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SCAMPI: A CODE PACKAGE FOR CROSS-SECTION PROCESSING

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ABSTRACT

The SCAMPI code package consists of a set of SCALE and AMPX modules that have been assembled to facilitate user needs for preparation of problem-specific, multigroup cross-section libraries. The function of each module contained in the SCAMPI code package is discussed, along with illustrations of their use in practical analyses. Ideas are presented for future work that can enable one-step processing from a fine-group, problem-independent library to a broad-group, problem-specific library ready for a shielding analysis.

I. INTRODUCTION

Multienery-group cross-section libraries are currently a necessity for using deterministic radiation transport codes. ANSI/ANS-6.1.2 cites the need for using problem-specific multigroup cross-section libraries in nuclear power plant radiation protection and shielding calculations. Other shielding applications have a similar sensitivity to processing of the cross sections to ensure proper treatment of the resonances and scattering matrices. However, the process of obtaining problem-specific cross sections can require the user to prepare the proper input to several computer codes in this multistep process. With this background, the Radiation Shielding Information Center (RSIC) requested that the Nuclear Engineering Applications (NEA) staff at Oak Ridge National Laboratory (ORNL) prepare a code package to facilitate the calculational procedure for creating problem-specific cross sections (working library) from problem-independent multigroup data (master library). The result is the SCAMPI (SCALE and AMPX Processing Interface) code package.¹

II. COMPONENTS OF SCAMPI

As indicated by the acronym, the SCAMPI system consists primarily of modules derived from the SCALE² and AMPX³ code systems. The AMPX system was conceived at ORNL in the late 1960s and has been continually maintained to provide a full range of code modules that (1) produce multigroup neutron, gamma-ray production, and/or gamma-ray interaction cross-section data from the Evaluated Nuclear Data Files (ENDF), (2) spectrally collapse cross sections to fewer groups, (3) perform resonance self-shielding of cross-section data, (4) execute a one-dimensional (1-D) discrete-ordinates calculation, and (5) perform miscellaneous cross-section operations (format conversion, consistency checks, listing, plotting, etc.). The cross-section libraries generated with AMPX can have two very general and flexible formats that are referred

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to as either a "master" or "working" library format. Working libraries are problem-specific and formatted for system analysis codes such as XSDRNPM.

Many of the AMPX modules used for problem-dependent processing and utility functions have been included in the SCALE code system. The SCALE code system was designed to perform criticality safety, radiation shielding, and source-term analyses using control sequences that automate the data processing and interface with system analysis modules. These control sequences use engineering data and keyword input to prepare the problem material and geometry specifications and then perform resonance self-shielding, Doppler broadening, and temperature interpolation of the thermal-scattering matrices to produce problem-dependent cross sections for the system analysis. Codes such as KENO V.a, KENO VI, MORSE-SGC, ORIGEN-S, and XSDRNPM are included in SCALE for system analysis.

The intent with SCAMPI is to provide users with a code package that included the AMPX modules needed to convert a fine-group, problem-independent master library into a broad-group, problem-specific, working-library format. The reasons for a new code package were the following:

1. A UNIX-based version operable on several workstation platforms would be needed prior to availability of the entire AMPX system.
2. There was a desire to include some of the simple, automated cross-section processing features available in the SCALE sequences.

The modules included in SCAMPI and a description of their functionality are provided in Table 1. The GIP module⁴ in SCAMPI is the only module not available in the SCALE or AMPX systems.

The SCALE control module called CSAS and its associated full-screen PC input processor, CSASIN,⁵ have been modified and included in SCAMPI to facilitate the creation of problem-specific cross-section libraries as a one-step process. Within SCAMPI, the CSAS module and the CSASIN input processor have been modified to provide the analysis sequences listed in Table 2. The input to CSAS consists of

1. keyword specification of the problem-independent cross-section library;
2. keyword specification of the geometry type—infinite homogeneous medium; a sphere, cylinder, or slab lattice cell; or a 1-D multiregion slab, cylinder, or sphere;
3. keyword specification of an alphanumeric material or nuclide identifier and associated properties (physical density or number density, isotopic abundance, weight percent of mixture, etc.) and mixture number; and
4. specification of region dimensions and materials, along with the model boundary conditions.

