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ENEA-Bologna Multi-Group Cross Section Libraries for LWR Shielding and Presure Vessel Dosimetry Applications

M. Pescarini, V. Sinitsa, R. Orsi, M. Frisoni

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ENEA-BOLOGNA MULTI-GROUP CROSS SECTION LIBRARIES FOR LWR SHIELDING AND PRESSURE VESSEL DOSIMETRY APPLICATIONS

M. Pescarini, V. Sinitsa, R. Orsi, M. Frisoni - ENEA

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Sommario

The ENEA-Bologna Nuclear Data Group produced two multi-group cross section libraries for nuclear fission applications, named VITJEFF311.BOLIB and BUGJEFF311.BOLIB. VITJEFF311.BOLIB is a fine-group coupled neutron/photon general-purpose library in AMPX format, based on the JEFF-3.1.1 evaluated nuclear data library and the Bondarenko (f-factor) neutron resonance self-shielding method. VITJEFF311.BOLIB was generated through the NJOY-99.259 nuclear data processing system in the neutron and photon energy group structures (199 n + 42 γ) of the VITAMIN-B6 similar library produced at ORNL. BUGJEFF311.BOLIB is a broad-group coupled neutron/photon working cross section library in FIDO-ANISN format, specifically dedicated to LWR shielding and pressure vessel dosimetry applications. It was generated in the same neutron and photon energy group structures (47 n + 20 γ) as the ORNL BUGLE-96 similar library, through problem-dependent cross section collapsing of the VITJEFF311.BOLIB library, performed with the updated and corrected ENEA-Bologna 2007 Revision of the ORNL SCAMPI nuclear data processing system. BUGJEFF311.BOLIB was tested on the PCA-Replica 12/13 and VENUS-3 engineering neutron shielding benchmark experiments (included in the SINBAD database), specifically conceived to check the nuclear data and the transport codes used in LWR radiation shielding and radiation damage analyses, through three-dimensional fixed source transport calculations with the TORT-3.2 discrete ordinates (S_N) code. BUGJEFF311.BOLIB was recently transferred to OECD-NEA Data Bank and is freely distributed with the designation NEA-1866/01 ZZ-BUGJEFF311.BOLIB.

Note

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ENEA-Bologna Multi-Group Cross Section Libraries for LWR Shielding and Pressure Vessel Dosimetry Applications

Massimo PESCARINI, Valentin SINITSA, Roberto ORSI, Manuela FRISONI

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1 - INTRODUCTION

Some years ago the ENEA-Bologna Nuclear Data Group started nuclear data processing and validation activities addressed to generate and/or to test broad-group coupled neutron/photon working cross section libraries, specifically dedicated to radiation shielding and radiation damage applications for the light water nuclear fission reactors (LWRs) and, in particular, to the reactor pressure vessel (RPV) dosimetry analyses. The generation of working cross section libraries in ENEA-Bologna was initially dedicated /1/ to the LWR radiation shielding and radiation damage applications since it was considered firstly important to produce working libraries for the most diffused types of nuclear power reactors all over the world. In fact about 82% of the 440 total world nuclear power reactor units are LWRs, i.e., 271 PWRs (about 62%) and 88 BWRs (about 20%), as reported in the July 20, 2011, updating of the IAEA-PRIS database.

It was considered important (see in particular /2/) to offer new updated working cross section libraries specifically addressed, in particular, to improve the calculation accuracy of the radiation damage parameters like fast neutron flux, fast neutron fluence, iron displacement per atom rate (DPA/s) and total iron displacement per atom (DPA) in the structural components of the future and present operating LWRs. In fact in this kind of applications even more accuracy is required than in radiation shielding calculations where more conservative calculation approaches are usually applied. For example, in radiation damage calculations for the most important LWR component, the reactor pressure vessel, the calculation accuracy obtained is a fundamental parameter, directly linked with the RPV End-of-Life (EoL) prediction which is in its turn connected with well known fundamental nuclear safety aspects and relevant economic impacts.

The present technical report summarizes the activities dedicated to generate a multi-purpose pseudo-problem-independent fine-group coupled neutron/photon cross section library in AMPX format for nuclear fission applications, named VITJEFF311.BOLIB, and a derived broad-group coupled neutron/photon working cross section library in FIDO-ANISN /3/ format for LWR shielding and pressure vessel dosimetry applications, named BUGJEFF311.BOLIB /4/, which was obtained through problem-dependent cross section collapsing of the VITJEFF311.BOLIB fine-group library.

In particular the ENEA-Bologna VITJEFF311.BOLIB library is based on the JEFF-3.1.1 /5/ /6/ (see also /7/) evaluated nuclear data library and on the Bondarenko /8/ (f-factor) method for the treatment of neutron resonance self-shielding and temperature effects.

The VITJEFF311.BOLIB library is a “pseudo-problem-independent” coupled neutron/photon library, i.e., a fine-group library prepared with enough detail in energy, temperatures and neutron resonance self-shielding so as to be applicable to a wide range of physical systems. VITJEFF311.BOLIB is characterized by the same neutron and photon energy group structures (199 neutron groups + 42 photon groups) as the ORNL DLC-0184/VITAMIN-B6 /9/ library in AMPX format, based on the ENDF/B-VI.3 /10/ evaluated data library.

The BUGJEFF311.BOLIB coupled working library adopts the neutron and photon energy group structures (47 neutron groups + 20 photon groups) of the ORNL DLC-0185/BUGLE-96 /9/ broad-group working library in FIDO-ANISN /3/ format, derived from the VITAMIN-B6 library and specifically conceived for the same previously cited applications in LWRs.

It is underlined, in particular, that broad-group working libraries, properly generated for the cited applications, are necessary to permit the use of the deterministic transport codes. The three-dimensional (3D) deterministic transport codes like, for example, the ORNL TORT /11/ discrete ordinates (S_N) code, can presently offer rigorous and reliable calculation solutions also for complex geometries, which could be described, up to few years ago, exclusively by the 3D stochastic transport codes like, for example, the LANL MCNP /12/ Monte Carlo code. In fact, if the 3D deterministic transport codes are properly assisted by dedicated pre/post-processor systems of programs (e.g., the ENEA-Bologna BOT3P /13/ /14/ /15/ /16/ and the Japanese TORTWARE /17/ systems) for the automatic generation and graphical verification of the spatial mesh grids of the reactor geometrical model, their performance can be highly competitive with that of the 3D Monte Carlo codes.

Despite the fact that, all over the world, the development of the 3D deterministic codes is going on and their use is increasingly appreciated also by the industrial organizations, it is not easy to find updated problem-dependent broad-group working cross section libraries for fission reactor shielding applications, free-released by the international distribution agencies (e.g., UNO-IAEA NDS, OECD-NEA Data Bank and ORNL-RSICC). In particular the packages of modular systems containing deterministic transport codes are distributed by the previously cited agencies without including working cross section libraries and this influences negatively the use and the diffusion of the deterministic transport culture and expertise. This is mainly due to the fact that, in order to generate a problem-dependent broad-group working cross section library for the previously mentioned applications, it is necessary to collapse the fine-group cross sections of a multi-purpose library, as recommended by specific standards. This operation is performed using problem-dependent neutron and photon spectra for the various spatial regions of a specific type of reactor, pre-calculated with typical compositional, geometrical and temperature parameters. These data are very often considered confidential and this implies that these libraries are mainly produced for internal use and commercial purposes within the industrial organizations.

In this contribution, based on the compositional, geometrical and temperature parameters reported in the BUGLE-96 /9/ library user’s manual for a typical PWR and a typical BWR, it was intentionally intended to follow the same data processing procedures and methodologies adopted at ORNL for the generation of the BUGLE-96 library which was widely and successfully used in LWR radiation shielding and radiation damage applications since 1996.
The LANL NJOY-99.259 /18/ and the ORNL SCAMPI /19/ nuclear data processing systems were selected and used to generate the group cross section libraries. NJOY-99.259 was

employed, in particular, for the generation of the VITJEFF311.BOLIB fine-group mother library. The so called ENEA-Bologna Revision 2007 /20/ of SCAMPI, an updated and corrected version specifically able, e.g., to process properly the recent nuclear data files of the JEFF-3.1.1 and ENDF/B-VII.0 /21/ evaluated data libraries, was used to generate the BUGJEFF311.BOLIB broad-group working library, through problem-dependent cross section collapsing. The AMPX format was adopted for the fine-group multi-purpose cross section library in order to have the compatibility with the AMPX-77 /22/ and SCAMPI nuclear data processing systems and with the SCALE-6 /23/ nuclear safety system, while the well known and diffused FIDO-ANISN format was selected for the broad-group working library.

Finally, a limited preliminary testing of the BUGJEFF311.BOLIB library was successfully performed with the 3D TORT-3.2 discrete ordinates transport code on the PCA-Replica 12/13 /24/ /25/ (Winfrith, UK) and VENUS-3 /26/ (Mol, Belgium) engineering neutron shielding benchmark integral experiments, whose compositional and geometrical specifications were taken from the fission reactor shielding section of the ORNL-RSICC/ OECD-NEA Data Bank SINBAD /27/ /28/ international database of shielding benchmark experiments. It is underlined that the testing of the BUGJEFF311.BOLIB library on the cited benchmark experiments is particularly meaningful since they were specifically conceived to verify and possibly to improve the accuracy of the calculation methodologies and nuclear data used in PWR radiation shielding and radiation damage calculations.

1.1 - Background

Since many years, at the international level, a decrease of open activity was observed /29/ for debating production, features and performances of energy group-averaged working cross section libraries dedicated to radiation shielding and radiation damage applications in nuclear fission reactors.

This situation is unjustified, taking into account the actual increased performances of computers and 3D deterministic transport codes, the potential availability of collapsed and self-shielded group cross section libraries for different spectral, compositional and temperature conditions and, finally, the requirements of the nuclear safety authorities which encourage nuclear safety calculations possibly performed with transport codes based on different methods (stochastic and deterministic).

The methodology for the generation of energy group-averaged cross section libraries for nuclear radiation protection calculations for nuclear power plants, recommended by the ANSI/ANS-6.1.2-1999 (R2009) /30/ American National Standard and adopted in the present work, consists of a two stage process: 1) the processing of evaluated data files into a fine-group, pseudo-problem-independent library, followed by 2) the collapsing of the fine-group library cross sections into the broad-group, problem-dependent cross sections of the desired working library for the specific application. The problem-dependent library is then derived from the fine-group library by taking into account temperature and neutron resonance self-shielding specifications and collapsing into a smaller number of groups. As underlined in the VITAMIN-B6 and BUGLE-96 /9/ library user’s manual, this approach removes from the end user the need to deal with the complex task of producing a group-averaged library from the evaluated data files, which contain a mix of point and functional data. This approach also reduces the user’s responsibility to the operation of a finite number of well-defined processing codes. Hence a higher level of standardization and reliability is achieved since the user can focus on only those features which are special to his application.

In other words, following the previously cited standard, a working cross section library for a specific application should not be obtained directly in broad-group (tenths of groups) energy structures, using generic neutron and photon weighting fluxes derived from analytical functions (e.g., Maxwellian thermal neutron spectrum, 1/E neutron slowing-down spectrum, neutron fission spectrum, 1/E photon spectrum, etc.). It is considered in fact, as a more accurate approach, to obtain the broad-group cross sections of the working libraries through proper cross section collapsing of fine-group (hundreds of groups) pseudo-problem independent cross section libraries, based, e.g., on the Bondarenko /8/ (f-factor) method for the treatment of neutron resonance self-shielding and temperature effects. It is recommendable, in particular, to collapse the fine-group cross sections using in-core and ex-core neutron and photon spectra, properly pre-calculated with a transport code for the specific compositional, geometrical and temperature data of the various spatial regions of a specific reactor type.

