

**BUGLE-96: A Revised Multigroup Cross Section Library
for LWR Applications Based on ENDF/B-VI Release 3***

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BUGLE-96: A REVISED MULTIGROUP CROSS SECTION LIBRARY FOR LWR APPLICATIONS BASED ON ENDF/B-VI RELEASE 3

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ABSTRACT

A revised multigroup cross-section library based on ENDF/B-VI Release 3 has been produced for light water reactor shielding and reactor pressure vessel dosimetry applications. This new broad-group library, which is designated BUGLE-96, represents an improvement over the BUGLE-93 library released in February 1994 and is expected to replace the BUGLE-93 data. The cross-section processing methodology is the same as that used for producing BUGLE-93 and is consistent with ANSI/ANS 6.1.2. As an added feature, cross-section sets having upscatter data for four thermal neutron groups are included in the BUGLE-96 package available from the Radiation Shielding Information Center. The upscattering data should improve the application of this library to the calculation of more accurate thermal fluences, although more computer time will be required. The incorporation of feedback from users has resulted in a data library that addresses a wider spectrum of user needs.

I. INTRODUCTION

In February 1994, the BUGLE-93¹ multigroup cross-section library for LWR shielding applications and reactor pressure vessel dosimetry was released through the Radiation Shielding Information Center. BUGLE-93 was developed using the ANS 6.1.2 recommended methodology² for producing multigroup cross sections for nuclear power plant shielding analyses. Additional data testing³ using the original BUGLE-93 release and the application of BUGLE-93 to reactor systems sensitive to the thermal flux have combined to suggest improvements to the original multigroup data. The timeliness of the improvements to BUGLE-93 were further influenced by the release of ENDF/B-VI Release 3.⁴

In the final BUGLE-93 report,⁵ the background for the development of the BUGLE series of data libraries and detailed specifications for the generation and testing of BUGLE-93 are documented. With respect to the fine-group VITAMIN-B6 library,⁶ there are no changes in the specifications. On the other hand, the broad-group specifications have been slightly modified with the exception of the materials and energy group structure which are unchanged. In the thermal neutron energy region, the shape of the weighting spectra now resembles a Maxwellian profile and the procedure used to self-shield the steel cross sections was improved. The list of response functions, units for kerma factors, library format and contents

have undergone significant change. This paper will summarize the differences between BUGLE-93 and the current version of the broad-group library which is designated as BUGLE-96.

II. BACKGROUND

BUGLE-93 was modeled after the successful BUGLE-80 and SAILOR libraries^{7,8} which were derived from the ENDF/B-IV- based VITAMIN-C fine-group library.⁹ In contrast to VITAMIN-B6, there were no upscatter data in the VITAMIN-C fine-group library. The development of BUGLE-93 was guided by the following considerations regarding the treatment of the thermal groups in VITAMIN-B6: (a) compatibility with the BUGLE-80 and SAILOR data libraries as requested by the LWR user community, (b) "plug-compatible" cross-section tables with previous LWR libraries and (c) a consensus of thought that below 0.1 MeV, the cross sections were unimportant for reactor pressure vessel dosimetry applications. The underlying motivation to remove the upscatter cross sections for the thermal neutron groups, particularly for two-dimensional transport analysis, was driven by the anticipation of increased execution times required to converge the upscatter groups.

Experience³ using the BUGLE-93 broad-group energy structure with thermal upscattering cross sections demonstrated better agreement for thermal responses. As a consequence of strong interest in the application of a broad-group library to calculate more accurate thermal fluences, our original approach to the LWR data library development task was reevaluated. With the inclusion of upscattering data for the thermal groups and other modifications in response to feedback from users, the BUGLE-96 data library package has enhancements to address a wider spectrum of user needs.

III. PREPARATION OF FINE-GROUP PROCESSED CROSS SECTIONS

The 1994 edition of the fine-group VITAMIN-B6 library, which was based on ENDF/B-VI Release 2, was the fine-group library from which BUGLE-93 was produced using the AMPX-77 code system¹⁰. This fine-group library, whose energy structure consists of 199 neutron energy groups and 42 gamma-ray energy groups, contains data for 127 nuclides, including over 60 new or extensively revised evaluations in ENDF/B-VI. Also, the cross section sets in this fine-group library contain upscatter data for 35 thermal neutron groups. The calculational procedure for developing problem-dependent cross-section libraries in the ANSI/ANS 6.1.2 standard calls for the existence of a fine-group problem-independent cross-section library.