With this input the CSAS module prepares input specifications for the functional modules accessed by each analysis sequence shown in Table 2. For each sequence, the BONAMI and NITAWL modules are accessed to perform problem-specific resonance self-shielding for neutron cross-section libraries that have Bondarenko factors, resonance parameters, or both. NITAWL also interpolates the available thermal scattering matrices to the temperature specified by the user. XSDRNPM is accessed if cell-averaged or

Table 1. A list of functional modules included in the SCAMPI code package

Module	Function
AIM	Converts master cross-section libraries from BCD (card-image) to binary format or vice versa
AJAX	Merges, collects, assembles, reorders, joins, and/or copies selected data sets from master libraries
ALE	Lists information and data from master or working libraries
ALPO	Converts AMPX working library to ANISN library format
BONAMI	Performs resonance self-shielding for nuclides that have Bondarenko shielding factors (f-factors) associated with their cross sections
CSAS	Modified SCALE control module that accesses the material information processor to create problem input and execute BONAMI, NITAWL, XSDRNPM, ICE, and ALPO in a sequence specified by the user
CORECTOL	Converts pre-AMPX77 master libraries to the AMPX-77 form
FILTER	"Filters" a library into a smaller subset (e.g., reducing a coupled neutron-gamma library to a neutron-only or gamma-only library)
GIP	Converts ANISN-formatted library to an energy-group organized library used by DORT
ICE	Uses AMPX working library to produce mixture cross sections in various working formats
LAVA	Converts an ANISN working library into an AMPX working library
MALOCS	Collapses AMPX master libraries based on specified energy spectrum
NITAWL	Applies Nordheim resonance self-shielding treatment to nuclides with resonance parameters included with their cross sections
PERFUME	Adjusts nonphysical Legendre polynomial fits to scattering matrices to produce acceptable distribution
RADE	Checks AMPX and ANISN libraries based on known physical properties, e.g., $\sigma_a = \sigma_c + \sigma_f$
SMILER	Converts NJOY-produced cross sections to an AMPX master format
UNITAB	Merges data from up to 12 different master libraries (e.g., combines neutron, gamma production, and gamma on separate libraries into one library)
WAX	Functions as AJAX but operates using working libraries
XSDRNPM	Functions as a 1-D discrete-ordinates code for solving eigenvalue or fixed source problems. Can produce energy- and spatially weighted cross sections

Table 2. Analysis sequences available in CSAS control module of SCAMPI

Control sequences	Functional modules executed by control sequence				
CSASI	BONAMI	NITAWL-II		ICE	ALPO
CSASIX	BONAMI	NITAWL-II	XSDRNPM	ICE	ALPO
CSASN	BONAMI	NITAWL-II			ALPO
CSAS1X	BONAMI	NITAWL-II	XSDRNPM		ALPO

region-averaged cross sections are needed. The ICE module is used to provide a mixed AMPX working library for use by XSDRNPM or a Monte-Carlo-formatted library for use by MORSE-SGC. For SCAMPI, the CSAS module was modified to include the ALPO module to create an ANISN-formatted library for use with shielding analysis codes such as DORT⁶ or ANISN.⁷ An ANISN-formatted library must be further modified with the GIP module to produce the group-organized cross-section library required by DORT.

Again, the CSAS control module is included in SCAMPI to provide an alternative procedure for straightforward, problem-specific processing of cross-sections. Within the SCAMPI driver, the SCAMPI modules can each be executed in a stand-alone fashion and linked together consecutively to create any specific execution path for processing cross-section libraries. If the CSAS module is used, the master libraries must have nuclide identifiers consistent with the scheme adopted for the SCALE system and discussed in the documentation for the Standard Composition Library. For master libraries with other identifiers, the identifiers can be changed using the AJAX module.

One significant code improvement provided in the SCAMPI package is a new version of the MALOCS program from AMPX. This new version is significantly different than the version provided in ref. 3. The major reason for the update was to provide the capability to correctly collapse Bondarenko factors (or f-factors) in a master library from a fine-group to broad-group structure using a specified flux spectrum. Whether libraries use resonance parameters or Bondarenko factors, the use of MALOCS means that a working library does not have to be created at the fine-group level.

III. TESTING OF SCAMPI

No cross-section libraries are available with the SCAMPI code package. However, SCAMPI has been tested using sample problems for the SCALE and AMPX systems and AMPX-formatted master libraries such as those released with SCALE and the VITAMIN-B6 library.⁸ Two sample problems are included in the SCAMPI package. These sample problems use the VITAMIN-B6 library to analyze the ZPR-6, Assembly 7 model and the CTR standard blanket model described in ref. 9. Testing was performed on IBM RS/6000, DEC Alpha, SUN, and HP workstations.

