport of neutrons in an iron sphere.

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1. Work partially supported by Defense Nuclear Agency under Subtask PC104.
2. Abstract of ORNL-TM-4235 (to be published).
3. University of Tennessee.
4. Columbia University.

4.5 AMPX: A MODULAR CODE SYSTEM FOR GENERATING COUPLED MULTIGROUP NEUTRON-GAMMA LIBRARIES FROM ENDF/B[1,2]

N. M. Greene,[3] J. L. Lucius,[3] W. E. Ford, III,[3] J. E. White,[3]
R. Q. Wright,[3] and L. M. Petrie[3]

AMPX is a modular system for producing coupled multigroup neutron-gamma cross-section sets. Usually basic cross-section data for AMPX are obtained from ENDF/B libraries, although some modules allow the users to select from alternate sources. Most commonly used operations required to generate and collapse multigroup cross-section sets are provided in the system.

AMPX is flexibly dimensioned; neutron group structures, gamma group structures, and expansion orders to represent anisotropic processes are all arbitrary and limited only by available computer core and budget. The basic processes provided will (1) generate multigroup neutron cross sections; (2) generate multigroup gamma cross sections; (3) generate gamma yields for gamma-producing neutron interactions; (4) combine neutron cross sections, gamma cross sections, and gamma yields into final "coupled sets"; (5) perform one-dimensional discrete ordinates transport or diffusion theory calculations for neutrons and gammas and, on option, collapse the cross sections to a broad-group structure, using the one-dimensional results as weighting functions; (6) plot cross sections, on option, to facilitate the "evaluation" of a particular multigroup set of data; (7) update and maintain multigroup cross-section libraries in such a manner as to make it not only easy to combine new data with previously processed data but also to do it in a single pass on the computer; and (8) output multigroup cross sections in convenient formats for other codes.

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1. Work supported by Defense Nuclear Agency under Subtask PEO74.
2. Abstract of ORNL-TM-3706 (AMPX-1) (1973).
3. Mathematics Division.

4.6 COMPARISON OF (n_{th},γ) YIELDS FROM THE CURRENT ENDF/B-III DATA WITH PUBLISHED DATA[1,2]

W. E. Ford, III[3]

As a first check of the ENDF/B-III photon production data available as of June, 1972, the number of photons per thermal-neutron capture was calculated for 50-keV gamma-ray energy bins and compared with published data. This comparison was done for ^{1}H(MAT 1148), ^{9}Be(1154), ^{14}N(1133), ^{16}O(1134), ^{23}Na(1156), ^{27}Al(1135), Si(1151), Cl(1149), K(1150), Ca(1152), Fe(1180), and Pb(1136).

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1. Work supported by Defense Nuclear Agency under Subtask PEO74.
2. Abstract of ORNL-TM-3910 (ENDF-172) (1972).
3. Mathematics Division.

4.7 THE TESTING OF PHOTON PRODUCTION DATA FROM ENDF/B-III MATERIAL 1135 (ALUMINUM)[1,2]

W. E. Ford, III[3]

Photon-production data in the Evaluated Nuclear Data File (ENDF/B-III) for ^{27}Al, MAT 1135, were tested by (1) comparing the thermal-neutron capture gamma-ray yields calculated with MAT 1135 with data from the literature, (2) comparing gamma-ray pulse-height spectra calculated with MAT 1135 with measured spectra, and (3) comparing the secondary gamma-ray production cross sections calculated with MAT 1135 data with cross sections from the literature.

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1. Work supported by Defense Nuclear Agency under Subtask PEO74.
2. Abstract of ORNL-TM-4032 (ENDF-180) (January 1973).
3. Mathematics Division.

4.8 GENERAL SENSITIVITY THEORY FOR RADIATION TRANSPORT[1,2]

E. M. Oblow, D. E. Bartine,[3] and F. R. Mynatt

The theoretical framework of a general approach to sensitivity analysis using adjoint functions is introduced and developed for practical application. Sensitivity and the context in which it is used is defined quantitatively in terms of adjoint functionals. The physical meaning and applicability of such a definition are then discussed with reference to both analytic and predictive studies. Connections are made between the general approach and perturbation theory for predictive applications. Specific formulations useful in cross-section sensitivity work are described in detail.

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1. Work supported by Defense Nuclear Agency under Subtask PC104.
2. Abstract of ORNL-TM-4110 (March 1973).
3. Mathematics Division.

4.9 SWANLAKE, A COMPUTER CODE UTILIZING ANISN RADIATION TRANSPORT CALCULATIONS FOR CROSS-SECTION SENSITIVITY ANALYSIS[1,2]

D. E. Bartine,[3] F. R. Mynatt, and E. M. Oblow

SWANLAKE calculates the sensitivity of a result, such as a dose or reaction rate, obtained from a one-dimensional discrete ordinates solution for the Boltzmann transport equation to the cross sections used in the calculation. This manual presents a brief discussion of the sensitivity function and the method used for its calculation, then gives detailed instructions concerning the required input data and a detailed description of the code output. The input and output of a sample problem are included, along with an interpretation of the results, as an aid to the prospective user. A derivation of the sensitivity function and a listing of computing time and core requirements for several problems are included as appendices.

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1. This work supported by Defense Nuclear Agency under Subtask PC104.
2. Abstract of ORNL-TM-3809 (1973).
3. Mathematics Division.

4.10 A SENSITIVITY ANALYSIS OF NEUTRON AND GAMMA TRANSPORT IN AIR[1,2]

D. E. Bartine,[3] F. R. Mynatt, and E. Oblow

The method for sensitivity analysis based on the use of the adjoint flux (see paper 4.9) has been used to study coupled neutron-gamma transport in air. The analysis consisted of determining the sensitivity of the total tissue dose at 2000 m in air to group-averaged sets of nitrogen and oxygen cross sections. While adjoint fluxes have been used in previous sensitivity studies of air,[4,5] the present approach offers an alternate definition of the sensitivity function designed for ease in physical interpretation and extends the method to include secondary gamma-ray sensitivity effects. In the sensitivity calculation, the importance of the individual reaction cross sections involved in transport is determined quantitatively as a function of energy. This information may then be used to assess the relevance of integral experiments for design problems, or, in conjunction with estimated cross-section errors, to determine the priorities by reaction type and energy range for future cross-section measurement and/or evaluation.

Equation 1 gives a very straightforward definition of a sensitivity function as the derivative of the calculated response, such as tissue dose, with respect to the lth moment of the cross section for scattering from energy group i to energy group j:

$$\frac{dR}{d\Sigma^l_{i\to j}} = \int_D \phi^{+l}_j \phi^l_i , \tag{1}$$

where D is the domain of $\Sigma_{i\to j}$. However, experience has shown that a better way to observe the sensitivity, and the way it is used in this study, is to give it as the derivative of the natural log of the response with respect to the natural log of the cross section:

$$\text{Sensitivity}\,(\Sigma^l_{i\to j}) \equiv \frac{d\,(\ln R)}{d\,(\ln \Sigma^l_{i\to j})} = \frac{\int_D \phi_j^{+l}\phi_i^l \Sigma^l_{i\to j}}{R}. \tag{2}$$

The uncertainty in R resulting from a given error in cross section, $\delta\Sigma_{i\to j}$, can be determined according to Eq. 3:

$$\delta R_{i\to j} = \sum_{l=0}^{l_{\max}} \int_D \phi_j^{+l}\phi_i^l \delta\Sigma^l_{i\to j}\,. \tag{3}$$

If the perturbed adjoint is used, the calculation is exact. For cross-section uncertainties that are small enough for the linear perturbation theory to be valid, the perturbed adjoint may be approximated by the unperturbed adjoint, and estimates of the resulting uncertainties can be obtained.

The initial set of problems presented here utilized 14-MeV, thermonuclear, and fission neutron sources and determined the tissue dose in air at 2000 m with the Snyder-Neufeld[6] response function for neutrons and the Henderson[7] response function for gamma rays. The flux calculations extended to 3000 m to allow for reflection. Figure 4.10.1 shows sensitivity profiles for the three cases considered, with each bar in the histograms representing the summed sensitivities for all the cross sections for a particular group divided by the lethargy width of that group; that is, the plots show the sensitivity of the problem to neutron total collision cross sections. The peaks generally correspond to cross-section minima, and the variation of the sensitivity profiles with source is evident, particularly at higher energies.

For the problem with a thermonuclear source, the sensitivity profiles were determined for each of the individual reaction cross sections in the ENDF/B-III listings for N-14, MAT 1133 (DNA MAT 4133), and O-16, MAT 1134 (DNA MAT 4134). In general, the sensitivity was high for the inelastic cross sections above 10 MeV, while the elastic cross-section sensitivity accounted for almost the total effect at lower energies.