These libraries are required to run the deterministic transport codes which are, e.g., included in the following systems of deterministic codes: the US packages DOORS-3.2 /31/ and PARTISN-5.97 /32/ or the Russian package CNCSN 2009 /33/, distributed by the OECD-NEA Data Bank and ORNL-RSICC. On the other hand these packages, unlike those which include Monte Carlo codes like MCNP /12/, do not contain any working cross section library. The production of fine-group coupled neutron/photon pseudo-problem-independent libraries, based on the Bondarenko /8/ neutron resonance self-shielding method (e.g., of the type similar to the VITAMIN-B6 /9/ library) continues in several research institutes (ENEA, KAERI, ORNL, etc.). On the other hand, the free availability of derived broad-group working libraries of collapsed and self-shielded cross sections (e.g., of the type similar to the BUGLE-96 /9/ or BUGJEFF311.BOLIB /4/ libraries) is practically absent.

The previously cited decrease of open activity dedicated to the generation of broad-group working cross section libraries for fission reactor shielding applications is very probably due to the fact that it is traditionally considered highly convenient to perform 3D radiation shielding analyses for complex geometries with the combinatorial geometry approach included in the Monte Carlo codes (e.g., MCNP) using continuous-energy (point-wise) processed cross section libraries, independent in practice from the specific neutron and photon spectral environment.

Differently from the 3D Monte Carlo codes using a single processed continuous-energy cross section library to treat the different spectral environments of interest, when deterministic transport codes are employed it is not practically meaningful to use only one broad-group spectrum-independent working cross section library for any kind of application.

As reported in the user's manual of the VITAMIN-B6 and BUGLE-96 libraries, the generation of group-averaged cross section libraries with broad-group energy structures is primarily justified for reasons of economy. Despite the impressive performance of modern supercomputers it is still often impractical to perform two and three-dimensional radiation transport analyses using point-wise data or finely structured multi-group data, especially if fine resolution is needed for the space or angular meshes. In particular the 3D deterministic

transport codes, could have convergence problems when fine-group working libraries are used together with hundreds of thousands of volumetric spatial meshes, possibly needed to describe accurately complex in-core and ex-core reactor geometrical models used to perform radiation shielding and radiation damage analyses.
Even for one-dimensional analyses, it is often more efficient to use few-group data to perform the initial scoping analysis and then advance to finer group data as accuracy requirements become more stringent. The establishment of reference broad-group libraries is desirable to avoid duplication of effort, both in terms of the library generation and verification, and to assure a common database for comparisons among participants to a specific calculation program.

Taking into account this background and following the previously cited recommended methodology of generating a broad-group working cross section library, dedicated to a specific reactor type, it is then necessary to know compositional, geometrical and temperature data, typical of the specific nuclear reactor, which are not normally freely released. These data, i.e., the typical homogenized atomic densities and the specific temperatures of the nuclide mixtures for the various in-core and ex-core spatial regions along the one-dimensional reactor radial geometry at the core midplane, are necessary for two fundamental reasons.

The first reason is that these data are necessary to pre-calculate the in-core and ex-core neutron and photon spectra in proper locations of each representative reactor zone of a specific reactor type in order to perform then a problem-dependent cross section collapsing of the fine-group cross sections of the pseudo-problem-independent mother library.

The second reason is that the mentioned data are necessary to calculate the correct problem-dependent neutron resonance self-shielding of the broad-group cross sections of the working library for a specific nuclear reactor type.

The fact that these data are still considered confidential by the industrial organizations implies that a wide and open data processing effort to produce this kind of libraries is not presently possible. This fact in its turn induces the risk that the culture and the technical expertise related to deterministic calculations may progressively disappear within the research and development organizations and university institutions whilst there is still the interest that they continue to be developed, within the industrial organizations, in a commercial and self-referential perspective that does not guarantee, in general, a completely satisfactory approach to nuclear safety.

Moreover, despite the free availability of systems (e.g., NJOY/TRANSX /18/ /34/, AMPX-77 /22/, SCAMPI /19/ /20/, SCALE /23/, etc.) which permit the problem-dependent nuclear data processing in order to obtain broad-group working libraries of collapsed and self-shielded cross sections from fine-group general-purpose cross section libraries, the expertise about the nuclear data processing systems and methods is not generally widespread at the industrial level.

When, on the contrary, the industrial organizations are equipped with the necessary human resources and technical tools to perform detailed nuclear data processing addressed to generate multi-purpose fine-group libraries and derived collapsed working libraries of self-shielded cross sections for a specific model of fission reactor (the so called "custom-made"

working cross section libraries), it is in any case necessary to follow the quality assurance approach.
This implies that, in order to reduce possible errors in the data entry during the problem-dependent data processing phase of a custom-made working library, it is in parallel recommended using of already processed working libraries dedicated to the same applications, with parameterized sets of self-shielded cross sections for a similar type of nuclear fission reactor.

In other words it is in any case important to verify and intercompare the results obtained with the custom-made working libraries together with the results obtained through working cross section libraries with parameterized sets of self-shielded cross section libraries, like BUGLE-96 or BUGJEFF311.BOLIB, dedicated, for example, to LWR shielding and pressure vessel dosimetry.

Concerning the deterministic codes, it is really an upsetting fact that the 3D deterministic transport codes currently cannot be fully used for the lack of broad-group working libraries also when their use should be strongly recommended and, in any case, competitive with the use of the 3D Monte Carlo stochastic codes. It is interesting to note that the industrial organizations presently continue to be interested in the use /35/ or even in the development /36/ of the 3D deterministic codes. Moreover they directly develop /37/ or outsource to external nuclear data processing working groups, under specific contracts, the broad-group working cross section libraries for radiation shielding and radiation damage calculations with the deterministic transport codes. In fact they must fulfil quality assurance procedures with respect to the nuclear safety authority requirements and when deterministic codes are employed there is no need, as in the case of the Monte Carlo codes, to justify the validity of the statistics adopted since the deterministic codes are based on rigorous analytical solutions of the neutral particle transport equations. Moreover it is underlined that the 3D deterministic codes applied to radiation shielding and radiation damage analyses assure, with only a single run, a simultaneous and accurate average dose determination in every spatial position of the reactor geometrical model. It is then very important to underline that the deterministic transport codes permit reliable and effective sensitivity and uncertainty analyses, particularly recommended in the data validation activity and in a modern and rigorous approach to the industrial project of a nuclear reactor.

The 3D deterministic transport codes (e.g., the TORT /11/ code in the DOORS /31/ package, the PARTISN /32/ parallel code, etc.), which necessarily use the group-wise cross section libraries, increased in recent years their calculation performances in an impressive way and expanded their applicability to handle complex geometries, reaching in many cases the detail offered by the 3D Monte Carlo codes (e.g., MCNP). This result was achieved through the use of pre/post-processor systems of ancillary programs (e.g., the ENEA-Bologna BOT3P /13/ distributed by OECD-NEA Data Bank and ORNL-RSICC), dedicated to the 2D and 3D deterministic transport codes. In particular, with the support of BOT3P, based on combinatorial geometry algorithms (see APPENDIX), it is now easily possible to generate automatically detailed spatial mesh grids not only for the 2D and 3D transport codes of the DOORS system but also for any other possible transport code (through simple interfaces dedicated to manage the BOT3P binary output files), together with the graphical verification of the input data of the geometrical model.

During the last 10-15 years, the 3D discrete ordinates (S_N) transport codes increased their competitiveness with respect to the corresponding 3D Monte Carlo stochastic codes, obtaining comparable or even more convenient performances in terms of CPU times, with the same calculation precision, similar description capability of complex geometries and suitable simulation of different neutron and photon spectral conditions. Moreover 3D discrete ordinates codes like the US ATTILA /38/ commercial code, with unstructured spatial grids (finite elements) can now treat not only the neutral but also the charged particle transport as the more conventional discrete ordinates codes of the Russian CNCSN 2009 /33/ system of deterministic codes with structured spatial grids: the 1D code ROZ-6.6, the 2D codes KASKAD-S-2.5 (serial) and KASKAD-S-3.0 (parallel multi-threaded) and the 3D codes KATRIN-2.0 (serial) and KATRIN-2.5 (parallel multi-threaded).

Since deterministic transport codes are going to be employed in the analysis of the Generation IV nuclear reactor projects within the European Union research activities, it would be highly recommended that a specific interest dedicated to the generation of broad-group working cross section libraries should be promoted.

During the last years, the ENEA-Bologna Nuclear Data Group has performed several actions addressed to generate practical tools to increase, in particular, the performance and competitiveness of the 2D and 3D deterministic transport codes, following the recommendations proposed by the OECD-NEA Data Bank.

1. Several fine-group cross section libraries /39/ /40/ /41/ /42/ /43/ /44/ for nuclear fission applications were generated and are presently freely distributed by OECD-NEA Data Bank and ORNL-RSICC.

2. A pre/post-processor system /13/ /14/ /15/ /16/ of programs for the automatic spatial mesh generation, dedicated to the 2D and 3D deterministic transport codes, was developed and it is now freely distributed by OECD-NEA Data Bank and ORNL-RSICC.

3. Transport analyses dedicated to fission reactor neutron shielding benchmark experiments /1/ /45/ /46/ /47/ /48/ /49/ were performed also within the activities /47/ of the OECD-NEA Nuclear Science Committee TFRDD Task Force /2/ on nuclear fission reactor ageing problems.

4. The whole set of the IRDF-2002 /50/ dosimetry cross sections were processed /51/ in the 47 neutron group structure of the BUGLE-96 cross section library using a flat neutron spectrum and weighting spectra calculated with JEFF-3.1.1 and ENDF/B-VII.0 data, at one quarter of the thickness of a typical PWR pressure vessel: these data are partially included in the package of the present BUGJEFF311.BOLIB library.

1.2 - JEFF-3.1/3.1.1 Evaluated Nuclear Data Library

The VITJEFF311.BOLIB fine-group mother library from which the BUGJEFF311.BOLIB /4/ library was generated, is based on the JEFF-3.1.1 /5/ evaluated nuclear data library which was released at the end of February 2009. With respect to the previous version JEFF-3.1 /7/, it contains a total of 23 modified evaluated data files: updated evaluated files for twelve isotopes (O-16, Zr-91, Zr-93, Zr-96, Tc-99, Ru-103, Cs-135, Pm-147, Pm-148g, Eu-154, Np-

237 and Pu-239) and corrected evaluated files for eleven isotopes (Cl-35, Ca-46, Cr-52, Fe-56, Mo-95, Rh-103, I-127, I-129, Ir-191, Ir-193, U-233).
For the next release, JEFF-3.2, more efforts on fission product evaluations, minor actinide evaluations and inclusion of more covariance data in the files are foreseen.
The other evaluated files of JEFF-3.1.1 are identical to those of the JEFF-3.1 evaluated nuclear data library, a version of the JEFF (Joint Evaluated Fission and Fusion) nuclear data file, released by the OECD-NEA Data Bank in May 2005. The JEFF project is a collaborative effort among the member countries of the OECD-NEA Data Bank to develop a reference nuclear data library. The JEFF library contains sets of evaluated nuclear data, mainly for fission and fusion applications; it contains a number of different data types, including neutron and proton interaction data, radioactive decay data, fission yield data, thermal scattering law data and photo-atomic interaction data.
While the objective of the previous JEF-2.2 library (1992) /52/ was to achieve improved performance for existing reactors and fuel cycles, its successor, the JEFF-3 project aims at providing users with a more extensive set of data for a wider range of applications. While existing reactors and fuel cycles remain the essential application areas of the nuclear data library, innovative reactor concepts (Generation-IV systems), transmutation of radioactive waste, fusion, medical applications and various non-energy related industrial applications are now also envisaged as scientific application areas that will make the use of the JEFF data.
Extensive benchmarking of the JEFF-3.1 data library was performed for both the general-purpose and the special-purpose sub-libraries. The official report ("The JEFF-3.1 Nuclear Data Library", OECD-NEA Data Bank, JEFF Report 21, 2006 /7/) presents only results from extensive benchmarking effort on criticality, effective delayed neutron parameters and shielding using a Monte Carlo approach (MCNP /12/ code). A wider validation of benchmark results using different methods (deterministic and Monte Carlo codes) for various integral quantities was promoted. The validation effort dedicated to the JEFF-3.1.1 updated and corrected data files for the 23 isotopes previously cited is described in "The JEFF-3.1.1 Nuclear Data Library", OECD-NEA Data Bank, JEFF Report 22 /5/.