IV. PROCESSING OF CROSS SECTIONS

Solution of the Boltzmann radiation transport equation using multienergy-group techniques remains of significant importance in the radiation shielding community. However, as evidenced by the above discussion that includes mention of various cross-section library formats and numerous codes that must be

executed to create a problem-specific library, the shielding analyst can often become somewhat confused about the process of obtaining accurate multigroup cross sections. The purpose of SCAMPI is to provide users with a means to create an accurate problem-dependent library from an accurate fine-group, problem-independent library. In fact the basic components of the library are based somewhat on the modules needed to create the BUGLE-93 library from the VITAMIN-B6 fine-group library.¹⁰ Some users see this process as so cumbersome that they elect to use an available problem-specific library [e.g., the BUGLE-80 (ref. 11) or BUGLE-93 (ref. 10)] with, perhaps, insufficient attention to its suitability for the problem at hand. Assuming that one starts with a fine-group, problem-independent library, it should be possible to create broad-group, problem-specific libraries based on a single input that specifies general information about the problem geometry and materials and the desired broad-group structure.

The CSAS module is an initial step towards providing an aid to the user who is not readily familiar with the various modules or the details of the process of preparing problem-specific cross sections. One limitation of the sequence is that it does not provide for the use of MALOCS to collapse libraries to a broad-group structure. Instead, the assumption is that the broad-group library input to CSAS is a pseudo-problem-independent library that has been collapsed from a fine-group library using a spectrum that is applicable to a wide class of problems. General use of the CSAS procedure in criticality, shielding, and depletion analyses within SCALE over the past 15 years has basically validated this assumption while helping to prevent the use of problem-specific libraries that are not applicable to the problem of concern. However, the approach applied in CSAS could be strengthened by providing additional execution paths that enable a collapse of the cross sections either before or after the resonance self-shielding steps.

V. APPLICATION OF SCAMPI

As noted above, the SCAMPI package contains all the modules needed to replicate the process used to create the BUGLE-93 library.¹⁰ This process begins with the fine-group, problem-independent VITAMIN-B6 library, performs resonance self-shielding with BONAMI, calculates flux spectra for particular locations of a generic model, and then collapses the cross sections to the 47 neutron 20 gamma BUGLE broad-group structure. To investigate the effect of altering this process, an application involving analysis of the Japan Power Demonstration Reactor¹² (JPDR) was selected. Figure 1 shows the 1-D model of the reactor used in the XSDRNPM calculation. Figure 2 shows the results of three different responses calculated with two different broad-group libraries as compared with the response results calculated from a reference fine-group library. The three responses investigated are the neutron fast flux greater than 1 MeV, the neutron dose, and the cobalt activation. The following three different cross-section libraries are used in the XSDRNPM analyses:

1. the fine-group VITAMIN-B6 library with resonance self-shielding via BONAMI (reference case);
2. a 67-neutron broad-group library output from the reference XSDRNPM case; and
3. a 67-neutron broad-group library created by first collapsing the VITAMIN-B6 library with MALOCS using the reference case spectrum located one-third into the pressure vessel followed by resonance self-shielding of the broad-group library.

The 67-neutron-group library created by XSDRNPM follows the basic process used to create the BUGLE-93 library (i.e., resonance self-shielding performed on the fine-group level). The use of MALOCS

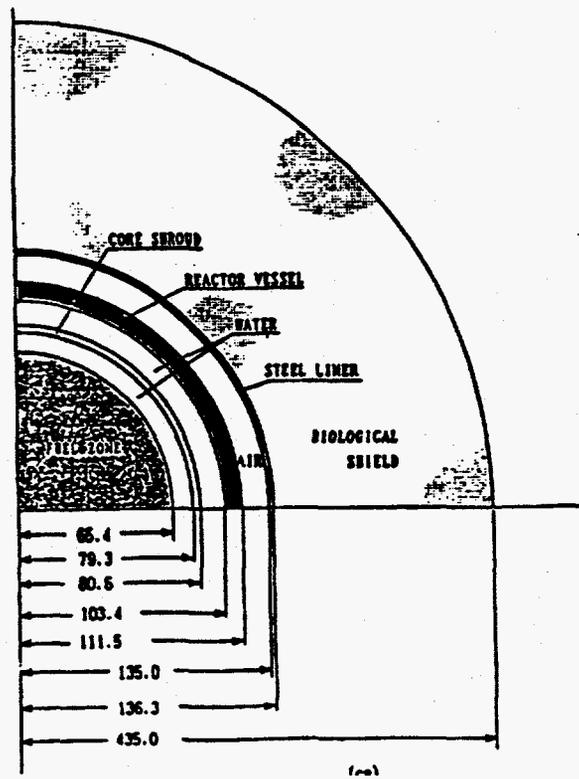


Fig. 1. One-dimensional cylindrical geometry model of JPDR at core midplane level.

