

**Final Deliverables for the ACTIV Code Project
(Project No. 05-07741)**

Appendix III

**Development of Activation Analysis Libraries
for Use with the ACTIV Code**

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Introduction

The nuclear data needed for detailed neutron activation studies fall into two general categories:

1. multigroup neutron cross sections for use in the transport calculations to compute the space and energy dependence of the neutron flux, and
2. multigroup activation cross sections (n,γ , n,p , $n,2n$, etc.) and decay data (natural abundances, half-lives, branching fractions, etc.) for all the important parent and daughter isotopes that can be generated via neutron activation.

If possible, the transport calculation and the activation analysis should be done with a consistent set of multigroup data. However, in practice, the two calculations are often done independently and are only loosely connected via a set of collapsed neutron flux information from the transport calculation that is used in zero-dimensional few-group codes that model and simulate the isotope transmutation schemes. Usually significant detail is lost in this space and energy collapsing process, which can lead to large uncertainties in the computed activities. This is especially true in regions where rapid changes in the neutron spectra cannot be treated adequately in a zero-dimensional model. In addition, the coupling process can be cumbersome, since it often requires a fair amount of manual intervention.

The new ACTIV code eliminates this separate coupling and collapsing process by simply performing the activation calculations with the full space and energy dependent fluxes from the transport code. The same geometry is modeled and the user can select any number of pointwise radial and axial traverses or zone average activations that he or she desires. Thus, all of the space-energy detail from the original transport calculation is preserved and included within the activation calculation – thereby, essentially removing all the uncertainty that is introduced in the traditional two-step process. Now, the only uncertainties remaining are those associated with the computed neutron fluxes, the base activation data, and, of course, the initial impurity concentrations present in the unirradiated structural materials.

For full benefit and minimal uncertainty, the activation cross sections used within ACTIV should be developed to be consistent with the multigroup data used in the transport theory calculations for the space-energy neutron flux distribution. If possible, the same base fine-group library, the same processing codes, and a set of similar assumptions should be used.

To achieve this level of compatibility, a reasonably general calculational procedure has been developed based on the assumed availability of a fine-group Master library and the use of the standard cross section processing codes and ORIGEN data libraries that are distributed as

part of the SCALE system (Ref. 1). The purpose of this document is to outline this general procedure and to identify some of the details associated with the development of a specific activation library for use with the BUGLE96 shielding library (Ref. 2). The steps involved in this specific example can be easily generalized for other situations.

Base Transport Theory Capability

The philosophy behind the development of the ACTIV code was based on the assumption that the owners of all nuclear power plants have a vessel surveillance program of some sort, that they all relate excor detector responses to variations in core arrangement, and that they all have concerns about dose to personnel and equipment in the ex-vessel regions, etc.. This need translates to the availability of some relatively detailed transport model to characterize the radiation environment (usually both neutron and gamma) in the excor and ex-vessel regions. The standard here appears to be multiple 2-D discrete ordinates models (R- θ and R-Z) using the DORT code (Ref. 3) with the BUGLE96 47/20 group coupled neutron gamma library (Ref. 2). The ACTIV code was developed to take advantage of the detailed information already available from these applications, with minimum duplication of effort and maximum use of existing capability.

The BUGLE96 data that are used for many of these analyses include information for 120 isotopes/materials in 47 neutron groups and 20 gamma groups. This broad-group data set was collapsed from the VITAMIN-B6 fine-group library (Ref. 4) which contains 199 neutron group and 42 gamma group information derived from the ENDF/B-VI nuclear data files. The BUGLE96 library was designed specifically for shielding applications focusing on fast neutron and gamma transport analyses, vessel damage studies, excor dosimetry evaluations, etc.. Its intended primary role was certainly not for determining thermal fluxes, thermal reaction rates, and thermal neutron activation – since there are only two energy groups below 0.4 eV. However, it has several positive attributes including the fact that it contains the latest ENDF data, it is readily available to the user community, it already has a wide user base, and the thermal group resolution and structure are more detailed than generally available in other zero-dimensional activation analysis codes. Thus, it was decided that the BUGLE96 structure would be a good choice for the development of a multigroup activation library for use with ACTIV. The space-dependent neutron fluxes in 47 energy groups would be determined from a DORT computation using BUGLE96 data, and the activation calculations would be performed using a consistent 47 group activation library within ACTIV.

Computational Procedure

A simplified schematic that illustrates the development of the activation library used within ACTIV is shown in Fig. 1. This figure summarizes the various steps involved for a general case starting from an available fine-group Master library. For the specific case of interest here, the broad-group libraries have the same neutron group structure as in BUGLE96 and the final activation library used in ACTIV is referred to as ACTXS47.LIB. The VITAMIN-B6 library is used as the reference fine-group dataset since this was the basis of the BUGLE96 library development (Ref. 2). A typical concrete spectrum is used as the weighting function (see below).