The content of the JEFF-3.1/3.1.1 evaluated nuclear data libraries is the following. The neutron general purpose library contains incident neutron data for 381 materials from H-1 to Fm-255. The activation library (based on the European Activation File, EAF-2003) contains 774 different targets from H-1 to Fm-257. The radioactive decay data library contains data for 3852 isotopes, of which 226 are stable. The proton special-purpose library contains incident proton data for 26 materials from Ca-40 to Bi-209. The thermal scattering law library covers 9 materials and the fission yield library covers 19 isotopes of neutron induced fission yield from Th-232 to Cm-245 and 3 isotopes with spontaneous fission yields (Cm-242, Cm-244 and Cf-252).
Concerning, in particular, the general purpose data library, new evaluations are included in JEFF-3.1 for the Ti isotopes (IRK-Vienna), the Ca, Sc, Fe, Ge, Pb and Bi isotopes (NRG-Petten), Rh-103, I-127, I-129, the Hf isotopes, U-236, U-237, U-238 and Am-241. For other isotopes more recent evaluations from other libraries were adopted.
Revised thermal scattering data have been produced for all important moderator and structural materials and this was included in JEFF-3.1 and remained unchanged in JEFF-3.1.1. The thermal scattering law library contains the following nine evaluations: hydrogen bound in water, hydrogen bound in zirconium hydride, hydrogen bound in polyethylene (CH_2) and CaH_2, deuterium bound in D_2O, Be-9, graphite, Mg-24 and finally calcium bound in CaH_2. All the cited data files are new evaluations, except Be-9 and hydrogen in polyethylene, which

are from the JEFF-3.0 /53/ library (April 2002). Many of the evaluations are the result of an IAEA co-ordinated project on thermal neutron scattering. Calculations for a variety of temperatures were made with the LEAPR module of the NJOY /18/ nuclear data processing system to obtain thermal scattering data that are accurate over a wider range of energy and momentum transfer.
The JEFF-3.1/3.1.1 libraries store all data in the internationally-accepted ENDF-6 /54/ format. Compared with JEF-2.2, a better agreement between JEFF-3.1/3.1.1-based calculations and measurements is expected in neutron transmission applications containing the following materials: Fe, O-16, Be-9, W and Na. For more details about the expected performance relative to JEF-2.2, concerning the LWR thermal reactor applications and the fast reactor applications, it is recommended to consult the official OECD-NEA Data Bank JEFF Reports 21 and 22 previously cited. Initial testing of the JEFF-3.1 file indicated that further improvements were needed in particular for Np-237 capture (updated in JEFF-3.1.1), Pu-239 fission and capture (updated in JEFF-3.1.1), Pu-242 capture, Am-241 capture, Fe-56 inelastic scattering (corrected in JEFF-3.1.1), fission product cross sections (capture cross section updated in JEFF-3.1.1 for Zr-93, Tc-99, Ru-103, Cs-135, Pm-147, Pm-148g and Eu-154), decay data and yields of short-lived fission products.

1.3 - Cross Section Processing and Testing

The calculation approach used to produce the BUGJEFF311.BOLIB /4/ library, based on the JEFF-3.1.1 /5/ evaluated nuclear data library, is consistent (see also 1.2) with the ANS standard "Neutron and Gamma-Ray Cross Sections for Nuclear Radiation Protection Calculations for Nuclear Power Plants" (ANSI/ANS-6.1.2-1999 (R2009) /30/). Specifically the JEFF-3.1.1 data were first processed into a fine-group cross section set similar to the VITAMIN-B6 /9/ pseudo-problem-independent library and then collapsed into a broad-group set similar to the BUGLE-96 /9/ working library, derived from VITAMIN-B6.

The selected approach employs both the following modular nuclear data processing systems LANL NJOY-99.259 /18/ and the ENEA-Bologna Revision 2007 /20/ of the ORNL SCAMPI /19/. Several modules of NJOY were used to process the neutron interaction, the photon production and the photon interaction data from the JEFF-3.1.1 formats to a group-averaged format.
In order to process correctly modern evaluated nuclear data like the JEFF-3.1.1 data files, it was necessary to develop an updated and corrected version of the SCAMPI system, originally developed at ORNL from the AMPX-77 /22/ system and already employed at ORNL to generate the BUGLE-96 library from the VITAMIN-B6 library. In particular, the previously cited so called "ENEA-Bologna 2007 Revision of SCAMPI", able to generate and to read data in AMPX format, was developed and was released to OECD-NEA Data Bank and ORNL-RSICC.
In particular the ENEA-Bologna 2007 Revision of SCAMPI, through the revised and corrected SMILER module, was employed to read the double-precision GENDF binary files from the NJOY-99.259 nuclear data processing system, to translate the intermediate NJOY file into the AMPX master format for the VITJEFF311.BOLIB fine-group library and, finally, to calculate the total (prompt + delayed) neutron fission spectra and average numbers of neutrons emitted per fission, taking into account that their delayed neutron components could not be previously obtained with the original ORNL SMILER version of the SCAMPI system.
The BONAMI module was used to self-shield the VITJEFF311.BOLIB cross sections taking

into account the compositional, geometrical and temperature specifications typical of PWR and BWR calculation models. These self-shielded cross sections in the VITJEFF311.BOLIB neutron and photon fine-group energy structures were used in transport calculations to determine the problem-dependent weighting spectra employed to generate the BUGJEFF311.BOLIB neutron and photon broad-group collapsed cross sections through the revised and corrected MALOCS module, which was used, in particular, to perform the cross section collapsing of the rectangular fission matrices.

A detailed description of the data processing performed for the generation of the VITJEFF311.BOLIB fine-group library is given in Chapter 2 while the specifications and processing methods used to generate the BUGJEFF311.BOLIB broad-group working library are described in Chapter 3. Finally, the results of a preliminary but important validation effort dedicated to the BUGJEFF311.BOLIB library is presented in Chapter 4.

2 - VITJEFF311.BOLIB FINE-GROUP LIBRARY SPECIFICATIONS

The BUGJEFF311.BOLIB /4/ working library was obtained through proper cross section collapsing of the VITJEFF311.BOLIB fine-group pseudo-problem-independent cross section library, based on the Bondarenko /8/ (f-factor) method for the treatment of neutron resonance self-shielding and temperature effects. This library, generated in ENEA-Bologna by the Nuclear Data Group, is a coupled neutron/photon library in AMPX format for nuclear fission applications, based on the OECD-NEA Data Bank JEFF-3.1.1 /5/ /6/ evaluated nuclear data library. It has the same neutron and photon energy group structures (199 neutron groups + 42 photon groups) and general basic features as the ORNL DLC-184/VITAMIN-B6 /9/ American library in AMPX format, based on the ENDF/B-VI Release 3 /10/ US evaluated nuclear data library.

The VITJEFF311.BOLIB library was generated through an updated automatic calculation procedure based on the LANL NJOY-99.259 /18/ nuclear data processing system, with the updating "upnea049", and the ENEA-Bologna 2007 Revision /20/ of the ORNL SCAMPI /19/ nuclear data processing system. VITJEFF311.BOLIB was extensively tested (see 2.9) on many thermal, intermediate and fast neutron spectrum criticality benchmark experiments.

A revised version of the SMILER module of the ENEA-Bologna 2007 Revision of the SCAMPI system was used to translate the fine-group data from the GENDF format into the AMPX master library format of the VITJEFF311.BOLIB library. In parallel, automatic multiplication of the term of ℓ-th order of the Legendre polynomial (P_ℓ) expansion of the scattering cross section matrix by the ($2\ell + 1$) factor was performed by the SMILER module for all the processed data files of the nuclides contained in the library.

The cross section files of VITJEFF311.BOLIB in AMPX format can be exclusively treated by the updated ENEA-Bologna 2007 Revision of the SCAMPI system which assures a high level of flexibility in the production of working cross section libraries and an evident consistency with the VITAMIN-B6 library generation methods. It is underlined, in particular, that the ENEA-Bologna revised version of the SMILER module, contained in the ENEA-Bologna 2007 Revision of the SCAMPI data processing system, permits to obtain separately the prompt neutron fission spectrum (MF=6 and MT=18), the delayed neutron fission spectrum (MF=5 and MT=455) and the total neutron fission spectrum needed, e.g., in the fixed source transport calculations for reactor radiation shielding applications. On the contrary, from the original ORNL SMILER version, used to generate VITAMIN-B6 and VITJEF22.BOLIB /39/, it is possible to obtain only the prompt neutron component of the fission spectrum.

At present, the availability of the VITJEFF311.BOLIB library permits to obtain derived collapsed working libraries of self-shielded cross sections, through the ENEA-Bologna 2007 Revision of the SCAMPI system. More specifically, the cross sections can be collapsed by the MALOCS module, can be self-shielded by the BONAMI module and finally can be generated in the AMPX or FIDO-ANISN /3/ format. The cross sections in AMPX format can be used by the XSDRNPM one-dimensional (1D) discrete ordinates transport code, included in the ORNL AMPX-77 /22/ and SCAMPI nuclear data processing systems, or in the ORNL SCALE-6 /23/ nuclear safety system. Concerning the cross sections in FIDO-ANISN format, they can be used by the discrete ordinates (S_N) deterministic codes ANISN-ORNL (1D), DORT (2D) and TORT (3D) of the DOORS /31/ system, by the PARTISN /32/ (1D, 2D and

3D) parallel time-dependent discrete ordinates system and, finally, by the 3D Monte Carlo stochastic code MORSE /55/.

2.1 - Name

The fine-group pseudo-problem-independent library which generated the BUGJEFF311.BOLIB /4/ broad-group working library is designated as VITJEFF311.BOLIB. "VIT" suggests that the main features of the library are similar to those of the ORNL VITAMIN-B6 /9/ library and to the ENEA fine-group libraries /39/ /42/ in AMPX format with the same neutron and photon energy group structures. The "JEFF311" designation conveniently reflects the origin of the evaluated data: the JEFF-3.1.1 evaluated nuclear data library /5/ /6/. Finally, "BOLIB" means BOlogna LIBrary and so it is indicative of the place of production of the library.

2.2 - Materials, Temperatures and Background Cross Sections

A set of 182 cross section files, derived from the JEFF-3.1.1 /5/ /6/ evaluated nuclear data library, was processed for the VITJEFF311.BOLIB fine-group library. In particular the complete list of the included nuclides is reported in TAB. 2.1 together with the corresponding Z atomic numbers, the JEFF-3.1.1 MAT numbers, the AMPX identifiers and a flag (YES/NO) indicating the presence of gamma ray production data in the specific evaluated nuclear data file. It is underlined that, in this set of processed data files, only three data files correspond to natural evaluated elements (C-nat, V-nat and Ga-nat) whereas the other ones correspond to single isotope evaluated data files.

The VITJEFF311.BOLIB library contains the following set of 12 nuclides whose evaluated files were updated or corrected in the JEFF-3.1.1 evaluated data library with respect to the corresponding files contained in the JEFF-3.1 evaluated data library: the O-16, Zr-91, Zr-96, Eu-154, Np-237 and Pu-239 data files were updated while the Cl-35 Ca-46, Cr-52, Fe-56, Mo-95 and U-233 data files were corrected (see also 1.2).

Concerning, in particular, the JEFF-3.1.1 Pu-239 nuclear data file, revised radiative capture (n,γ) MT=102 and fission (n,f) MT=18 cross sections below 0.0253 eV, in the sub-thermal neutron energy region, were introduced together with revised ν_p (mean number of prompt neutrons per fission) MT=456 data up to 20 eV, with respect to the corresponding JEFF-3.1 Pu-239 nuclear data file.
The revised JEFF-3.1.1 Pu-239 evaluated data file is expected to correct, in particular, the reported /5/ k-effective (k_{eff}) overestimation in criticality calculations for MOX fuel and Pu solutions in thermal neutron spectrum (see also 1.2 and 2.9).