In addition to the sensitivity profiles, Eq. 3, with the unperturbed adjoint flux, was employed to predict the effects of a uniform increase of all cross sections. The linear predictions showed good agreement

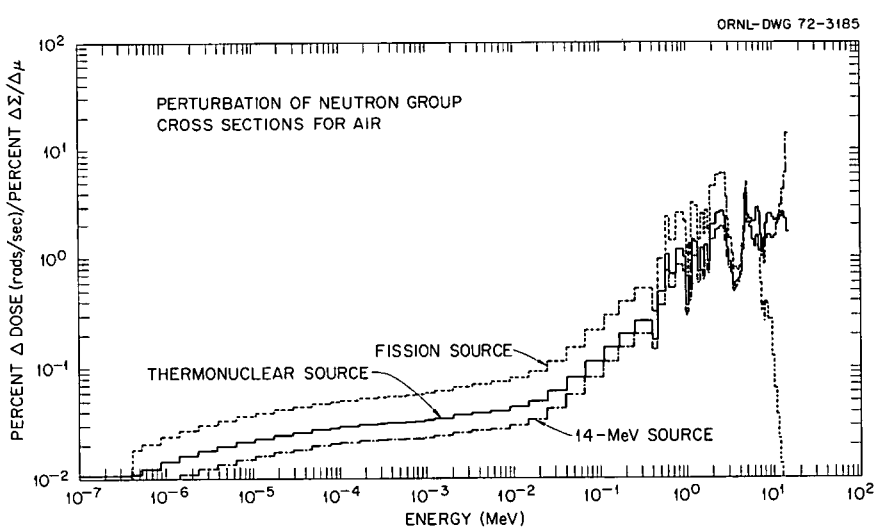

Fig. 4.10.1. Total collision cross-section sensitivity profile for three sources in air.

with modified transport calculations for small cross-section uncertainties (for 1% increase in all cross sections, the predicted dose decrease of 7.4% compares with a recalculated decrease of 7.1%), but relatively poorer agreement for larger cross-section uncertainties (for 10% increase in all cross sections, the predicted dose decrease is 74% compared with a recalculated decrease of 48%), indicating nonlinear effects.

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1. Work supported by Defense Nuclear Agency under Subtask PC104.
2. Paper presented at American Nuclear Society Meeting, November 12–17, 1972; published in *Trans. Am. Nucl. Soc.* **15**, 959 (1972).
3. Mathematics Division.
4. P. C. E. Hemment et al., *The Multigroup Neutron Transport Perturbation Program DUNDEE,* AWRE Report 040/66 (1966).
5. D. L. Prezbindowski and H. A. Sandmeier, "The Effects of Cross-Section Inaccuracies on Integral Data," *Trans. Am. Nucl. Soc.* **11**, 193 (1968).
6. W. S. Snyder and C. Neufeld, *Radiat. Res.* **6**(1), 67 (1957).
7. B. J. Henderson, *Conversion of Neutron and Gamma-Ray Flux to Absorbed Dose Rate,* XDC 59-8-179 (1959).

4.11 CROSS-SECTION SENSITIVITY ANALYSIS FOR DISCRETE ORDINATES CALCULATIONS[1,2]

D. E. Bartine,[3] E. M. Oblow, and F. R. Mynatt

Cross-section sensitivity analysis refers to a determination of how sensitive a calculated quantity or result is to microscopic cross-section data utilized in the calculation. Previous work in this field has employed both direct substitution methods[4-7] and perturbation theory.[8-10] The sensitivity function used in the work reported here represents an application of earlier perturbation approaches (see papers 4.8 and 4.9). The sensitivity of a result, R, to a particular cross section, X, at energy E may be expressed as:

$$P_X(E) = \int_{\mathbf{r}} dr \int_{\Omega} d\Omega \left[-\Phi^+(\mathbf{r},E,\Omega)\Sigma_{X_T}(\mathbf{r},E)\Phi(\mathbf{r},E,\Omega) + \int_{\Omega'} \int_{E'} d\Omega' dE' \, \Phi^+(\mathbf{r},E',\Omega')\Sigma_X(\mathbf{r},E\to E',\Omega\cdot\Omega')\Phi(\mathbf{r},E,\Omega) \right] \Big/ R \,, \qquad (1)$$

where

$\Phi^+(\mathbf{r},E,\Omega)$ = unperturbed adjoint flux,

$\Phi(\mathbf{r},E,\Omega)$ = unperturbed forward flux,

$\Sigma_{X_T}(E)$ = total cross section for reaction type X,

$\Sigma_X(\mathbf{r},E\to E',\Omega\cdot\Omega')$ = scattering cross section from energy E to E' for reaction type X,

R = integrated response.

All the above quantities are defined for the specific problem under consideration.

R is defined as:

$$R = \int_E dE \int_{\mathbf{r}} dr \int_{\Omega} d\Omega \, D(\mathbf{r},E,\Omega)\Phi(\mathbf{r},E,\Omega) \,, \qquad (2)$$

where $D(\mathbf{r},E,\Omega)$ is the response function, for example, a flux-to-dose conversion factor.

The sensitivity definition of Eq. 1 has been found to be convenient for identification of the most important cross sections for a given problem. A plot of the sensitivity function versus energy is referred to as a sensitivity profile, and indicates cross-section importance as a function of the energy of the incident particle. This "fingerprint" of the calculation has many potential uses since it quantitatively focuses attention on the important cross-section data. These uses consist partly of indication of need for specific

cross-section evaluation and measurements, the correlation of integral experiments and design problems, and the prediction of overall uncertainty in a design problem.

Equation 1 can also be integrated over the incident energy E to give the total sensitivity of the problem to the cross sections for reaction type X. The effect of Legendre series truncation for a multigroup P_l cross-section set may also be evaluated by examining sensitivity as a function of the number of expansion terms.

As an example, one problem investigated was a one-dimensional air-transport problem with a thermonuclear neutron source (see paper 4.10). The response function was that for tissue dose in air at 2000 m with the Snyder-Neufeld response function for neutrons[11] and the Henderson response function for gamma rays.[12] Sensitivity profiles were determined for individual reaction cross sections in the ENDF/B-III listings for N-14, MAT 1133 (DNA MAT 4133) and O-16, MAT 1134 (DNA MAT 4134). A rough nitrogen error file[13] was used, along with the results of the cross-section sensitivity code, to estimate the uncertainty in the total dose due to uncertainties in specific reaction cross sections. In obtaining the total problem variance, the individual components were combined appropriately to account for the strong covariance introduced by deriving certain cross sections; e.g., the elastic cross section is often obtained by subtracting the nonelastic from the total. Table 4.11.1 shows the energy-integrated sensitivity for specific cross sections for this problem. While the significance of the elastic cross sections is clear, the full analysis also indicates the importance of other cross sections, such as nitrogen inelastic above 10 MeV and nitrogen $(n,X\gamma)$ reactions, especially $(n,\alpha\gamma)$ reactions, from 2 to 5 MeV.

This method of analysis is applicable to a wide range of problems, and has been used for a study of deep neutron penetration in a sodium-iron system (see Section 8) and in a preliminary CTR blanket study.[14] Information from this prototype sensitivity analysis is being used to assist the specification of ENDF error file formats. The full potential of the sensitivity analysis technique will not be realized until the use of the ENDF error files for the prediction of design problem uncertainties is routine and techniques are fully developed to obtain and test error files using integral experiments. Sensitivity analysis routines are being developed for time-dependent and two-dimensional problems.

Table 4.11.1. Sensitivity of total tissue dose to specific reaction cross sections for nitrogen and oxygen

Reaction cross sections	Sensitivity (relative importance)		
	N_2	O_2	Air (total)
$\Sigma^a_{coll(n+\gamma)}$	−6.08[b]	−1.42	−7.50
$\Sigma_{coll(n)}$	−5.25	−1.16	−6.41
$\Sigma_{coll(\gamma)}$	−0.83	−0.26	−1.09
Σ_{el}	−3.17	−0.94	−4.11
Σ_{inel}	−0.55	−0.09	−0.64
Σ_{absn}	−1.53	−0.13	−1.66
$\Sigma_{(n,\gamma)}$	+0.12[c]	0.00	+0.12
$\Sigma_{(n,p)}$	−0.45	−0.01	−0.46
$\Sigma_{(n,d)}$	−0.10	0.00	−0.10
$\Sigma_{(n,t)}$	−0.08		−0.08
$\Sigma_{(n,p)} + \Sigma_{(n,d)} + \Sigma_{(n,t)}$	−0.63	−0.01	−0.64
$\Sigma_{(n,\alpha)}$	−1.00	−0.12	−1.12
$\Sigma_{(n,2\alpha)}$	−0.02		−0.02

[a]Total cross section for the collision of neutrons and secondary gamma rays.

[b]Negative sensitivity indicates an increase in cross section causes a decrease in the dose.

[c]Positive sensitivity indicates an increase in cross section causes an increase in the dose.

1. Work supported by Defense Nuclear Agency under Subtask PC104.

2. Paper presented at American Nuclear Society Meeting, June 10–15, 1973; published in *Trans. Am. Nucl. Soc.* **16**, 345 (1973).

3. Mathematics Division.

4. G. E. Hansen and H. A. Sandmeier, *The Effect of Basic Neutron Reaction Cross Sections of Nitrogen* (n,n'), $(n,2n)$, (n,γ), (n,p), *and* (n,α) *on High Energy Neutron Penetration in Air,* LA-3810, Los Alamos Scientific Laboratory (1967).

5. E. A. Straker, *Sensitivity of Neutron Transport in Oxygen to Various Cross-Section Sets,* ORNL-TM-2252 (1968).

6. W. E. Preeg, *Flux Sensitivity to Cross-Section Data for Iron and Oxygen,* Doctoral Thesis, Columbia University (1970).

7. S. Hui, D. Spielberg, H. Steinberg, E. S. Troubetzkoy, and M. Kalos, *SAMCEP: An Application of Correlated Monte Carlo to the Simultaneous Solution of Multiple, Perturbed, Time-Dependent Neutron Transport Problems on Complex Three-Dimensional Geometry,* BRL-CR-62, Ballistic Research Laboratories, Aberdeen Proving Ground (1972).

8. L. N. Usachev, "Perturbation Theory for the Breeding Ratio," *J. Nucl. Energy* **A/B 18**, 571 (1964).

9. P. C. E. Hemment et al., *The Multigroup Neutron Transport Perturbation Program DUNDEE,* AWRE Report 040/66 (1966).

10. D. L. Prezbindowski and H. A. Sandmeier, "The Effects of Cross-Section Inaccuracies on Integral Data," *Trans. Am. Nucl. Soc.* **11**, 193 (1968).