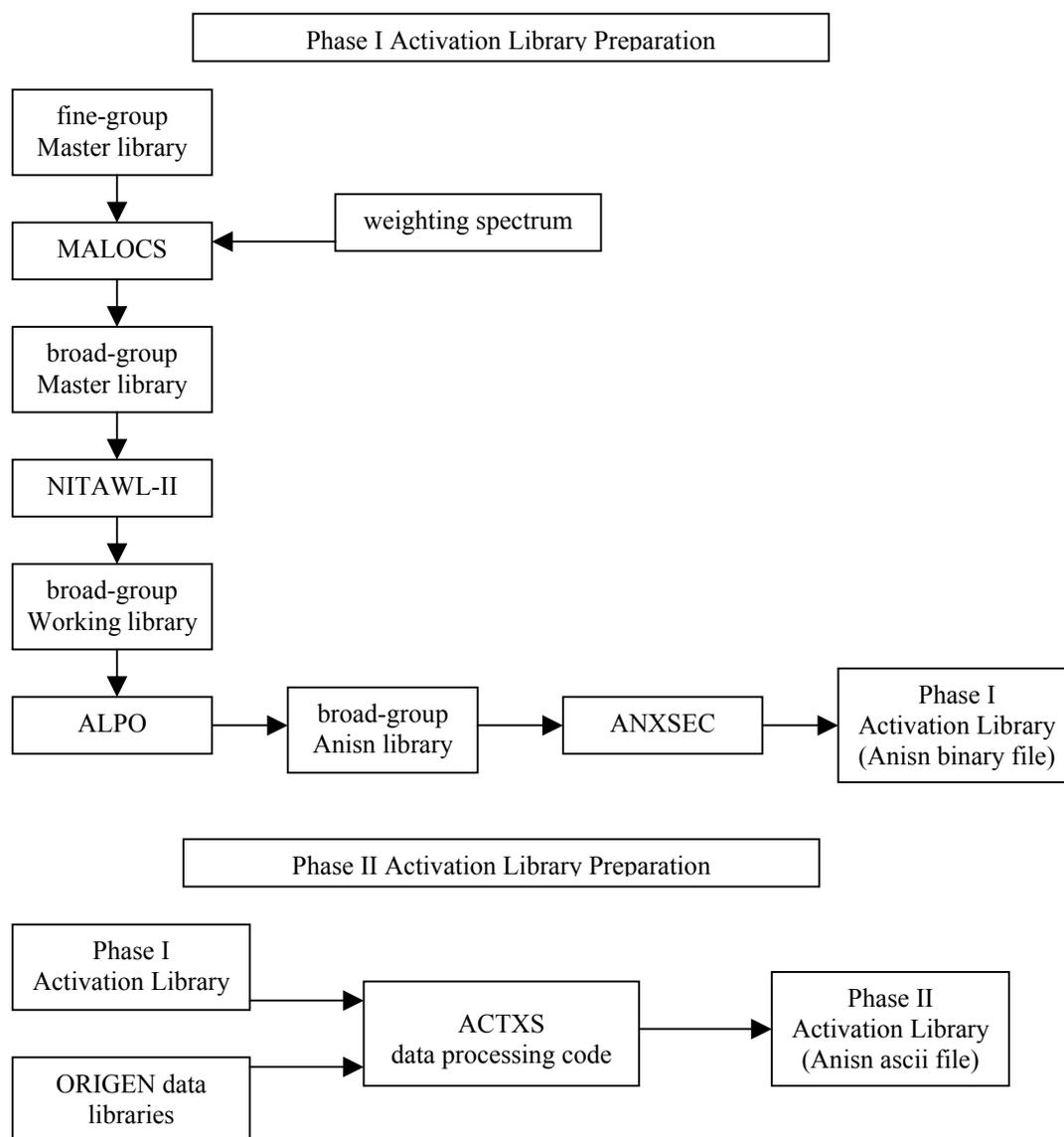


Fig. 1. Simplified schematic for generation of the activation library for ACTIV.

The overall process is broken into two steps or phases. The first step involves the collapse of the infinitely dilute data in the fine-group library into the desired broad group structure and subsequent format changes to put the Phase I Activation Library into proper form. This involves the elimination of lots of unnecessary information (gamma cross sections, scattering data, etc.) and the storage of the remaining activation cross sections in ANISN format. In particular, ten reaction cross sections are extracted from the collapsed library and stored in a format suitable for use in ACTIV. The specific reactions and the associated ENDF MT numbers (see Ref. 1) that are included in the activation library are listed in Table 1. The first eight of these cross sections are the only neutron activation reactions that are treated in ACTIV.

Table 1. Reaction cross sections included in the activation library.