The Bondarenko /8/ (f-factor) method was used for handling neutron resonance self-shielding and temperature effects. As for VITAMIN-B6 /9/, all the 176 standard (not bound) nuclides were processed at the 4 temperatures of 300 °K, 600 °K, 1000 °K and 2100 °K and most materials were processed with 6 to 8 values for the background cross section σ_0. These parameters are indicated in detail in TAB. 2.2, where it is possible to verify that nearly all materials were processed with the following values of σ_0: 1, 10, 1.0E+2, 1.0E+3, 1.0E+4 and 1.0E+10 barns.

With respect to the σ_0 values used in the generation of the Fe-56 processed files in the VITAMIN-B6 (AMPX format), VITJEF22.BOLIB /39/ (AMPX format) and MATJEF22.BOLIB /40/ (MATXS format) older libraries, an additional σ_0 numerical value equal to 0.01 barns was used in the production of the Fe-56 processed file included in VITJEFF311.BOLIB as it was done for the VITJEFF31.BOLIB /42/ (AMPX format) and the MATJEFF31.BOLIB /43/ (MATXS format) libraries. This additional σ_0 numerical value improves further, through a more precise self-shielding factor interpolation, the neutron self-shielding of the Fe-56 cross sections in natural iron. Moreover the possibility of a more accurate self-shielding calculation for Fe-56 was considered useful also in LWR radiation damage analyses in the carbon steel of the pressure vessel and in the stainless steel of the reactor internals (see also 3.3).

For consistency with most other similar libraries, it was decided to use infinitely dilute background cross sections (σ_0 =1.0E+10 barns) for nuclides with the atomic number Z less than 7, with the exception of B-11. Hence, only a background cross section with a numerical value of 1.0E+10 barns was used for each of these nuclides.

Thermal scattering cross sections were produced for six additional bound nuclides which were processed at all the temperatures (see TAB. 2.3) available in the JEFF-3.1.1 thermal scattering law data file (see /5/ and /7/): H-1 in light water, H-1 in polyethylene, H-1 in zirconium hydride (not contained in the VITAMIN-B6, VITJEF22.BOLIB and MATJEF22.BOLIB libraries), H-2 in heavy water, C in graphite and Be in beryllium metal.
It is important to note that in total reactor power and heating calculations, the corresponding results can be heavily affected by the lack of gamma production data in some JEFF-3.1.1 evaluated data files. Concerning this, it is recommended to verify carefully if the JEFF-3.1.1 data files of the nuclides involved in the calculations include gamma production data (see TAB. 2.1).

TAB. 2.1

JEFF-3.1.1 Nuclides Processed for the VITJEFF311.BOLIB Library.

Z	Nuclide	JEFF-3.1.1 MAT	AMPX Identifier	Gamma Ray Production
1	H-H_2O	125/1	1001	YES
	H-CH_2	125/37	1901	YES
	H-ZrH	125/7	1401	YES
	D-D_2O	128/11	1002	YES
	H-3	131	1003	NO
2	He-3	225	2003	NO
	He-4	228	2004	NO
3	Li-6	325	3006	YES
	Li-7	328	3007	YES
4	Be-9	425	4009	YES
	Be-9 (Thermal)	425/26	4309	YES
5	B-10	525	5010	YES
	B-11	528	5011	YES
6	C-nat	600	6012	YES
	C-nat (Graphite)	600/31	6312	YES
7	N-14	725	7014	YES
	N-15	728	7015	YES
8	O-16	825	8016	YES
	O-17	828	8017	NO
9	F-19	925	9019	YES
11	Na-23	1125	11023	YES
12	Mg-24	1225	12024	YES
	Mg-25	1228	12025	YES
	Mg-26	1231	12026	YES
13	Al-27	1325	13027	YES
14	Si-28	1425	14028	YES
	Si-29	1428	14029	YES
	Si-30	1431	14030	YES
15	P-31	1525	15031	YES
16	S-32	1625	16032	YES
	S-33	1628	16033	YES
	S-34	1631	16034	YES
	S-36	1637	16036	YES
17	Cl-35	1725	17035	YES
	Cl-37	1731	17037	YES
19	K-39	1925	19039	YES
	K-40	1928	19040	YES
	K-41	1931	19041	YES
20	Ca-40	2025	20040	YES
	Ca-42	2031	20042	YES
	Ca-43	2034	20043	YES
	Ca-44	2037	20044	YES
	Ca-46	2043	20046	YES
	Ca-48	2049	20048	YES
22	Ti-46	2225	22046	YES
	Ti-47	2228	22047	YES
	Ti-48	2231	22048	YES
	Ti-49	2234	22049	YES
	Ti-50	2237	22050	YES

TAB. 2.1 Continued

JEFF-3.1.1 Nuclides Processed for the VITJEFF311.BOLIB Library.

Z	Nuclide	JEFF-3.1.1 MAT	AMPX Identifier	Gamma Ray Production
23	V-nat	2300	23000	YES
24	Cr-50	2425	24050	YES
	Cr-52	2431	24052	YES
	Cr-53	2434	24053	YES
	Cr-54	2437	24054	YES
25	Mn-55	2525	25055	YES
26	Fe-54	2625	26054	YES
	Fe-56	2631	26056	YES
	Fe-57	2634	26057	YES
	Fe-58	2637	26058	YES
27	Co-59	2725	27059	YES
28	Ni-58	2825	28058	YES
	Ni-60	2831	28060	YES
	Ni-61	2834	28061	YES
	Ni-62	2837	28062	YES
	Ni-64	2843	28064	YES
29	Cu-63	2925	29063	YES
	Cu-65	2931	29065	YES
31	Ga-nat	3100	31000	YES
39	Y-89	3925	39089	YES
40	Zr-90	4025	40090	YES
	Zr-91	4028	40091	YES
	Zr-92	4031	40092	YES
	Zr-94	4037	40094	YES
	Zr-96	4043	40096	YES
41	Nb-93	4125	41093	YES
42	Mo-92	4225	42092	YES
	Mo-94	4231	42094	YES
	Mo-95	4234	42095	YES
	Mo-96	4237	42096	YES
	Mo-97	4240	42097	YES
	Mo-98	4243	42098	YES
	Mo-100	4249	42100	YES
47	Ag-107	4725	47107	NO
	Ag-109	4731	47109	NO
48	Cd-106	4825	48106	NO
	Cd-108	4831	48108	NO
	Cd-110	4837	48110	NO
	Cd-111	4840	48111	NO
	Cd-112	4843	48112	NO
	Cd-113	4846	48113	NO
	Cd-114	4849	48114	NO
	Cd-115m	4853	48115	NO
	Cd-116	4855	48116	NO
49	In-113	4925	49113	NO
	In-115	4931	49115	NO
50	Sn-112	5025	50112	NO
	Sn-114	5031	50114	NO
	Sn-115	5034	50115	NO

TAB. 2.1 Continued

JEFF-3.1.1 Nuclides Processed for the VITJEFF311.BOLIB Library.

Z	Nuclide	JEFF-3.1.1 MAT	AMPX Identifier	Gamma Ray Production
	Sn-116	5037	50116	NO
	Sn-117	5040	50117	NO
	Sn-118	5043	50118	NO
	Sn-119	5046	50119	NO
	Sn-120	5049	50120	NO
	Sn-122	5055	50122	NO
	Sn-123	5058	50123	NO
	Sn-124	5061	50124	NO
	Sn-125	5064	50125	NO
	Sn-126	5067	50126	NO
56	Ba-138	5649	56138	NO
63	Eu-151	6325	63151	YES
	Eu-152	6328	63152	NO
	Eu-153	6331	63153	NO
	Eu-154	6334	63154	NO
	Eu-155	6337	63155	NO
64	Gd-152	6425	64152	NO
	Gd-154	6431	64154	NO
	Gd-155	6434	64155	NO
	Gd-156	6437	64156	NO
	Gd-157	6440	64157	NO
	Gd-158	6443	64158	NO
	Gd-160	6449	64160	NO
68	Er-162	6825	68162	YES
	Er-164	6831	68164	YES
	Er-166	6837	68166	YES
	Er-167	6840	68167	YES
	Er-168	6843	68168	YES
	Er-170	6849	68170	YES
72	Hf-174	7225	72174	YES
	Hf-176	7231	72176	YES
	Hf-177	7234	72177	YES
	Hf-178	7237	72178	YES
	Hf-179	7240	72179	YES
	Hf-180	7243	72180	YES
73	Ta-181	7328	73181	YES
	Ta-182	7331	73182	NO
74	W-182	7431	74182	YES
	W-183	7434	74183	YES
	W-184	7437	74184	YES
	W-186	7443	74186	YES
75	Re-185	7525	75185	NO
	Re-187	7531	75187	NO
79	Au-197	7925	79197	YES
82	Pb-204	8225	82204	YES
	Pb-206	8231	82206	YES
	Pb-207	8234	82207	YES
	Pb-208	8237	82208	YES
83	Bi-209	8325	83209	YES

TAB. 2.1 Continued

JEFF-3.1.1 Nuclides Processed for the VITJEFF311.BOLIB Library.

Z	Nuclide	JEFF-3.1.1 MAT	AMPX Identifier	Gamma Ray Production
90	Th-230	9034	90230	NO
	Th-232	9040	90232	YES
91	Pa-231	9131	91231	NO
	Pa-233	9137	91233	NO
92	U-232	9219	92232	NO
	U-233	9222	92233	YES
	U-234	9225	92234	NO
	U-235	9228	92235	YES
	U-236	9231	92236	YES
	U-237	9234	92237	YES
	U-238	9237	92238	YES
93	Np-237	9346	93237	YES
	Np-238	9349	93238	NO
	Np-239	9352	93239	NO
94	Pu-236	9428	94236	NO
	Pu-237	9431	94237	NO
	Pu-238	9434	94238	NO
	Pu-239	9437	94239	NO
	Pu-240	9440	94240	YES
	Pu-241	9443	94241	NO
	Pu-242	9446	94242	YES
	Pu-243	9449	94243	YES
	Pu-244	9452	94244	NO
95	Am-241	9543	95241	NO
	Am-242	9546	95242	NO
	Am-242m	9547	95601	NO
	Am-243	9549	95243	NO
96	Cm-241	9628	96241	NO
	Cm-242	9631	96242	YES
	Cm-243	9634	96243	YES
	Cm-244	9637	96244	YES
	Cm-245	9640	96245	NO
	Cm-246	9643	96246	YES
	Cm-247	9646	96247	YES
	Cm-248	9649	96248	YES

TAB. 2.2

Background Cross Sections Values at which Bondarenko Factors Are Tabulated
in the VITJEFF311.BOLIB Library.
All Nuclides Were Processed at Four Temperatures: 300 °K, 600 °K, 1000 °K and 2100 °K.