Since the release of BUGLE-93, there have been some changes in the computing environment used for cross-section processing. Most of the changes are related to differences in computer hardware and to improvements in the calculational tools. The 1994 version of the VITAMIN-B6 library was processed using a late 1993 version of NJOY91. For the current work, seven nuclides from ENDF/B-VI.3 were processed into multigroup form with NJOY94.10¹¹ using the fine-group VITAMIN-B6 specifications. BUGLE-96 contains new evaluated data for H-2, N-14, Al-27, Ba-138, U-235, Pu-241, and Am-241. Details associated with the new evaluations are given in Table 1. Simple physics checks on the new fine-group data in AMPX master format revealed a problem with the Am-241 fission spectrum. A recently suggested correction to NJOY94.10 from MacFarlane¹² led to the creation of a modified version of NJOY94.10. The reprocessing of ENDF/B-VI.3 Am-241 with the updated NJOY94.10 produced a fission spectrum with a more reasonable shape.

The migration of some cross-section activities at ORNL to a workstation environment has resulted in the creation of a new code package called SCAMPI¹³ which is a subset of the AMPX-77 system with some improvements arising from the SCALE project.¹⁴ The seven new evaluations in AMPX format were used to produce a revised fine-group VITAMIN-B6 master library using the SCAMPI code package. These seven nuclides superceded nuclear data in the 1994 edition of VITAMIN-B6. The identifiers of the nuclides in the fine-group library were changed to conform with the SCALE ZA nomenclature to facilitate ENDF/B-VI data testing activities within the SCALE project.

Table 1. ENDF/B-VI Release 3 Nuclides

Z	Nuclide	MAT	MOD	ENDF Tape
1	H-2	128	2	134
7	N-14	725	3	134
13	Al-27	1325	1	134
56	Ba-138	5649	2	134
92	U-235	9228	4	135
94	Pu-241	9443	3	135
95	Am-241	9543	3	135

IV. PREPARATION OF PROBLEM-DEPENDENT DATA

All computational tools used to self-shield, temperature-correct, and collapse the fine-group library into the broad-group format were part of the SCAMPI package operational on an IBM/RISC 6000 workstation cluster. The development of the SCAMPI package was stimulated by the need for access to tested operational modules to perform the above mentioned tasks in a workstation environment.

Starting with the revised VITAMIN-B6 master library, the next step was the production of a self-shielded cross-section library for the LWR models used to determine the collapsing flux spectra. These models, which correspond to the models used in the SAILOR report, are shown in Figure 1. Unlike the BUGLE-93 production procedure, the SAILOR approach (50-50 mixture of water and steel) for self-shielding the steel constituents was abandoned. The adopted approach can be seen in Figure 2 which illustrates the revised procedure for calculating the LWR-specific flux spectra. Note the BONAMI path labeled "C/S Steels" in Figure 2. The constituents of carbon and stainless steels were self-shielded in a mixture containing only steel. A reanalysis of Arkansas Power and Light's Arkansas Nuclear One-1 Reactor (ANO-1) using scaled one-dimensional methods and preliminary ENDF/B-VI iron cross sections prepared using this approach showed significant improvements in the agreement with measured dosimeter data.¹⁵ Other than steel, the specific nuclides in the PWR and BWR regions were resonance self-shielded and corrected for temperature effects using the same procedure as BUGLE-93.

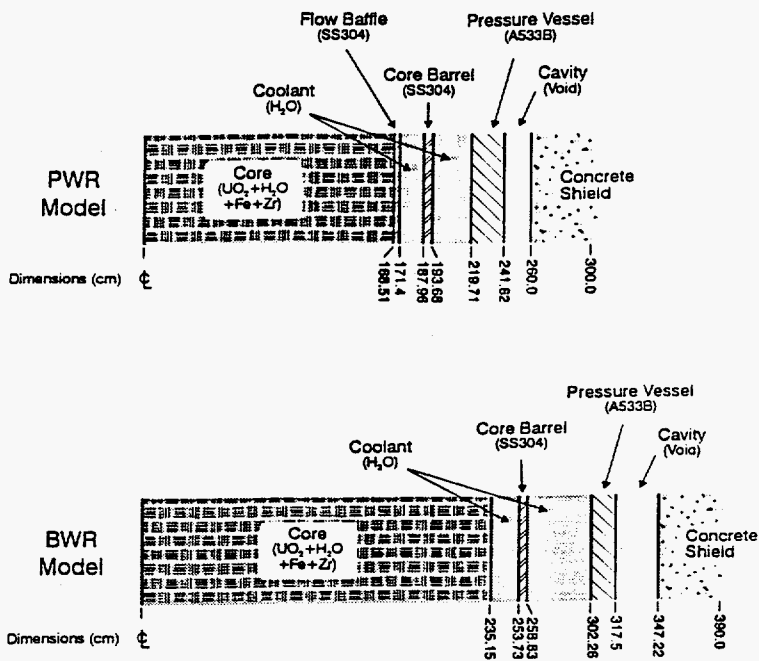


Figure 1. One-dimensional models used to calculate the specific flux spectra for collapsing BUGLE-96 cross sections from VITAMIN-B6.