ENDF MT No.	102	107	103	16	104	105	18	27	1452	1
Reaction	n, γ	n, α	n,p	n,2n	n,d	n,t	n,f	n,abs	$v\sigma_f$	σ_T

The MALOCS, NITAWL-II, and ALPO codes identified in Fig. 1 as part of the Phase I processing sequence are included within the SCALE 4.3 package. The ANXSEC code was written at UMass-Lowell to perform a variety of manipulations on ANISN-formatted libraries, and it is distributed as part of the ACTIV code package. As indicated in the sketch, the primary function of each of these codes is as follows:

- MALOCS collapse fine-group master library to desired broad group structure using an input fine-group weight function.
- NITAWL-II convert broad-group master library to working library format (note that no resonance processing is performed since we desire infinitely dilute activation cross sections).
- ALPO convert the working library into ANISN format with “extra” cross sections (as noted above) added to the top of the normal ANISN cross section tables.
- ANXSEC truncate ANISN table width and length to eliminate unnecessary gamma cross sections and scattering data.

The second step in the generation of an activation library combines the data from Phase I with a variety of information from the ENDF\B-VI version of the ORIGEN data libraries distributed as part of the SCALE 4.3 package. In particular, two card image libraries (see Ref. 1 for more details) are used here, as follows:

- END6DEC decay database for the light elements, actinides, and fission products.
- XSECTPHO nuclear data libraries and photon yield libraries for the light elements, actinides, and fission products.

These libraries are read and the hollerith names, natural isotopic abundances, decay data, and appropriate branching fractions are extracted for the isotopes of interest. The processing of the ORIGEN data files is performed in the ACTXS code. This module was written at UMass-Lowell as a tool for integrating all the necessary nuclear data from the Phase I activation library and the two ORIGEN libraries into a single file for use in ACTIV. For the development associated with the BUGLE96 compatible activation library, the final product is the ACTXS47.LIB file.

The user interface to ACTXS simply includes a list of the IDs for the nuclides of interest and the corresponding material number on the Phase I ANISN-formatted library. The base isotope ID uses the ZA number of the particular isotope, where

$$ID = Z * 10000 + A * 10 + IS$$

- and Z = atomic number
 A = atomic weight
 $IS = 0/1$ to indicate the ground/metastable state.

The input libraries are searched for the nuclides of interest and, if found, the pertinent data are added to the final Phase II activation library written in ANISN ascii format. Note that, in the ORIGEN libraries, the data associated with the first occurrence of the nuclide ID are used and, at present, only the light element and actinide portions of the libraries are searched (since the emphasis in ACTIV is on the excore structural regions, it does not treat fission product production paths - thus there is no need for fission product isotopes in the final activation library).

Approximately 800 isotopes were included in the desired nuclide list for the final ACTXS47.LIB file. Since the ORIGEN libraries are very comprehensive, natural abundances, decay data, and branching fractions were obtained for all of these isotopes. However, nonzero activity cross sections for only about 100 isotopes were obtained from the base VITAMIN-B6 library data. Appropriate flags identifying the content of the library are incorporated directly within the final library. In this way, ACTIV knows what information is available and it simply eliminates any transmutation paths that are not compatible with the existing library data.

The final library has a relatively simple structure and it is written in ascii format. This allows for simple editing of the file to modify existing data or to add additional information from other sources as needed.