Nuclide	Background Cross Sections [barns]											Legendre
	1.E+10	1.E+6	1.E+5	1.E+4	1000.	300.	100.	50.	10.	1.	0.01	Order
H-1	1.E+10											7
H-2	1.E+10											7
H-3	1.E+10											7
He-3	1.E+10											7
He-4	1.E+10											7
Li-6	1.E+10											7
Li-7	1.E+10											7
Be-9	1.E+10											7
B-10	1.E+10											7
B-11	1.E+10				1000.		100.		10.	1.		7
C-nat	1.E+10											7
N-14	1.E+10				1000.		100.		10.	1.		7
N-15	1.E+10				1000.		100.		10.	1.		7
O-16	1.E+10				1000.		100.		10.	1.		7
O-17	1.E+10				1000.		100.		10.	1.		7
F-19	1.E+10				1000.		100.		10.	1.		7
Na-23	1.E+10				1000.	300.	100.	50.	10.	1.		7
Mg-24	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Mg-25	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Mg-26	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Al-27	1.E+10			1.E+4	1000.		100.	50.	10.	1.		7
Si-28	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Si-29	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Si-30	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
P-31	1.E+10			1.E+4	1000.		100.		10.	1.		7
S-32	1.E+10			1.E+4	1000.		100.		10.	1.		7
S-33	1.E+10			1.E+4	1000.		100.		10.	1.		7
S-34	1.E+10			1.E+4	1000.		100.		10.	1.		7
S-36	1.E+10			1.E+4	1000.		100.		10.	1.		7
Cl-35	1.E+10			1.E+4	1000.		100.		10.	1.		7
Cl-37	1.E+10			1.E+4	1000.		100.		10.	1.		7
K-39	1.E+10			1.E+4	1000.		100.		10.	1.		7
K-40	1.E+10			1.E+4	1000.		100.		10.	1.		7
K-41	1.E+10			1.E+4	1000.		100.		10.	1.		7
Ca-40	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ca-42	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ca-43	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ca-44	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ca-46	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ca-48	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ti-46	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ti-47	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ti-48	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ti-49	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ti-50	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
V-nat	1.E+10			1.E+4	1000.		100.		10.	1.		7
Cr-50	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Cr-52	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Cr-53	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Cr-54	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Mn-55	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Fe-54	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Fe-56	1.E+10		1.E+5	1.E+4	1000.		100.	50.	10.	1.	0.01	7
Fe-57	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Fe-58	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Co-59	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ni-58	1.E+10		1.E+5	1.E+4	1000.		100.	50.	10.	1.		7
Ni-60	1.E+10		1.E+5	1.E+4	1000.		100.	50.	10.	1.		7
Ni-61	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7

TAB. 2.2 Continued

Background Cross Sections Values at which Bondarenko Factors Are Tabulated
in the VITJEFF311.BOLIB Library.
All Nuclides Were Processed at Four Temperatures: 300 °K, 600 °K, 1000 °K and 2100 °K.

Nuclide	Background Cross Sections [barns]											Legendre
	1.E+10	1.E+6	1.E+5	1.E+4	1000.	300.	100.	50.	10.	1.	0.01	Order
Ni-62	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ni-64	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Cu-63	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Cu-65	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		7
Ga-nat	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Y-89	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Zr-90	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Zr-91	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Zr-92	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Zr-94	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Zr-96	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Nb-93	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Mo-92	1.E+10		1.E+5	1.E+4	1000.		100.					5
Mo-94	1.E+10		1.E+5	1.E+4	1000.		100.					5
Mo-95	1.E+10		1.E+5	1.E+4	1000.		100.					5
Mo-96	1.E+10		1.E+5	1.E+4	1000.		100.					5
Mo-97	1.E+10		1.E+5	1.E+4	1000.		100.					5
Mo-98	1.E+10		1.E+5	1.E+4	1000.		100.					5
Mo-100	1.E+10		1.E+5	1.E+4	1000.		100.					5
Ag-107	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Ag-109	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-106	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-108	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-110	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-111	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-112	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-113	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-114	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-115m	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Cd-116	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
In-113	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
In-115	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-112	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-114	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-115	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-116	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-117	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-118	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-119	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-120	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-122	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-123	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-124	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-125	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Sn-126	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Ba-138	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Eu-151	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Eu-152	1.E+10	1.E+6	1.E+5	1.E+4	1000.		100.					5
Eu-153	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Eu-154	1.E+10	1.E+6	1.E+5	1.E+4	1000.		100.					5
Eu-155	1.E+10	1.E+6	1.E+5	1.E+4	1000.		100.					5
Gd-152	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Gd-154	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Gd-155	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Gd-156	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Gd-157	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Gd-158	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Gd-160	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5

TAB. 2.2 Continued

Background Cross Sections Values at which Bondarenko Factors Are Tabulated
in the VITJEFF311.BOLIB Library.
All Nuclides Were Processed at Four Temperatures: 300 °K, 600 °K, 1000 °K and 2100 °K.

Nuclide	Background Cross Sections [barns]											Legendre
	1.E+10	1.E+6	1.E+5	1.E+4	1000.	300.	100.	50.	10.	1.	0.01	Order
Er-162	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Er-164	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Er-166	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Er-167	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Er-168	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Er-170	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Hf-174	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Hf-176	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Hf-177	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Hf-178	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Hf-179	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Hf-180	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Ta-181	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Ta-182	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
W-182	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
W-183	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
W-184	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
W-186	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Re-185	1.E+10	1.E+6	1.E+5	1.E+4	1000.		100.					5
Re-187	1.E+10	1.E+6	1.E+5	1.E+4	1000.		100.					5
Au-197	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Pb-204	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Pb-206	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Pb-207	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Pb-208	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Bi-209	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Th-230	1.E+10	1.E+6	1.E+5	1.E+4	1000.		100.					5
Th-232	1.E+10			1.E+4	1000.	300.	100.	50.	10.	1.		5
Pa-231	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Pa-233	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
U-232	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
U-233	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
U-234	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
U-235	1.E+10	1.E+6	1.E+5	1.E+4	1000.		100.	50.				5
U-236	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
U-237	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
U-238	1.E+10			1.E+4	1000.	300.	100.	50.	10.	1.		5
Np-237	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Np-238	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Np-239	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Pu-236	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Pu-237	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Pu-238	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Pu-239	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Pu-240	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Pu-241	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Pu-242	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Pu-243	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Pu-244	1.E+10		1.E+5	1.E+4	1000.		100.		10.	1.		5
Am-241	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Am-242	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Am-242m	1.E+10		1.E+5	1.E+4	1000.							5
Am-243	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Cm-241	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Cm-242	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Cm-243	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Cm-244	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Cm-245	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5

TAB. 2.2 Continued

Background Cross Sections Values at which Bondarenko Factors Are Tabulated
in the VITJEFF311.BOLIB Library.
All Nuclides Were Processed at Four Temperatures: 300 °K, 600 °K, 1000 °K and 2100 °K.

Nuclide	Background Cross Sections [barns]											Legendre
	1.E+10	1.E+6	1.E+5	1.E+4	1000.	300.	100.	50.	10.	1.	0.01	Order
Cm-246	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Cm-247	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5
Cm-248	1.E+10		1.E+5	1.E+4	1000.		100.	50.				5

TAB. 2.3

Processed Thermal Scattering Data in the VITJEFF311.BOLIB Library.

Thermal scattering cross sections for the following bound nuclides were produced, through the THERMR module of NJOY, from the scattering matrices S(α,β) at various temperatures, included in the original JEFF-3.1.1 thermal scattering law data file:

H-1 in H_2O (light water)
H-1 in CH_2 (polyethylene)
H-1 in ZrH (zirconium hydride)
H-2 in D_2O (heavy water)
C (graphite)
Be (beryllium metal)

Nuclide	Temperature [°K]
H-1 in H_2O	293.6 323.6 373.6 423.6 473.6 523.6 573.6 623.6 647.2 800. 1000.
H-1 in CH_2	293.6 350.
H-1 in ZrH	293.6 400. 500. 600. 700. 800. 1000. 1200.
H-2 in D_2O	293.6 323.6 373.6 423.6 473.6 523.6 573.6 643.9
C	293.6 400. 500. 600. 700. 800. 1000. 1200. 1600. 2000. 3000.
Be	293.6 400. 500. 600. 700. 800. 1000. 1200.

2.3 - Energy Group Structure

The VITJEFF311.BOLIB library adopts the same neutron and photon energy group structures as the VITAMIN-B6 /9/ library with 199 neutron energy groups (see TAB. 2.4) and 42 photon energy groups (see TAB. 2.5). The neutron and photon energy ranges are respectively included within 1.0E-05 eV and 1.9640E+07 eV for neutrons and within 1.0E+03 eV and 3.0E+07 eV for photons.

As reported in the VITAMIN-B6 library user's manual, this 199 neutron group structure was constructed as a compromise and improvement over the 174 neutron group structure used for the VITAMIN-E /56/ fine-group library, primarily conceived to treat fast neutron spectrum applications, and the 27 neutron group structure of the 27-neutron-group library, included in the SCALE /23/ system, suitable to treat criticality safety problems and out-of-core radiation shielding applications. The 27-neutron-group library has, in particular, a favourable neutron group discretization in the thermal neutron energy range whilst the resolution in the fast neutron energy range above 0.1 MeV results to be inadequate. Therefore the choice of the 199 group structure permits to treat not only fast neutron spectrum applications, through the proper neutron group structure at higher energies typical of VITAMIN-E, but also to treat physical systems with thermal neutron spectra, through the adequate group structure at lower energies of the 27-neutron-group library. Like the VITAMIN-B6 library, the VITJEFF311.BOLIB thermal neutron energy range, i.e. the range of the neutron energy groups which include upscatter, contains 36 groups and has 5.043 eV as the uppermost boundary. In particular, the thermal neutron group energy limits are listed in TAB. 2.6. As underlined in the VITAMIN-B6 library user's manual, by combining the best features of the VITAMIN-E with the 27-group neutron energy grids, the best options were obtained for creating a problem-independent energy grid for a variety of reactor designs, including thermal (water or graphite-moderated) and fast reactor systems. Consequently, problem-dependent cross section libraries can be easily derived from VITJEFF311.BOLIB, through the ENEA-Bologna 2007 Revision /20/ of the SCAMPI /19/ data processing system, without having to repeat the multi-group averaging directly from the JEFF-3.1.1 files.

The full VITJEFF311.BOLIB library neutron energy group structure given in TAB. 2.4 is identical to the corresponding structure of the VITAMIN-B6 library. The 199 group energy limits are based on the 175 groups in VITAMIN-J /57/ (an OECD-NEA Data Bank library based on the VITAMIN-C /58/ and VITAMIN-E structures) with an expanded number of thermal groups as discussed above. At higher energies, the boundaries are almost identical with the earlier VITAMIN libraries, which consist of a basic 100-group-mesh of equal lethargy width plus numerous additional boundaries to resolve resonance minima that are important for radiation shielding calculations.

The full VITJEFF311.BOLIB library photon energy group structure given in TAB. 2.5 is identical to the corresponding structure of the VITAMIN-B6 library. It is based on a combination of the 42 photon groups in the VITAMIN-J structure and the 18 group structure in the SCALE shielding library. The top energy group extends to 30 MeV, which allows proper representation of high energy gamma rays from neutron capture at high energies. Although the cross section for capture at neutron energies between 20 and 30 MeV is small, such a reaction in some materials can produce gamma rays with energies between 20 and 30 MeV, as reported in the VITAMIN-B6 library user's manual.

TAB. 2.4

Neutron Group Energy Boundaries for the VITJEFF311.BOLIB Library.