11. W. S. Snyder and C. Neufeld, *Radiat. Res.* **6**(1), 67 (1957).

12. B. J. Henderson, *Conversion of Neutron and Gamma-Ray Flux to Absorbed Dose Rate,* XDC 59-8-179, General Electric Co. (1959).

13. P. G. Young and D. G. Foster, Jr., *An Evaluation of the Neutron and Gamma-Ray Production Cross Sections for Nitrogen,* LA-4725, Los Alamos Scientific Laboratory (1972).

14. D. E. Bartine, R. G. Alsmiller, Jr., E. Oblow, and F. R. Mynatt, "Cross-Section Sensitivity of Breeding Ratio in a Fusion-Reactor Blanket," *Trans. Am. Nucl. Soc.* **16**, 8 (1973).

4.12 MONTE CARLO CALCULATIONS OF THE TIME-DEPENDENT SPECTRA OF NEUTRONS AND SECONDARY GAMMA RAYS PRODUCED IN A CONCRETE SHIELD BY A PULSED NEUTRON BEAM[1,2]

E. A. Straker,[3] G. W. Morrison,[4] C. L. Thompson,[4]
M. B. Emmett,[4] and C. E. Burgart[3]

An analysis of the Gulf Radiation Technology concrete experiment has been performed with the NUSECT-O6R-ACTIFK-OGRE4D Monte Carlo transport system and Young's evaluated cross sections for concrete. The experiment consisted of measurements of the time-dependent count rates and energy spectra of neutrons and secondary gamma rays behind concrete slabs placed in a pulsed neutron beam. The calculated neutron count rates for a 40.64-cm-thick concrete slab were in reasonable agreement with the data, but the gamma-ray count rates were too low by a factor of 2 for times greater than 2.4 μsec. The calculated neutron and gamma-ray energy spectra for fixed time intervals did not agree very well with the measured spectra either in shape or in magnitude. Calculations for an 81.32-cm-thick slab resulted in even larger disagreement, particularly for gamma rays. This disagreement may be attributable to gamma-ray emission anisotropy not represented in the cross sections, to the neglect in the calculations of interactions in the detector, or to undersampling of important events. Another possible source of error is the lack of sufficient data on gamma rays produced in trace elements and in silicon.

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1. Work supported by Defense Nuclear Agency under Subtask PEO83.

2. Abstract of ORNL-TM-4114 (to be published).

3. Now at Science Applications, Inc.

4. Mathematics Division.

4.13 MONTE CARLO CALCULATIONS AND SENSITIVITY STUDIES OF THE TIME-DEPENDENT NEUTRON SPECTRA MEASURED IN THE LLL PULSED-SPHERE PROGRAM[1,2]

S. N. Cramer,[3] R. W. Roussin, and E. M. Oblow

Calculations of the time-dependent neutron spectra measured in the LLL pulsed-sphere experiments have been performed using the O6R Monte Carlo code. The materials investigated were Fe, N, O, H_2O, and Li. The cross sections used were evaluations from the Defense Nuclear Agency Working Cross Section Library. Agreement between calculation and experiment was generally fair with rather poor agreement for the iron spheres. It is shown that a time-independent analysis is adequate to determine the energy spectra of neutrons.

Sensitivity studies were performed to determine the number, sequence, and type of collisions, as well as the reaction energy and angle of scattering, of all neutrons contributing to the detector response. Nonelastic scattering events have been separated according to the excitation of discrete levels and the models used in describing the continuum. Calculations were also performed to determine the effect of source assembly, detector collimator, and detector response function. Results of these calculations are presented in graphical form. Special sensitivity calculations were carried out for the iron spheres in an effort to isolate the cause of the large disagreement between experiment and calculation, and it appears that the trouble can be traced to the continuum inelastic-scattering data.

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1. Work supported by Defense Nuclear Agency under Subtask PEO83.
2. Abstract of ORNL-TM-4072 (March 1973).
3. Mathematics Division.

4.14 CALCULATIONAL ANALYSIS OF NEUTRON AND GAMMA-RAY TRANSPORT EXPERIMENTS IN CARBON[1,2]

S. N. Cramer[3] and E. M. Oblow

Calculations were made for comparison with a recent series of experiments involving neutron transport through carbon performed at ORNL (see paper 3.6) and neutron and gamma transport through carbon performed at GRT.[4] The GRT experiment consisted of a 15-cm-diam carbon sphere pulsed with a monodirectional white source of neutrons with neutron and gamma-ray detectors oriented at 30, 55, 90, and 125 deg with respect to the incident beam direction. The ORNL experiment was similar except for a change to ring geometry and the detection of neutrons only. In the latter experiment, a pulsed monodirectional neutron beam was incident on the face of a 10-in.-OD, 6-in.-ID annular ring 2 in. thick, with detectors located at various positions along the axis of the ring.

Figure 4.14.1 shows the counts per incident neutron as a function of incident neutron energy recorded in the GRT experiment at 55 deg, compared with calculated results from the MORSE Monte Carlo code. The neutron spectrum unfolded from incident neutron energies in the 9- to 10-MeV range from the ORNL experiment at 90 deg is compared with MORSE calculations in Fig. 4.14.2. All calculations used the ENDF/B-III carbon data, MAT 1165.[5]

The neutron count-rate results shown in Fig. 4.14.1 are representative of neutron calculational comparisons with both experiments. The agreement is generally good below 4 MeV, with significant disagreements appearing only after the 4.43-MeV inelastic threshold. The cause of the disagreements appears to be inelastic angular distribution data as seen in Fig. 4.14.2, typical of the unfolded spectra comparisons. The low-energy peak in this latter figure (where the disagreement is pronounced) arises from 9- to 10-MeV neutrons inelastically scattering to about 4 MeV. Disagreements arising from elastic scattering appeared in other results at high energies.

Far larger disagreements (the calculations being low by a factor of 2 over a wide energy range) appeared in the gamma count rate comparisons for the GRT experiment. Analysis of these discrepancies to date indicate that the results do not reflect discrepancies in the gamma-ray-production data. Rather, the

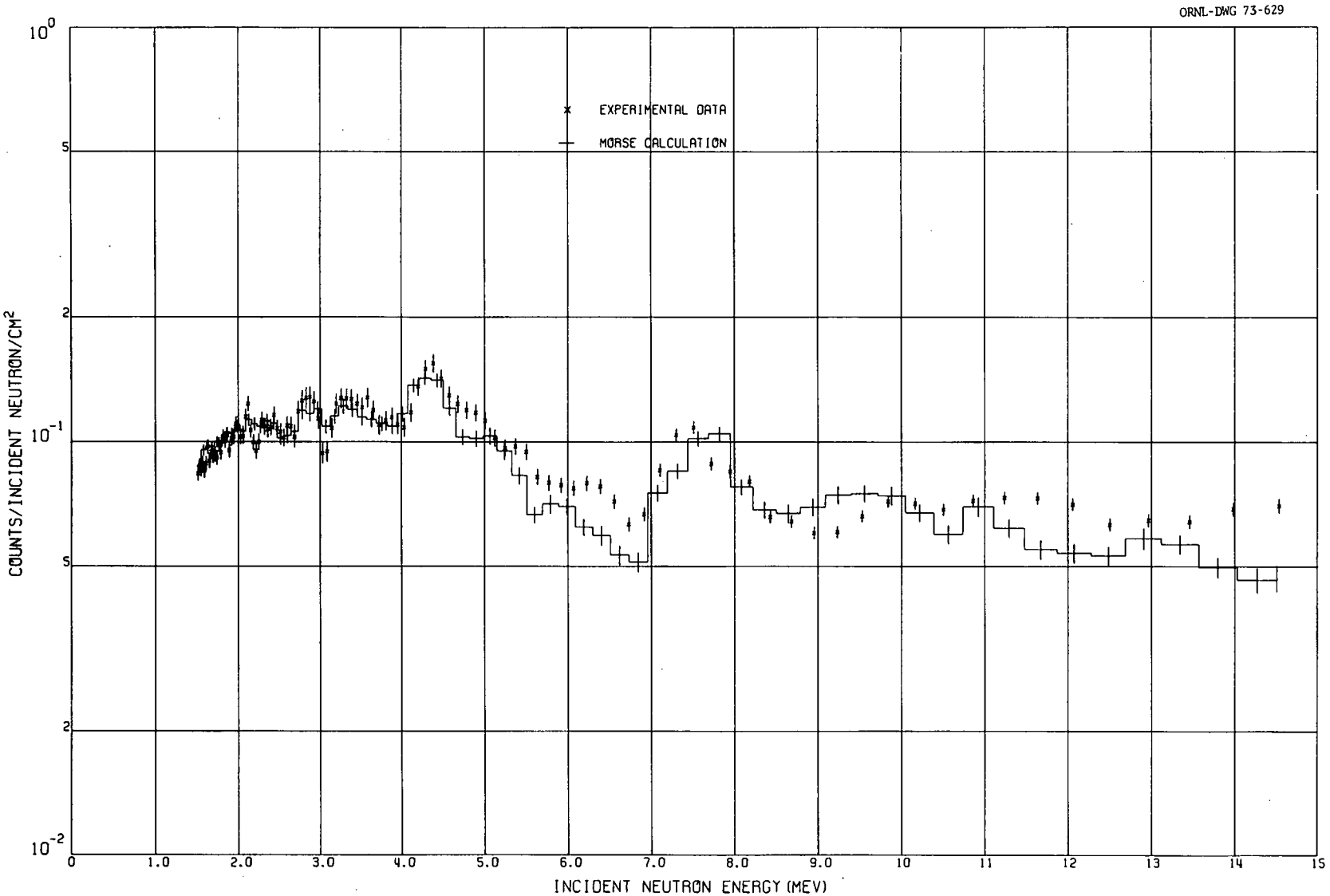

Fig. 4.14.1. Morse calculation of GRT carbon experiment at 55 deg detector orientation.