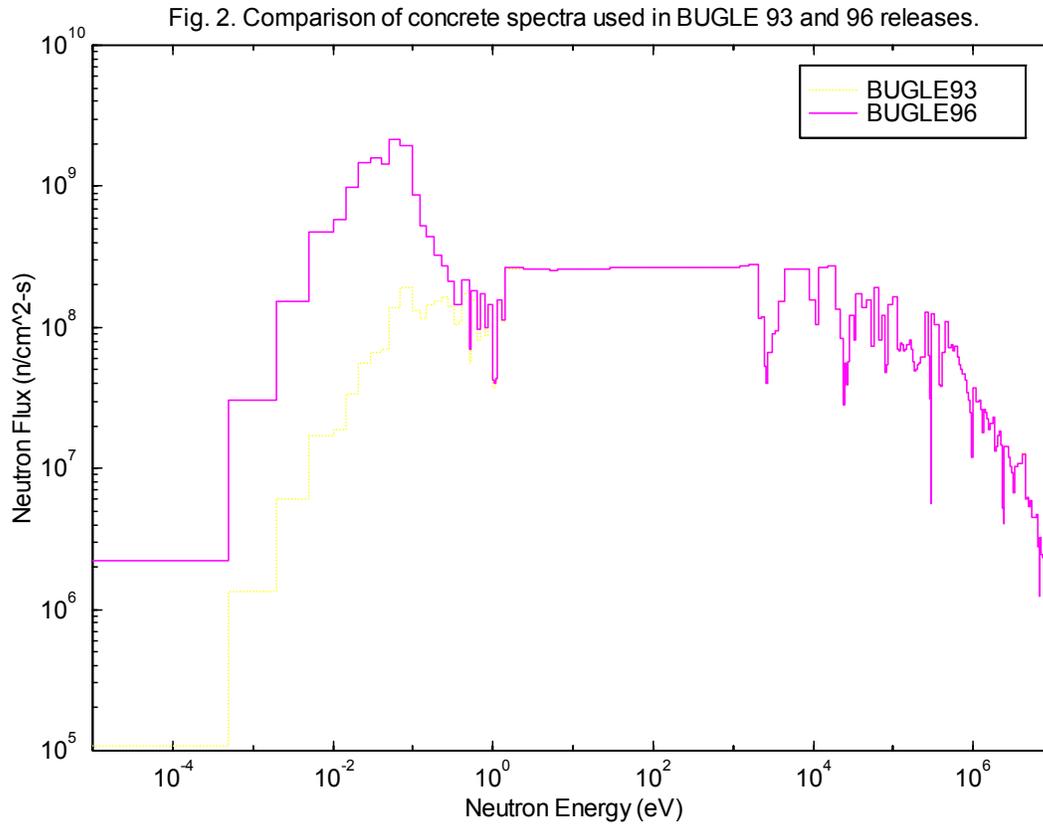
Weight Function for ACTXS47.LIB

As indicated above, the MALOCS code is used to collapse the original fine-group structure to the desired broad-group format. For the development of the ACTXS47.LIB dataset, a "typical spectrum" found in the excore regions of an LWR was chosen as the desired weight function. A "typical spectrum" is actually a hard quantity to define precisely, since the actual neutron spectrum can vary significantly from region to region. However, for this case, the 47 group structure in the resultant broad-group library still has enough energy resolution that the collapsed cross sections are not overly sensitive to the specifics of the weight function (as long as it is reasonable).

With this in mind, it was decided that the same concrete weight function that was used to generate part of the BUGLE96 data from VITAMIN-B6 would be used here. Following the details given in Ref. 2, a typical 1-D PWR system was modeled in the XSDRN code (Ref. 1) and the neutron and gamma spectra were generated throughout the core and excore regions. The resultant neutron spectrum in the concrete bioshield (at mesh #106 in the 1-D XSDRN model) was used as the weight function in the generation of ACTXS47.LIB. This procedure is fully consistent with the methods and assumptions used in the generation of BUGLE96.

Note that the actual implementation of this process was done in two steps. The BUGLE93 report explicitly tabulates the concrete spectrum at mesh point 106, but the BUGLE96 update documentation does not have this information. Therefore, as a check on the overall procedure, an XSDRN calculation with only one outer iteration was performed first. This calculation reproduced nearly exactly the spectrum given in the original BUGLE93 report (ORNL-6795), thus verifying the equivalency of the current setup and the BUGLE93 development. With this verification complete, a second XSDRN run was made that allows multiple outer iterations to properly converge the thermal flux (this correction was made in the BUGLE96 release). The differences in the computed spectra are quite significant in the thermal

region as illustrated in Fig. 2. The concrete spectrum denoted as BUGLE96 in Fig.2 is the one used to collapse the VITAMIN-B6 library to 47 groups to produce ACTXS47.LIB.



Summary

This brief report documents the general procedure used to develop activation analysis libraries compatible with the ACTIV code. It identifies and explains how the SCALE 4.3 processing codes and data libraries are used, and it also overviews the function of the ACTXS code which was written as part of this development effort.

A specific example is also discussed to give the general procedure some specificity. In this case, the base VITAMIN-B6 fine-group library was used to generate a 47 group activation library, ACTXS47.LIB, that is fully compatible with the popular BUGLE96 shielding library. With this new library, the combination of BUGLE96 and DORT (for the neutron transport calculations) and ACTXS47.LIB and ACTIV (for the activation computations) represent a powerful tool for addressing a whole range of activation analysis situations.

References

1. "SCALE 4.3 - Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation for Workstations and Personal Computers," Radiation Shielding Information Computational Center, CCC-545 (1997).
2. "BUGLE-96 - Coupled 47 Neutron, 20 Gamma-Ray Group Cross Section Library from ENDF/B-VI for LWR Shielding and Pressure Vessel Dosimetry Applications," Radiation Shielding Information Computational Center, DLC-185 (1996).
3. "DOORS3.1 - One, Two, and Three Dimensional Discrete Ordinates Neutron/Photon Transport Code System," Radiation Shielding Information Computational Center, CCC-650 (1996).
4. "VITAMIN-B6 - A Fine-Group Cross Section Library Based on ENDF/B-VI Release 3 for Radiation Transport Applications," Radiation Shielding Information Computational Center, DLC-184 (1996).