Group	Upper Energy [eV]	Energy Width [eV]	Upper Lethargy	Lethargy Width
1	1.9640E+07	2.3080E+06	-6.7498E-01	0.1250
2	1.7332E+07	4.2700E+05	-5.4997E-01	0.0249
3	1.6905E+07	4.1800E+05	-5.2502E-01	0.0250
4	1.6487E+07	8.0400E+05	-4.9999E-01	0.0500
5	1.5683E+07	7.6500E+05	-4.4999E-01	0.0500
6	1.4918E+07	3.6800E+05	-3.9998E-01	0.0250
7	1.4550E+07	3.5900E+05	-3.7501E-01	0.0250
8	1.4191E+07	3.5100E+05	-3.5002E-01	0.0250
9	1.3840E+07	3.4100E+05	-3.2498E-01	0.0249
10	1.3499E+07	6.5900E+05	-3.0003E-01	0.0501
11	1.2840E+07	3.1700E+05	-2.4998E-01	0.0250
12	1.2523E+07	3.0900E+05	-2.2498E-01	0.0250
13	1.2214E+07	5.9600E+05	-2.0000E-01	0.0500
14	1.1618E+07	5.6600E+05	-1.4997E-01	0.0499
15	1.1052E+07	5.3900E+05	-1.0003E-01	0.0500
16	1.0513E+07	5.1300E+05	-5.0027E-02	0.0500
17	1.0000E+07	4.8770E+05	0.0000E+00	0.0500
18	9.5123E+06	4.6390E+05	4.9999E-02	0.0500
19	9.0484E+06	4.4130E+05	9.9997E-02	0.0500
20	8.6071E+06	4.1980E+05	1.5000E-01	0.0500
21	8.1873E+06	3.9930E+05	2.0000E-01	0.0500
22	7.7880E+06	3.7980E+05	2.5000E-01	0.0500
23	7.4082E+06	3.6130E+05	3.0000E-01	0.0500
24	7.0469E+06	3.4370E+05	3.5000E-01	0.0500
25	6.7032E+06	1.1080E+05	4.0000E-01	0.0167
26	6.5924E+06	2.1610E+05	4.1667E-01	0.0333
27	6.3763E+06	3.1100E+05	4.5000E-01	0.0500
28	6.0653E+06	2.9580E+05	5.0000E-01	0.0500
29	5.7695E+06	2.8140E+05	5.5000E-01	0.0500
30	5.4881E+06	2.6760E+05	6.0000E-01	0.0500
31	5.2205E+06	2.5460E+05	6.4999E-01	0.0500
32	4.9659E+06	2.4220E+05	6.9999E-01	0.0500
33	4.7237E+06	2.3040E+05	7.4999E-01	0.0500
34	4.4933E+06	4.2760E+05	8.0000E-01	0.1000
35	4.0657E+06	3.8690E+05	9.0000E-01	0.1000
36	3.6788E+06	3.5010E+05	1.0000E+00	0.1000
37	3.3287E+06	1.6230E+05	1.1000E+00	0.0500
38	3.1664E+06	1.5450E+05	1.1500E+00	0.0500
39	3.0119E+06	1.4680E+05	1.2000E+00	0.0500
40	2.8651E+06	1.3980E+05	1.2500E+00	0.0500
41	2.7253E+06	1.3290E+05	1.3000E+00	0.0500
42	2.5924E+06	1.2640E+05	1.3500E+00	0.0500
43	2.4660E+06	8.0800E+04	1.4000E+00	0.0333
44	2.3852E+06	1.9900E+04	1.4333E+00	0.0084
45	2.3653E+06	1.9600E+04	1.4417E+00	0.0083
46	2.3457E+06	3.8800E+04	1.4500E+00	0.0167
47	2.3069E+06	7.5600E+04	1.4667E+00	0.0333
48	2.2313E+06	1.0880E+05	1.5000E+00	0.0500
49	2.1225E+06	1.0350E+05	1.5500E+00	0.0500

TAB. 2.4 Continued

Neutron Group Energy Boundaries for the VITJEFF311.BOLIB Library.

Group	Upper Energy [eV]	Energy Width [eV]	Upper Lethargy	Lethargy Width
50	2.0190E+06	9.8500E+04	1.6000E+00	0.0500
51	1.9205E+06	9.3700E+04	1.6500E+00	0.0500
52	1.8268E+06	8.9100E+04	1.7000E+00	0.0500
53	1.7377E+06	8.4700E+04	1.7500E+00	0.0500
54	1.6530E+06	8.0600E+04	1.8000E+00	0.0500
55	1.5724E+06	7.6700E+04	1.8500E+00	0.0500
56	1.4957E+06	7.3000E+04	1.9000E+00	0.0500
57	1.4227E+06	6.9300E+04	1.9500E+00	0.0500
58	1.3534E+06	6.6000E+04	2.0000E+00	0.0500
59	1.2874E+06	6.2800E+04	2.0500E+00	0.0500
60	1.2246E+06	5.9800E+04	2.1000E+00	0.0500
61	1.1648E+06	5.6800E+04	2.1500E+00	0.0500
62	1.1080E+06	1.0540E+05	2.2000E+00	0.1000
63	1.0026E+06	4.0960E+04	2.3000E+00	0.0417
64	9.6164E+05	5.4460E+04	2.3417E+00	0.0583
65	9.0718E+05	4.4240E+04	2.4000E+00	0.0500
66	8.6294E+05	4.2090E+04	2.4500E+00	0.0500
67	8.2085E+05	4.0030E+04	2.5000E+00	0.0500
68	7.8082E+05	3.8080E+04	2.5500E+00	0.0500
69	7.4274E+05	3.6230E+04	2.6000E+00	0.0500
70	7.0651E+05	3.4450E+04	2.6500E+00	0.0500
71	6.7206E+05	3.2780E+04	2.7000E+00	0.0500
72	6.3928E+05	3.1180E+04	2.7500E+00	0.0500
73	6.0810E+05	2.9660E+04	2.8000E+00	0.0500
74	5.7844E+05	2.8210E+04	2.8500E+00	0.0500
75	5.5023E+05	2.6830E+04	2.9000E+00	0.0500
76	5.2340E+05	2.5530E+04	2.9500E+00	0.0500
77	4.9787E+05	4.7380E+04	3.0000E+00	0.1000
78	4.5049E+05	4.2870E+04	3.1000E+00	0.1000
79	4.0762E+05	1.9880E+04	3.2000E+00	0.0500
80	3.8774E+05	1.8910E+04	3.2500E+00	0.0500
81	3.6883E+05	3.5100E+04	3.3000E+00	0.1000
82	3.3373E+05	3.1760E+04	3.4000E+00	0.1000
83	3.0197E+05	3.4800E+03	3.5000E+00	0.0116
84	2.9849E+05	1.2800E+03	3.5116E+00	0.0043
85	2.9721E+05	2.6900E+03	3.5159E+00	0.0091
86	2.9452E+05	7.2700E+03	3.5250E+00	0.0250
87	2.8725E+05	1.4010E+04	3.5500E+00	0.0500
88	2.7324E+05	2.6000E+04	3.6000E+00	0.1000
89	2.4724E+05	1.2060E+04	3.7000E+00	0.0500
90	2.3518E+05	1.1470E+04	3.7500E+00	0.0500
91	2.2371E+05	1.0910E+04	3.8000E+00	0.0500
92	2.1280E+05	1.0380E+04	3.8500E+00	0.0500
93	2.0242E+05	9.8700E+03	3.9000E+00	0.0500
94	1.9255E+05	9.3900E+03	3.9500E+00	0.0500
95	1.8316E+05	8.9400E+03	4.0000E+00	0.0500
96	1.7422E+05	8.4900E+03	4.0500E+00	0.0500
97	1.6573E+05	8.0900E+03	4.1000E+00	0.0500
98	1.5764E+05	7.6800E+03	4.1500E+00	0.0500

TAB. 2.4 Continued

Neutron Group Energy Boundaries for the VITJEFF311.BOLIB Library.

Group	Upper Energy [eV]	Energy Width [eV]	Upper Lethargy	Lethargy Width
99	1.4996E+05	7.3200E+03	4.2000E+00	0.0500
100	1.4264E+05	6.9500E+03	4.2500E+00	0.0500
101	1.3569E+05	6.6200E+03	4.3000E+00	0.0500
102	1.2907E+05	6.3000E+03	4.3500E+00	0.0500
103	1.2277E+05	5.9800E+03	4.4000E+00	0.0500
104	1.1679E+05	5.7000E+03	4.4500E+00	0.0500
105	1.1109E+05	1.3053E+04	4.5000E+00	0.1250
106	9.8037E+04	1.1520E+04	4.6250E+00	0.1250
107	8.6517E+04	4.0140E+03	4.7500E+00	0.0475
108	8.2503E+04	3.0040E+03	4.7975E+00	0.0371
109	7.9499E+04	7.5010E+03	4.8346E+00	0.0991
110	7.1998E+04	4.6190E+03	4.9337E+00	0.0663
111	6.7379E+04	1.0817E+04	5.0000E+00	0.1750
112	5.6562E+04	4.0870E+03	5.1750E+00	0.0750
113	5.2475E+04	6.1660E+03	5.2500E+00	0.1250
114	4.6309E+04	5.4410E+03	5.3750E+00	0.1250
115	4.0868E+04	6.5610E+03	5.5000E+00	0.1750
116	3.4307E+04	2.4790E+03	5.6750E+00	0.0750
117	3.1828E+04	3.3270E+03	5.7500E+00	0.1104
118	2.8501E+04	1.5010E+03	5.8604E+00	0.0541
119	2.7000E+04	9.4200E+02	5.9145E+00	0.0355
120	2.6058E+04	1.2700E+03	5.9500E+00	0.0500
121	2.4788E+04	6.1200E+02	6.0000E+00	0.0250
122	2.4176E+04	5.9700E+02	6.0250E+00	0.0250
123	2.3579E+04	1.7040E+03	6.0500E+00	0.0750
124	2.1875E+04	2.5700E+03	6.1250E+00	0.1250
125	1.9305E+04	4.2710E+03	6.2500E+00	0.2500
126	1.5034E+04	3.3250E+03	6.5000E+00	0.2500
127	1.1709E+04	1.1140E+03	6.7500E+00	0.1000
128	1.0595E+04	1.4762E+03	6.8500E+00	0.1500
129	9.1188E+03	2.0171E+03	7.0000E+00	0.2500
130	7.1017E+03	1.5709E+03	7.2500E+00	0.2500
131	5.5308E+03	1.2234E+03	7.5000E+00	0.2500
132	4.3074E+03	6.0000E+02	7.7500E+00	0.1500
133	3.7074E+03	3.5280E+02	7.9000E+00	0.1000
134	3.3546E+03	3.1920E+02	8.0000E+00	0.1000
135	3.0354E+03	2.8890E+02	8.1000E+00	0.1000
136	2.7465E+03	1.3390E+02	8.2000E+00	0.0500
137	2.6126E+03	1.2740E+02	8.2500E+00	0.0500
138	2.4852E+03	2.3650E+02	8.3000E+00	0.1000
139	2.2487E+03	2.1400E+02	8.4000E+00	0.1000
140	2.0347E+03	4.5010E+02	8.5000E+00	0.2500
141	1.5846E+03	3.5050E+02	8.7500E+00	0.2500
142	1.2341E+03	2.7298E+02	9.0000E+00	0.2500
143	9.6112E+02	2.1260E+02	9.2500E+00	0.2500
144	7.4852E+02	1.6557E+02	9.5000E+00	0.2500
145	5.8295E+02	1.2895E+02	9.7500E+00	0.2500
146	4.5400E+02	1.0043E+02	1.0000E+01	0.2500
147	3.5357E+02	7.8210E+01	1.0250E+01	0.2500

TAB. 2.4 Continued

Neutron Group Energy Boundaries for the VITJEFF311.BOLIB Library.