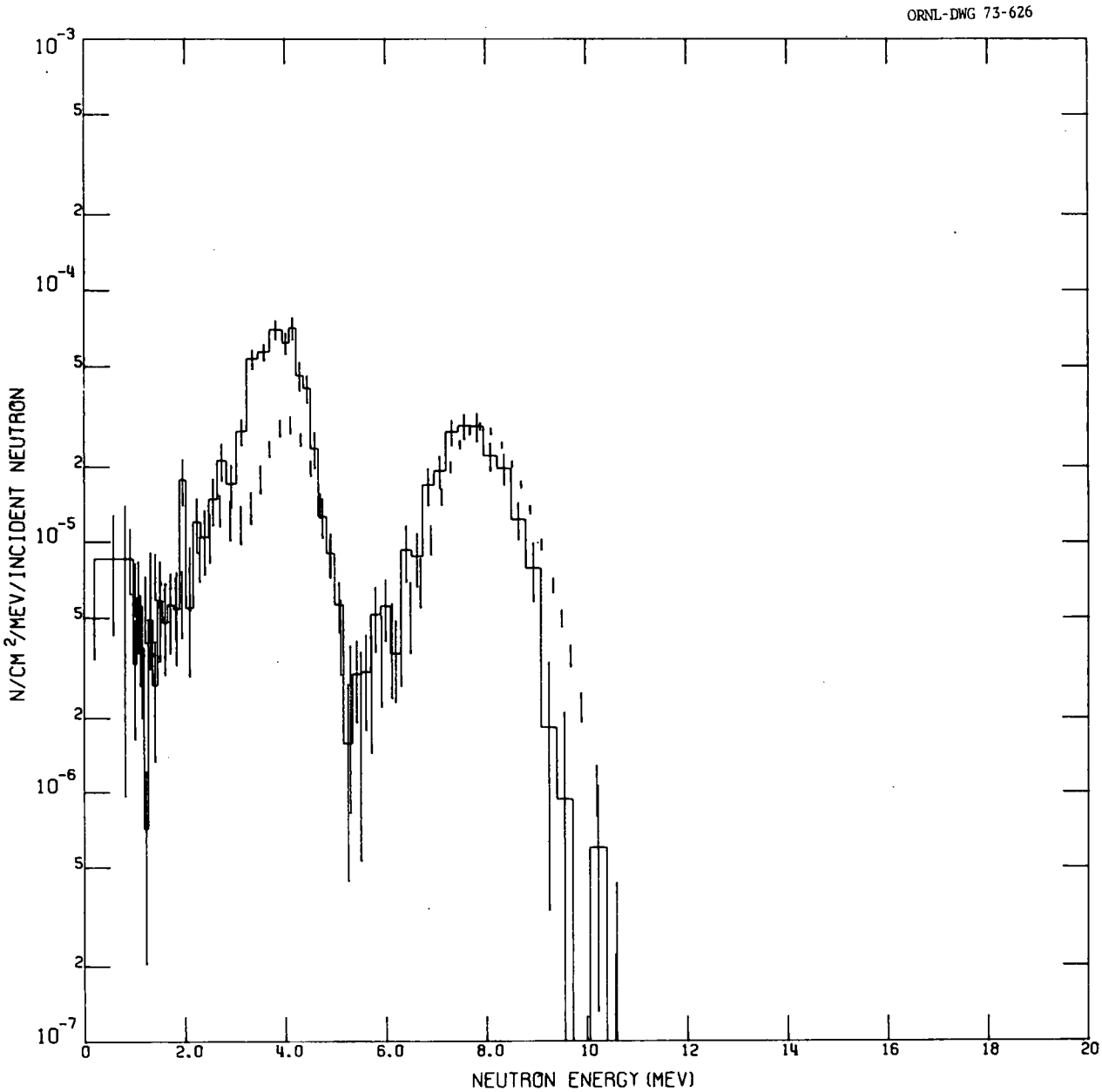

Fig. 4.14.2. Morse calculation of ORNL unfolded spectrum from carbon experiment with detector inside the ring (E_n = 9.001 to 9.971 MeV).

reported gamma efficiencies of the detector or the neutron-induced gammas in the detector and in the surrounding room are suspect.

1. Work supported by Defense Nuclear Agency under Subtask PEO83.
2. Paper presented at American Nuclear Society Meeting, June 10–15, 1973; published in *Trans. Am. Nucl. Soc.* **16**, 349 (1973).
3. Mathematics Division.
4. L. Harris, Jr., G. D. Trimble, and J. C. Young, *Integral Experiment to Test Gamma-Ray Production and Neutron Scattering Cross Sections,* Gulf-RT-A12292, Gulf Radiation Technology (1972).
5. *Data Formats and Procedures for the ENDF Neutron Cross Section Library*, M. K. Drake, ed., BNL-50274, ENDF 102, Vols. I and II.

4.15 TIME-DEPENDENT NEUTRON AND SECONDARY GAMMA-RAY TRANSPORT IN INFINITE HOMOGENEOUS AIR – COMPARISON OF TWO CROSS-SECTION SETS[1,2]

W. W. Engle, Jr., and F. R. Mynatt

Time-dependent ANISN calculations have been performed for the transport of neutrons and secondary gamma rays in infinite homogeneous air for the purpose of determining the effects of using the most recent ENDF/B-III data from Young and Foster compared with the much used multigroup cross-section set prepared by Straker. A hybrid set containing the neutron cross sections from ENDF-III and the gamma-ray production from the Straker set were also used. The calculation extended to a range of 3000 m and 10 sec elapsed time. Both a 14-MeV and a "typical" thermonuclear source were used. Results for several response functions were calculated and are presented graphically in both time-dependent and time-independent modes.

1. Work supported by Defense Nuclear Agency under Subtask PBO50.
2. Abstract of ORNL-TM-3932 (September 1972).

4.16 CALCULATIONS OF THE PENETRATION OF NUCLEAR WEAPONS RADIATION INTO A MISSILE SILO[1,2]

F. R. Mynatt, T. J. Hoffman,[3] J. V. Pace, III,[4]
C. E. Burgart,[3] and L. S. Abbott

A series of calculations have been performed which comprise a study of the vulnerability of Minuteman missile silos to neutrons and gamma rays streaming through regions of the structure having complex geometries as compared to radiation transmitted through the silo cover. The radiation incident on the silo was obtained from calculations with the two-dimensional discrete ordinates code DOT for a point thermonuclear neutron source in an air-over-ground geometry. Insofar as possible, both the DOT code and the three-dimensional Monte Carlo code MORSE were used to evaluate streaming paths within the silo in order to provide verification through cross-checks. The quantities compared were the ionization induced in silicon by secondary gamma rays produced in the atmosphere and silo structure and the ionization and displacement induced by the source neutrons. Most of the comparisons were made at points on the silo axis. The majority of the analysis was on a time-integrated basis, although time-dependent MORSE calculations were performed for the most important streaming problems.

1. Work supported by Defense Nuclear Agency under Subtask PBO50.
2. Abstract of ORNL-TM-4021 (to be published).
3. Now at Science Applications, Inc.
4. Mathematics Division.

5. Radiation Shielding Information Center

5.0. INTRODUCTION, FUNCTIONS, AND SUMMARY OF OPERATIONS[1]

B. F. Maskewitz, D. K. Trubey, R. W. Roussin, F. H. Clark, F. S. Alsmiller, R. T. Santoro, W. Zobel, C. M. Anthony, H. E. Comolander, J. Gurney, A. B. Gustin, H. R. Hendrickson, V. Z. Jacobs, M. W. Landay, M. B. Nicholson, and J. B. Wright

The Radiation Shielding Information Center (RSIC) continues to serve the international scientific community. Functioning as a scientific institute, it serves those engaged in research and development for the design of shields that provide protection from biological and physical damage due to penetrating ionizing radiation. The Center is sponsored by the Atomic Energy Commission (AEC), the Defense Nuclear Agency (DNA), and the National Aeronautics and Space Administration (NASA). In serving the interests of these agencies, RSIC is concerned with shielding against the radiations from nuclear reactors, nuclear weapons, radioisotopes, and accelerators, and the radiations present in space.

The RSIC Directory

The RSIC Storage and Retrieval Information System (SARIS)[2] is used routinely for producing lists of persons with particular interests and mailing labels for the RSIC distribution, keeping current a customer address and telephone directory, and an inventory of the codes and data collections.

The directory contains over 2200 names and addresses of persons and organizations interested in shielding. About two-thirds are persons who receive the monthly newsletter and optionally receive other material such as the Selective Dissemination of Information (SDI), which provides computer-printed abstracts of added literature to those interested in particular subjects. The number of persons has been increasing slowly, even though many additions are made, since names of persons no longer interested are removed each year.

Literature Review and Indexing

The RSIC monthly newsletter lists the current accession of literature in the process of review. During the year approximately 900 papers, reports, and books on reactor and weapons shielding and 130 on space and accelerator shielding were announced and subsequently reviewed. More than half of these were indexed according to the RSIC subject category classification scheme and entered into the SARI system which presently has about 4000 abstracts. An additional 215 documents describing computer codes for use in shielding research were reviewed, indexed, and announced in the newsletter.