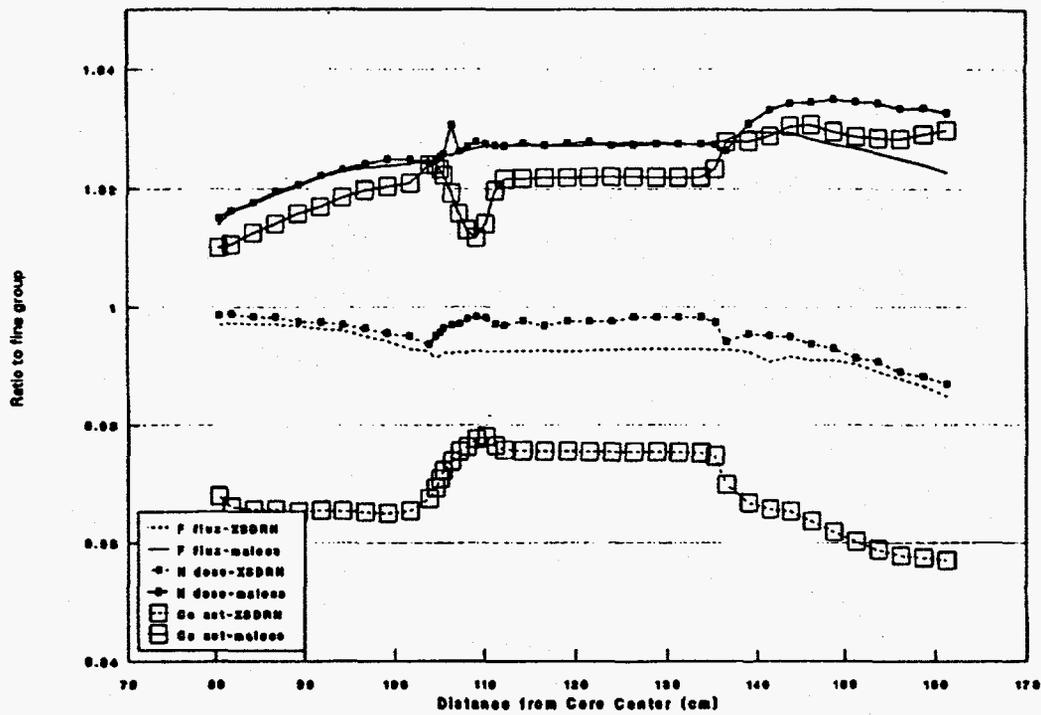


Fig. 2. Response differences due to cross-section processing.

to create a 67-neutron-group master library from a generic reactor shielding spectrum is the process typically used in the SCALE code system (i.e., resonance self-shielding performed on the broad-group level) and available in SCAMPI via the use of the CSAS module.

The results shown in Fig. 2 indicate the three responses are fairly insensitive to the two procedures used here for the creation of problem-specific, broad-group libraries. The XSDRNPM-collapsed procedure provides more accurate results in comparison to the reference case for the fast flux and neutron dose responses. However, the alternative procedure using a pseudo-problem-independent broad-group library is within 3% of the reference case results. Indeed, for the cobalt activation response, the generic broad-group library provides better agreement with the reference case than does the XSDRNPM-collapsed library. Of further interest would be the use of these two broad-group libraries to analyze different reactor shielding structures. For some cases it could well be that the XSDRNPM-collapsed library would be less accurate than the generic broad-group library because of the ability to readily use problem-specific parameters in the self-shielding process.

The results shown in Fig. 2 indicate that if a spectrum that is characteristic of a class of problems is used to collapse a problem-independent fine-group library, then the resulting broad-group library can be accurately applied to that class of shielding analysis problems, and problem-specific resonance self-shielding can be readily performed at the broad-group level.

VI. SUMMARY

The SCAMPI code package has been assembled to provide ready access to the calculational tools needed to process fine-group, problem-independent libraries into problem-specific, broad-group libraries. A control module to automate resonance self-shielding of fine-group libraries or generic broad-group libraries has been included. Further enhancements of this control module could provide users with an easy-to-use tool for one-step processing of data for each specific problem of concern. Particularly, the control module would have to include the option to collapse cross sections based on specified or calculated flux spectra. Inclusion of GIP into the analysis sequence accessed by the control module would also be beneficial.

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