Group	Upper Energy [eV]	Energy Width [eV]	Upper Lethargy	Lethargy Width
148	2.7536E+02	6.0910E+01	1.0500E+01	0.2500
149	2.1445E+02	4.7430E+01	1.0750E+01	0.2500
150	1.6702E+02	3.6950E+01	1.1000E+01	0.2500
151	1.3007E+02	2.8770E+01	1.1250E+01	0.2500
152	1.0130E+02	2.2407E+01	1.1500E+01	0.2500
153	7.8893E+01	1.7451E+01	1.1750E+01	0.2500
154	6.1442E+01	1.3591E+01	1.2000E+01	0.2500
155	4.7851E+01	1.0585E+01	1.2250E+01	0.2500
156	3.7266E+01	8.2430E+00	1.2500E+01	0.2500
157	2.9023E+01	6.4200E+00	1.2750E+01	0.2500
158	2.2603E+01	4.9990E+00	1.3000E+01	0.2500
159	1.7604E+01	3.8940E+00	1.3250E+01	0.2500
160	1.3710E+01	3.0330E+00	1.3500E+01	0.2500
161	1.0677E+01	2.3617E+00	1.3750E+01	0.2500
162	8.3153E+00	1.8393E+00	1.4000E+01	0.2500
163	6.4760E+00	1.4325E+00	1.4250E+01	0.2500
164	5.0435E+00	1.1156E+00	1.4500E+01	0.2500
165	3.9279E+00	8.6890E-01	1.4750E+01	0.2500
166	3.0590E+00	6.7660E-01	1.5000E+01	0.2500
167	2.3824E+00	5.2700E-01	1.5250E+01	0.2500
168	1.8554E+00	4.1040E-01	1.5500E+01	0.2500
169	1.4450E+00	1.4500E-01	1.5750E+01	0.1060
170	1.3000E+00	1.7470E-01	1.5856E+01	0.1440
171	1.1253E+00	4.5300E-02	1.6000E+01	0.0410
172	1.0800E+00	4.0000E-02	1.6041E+01	0.0380
173	1.0400E+00	4.0000E-02	1.6079E+01	0.0390
174	1.0000E+00	1.2357E-01	1.6118E+01	0.1320
175	8.7643E-01	7.6430E-02	1.6250E+01	0.0910
176	8.0000E-01	1.1744E-01	1.6341E+01	0.1590
177	6.8256E-01	5.7500E-02	1.6500E+01	0.0880
178	6.2506E-01	9.3480E-02	1.6588E+01	0.1620
179	5.3158E-01	3.1580E-02	1.6750E+01	0.0610
180	5.0000E-01	8.6010E-02	1.6811E+01	0.1890
181	4.1399E-01	4.7190E-02	1.7000E+01	0.1210
182	3.6680E-01	4.1800E-02	1.7121E+01	0.1210
183	3.2500E-01	5.0000E-02	1.7242E+01	0.1670
184	2.7500E-01	5.0000E-02	1.7409E+01	0.2010
185	2.2500E-01	4.1000E-02	1.7610E+01	0.2010
186	1.8400E-01	3.4000E-02	1.7811E+01	0.2040
187	1.5000E-01	2.5000E-02	1.8015E+01	0.1830
188	1.2500E-01	2.5000E-02	1.8198E+01	0.2230
189	1.0000E-01	3.0000E-02	1.8421E+01	0.3560
190	7.0000E-02	2.0000E-02	1.8777E+01	0.3370
191	5.0000E-02	1.0000E-02	1.9114E+01	0.2230
192	4.0000E-02	1.0000E-02	1.9337E+01	0.2880
193	3.0000E-02	9.0000E-03	1.9625E+01	0.3560
194	2.1000E-02	6.5000E-03	1.9981E+01	0.3710
195	1.4500E-02	4.5000E-03	2.0352E+01	0.3710
196	1.0000E-02	5.0000E-03	2.0723E+01	0.6930

TAB. 2.4 Continued

Neutron Group Energy Boundaries for the VITJEFF311.BOLIB Library.

Group	Upper Energy [eV]	Energy Width [eV]	Upper Lethargy	Lethargy Width
197	5.0000E-03	3.0000E-03	2.1416E+01	0.9170
198	2.0000E-03	1.5000E-03	2.2333E+01	1.3860
199	5.0000E-04	4.9000E-04	2.3719E+01	3.9120
	Lower Energy		Lower Lethargy	
	1.0000E-05		2.7631E+01	

TAB. 2.5

Photon Group Energy Boundaries for the VITJEFF311.BOLIB Library.

Group	Upper Energy [eV]	Energy Width [eV]	Upper Lethargy	Lethargy Width
1	3.0000E+07	1.0000E+07	-1.0986E+00	0.4055
2	2.0000E+07	6.0000E+06	-6.9315E-01	0.3567
3	1.4000E+07	2.0000E+06	-3.3647E-01	0.1542
4	1.2000E+07	2.0000E+06	-1.8232E-01	0.1823
5	1.0000E+07	2.0000E+06	0.0000E+00	0.2231
6	8.0000E+06	5.0000E+05	2.2314E-01	0.0645
7	7.5000E+06	5.0000E+05	2.8768E-01	0.0690
8	7.0000E+06	5.0000E+05	3.5667E-01	0.0741
9	6.5000E+06	5.0000E+05	4.3078E-01	0.0800
10	6.0000E+06	5.0000E+05	5.1083E-01	0.0870
11	5.5000E+06	5.0000E+05	5.9784E-01	0.0953
12	5.0000E+06	5.0000E+05	6.9315E-01	0.1054
13	4.5000E+06	5.0000E+05	7.9851E-01	0.1178
14	4.0000E+06	5.0000E+05	9.1629E-01	0.1335
15	3.5000E+06	5.0000E+05	1.0498E+00	0.1542
16	3.0000E+06	5.0000E+05	1.2040E+00	0.1823
17	2.5000E+06	5.0000E+05	1.3863E+00	0.2231
18	2.0000E+06	3.4000E+05	1.6094E+00	0.1863
19	1.6600E+06	1.6000E+05	1.7958E+00	0.1014
20	1.5000E+06	1.6000E+05	1.8971E+00	0.1128
21	1.3400E+06	1.0000E+04	2.0099E+00	0.0075
22	1.3300E+06	3.3000E+05	2.0174E+00	0.2852
23	1.0000E+06	2.0000E+05	2.3026E+00	0.2231
24	8.0000E+05	1.0000E+05	2.5257E+00	0.1335
25	7.0000E+05	1.0000E+05	2.6593E+00	0.1542
26	6.0000E+05	8.8000E+04	2.8134E+00	0.1586
27	5.1200E+05	2.0000E+03	2.9720E+00	0.0039
28	5.1000E+05	6.0000E+04	2.9759E+00	0.1252
29	4.5000E+05	5.0000E+04	3.1011E+00	0.1178
30	4.0000E+05	1.0000E+05	3.2189E+00	0.2877
31	3.0000E+05	1.0000E+05	3.5066E+00	0.4055
32	2.0000E+05	5.0000E+04	3.9120E+00	0.2877
33	1.5000E+05	5.0000E+04	4.1997E+00	0.4055
34	1.0000E+05	2.5000E+04	4.6052E+00	0.2877
35	7.5000E+04	5.0000E+03	4.8929E+00	0.0690
36	7.0000E+04	1.0000E+04	4.9618E+00	0.1542
37	6.0000E+04	1.5000E+04	5.1160E+00	0.2877
38	4.5000E+04	5.0000E+03	5.4037E+00	0.1178
39	4.0000E+04	1.0000E+04	5.5215E+00	0.2877
40	3.0000E+04	1.0000E+04	5.8091E+00	0.4055
41	2.0000E+04	1.0000E+04	6.2146E+00	0.6931
42	1.0000E+04	9.0000E+03	6.9078E+00	2.3026
	Lower Energy		Lower Lethargy	
	1.0000E+03		9.2103E+00	

TAB. 2.6

VITJEFF311.BOLIB Library Thermal Neutron Energy Range.

Group	Upper Energy [eV]	Lethargy Width	Group	Upper Energy [eV]	Lethargy Width
164	5.04350	0.250	182	0.36680	0.121
165	3.92790	0.250	183	0.32500	0.167
166	3.05900	0.250	184	0.27500	0.201
167	2.38240	0.250	185	0.22500	0.201
168	1.85540	0.250	186	0.18400	0.204
169	1.44500	0.106	187	0.15000	0.183
170	1.30000	0.144	188	0.12500	0.223
171	1.12530	0.041	189	0.10000	0.356
172	1.08000	0.038	190	0.07000	0.337
173	1.04000	0.039	191	0.05000	0.223
174	1.00000	0.132	192	0.04000	0.288
175	0.87643	0.091	193	0.03000	0.356
176	0.80000	0.159	194	0.02100	0.371
177	0.68256	0.088	195	0.01450	0.371
178	0.62506	0.162	196	0.01000	0.693
179	0.53158	0.061	197	0.00500	0.917
180	0.50000	0.189	198	0.00200	1.386
181	0.41399	0.121	199	0.00050	3.912
				Lower Energy	
				0.00001	

2.4 - Weighting Function

The neutron and photon weighting functions used to produce the VITJEFF311.BOLIB library cross sections are the same as those employed in the generation of the VITAMIN-B6 /9/ cross sections.
The neutron weighting function is of the form typically chosen for fission reactor shielding problems, i.e., it consists of a smoothly varying combination of a Maxwellian thermal spectrum, a fission spectrum, and a “l/E” slowing down spectrum. This corresponds to the IWT=4 option in the GROUPR module of the NJOY /18/ system. The breakpoint energies for the 3-region spectrum are similar to those used in VITAMIN-C /58/. The breakpoint energy between the Maxwellian and l/E shapes is 0.125 eV. The fission temperature has been adjusted to better reflect the neutron spectrum in a thermal reactor (θ = 1.273 MeV). The use of a large number of energy groups should make the exact functional form and energy break points less important compared to generating a broad-group library directly from JEFF data. The functional form of the weighting spectrum is given by the following:

Functional Form	Energy Limits	Groups
1. Maxwellian Thermal Spectrum (kT = 0.025 eV)		
$W_1(E) = C_1Ee^{-E/kT}$	1.0E-5 eV to 0.125 eV	188-199
2. “l/E” Slowing-Down Spectrum		
$W_2(E) = C_2/E$	0.125 eV to 820.8 keV	67-187
3. Fission Spectrum (θ = 1.273 MeV)		
$W_3(E) = C_3E^{1/2}\, e^{-E/\theta}$	820.8 keV to 20 MeV	1-66

A continuous weighting spectrum is achieved with the following constants: C_1 = 9498.4 eV^{-2}, C_2 = 1.0 and C_3 = 2.5625 MeV$^{-1.5}$. The neutron weighting function is shown in FIG. 2.1 and listed in TAB. 2.7 in a 199 group representation.

The photon weighting spectrum consists of a l/E spectrum with a “roll-off” of the spectrum at lower energies to represent photoelectric absorption and a similar drop-off of the spectrum at higher energies corresponding to the Q-value for neutron capture. This corresponds to the IWT=3 input option in the GAMINR module of the NJOY system. The gamma ray weighting function is shown in FIG. 2.2 and listed in TAB. 2.8 in a 42 group representation.

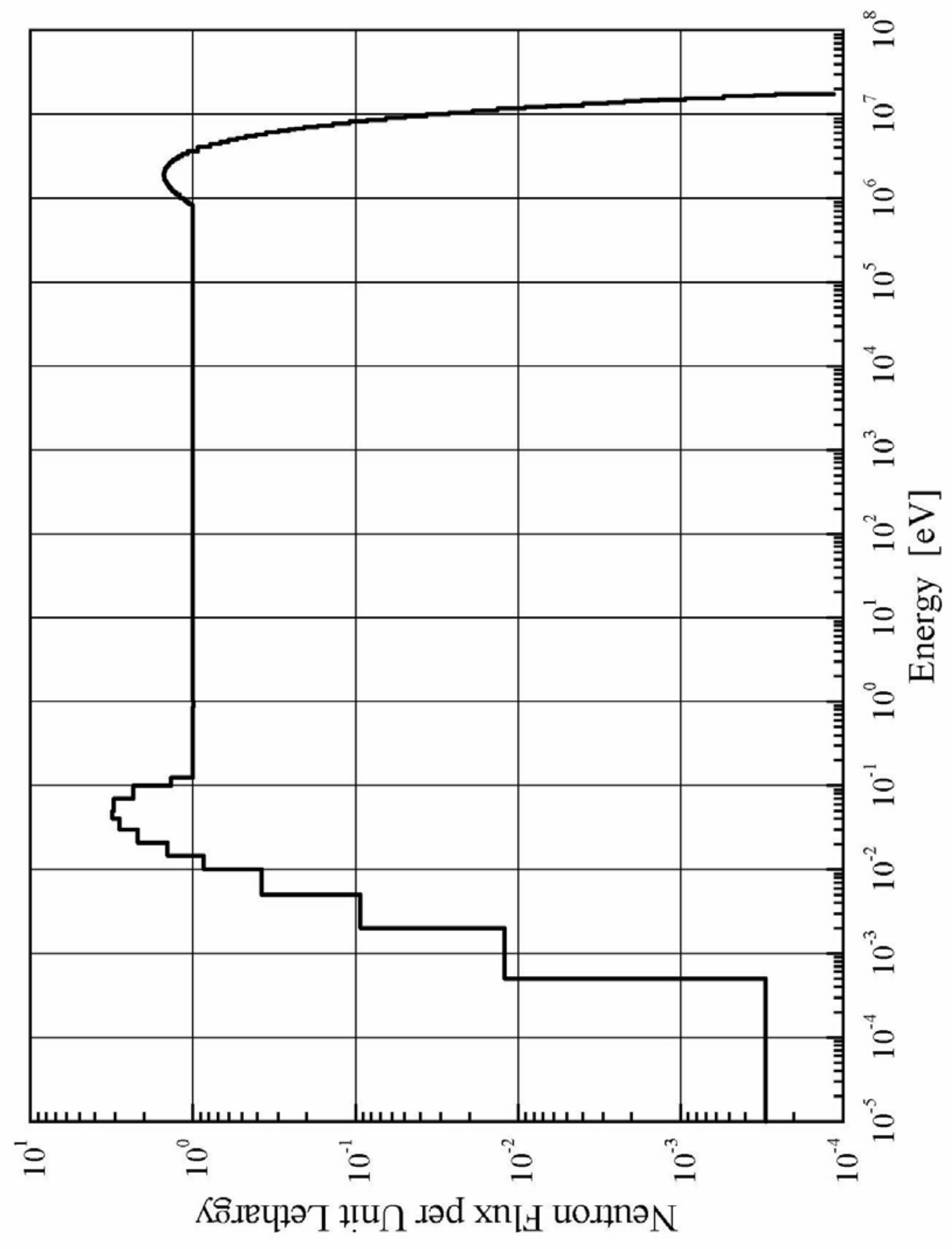


FIG. 2.1 199 Group Representation of Standard Weighting Spectrum Used to Create VITJEFF311.BOLIB Neutron Cross Sections from JEFF-3.1.1 Pointwise Data.