Selective Dissemination of Information (SDI)

The number of persons taking advantage of the SDI service increased during the year. Currently, 243 profiles are serviced through SARIS. An additional 126 retrospective searches were performed on requests received in the report period.

Computer Information Storage and Retrieval Development

The RSIC Storage and Retrieval Information System (SARIS) has been fully operational since 1969. It is a batch-type program running at the Oak Ridge Computing Technology Center (CTC). The data base is

stored on tape. Input consists of punched cards or Magnetic Tape Selectric Typewriter (MT/ST) cartridge tapes. Programming was completed to implement several improvements to make file maintenance and search input preparation easier. In addition, the capability to use key term descriptors and add text information was implemented to the customer data as described in ref. 3.

Computer terminal operations. A General Electric TermiNet 300 communication terminal was installed to facilitate on-line data creation, editing, and retrieval. The terminal, which replaced the IBM 2741 used previously, operates with the ASCII code allowing access to the ORNL DEC System 10 (PDP-10) at up to 30 characters per second. It can also access directly the ORNL IBM 360/75 at 10 cps. The terminal has a tape cassette unit which facilitates efficient off-line data creation. The Conversational Remote Batch Entry (CRBE) system, operating normally on the ORNL IBM 360/75 computer, and the DEC System 10 allow the terminal user to create data, edit it, store it on disk, and submit jobs. The objective is to increase efficiency by reducing the various typing and keypunching operations involved in literature control (card files, records, and ordering forms) and computer input. To this end, citations of the literature ordered since January 1972 were entered into CRBE files, corrected as necessary, printed out for the Newsletter accession list, indexed by the BIRS program (see below), filed on longer term tape storage, and processed for ADSEP input (see below). Data on the RSIC computer code collection was also entered and indexed by BIRS.

The terminal has a typewriter-like character set which makes the creation of upper and lower case text information easy to implement.

The new connection from the DEC System 10 to the CTC computers now permits on-line creation of job control and input data and direct job submission for the SARIS programs.

BIRS program. The Michigan State University Basic Information Retrieval System (BIRS),[4] version 4.0, is a general-purpose file maintenance, indexing, and retrieval system, having more than 100 commands available which control the operations. The program and information data files are stored on private disk. BIRS jobs are easily set up and submitted through CRBE, normally processing text data stored on CRBE disk files. The main use of BIRS by RSIC is to produce indices to newly created data or other files not available in the SARIS data base. It will not replace SARIS because of the many SARIS features which continue to be needed, but it is useful as an additional tool. It uses a delimiter to identify data elements and therefore can process the data in the ORNL "general external format."[5]

ORCHIS project. The ORNL Mathematics Division, supported by various programs, is developing a comprehensive information system called ORCHIS (Oak Ridge Computerized Hierarchical Information System[6]). Several components of the system are being evaluated for possible RSIC routine use. For example, the cathode ray tube RECON terminal, located at the ORNL Library, is used to search *Nuclear Science Abstracts* when searches are required such as those in areas at the periphery of RSIC scope. The *Nuclear Science Abstracts* tapes are processed routinely to provide RSIC (and others) with citations of interest.

The ORLOOK program offers the capability of using a deallocated CRBE terminal for conversational search of text. Text in "generalized external format" is processed by the ADSEP[6,7] program for on-line data cell storage. Literature citations on the subject of computer codes published in the Newsletter have been processed by ADSEP and are now available as a data base for interactive searching by ORLOOK. Keyword descriptors were added to facilitate searches by subject.

A batch version of ORLOOK is also used to perform logical searches of smaller amounts of text data held on CRBE disk files or on tape. The most used file is a list of the RSIC Computer Code Collection (CCC) which has keywords. The output is routed to the terminal.

Computer Code Collection

The computer code collection continues to grow. Those packaged as CCC codes[8] perform radiation transport calculations; the PSR codes[9] perform calculations of an auxiliary nature such as cross-section processing. Since last reporting, 31 new CCC packages and 22 new PSR packages have been added to the collection. In addition, 12 new hardware versions to existing code packages have been returned to RSIC, tested and packaged, and 21 updates were made to existing packages.

The term "code package" is used by RSIC to describe a miscellaneous grouping of materials which, when interpreted and used correctly in connection with a digital computer, enables the scientist-user to solve technical problems in the area for which the material was designed. In general, an RSIC "code package" consists of: (a) written material – reports, instructions, data sheets, listings of data, and any other useful material; (b) other materials – punched card decks, or, more often, a reel of magnetic tape on which the source card decks, sample problem input, including any available libraries of data, and the formatted output from the sample problem are written. Not only is the main code of interest included in the package, but any auxiliary routine which has been made available to RSIC is also included. In many cases, several versions are available. Included in the 211 computer code packages (CCC's), there are a total of 356 separate versions; in the 59 peripheral-to-shielding packages (PSR's), there are a total of 90 versions.

The Data Library Collection (DLC)

Eleven new data libraries were added and several existing ones were updated and improved during the past year. A total of 343 separate shipments of these data sets were made. Abstracts of the current series are published in ref. 10.

The philosophy behind the packaging and distributing of these data libraries is to preserve and make available in an easily usable form data which may be useful to those utilizing or performing radiation transport calculations. Since this usually involves the use of large computer programs, several of these libraries are multigroup cross sections in the format utilized by many such programs. In addition, a data library may consist of voluminous results from particular calculations or input data that can be used to reproduce benchmark calculations.

Data libraries on magnetic tape or in other forms are packaged, maintained, and distributed in a manner analogous to computer code distribution. Each library carries a Data Library Collection (DLC) number and is packaged as a unit. In addition to the data, the package contains a handling program and documentation, including an RSIC-prepared abstract. Additions to and revisions of the DLC's are announced in the RSIC Newsletter. New abstracts are distributed with the Newsletter.

During the next year it is expected that we will acquire and package neutron and gamma-ray cross-section data sets which have proved useful for analyzing benchmark experiments in important shielding materials, such as nitrogen, oxygen, sodium, and iron.

Defense Nuclear Agency Cross Section Library

RSIC continued serving as a depository for the DNA cross-section data,[11] which is a working library (in ENDF format)[12] subject to modification and revision at as fast a rate as necessary. The key to this approach is the selected evaluator, a person responsible who will authorize and document changes in evaluations for particular elements. The evaluations are for those materials of interest to DNA and emphasis is apt to be placed on neutron energies up to 20 MeV and on secondary gamma-ray production.

The clearinghouse for the program is RSIC. Initial versions of evaluations are received, processed through checking codes to eliminate obvious format errors, and modified as necessary in collaboration with the evaluator. Next DNA Phase I data testing is performed whereby selected reviewers will be provided with listings, output from checking codes, graphics, etc., and asked to review the data and feed back their comments. These are relayed to the evaluator and, upon his instruction, appropriate changes are made.

The data, along with available documentation, are distributed upon request. The users are asked to feed back any comments they have through using the data.

The official DNA library is maintained at RSIC. Changes to it are initiated only by the evaluator and each change is documented so that users can at any time refer to an identifiable data set when reporting results of their calculations.

Because the data are apt to be revised with some frequency, each evaluation is designated by a DNA MAT number and a MOD number. The DNA MAT number is equal to ENDF MAT number plus three thousand for those evaluations which are submitted for inclusion in the ENDF/B library. The MOD number designates the number of times the DNA evaluation has been modified since its initial availability through RSIC.

The current contents of the DNA library are listed in Table 5.0.1.

Table 5.0.1. Contents of Defense Nuclear Agency working cross-section library

Material	Evaluators	MAT	MOD	Date
Nitrogen[a]	Young, Foster – LASL	4133	3	2-72
Oxygen[a]	Young, Foster – LASL	4134	1	2-72
Aluminum[a]	Foster, Young – LASL	4135	2	2-72
Lead	Fu, Perey – ORNL	4136	4	11-72
Hydrogen[a,b]	Stewart, LaBauve, Young – LASL	4148	1	2-72
Silicon[c]	Drake, Kinsey – BNL	4151	2	10-72
Calcium	Fu, Perey – ORNL	4152	3	2-73
Beryllium[b]	Howerton, Perkins – LLL	4154	1	3-73
Sodium[a]	Paik, Pitterle, Perey – WARD, ORNL	4156	0	2-72
Tritium[b]	Stewart – LASL	4169	0	9-72
Tantalum[b]	Howerton, Perkins, MacGregor – LLL	4179	1	1-73
Iron	Penny, Kinney, Wright, Perey, Fu – ORNL	4180	1	8-72
U-238[b]	Howerton, MacGregor – LLL	4187	1	3-73
U-235[b]	Howerton, MacGregor – LLL	4188	1	3-73
Pu-239	Stewart, Hunter – LASL	4539	0	3-73
Pu-240	Stewart, Hunter – LASL	4540	0	3-73
Mg	Drake, Fricke – SAI	4512	0	4-73
Cu	Drake, Fricke – SAI	4529	0	4-73

[a]These evaluations, or particular MOD numbers, are the same as ENDF/B Version III (January 1972).

[b]These evaluations on the disk have Legendre coefficients for representing elastic scattering angular distributions; the originals used tabulated distributions.

[c]The silicon evaluation work will now be done at ORNL (see paper 3.0).

Shielding Subcommittee, Cross Section Evaluation Working Group

RSIC continues to collaborate with the National Neutron Cross Section Center (NNCSC) at Brookhaven National Laboratory (BNL) and the Cross Section Evaluation Working Group (CSEWG) Shielding Subcommittee. The Center's role in the activity is to assist in the acquisition, check-out, and review of "shielding" cross sections in ENDF format which will ultimately be placed in the ENDF/B file. In this context, "shielding" cross sections are evaluations performed in the shielding, radiation effects, or weapons community which are likely to have an emphasis on gamma-ray production cross sections, gamma-ray interaction cross sections, and neutron cross sections in the energy range of interest for shielding with detailed energy and angular distribution resolution.