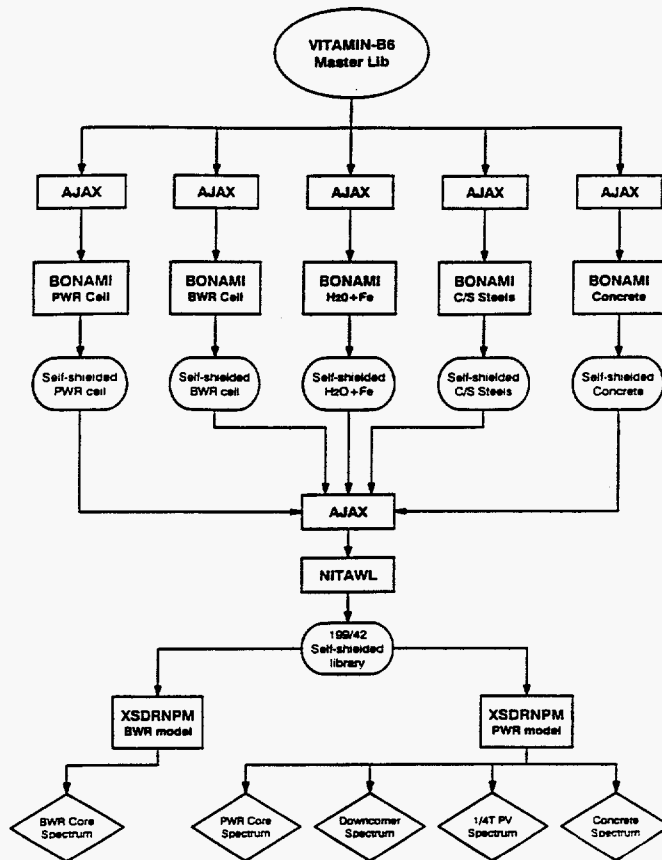


Figure 2. Procedure for calculating BWR- or PWR-specific flux spectra.

After obtaining the flux spectra, the next stage of the collapsing procedure included the MALOCS module which performed the group collapse. For BUGLE-96, this stage was performed twice. A schematic diagram of the collapsing procedure is given in Figure 3. The first pass was to regenerate the files needed to replace BUGLE-93 (no thermal upscattering cross sections). The authors expect that a sizable segment of the user community has interest in using this form of the data. The second pass was to produce a broad-group library designated as BUGLE-96T which includes thermal upscattering data. The difference between the production of the collapsed data for BUGLE-96 and BUGLE-96T is a single parameter in the MALOCS module.

Feedback from users of BUGLE-93 led to the collection of the following concerns which were corrected in BUGLE-96. Improvements to the broad-group data include accommodations for:

- Missing photon absorption cross sections,
- Consistent units for gamma-ray kerma factors per atom ($\text{eV}\cdot\text{b}$ rather than $\text{MeV}\cdot\text{b}$),
- Temperature dependence for special weighted cross sections,
- Correcting an error in the thermal range caused by a programming bug in the MALOCS module of AMPX-77,
- Providing some analysts a choice of using or not using thermal upscattering data,
- Correcting the convergence problem in the thermal energy region of the 1-D transport cases used to determine the collapsing spectra.

In the thermal region, the significance of the convergence problem can be seen in Figure 4. A comparison is made between the downcomer flux spectrum used to produce BUGLE-93 and the downcomer flux spectrum used to produce BUGLE-96. Note the Maxwellian flux shape that is clearly evident now.