Evaluations were received by RSIC during the year, processed through checking codes, modified as necessary, and forwarded to NNCSC for inclusion in the ENDF/B library, Version IV of ENDF/B, which is expected to be distributed in January 1974, will contain more evaluations, including secondary gamma-ray production data. These will include data for ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, V, ^{6}Li, ^{7}Li, ^{12}C, Cu, and Mg.

Future efforts of the CSEWG Shielding Subcommittee will focus on recommending appropriate experiments for Phase II Integral Data Testing of the "shielding" evaluations. Other efforts will involve reviewing photon interaction libraries, devising formats for charged-particle- and gamma-ray-induced reactions, and improving and expanding the ENDF/B library to meet the needs of shielding calculations.

ORNL Cross Section Steering Committee (ORNL-CSSC)

The ORNL Cross Section Steering Committee (CSSC) was discontinued. It had as its charter the promotion of information exchange and the reduction of duplication of effort in manipulating and using cross-section data at ORNL. RSIC continues to try to meet these needs.

RSIC acts as the local clearinghouse for all ENDF data and codes distributed to ORNL by NNCSC. The Center also promotes the various computer programming efforts which are useful to the program of the Shielding Subcommittee of CSEWG.

Annual Summary of Operations and Services

During the 12 months of 1972 a total of 2775 separate letters/telephone calls of request were logged into the Center, an average of about 230/month, and an increase of about 20% over that of the previous year. These requests resulted in 4607 separate actions. General information requests accounted for 986 of the communications, while 1684 were concerned with information about and requests for data and/or code packages.

RSIC shipped 654 separate code packages (including full documentation) – an average of 2.5 per working day, and 343 separate data library packages – an average of 6.5 data shipments per work-week.

Other items mailed to requesters include RSIC publications, shielding documents (e.g., code documents not counted in code package shipments), and packets of RSIC introductory literature. These totaled 1283.

A number of calls were serviced in which staff members assisted a requester as he was learning to use a specific program. Research was done and advice and descriptive material were given to help in the selection of computer codes to fit the requester's problem and his local computer environment.

In 986 instances, time was spent by RSIC staff members in assisting the requester to solve his shielding problem – giving general advice and counsel. Of these, at least 491 research efforts were nontrivial, requiring technical expertise, considerable time, and occasionally a need to use the computer to find solutions to the requester's difficulty.

In addition to the above, RSIC performed data handling activities involving the use of the computer in connection with the National Neutron Cross Section Center (NNCSC), the Shielding Subcommittee of the Cross Section Evaluation Working Group (CSEWG), and for the Clearinghouse activities associated with the DNA Cross Section Working Library.

RSIC received 138 visitors for orientation and/or to use the facility. Eleven visitors were from foreign countries: two from Germany; one each from Canada, India, France, Japan, Romania, Scotland, Egypt, Greece, and the NEA Computer Programme Library in Italy. Extended visits were made to do technical work by scientists from Germany, Turkey, the University of Illinois, and the University of Wisconsin.

Most recent statistics (1972) indicate that RSIC processes ~230 letters of request per month on an average, requiring ~400 separate actions to satisfy the requests. The actions range from the trivial, i.e., mailing a document or sending a code and/or a data package, to requests for technical information requiring time spent by a senior technical research staff member, and sometimes requiring the use of a computer to do calculations. On an average, 2.5 code packages are shipped each working day, and approximately 6.5 data packages per week.

Two areas given priority within RSIC operations are:

1. Effective and expeditious review of all relevant published technical information, and selection and processing of that pertinent to shielding research or design.
2. Quick response to customer inquiry with a serious effort to supply the best information and advice available.

Standards

Previous work on standards has been associated with the American Nuclear Society (ANS) Standards Subcommittees ANS-6, Shielding, and ANS-10. Mathematics and Computation. The goal of ANS-6 is to establish standards in connection with radiation shields, to provide shielding information to other standards groups, and to prepare recommended sets of shielding data and test problems. Previous work has been reported in ref. 13.

In February of 1972, D. K. Trubey was appointed chairman of ANS-6. The immediate work was to reorganize the committee since nearly all previous members had resigned. Chairmen and working group members were recruited, largely during the summer of 1972. The chairmen and objectives are as follows:

ANS-6.1. Shielding Cross Sections

M. E. Battat, Los Alamos Scientific Laboratory

A study is being made which could lead toward selecting reference data for use as neutron and gamma-ray response functions (e.g., fluence-to-dose), and certain group cross sections (e.g., elemental data for concrete).

ANS-6.2. Benchmark Problems

G. L. Simmons, Science Applications, Inc.

Additional benchmark problems are being prepared for publication in ORNL-RSIC-25.

ANS-6.3. Shield Performance Evaluation

P. J. Persiani, Argonne National Laboratory

The standard "Program for Testing of Biological Shielding in Nuclear Reactor Plants," ANSI N18.9 – 1972, was approved by ANSI and published in 1972. It has not been endorsed by the AEC Directory of Regulatory Standards for use as a guide for power plants. The committee is investigating the standards applicability with intentions of revising as necessary.

ANS-6.4. Shield Materials

B. A. Engholm, Gulf General Atomic (Concrete)

The committee prepared a draft of a standard with individual members preparing various sections. The emphasis of the standard will be on radiation analysis and design of concrete shields for nuclear power plants.

G. L. Stukenbroeker, NL Industries

A survey was taken of the lead industry (producers and users) to determine the need for lead shielding standards.

ANS-6.5. Shielding Nomenclature

H. E. Hungerford

Definitions of shielding terms are being drafted for consideration by ANS-6.

The purpose of ANS-10 is to recommend practices which will facilitate the exchange of computer programs among the users and simplify the conversion of existing programs at a given laboratory when there is a change in computers. Specifically, the intent is to provide standards for documentation, programming practices, and test problems. An RSIC staff member has worked with this effort since its inception. Progress was made toward revising and updating ANS-STD.2-1967, "A Code of Good Practices for the Documentation of Digital Computer Programs."

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1. Work partially supported by the Defense Nuclear Agency (DNA) under Subtask PB052-03 and by National Aeronautics and Space Administration (NASA) under NASA Order H-79272A.

2. J. G. Jones, D. K. Trubey, and J. Gurney, *RSIC Storage and Retrieval Information System (SARIS),* ORNL-TM-2719 (1969); J. G. Jones and R. O. Green, *Radiation Shielding Information Center Program Set-Up Instruction Manual,* CTC-INF-1017 (1971); and J. G. Jones, R. O. Green, and S. L. Young, *RSIC User Documentation,* CTC-48 (1971).

3. D. K. Trubey, J. G. Jones, and R. O. Green, Jr., *The 1971 EIS Directory Program: A Synopsis,* ORNL-EIS-71-4 (1972).

4. John F. Vinsonhaler, John M. Hafterson, and Stuart W. Thomas, Jr., eds., *BIRS Technical Manual, Basic Information Retrieval System,* Vol. I-XII, Information Systems Laboratory, College of Education, Michigan State University (1970).

5. C. J. Oen, N. F. Sollins, and D. K. Trubey, *Guide to the Generalized Bibliographic Format for the Environmental Information System,* ORNL-EIS-71-3 (1972).

6. A. A. Brooks, ed., *ORCHIS Interim Technical Report – Collected Memos and Cumulative Bibliography,* ORNL-TM-3727 (August 1972).

7. A. A. Brooks, *ADSEP – An Automated Data Set Editing Program,* CTC-34 (May 1970).

8. Betty F. Maskewitz, *Abstracts of Digital Computer Code Packages Assembled by the Radiation Shielding Information Center,* ORNL-RSIC-13, Vols. I, II, and III; see also B. F. Maskewitz, F. H. Clark, and D. K. Trubey, "Computer Codes for Shielding and Related Calculations – 1972," *Nucl. Eng. Design* 22, 334 (1972).

9. B. F. Maskewitz, *Abstracts of the Peripheral Shielding Code Packages Assembled by the Radiation Shielding Information Center,* ORNL-RSIC-31 (1972).

10. R. W. Roussin, *Abstracts of the Data Library Packages Assembled by the Radiation Shielding Information Center,* ORNL-RSIC-30 (Vol. I), March 1972.

11. R. W. Roussin, *Defense Nuclear Agency Working Cross Section Library: Description and Contents,* ORNL-RSIC-34 (October 1972).

12. M. K. Drake, ed., *Data Formats and Procedures for the ENDF Neutron Cross Section Library,* BNL-50274 (ENDF-102, Vol. I), October 1970, and Donald J. Dudziak, Compiler, *ENDF Formats and Procedures for Photon Production and Interaction Data,* LA-4549 (ENDF-102, Rev., Vol. II), July 1971.

13. H. Clyde Claiborne, D. J. Dudziak, and N. M. Schaeffer, *Activities of the ANS-6 Subcommittee on Radiation Shielding Standards,* ORNL-TM-3251 (1970).

5.1. ABSTRACTS OF DIGITAL COMPUTER CODE PACKAGES ASSEMBLED BY THE RADIATION SHIELDING INFORMATION CENTER (Volume III)[1,2]

B. F. Maskewitz

This volume of ORNL-RSIC-13 is the third in a series in which abstracts of codes included in the RSIC Computer Code Collection are published. It contains CCC-116 through CCC-168, all of which were packaged during 1970–1972. Volume I contains abstracts for CCC-1 through CCC-58, packaged in 1966–1967, and Volume II contains abstracts for CCC-59 through CCC-115, packaged in 1968–1969. Since this volume has been issued in a loose-leaf binder, additional abstracts may be added to it. The main purpose of the abstracts is to give a potential code user several criteria for deciding whether he wishes to request the code package. Letters of request for code packages should be accompanied by the number of reels of magnetic tape indicated in the abstract, along with a statement as to how the tapes should be written.

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1. Work partially supported by the Defense Agency under Subtask PB052-03 and by the National Aeronautics and Space Administration under Order H-79272A.

2. Abstract of ORNL-RSIC-13, Vol. III (August 1972).

5.2. ABSTRACTS OF THE DATA LIBRARY PACKAGES ASSEMBLED BY THE RADIATION SHIELDING INFORMATION CENTER (Volume I Update)[1,2]

R. W. Roussin

Nine data sets have been added to RSIC's Data Library Collection, bringing the total to 25. These additional data sets have been distributed with the RSIC Newsletter for insertion into the looseleaf binder in which the first 16 abstracts of Volume I were published. Each data set carries a Data Library Collection (DLC) number and is packaged as a unit. In general a data set consists of a cross-section library or of the results from a large transport calculation, but other types of data are also included. As with the code packages, a particular data package will not remain static, but will be subject to revision, updating, and expansion.

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1. Work partially supported by the Defense Nuclear Agency under subtask PB052-03 and by the National Aeronautics and Space Administration under Order H-79272.

2. Additions to ORNL-RSIC-30, Vol. I, which was published in March 1972.

5.3 ABSTRACTS OF PERIPHERAL SHIELDING CODE PACKAGES ASSEMBLED BY THE RADIATION SHIELDING INFORMATION CENTER[1,2]

B. F. Maskewitz

This book of abstracts describes 25 computer code packages considered to be useful tools for shielding research. In order to distinguish between complex radiation transport programs designated by CCC numbers, these codes are designated as *P*eripheral to *S*hielding *R*outines (PSR's). They differ from the auxiliary routines included with the CCC abstracts in that they are not associated with specific CCC

packages. As with other types of abstracts issued by RSIC, these abstracts have been published in a looseleaf binder so that other abstracts can be added as they are issued.

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1. Work partially supported by National Aeronautics and Space Administration under Order H-79272A and Defense Nuclear Agency under Subtask PB052-03.
2. Abstract of ORNL-RSIC-31, Vol. I (March 1973).

5.4. DEFENSE NUCLEAR AGENCY WORKING CROSS-SECTION LIBRARY: DESCRIPTION AND CONTENTS[1,2]

R. W. Roussin

RSIC serves as a repository for the Defense Nuclear Agency (DNA) cross-section library. This is a working library in ENDF format and each cross-section set can be revised whenever the authorized evaluator deems changes to be necessary. This report, which has been issued in a looseleaf binder to accommodate additions, lists the initial contents of the Library, describes the data formats and procedures to be used, gives a history of the modifications made to DNA evaluations to date, and gives the listings of file 1 from each tape in the Library. Liaison with the ENDF/B Library is maintained, and the evaluations are identified with numbers that correspond to similar data in the ENDF/B Library. In this initial issue, data sets are included for N, O, Al, Pb, H, Si, Ca, Be, Na, Ta, Fe, ^{238}U, and ^{235}U.

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1. This work supported by Defense Nuclear Agency under Subtask PB052-03.
2. Abstract of ORNL-RSIC-34, Vol. I (October 1972).

5.5. SHIELDING OF MANNED SPACE VEHICLES AGAINST PROTONS AND ALPHA PARTICLES[1,2]

R. G. Alsmiller, Jr., R. T. Santoro, J. Barish,[3] and H. C. Claiborne

In this report the available information on the shielding of manned space vehicles against protons and alpha particles is summarized. The emphasis in the report is on shielding against Van Allen belt protons and against solar-flare protons and alpha particles, but information on shielding against galactic cosmic rays is also presented.

The report is primarily intended as a handbook for nonexperts in space shielding. For the most part, the approximation methods discussed are those that are standard in the space-shielding literature. However, a large amount of numerical data, not previously published, on the validity of the various approximation methods is presented, and these data may be of interest to those who are familiar with space shielding.

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1. Work supported by National Aeronautics and Space Administration under Orders H-38280A and H-79272A.
2. Abstract of ORNL-RSIC-35 (November 1972); same as paper 1.8, but repeated here to reflect full picture of RSIC activities in this section.
3. Mathematics Division.

5.6. SHIELDING AGAINST INITIAL RADIATIONS FROM NUCLEAR WEAPONS[1,2]

L. S. Abbott

Neutrons and gamma rays released by in-air detonations of nuclear weapons undergo various types of interactions with the surrounding environment, some of which result in additional radiations being born at points far removed from the original burst location. In the absence of adequate weapons test data, designers of shields to attenuate the initial radiations (those born within the first minute) must rely on information gained from "transport" calculations performed on large electronic computers. In such calculations the detonation and surrounding materials, including the proposed shielded structure, are mocked up as accurately as is possible and practicable, and the intensities of the radiations reaching specified locations

within the structures are computed. Such calculations are extremely difficult and very time-consuming, and much of the shielding research effort during the past decade has been devoted to the development of adequate transport methods and of the necessary input data that describe neutron and gamma-ray interactions in the pertinent materials. A major result has been the successful application of the discrete ordinates and Monte Carlo transport methods to a limited number of weapons radiation shielding problems. This report, which includes an elementary description of weapons radiations and their interactions, summarizes these problems and points out both their uses and and their limitations.

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1. Work supported by U.S. Corps of Engineers, Omaha District, Omaha, Nebraska, and Defense Nuclear Agency under Subtask PB052.
2. Abstract of ORNL-RSIC-36 (July 1973).

5.7. CALCULATIONS OF THE TRANSPORT OF NEUTRONS AND SECONDARY GAMMA RAYS THROUGH CONCRETE FOR INCIDENT NEUTRONS IN THE ENERGY RANGE 15 TO 75 MeV[1,2]

R. W. Roussin, R. G. Alsmiller, Jr., and J. Barish[3]

Earlier work by Alsmiller et al. considered coupled neutron and secondary-gamma-ray transport through a thick shield of silicon dioxide with 5% water by weight for neutron sources with energies of 50, 100, 200, 300, and 400 MeV. In that work, the approximation was made that gamma rays were produced only by neutron capture. In the present work, coupled neutron and secondary-gamma-ray transport through a thick shield of concrete for neutron sources with energies of 15, 25, and 75 MeV is considered. In this study, gamma-ray production for all interactions involving neutrons with energies up to 15 MeV was included; i.e., the approximation made here is that gamma-ray production can be neglected for interactions by neutrons with energies >15 MeV.

For incident neutron energies of 15, 25, 50, and 75 MeV, results of total and gamma-ray dose equivalents are given as a function of depth into the slab. For the 50- and 75-MeV incident neutron energies, the gamma-ray dose equivalent was found to be no more than 5% of the total dose equivalent at all depths considered ($\leqslant 1500$ g/cm^2). For the 15- and 25-MeV incident neutron energies, however, the gamma-ray dose equivalent dominates at greater depths into the slab. A conservative estimate of the effect of including gamma rays produced in interactions with neutrons of energies >15 MeV indicates that the calculated total dose equivalent would increase by no more than 5%.

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1. Work partially funded by Defense Nuclear Agency under Subtask PB052-03 and partially by National Aeronautics and Space Administration under Order H-79272A.
2. Abstract of *Nucl. Eng. Design* **24**, 250–57 (1973) and of ORNL-TM-3659 (Revised) (November 1972).
3. Mathematics Division.

5.8. COMPARISON OF TRANSPORT AND DIFFUSION THEORY FOR FAST REACTOR SHIELDING CALCULATIONS[1]

S. Sahin[2]

The purpose of this study is to compare the results of transport theory with those of diffusion theory for certain configurations of shields for sodium-cooled fast breeder reactors. Substantial cost savings are possible if diffusion theory can be used to calculate neutron penetration in reactor shielding.

Neutron spectra characteristic of the proposed Fast Flux Test Facility Reactor (FFTFR) are assumed as the neutron source. The shields consist of various combinations of iron and sodium, the principal shielding materials in fast reactors between the core and the biological shield.

In the calculations, we used the ANISN one-dimensional S_N program with the current 100-energy-group Radiation Shielding Information Center DLC-2/99G cross-section library. For integration of the angular

flux, Gaussian quadrature with 16 angular sections (N = 16) was employed. Anisotropic scattering cross sections were represented by the P_5 approximation.

Other limited studies of the differences between transport and diffusion theory have been made in this context. However, we have emphasized the effects on measurable quantities outside the sodium-iron region and interior to the biological shield. These measurables have included a manganese low-energy resonance flux (i.e., activation detector) and high-energy sulfur, ^{238}U, and iron threshold detectors. Also, we provide a tissue dose response and an energy integral which is an index of potential damage flux. In the cited region and in others, detailed neutron energy spectra are provided.

Further, we investigated effects on the tissue dose outside the concrete biological shield; and for an integral quantity evaluated throughout the shielding material, we investigated the neutron absorption.

Our study leads us to the following conclusions:

The higher the neutron energy and the deeper the neutron penetration in the shielding material, the worse is the diffusion theory description of the differential neutron spectra. If the shield consists of both iron and sodium zones, the use of diffusion theory is unacceptable. Neutron absorption, calculated by diffusion theory, throughout the shielding region is satisfactory if the shielding consists entirely of sodium or entirely of iron and is of medium thickness. In thin or thick shielding, or in several material zones, the diffusion theory neutron absorption spatial dependence is greatly in error. The diffusion theory damage flux and tissue dose response outside of the iron-sodium region is drastically low if the shielding is thick and consists of several material zones. Even for one zone, there are remarkable errors if it is thick.