V. LIBRARY VERIFICATION

The BUGLE-93 cross-section library was extensively verified using three levels of testing, which included: (1) automatic diagnostic software to check for internal consistency of the data files, (2) numerical and graphical comparisons with other cross-section data, and (3) computational analyses of more than 30 integral benchmark experiments. The benchmark testing was a significant effort comparable to the level of effort needed to process the library. It not only helped to verify the processing of the multigroup cross sections, but also to demonstrate the impact of changes in the ENDF/B-VI data for a range of transport and physics analyses. Much of this benchmark testing of BUGLE-93 remains valid for BUGLE-96, especially for those applications which are sensitive only to data above the thermal energy range. A few selected benchmarks have been recalculated using BUGLE-96 data and it is expected that additional benchmarks will be analyzed in the near future.

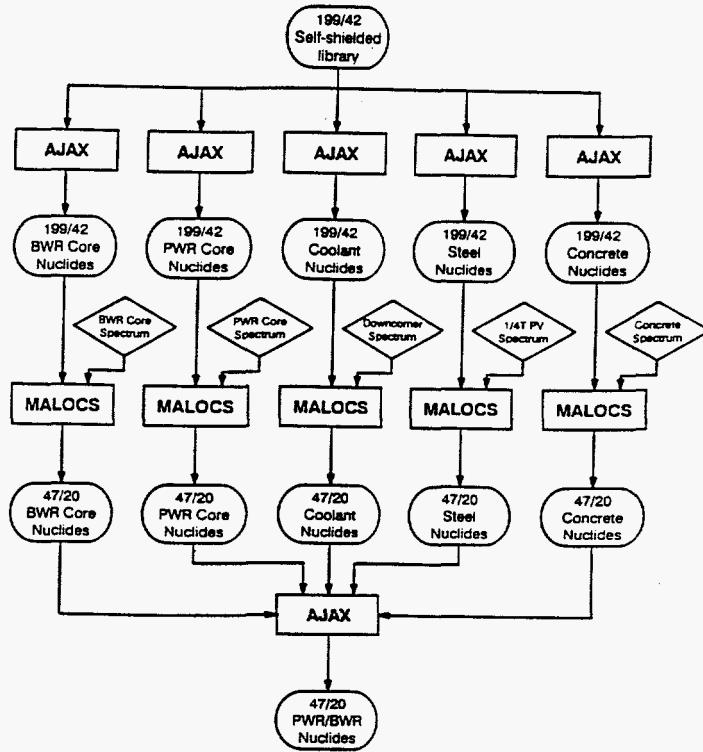


Figure 3. Procedure for collapsing fine-group cross sections using BWR- or PWR-specific flux spectra.

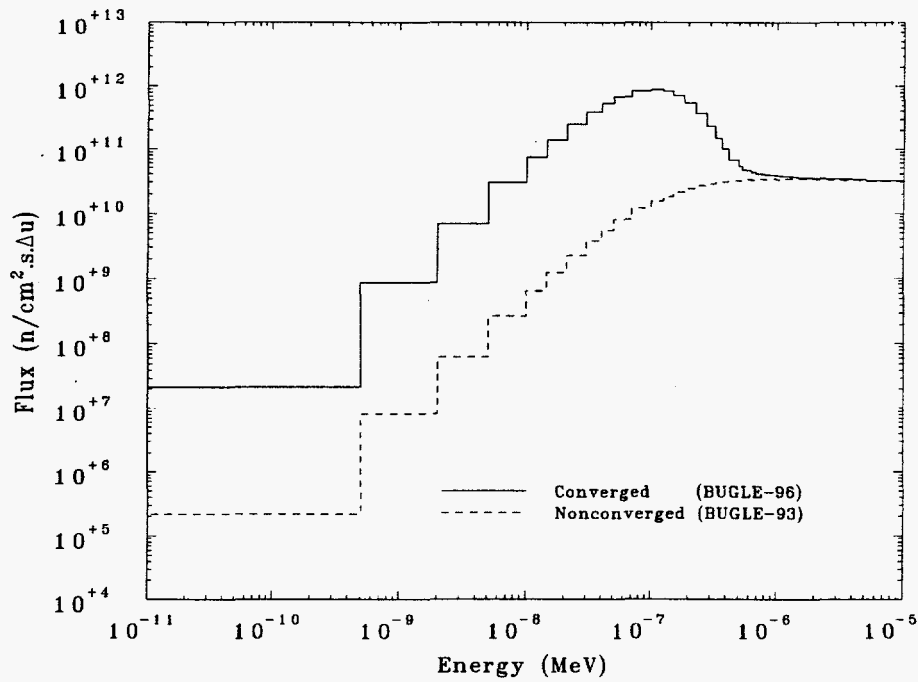


Figure 4. Comparison of converged and nonconverged thermal neutron flux at the downcomer location of the PWR model.