The spectra calculated by diffusion theory outside the iron-sodium shield is underestimated compared with that of transport theory. Therefore, the tissue dose response beyond the biological shield is also underestimated.

The response of threshold detectors outside reasonably thick iron-sodium shields is also calculated much too low by use of diffusion theory.

A computer program (APSAI) was developed in the course of this work to read the flux values from ANISN output tapes and process and make machine plots of it (see paper 5.9). The program computes energy integrals of the fluxes with an arbitrary weight function supplied by the user.

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1. Abstract of paper submitted for publication in *Atomkernenergie,* June 1973.
2. Present address: Karadeniz Teknik Universitesi, Trabzon, Turkey.

5.9. APSAI: A COMPUTER CODE FOR PLOTTING FLUXES AND ABSORPTION DENSITIES GENERATED BY THE ANISN CODE[1]

S. Sahin

APSAI is a program to plot energy- or geometry-dependent neutron fluxes and adsorption densities which were already produced through an ANISN calculation. It permits the plotting of several curves from different cases, which must have the same energy group and mesh interval structure, on the same graph, in order to facilitate a comparison between them. Further, APSAI calculates the damage flux and activities at the outer boundary. APSAI uses the INTRIGUE-II-C package for plotting. Pen-and-ink or cathode-ray-tube (CRT) plotting are both possible.

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1. Abstract of ORNL-TM-4273 (July 1973).
2. Present address: Karadeniz Teknik Universitesi, Trabzon, Turkey.

5.10. MACK: A COMPUTER PROGRAM TO CALCULATE NEUTRON ENERGY RELEASE PARAMETERS (FLUENCE-TO-KERMA FACTORS) AND MULTIGROUP NEUTRON REACTION CROSS SECTIONS FROM NUCLEAR DATA IN ENDF FORMAT[1,2]

M. A. Abdou,[3] C. W. Maynard,[3] and R. Q. Wright[4]

A model for calculating neutron energy release parameters (fluence-to-kerma factors) is discussed. The computer program MACK designed to calculate pointwise neutron fluence-to-kerma factors from nuclear data in ENDF format is described.

MACK calculates the following: (1) pointwise cross sections at an arbitrary energy mesh, (2) cross sections from resonance parameters in the resolved and unresolved resonance regions, (3) energy group cross sections by reaction, (4) pointwise kerma factors, and (5) multigroup kerma factors. The energy point mesh and group structure can be arbitrarily set by the user. Kerma factors and cross sections can be averaged over an arbitrary input weighting function or any of several built-in functions.

The kerma factors and cross sections by reaction are of prime importance in calculating heating, dose, and reaction rates of interest in any nuclear system.

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1. Work partially supported by Defense Nuclear Agency under Subtask PB052-03.
2. Abstract of ORNL-TM-3994 (July 1973) and of University of Wisconsin Fusion Design Memo 37; packaged in RSIC as PSR-52.
3. University of Wisconsin.
4. Mathematics Division.

5.11. THE MAINTAIN CODE FOR USE IN MAINTAINING CARD IMAGE FILES ON TAPE[1]

D. K. Trubey

The ORNL Conversational Remote Batch Entry (CRBE) system and ORNL DEC System 10 are useful for on-line creating, editing, and storing text data on disk. The on-line storage space is limited, however, and it is therefore necessary to copy data on tape for off-line longer-term storage. The MAINTAIN code was written for this purpose. Commands, similar to those of CRBE, control the operations of the program. Each command consists of $$ plus three more characters in columns 1–5. Additional characters may be added if desired. These commands and their uses are:

Command	Result
(1) $$NEW	Add new data to tape from a CRBE file, initializing the tape
(2) $$ADD	Copy old tape and add a new file to the new tape
(3) $$PRINT	Use line printer to print a particular tape file or the whole tape
(4) $$FETCH	Copy a tape file to an on-line disk for CRBE editing
(5) $$REPLACE	Copy old tape but replace a particular file with new data on the new tape
(6) $$PURGE	Copy old tape but delete a particular file
(7) $$COPY	Copy selected files of old tape to a new tape
(8) $$CADSEP	Copy selected files of old tape to a new tape in ADSEP format
(9) $$CHECK	Check first record of old tape to be sure of data

The revised version of the program has additional commands and may revise or recover data from any card image tape. The additional commands are:

(10) $$BRING	Same as $$FETCH except omits file name record and "end-of-file" record
(11) $$INSERT	Insert 1 or more records following a designated record
(12) $$COLUMN	Define the number of columns to be searched on each record
(13) $$DIRECTORY	Print the list of file names of all the files on the tape
(14) $$PUBLISH	Print all files with a directory which indexes each file by page number in the printout
(15) $$CHANGE	Change job control records for use
(16) $$OPTION	Select the optional use for arbitrary "end-of-file" records

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1. Abstract of ORNL-TM-4291 (to be published); revised version of ORNL-CF-72-5-24 (1972).

5.12. ADLER-III: A PROGRAM TO CALCULATE CROSS SECTIONS FROM ADLER-ADLER RESONANCE PARAMETERS[1,2]

R. Q. Wright[3]

ADLER-III is a revision and extension of the ADLER program described in "ENDF/B Processing Codes for the Resonance Region," BNL-50296 (ENDF 148) by M. R. Bhat. The program calculates total, capture, and fission cross sections according to the Adler-Adler formalism using the corresponding parameters from file 2 of ENDF/B data. Doppler broadening is provided through the use of the ψ and φ functions. The program can read the resonance parameters from an ENDF/B tape (BCD mode) or the resonance parameters may be input on cards if desired.

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1. Work partially supported by Defense Nuclear Agency under Subtasks PB052-03 and PE074.

2. Abstract of TM-4257 (ENDF-191) (June 1973); packaged in RSIC as PSR-58.

3. Mathematics Division.

5.13. THE EXREM III COMPUTER CODE FOR ESTIMATING EXTERNAL RADIATION DOSES TO POPULATIONS[1]

D. K. Trubey

The EXREM computer code[2] is used to estimate the dose equivalent rate and the total dose equivalent from beta and gamma radiation resulting from submersion in contaminated water, submersion in contaminated air, and exposure to a contaminated surface. There can be more than one environmental release, and exposure can begin at any time after the first release. Contributions are considered from environmental releases and from nuclide decay chains. For a particular problem, the user may choose to calculate either the dose rates, the total doses, or both for any of three modes of exposure. A separate solution array is printed for each mode of exposure.

The EXREM II code has been available from RSIC but since the available nuclide decay data is rather out of date, and there is need to include positron and electron radiation, it was determined to assemble a new data base for nuclides of interest in environmental impact studies and revise the code.

The new data base now includes 164 nuclides comprising 130 decay chains. Spectral data include up to 30 gamma rays, 15 beta rays, 3 positrons, and 30 electrons for each nuclide. The data are based on recently published evaluations or on unpublished data made available by the ORNL Information Center for Internal Exposure. Care is taken to include x rays, conversion, and Auger electrons.

The new version of the code, to be called EXREM III, treats electrons and positrons in addition to beta rays and photons. The average energy of the positrons is calculated slightly differently from that of beta rays; the total energy of the electrons is taken for calculating the dose, rather than the average energy as in the case of beta rays.

Data management and input have been extensively revised. The first input is the entire nuclear data base (or the data can be available on disk). This is followed by the remaining input data which include the selected nuclide names (e.g., C060) but no additional nuclear data. The input parameters are given in free form by incorporating the FREEFORM[3] subroutines.

The major internal data arrays have been variably dimensioned. The large arrays depend on limits (e.g., maximum number of gamma rays or beta rays per nuclide) which are set in a BLOCK DATA subroutine or, in the cases of NRNUC (the number of nuclides in the problem), MAXCHN (the maximum number of decay chains), and NLOC (the number of dose locations), are set with input parameters. The total size of the variably dimensioned storage is set in a special subroutine which allows the size of the code to be changed easily. EXREM III will be made available from RSIC.

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1. Work sponsored by ORNL Environmental Sciences Division.

2. W. D. Turner, "The EXREM II Computer Code for Estimating Doses to Populations for Construction of a Sea-Level Canal with Nuclear Explosives," CTC-8 (1969).

3. R. C. Durfee, "FORTRAN Free-Form Input," internal ORNL memorandum, CF 70-1-45 (1970).

5.14. OTHER PUBLICATIONS BY RSIC STAFF MEMBERS

In addition to the program represented by the preceding abstracts, RSIC members participate in on-going shielding research programs not considered an integral part of RSIC itself. RSIC staff members are also frequently called upon for pre- or post-reviews of shielding publications. Two publications which have fallen in this category the past year are the following:

Monte Carlo Calculations and Sensitivity Studies of the Time-Dependent Neutron Spectra Measured in the LLL Pulsed Sphere Program, by S. N. Cramer, R. W. Roussin, and E. M. Oblow, ORNL-TM-4072 (March 1973). Abstract given in paper 4.13 of this report. Staff participant: RWR

Book Review by D. K. Trubey: *Engineering Compendium on Radiation Shielding. Vol. III: Shield Design and Engineering,* ed. by R. G. Jaeger, E. P. Blizard, A. B. Chilton, M. Grotenhuis, A. Honig, Th. A. Jaeger, and H. H. Eisenlohr, Springer-Verlag, Berlin-Heidelberg-New York, 1970; XII, 478 pages, 506 figures, U.S. $68. Review published in *Nucl. Eng. Design* **24**, 451 (1973).

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