In addition to the few benchmark tests, verification of the BUGLE-96 library has included the first two levels of verification described above, i.e. automated software checking and comparisons with other cross-section data. The first step in the data verification process made use of the RADE diagnostic module in the AMPX-77 system. Also, data were compared with previous results at several steps during the processing. These periodic comparisons are an important step in the processing, since it frequently happens that even minor changes to the processing codes, which are intended to fix a specific problem, may cause unexpected changes in other portions of the processed data files.

One useful check is to compare the PWR- and BWR-specific fine-group flux spectra, which were used to collapse the special weighted cross sections, to the corresponding spectra produced by recalculating the one-dimensional PWR and BWR reactor models with the collapsed broad-group cross sections. This was done for each of the five weighting spectra. Figure 5 shows the comparison of the VITAMIN-B6 and the BUGLE-96 spectra at the 1/4T position in the pressure vessel of the PWR model. The broad-group results appear to reproduce the fine-group results very well. Note that the spectra are plotted on a "per unit energy" basis, which is appropriate for comparing the integrated areas under the histograms.

Further data testing of the BUGLE-96 library is expected and desirable. However, it is felt that sufficient testing has been performed to reasonably assure that the correct methodology was used to process the library.

VI. SUMMARY AND CONCLUSIONS

All significant evaluations in ENDF/B-VI Release 3 have been incorporated into BUGLE-96 in the spirit of continuing to provide radiation transport analysts with the most currently available nuclear data. BUGLE-96 represents an improvement over the previous BUGLE-93 library particularly for applications sensitive to the thermal flux. The inclusion of thermal upscattering data in one form of the BUGLE-96 package contributed to RSIC should help users obtain a more accurate thermal fluence. The authors continue to encourage feedback from the user community on the performance of nuclear data customized for LWR applications.

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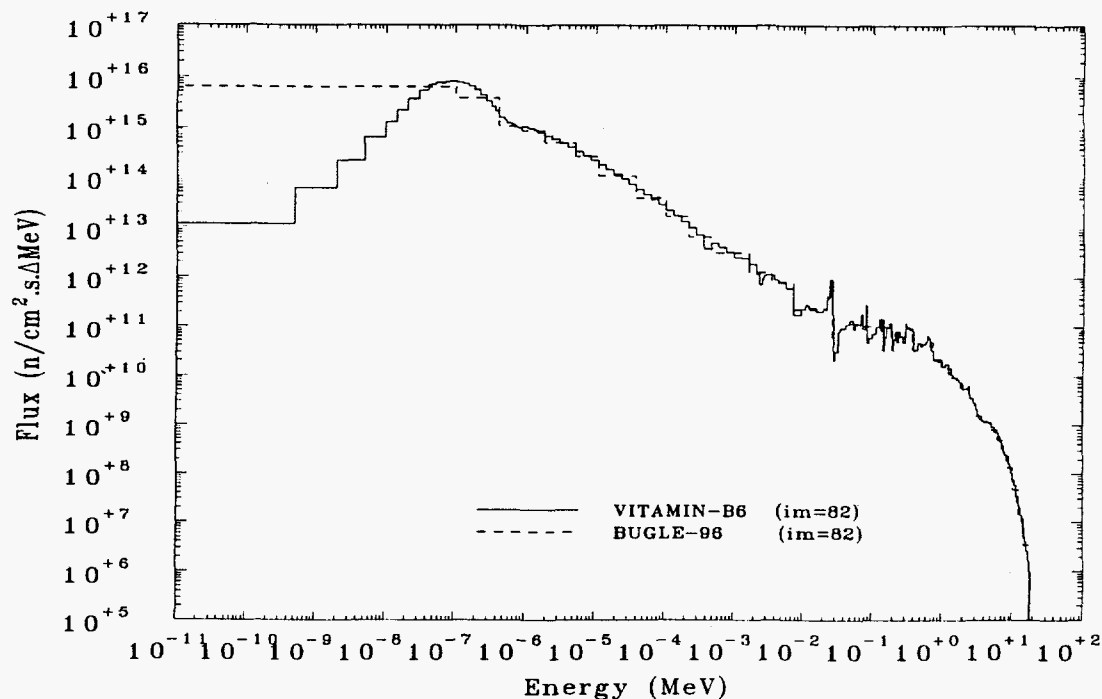


Figure 5. Comparison of VITAMIN-B6 and BUGLE-96 spectra at the 1/4T position in the pressure vessel.

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