TAB. 2.7

Neutron Energy Weighting Spectrum for the VITJEFF311.BOLIB Library.

Group	Weight	Group	Weight	Group	Weight
1	1.423E-05	51	7.543E-02	101	5.002E-02
2	6.578E-06	52	7.516E-02	102	5.004E-02
3	8.861E-06	53	7.461E-02	103	4.994E-02
4	2.733E-05	54	7.389E-02	104	5.004E-02
5	4.690E-05	55	7.295E-02	105	1.250E-01
6	3.419E-05	56	7.181E-02	106	1.250E-01
7	4.380E-05	57	7.031E-02	107	4.751E-02
8	5.590E-05	58	6.888E-02	108	3.709E-02
9	7.036E-05	59	6.723E-02	109	9.911E-02
10	1.991E-04	60	6.552E-02	110	6.631E-02
11	1.368E-04	61	6.354E-02	111	1.750E-01
12	1.684E-04	62	1.211E-01	112	7.500E-02
13	4.576E-04	63	4.809E-02	113	1.250E-01
14	6.684E-04	64	6.474E-02	114	1.250E-01
15	9.574E-04	65	5.321E-02	115	1.750E-01
16	1.342E-03	66	5.108E-02	116	7.500E-02
17	1.843E-03	67	5.000E-02	117	1.104E-01
18	2 482E-03	68	5.000E-02	118	5.410E-02
19	3.285E-03	69	5.001E-02	119	3.551E-02
20	4.272E-03	70	4.999E-02	120	4.997E-02
21	5.465E-03	71	5.001E-02	121	2.500E-02
22	6.882E-03	72	5.000E-02	122	2.500E-02
23	8.540E-03	73	5.000E-02	123	7.501E-02
24	1.045E-02	74	5.000E-02	124	1.250E-01
25	3.951E-03	75	4.999E-02	125	2.501E-01
26	8.659E-03	76	5.001E-02	126	2.500E-01
27	1.503E-02	77	1.000E-01	127	9.998E-02
28	1.769E-02	78	1.000E-01	128	1.500E-01
29	2.058E-02	79	5.000E-02	129	2.500E-01
30	2.368E-02	80	5.000E-02	130	2.500E-01
31	2.697E-02	81	1.000E-01	131	2.500E-01
32	3.041E-02	82	1.000E-01	132	1.500E-01
33	3.397E-02	83	1.159E-02	133	1.000E-01
34	7.885E-02	84	4.297E-03	134	9.999E-02
35	9.338E-02	85	9.092E-03	135	1.000E-01
36	1.073E-01	86	2.499E-02	136	4.998E-02
37	5.848E-02	87	5.000E-02	137	4.999E-02
38	6.148E-02	88	9.999E-02	138	1.000E-01
39	6.413E-02	89	5.001E-02	139	1.000E-01
40	6.666E-02	90	5.000E-02	140	2.500E-01
41	6.879E-02	91	5.000E-02	141	2.500E-01
42	7.065E-02	92	5.001E-02	142	2.500E-01
43	4.797E-02	93	4.999E-02	143	2.500E-01
44	1.216E-02	94	5.000E-02	144	2.500E-01
45	1.212E-02	95	5.004E-02	145	2.500E-01
46	2.439E-02	96	4.996E-02	146	2.500E-01
47	4.909E-02	97	5.005E-02	147	2.500E-01
48	7.440E-02	98	4.995E-02	148	2.500E-01
49	7.503E-02	99	5.004E-02	149	2.500E-01
50	7.539E-02	100	4.995E-02	150	2.500E-01

TAB. 2.7 Continued

Neutron Energy Weighting Spectrum for the VITJEFF311.BOLIB Library.

Group	Weight	Group	Weight	Group	Weight
151	2.500E-01	168	2.500E-01	185	2.012E-01
152	2.500E-01	169	1.057E-01	186	2.043E-01
153	2.500E-01	170	1.443E-01	187	1.823E-01
154	2.500E-01	171	4.109E-02	188	3.037E-01
155	2.500E-01	172	3.774E-02	189	8.282E-01
156	2.500E-01	173	3.922E-02	190	1.038E+00
157	2.500E-01	174	1.319E-01	191	7.060E-01
158	2.500E-01	175	9.125E-02	192	8.174E-01
159	2.500E-01	176	1.588E-01	193	7.820E-01
160	2.500E-01	177	8.800E-02	194	5.360E-01
161	2.500E-01	178	1.620E-01	195	3.194E-01
162	2.500E-01	179	6.125E-02	196	2.614E-01
163	2.500E-01	180	1.888E-01	197	8.601E-02
164	2.500E-01	181	1.210E-01	198	1.684E-02
165	2.500E-01	182	1.210E-01	199	1.171E-03
166	2.500E-01	183	1.671E-01		
167	2.500E-01	184	2.007E-01		

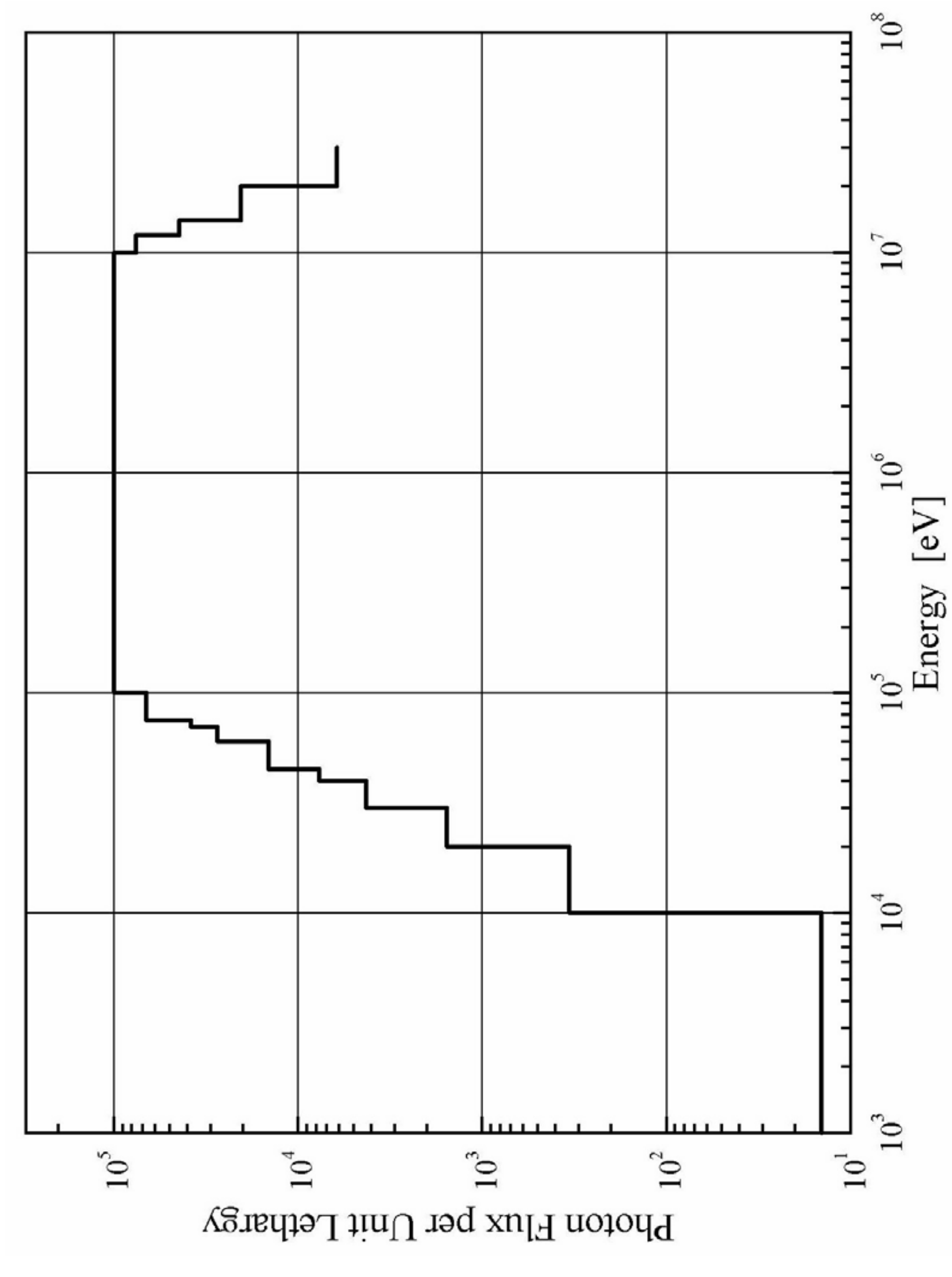


FIG. 2.2 42 Group Representation of Standard Weighting Spectrum Used to Create VITJEFF311.BOLIB Photon Cross Sections from JEFF-3.1.1 Pointwise Data.

TAB. 2.8

Photon Energy Weighting Spectrum for the VITJEFF311.BOLIB Library.

Group	Weight	Group	Weight	Group	Weight
1	2.498E+03	15	1.542E+04	29	1.178E+04
2	7.298E+03	16	1.824E+04	30	2.877E+04
3	6.824E+03	17	2.232E+04	31	4.055E+04
4	1.387E+04	18	1.864E+04	32	2.877E+04
5	2.232E+04	19	1.014E+04	33	4.055E+04
6	6.455E+03	20	1.128E+04	34	1.927E+04
7	6.901E+03	21	7.491E+02	35	2.629E+03
8	7.413E+03	22	2.852E+04	36	4.233E+03
9	8.006E+03	23	2.232E+04	37	4.163E+03
10	8.703E+03	24	1.335E+04	38	9.042E+02
11	9.534E+03	25	1.542E+04	39	1.233E+03
12	1.054E+04	26	1.586E+04	40	6.333E+02
13	1.178E+04	27	3.914E+02	41	2.333E+02
14	1.336E+04	28	1.252E+04	42	3.330E+01

2.5 - Legendre Order of Scattering

The order of scattering used for both neutrons and photons is P_7, for nuclides with Z=l through Z=29 (copper) and P_5 for the remainder of the nuclides. In particular, the previous values corresponding to L=ℓ-max, the maximum order of the Legendre polynomial (P_ℓ) expansion of the scattering cross section matrix, available for each nuclide of the library, are listed in TAB. 2.2.
Most calculations are likely to be done with P_3 scattering, but for some problems, e.g., when single scatter events dominate, higher orders may be required as stated in the VITAMIN-B6 /9/ library user's manual. For the same nuclide, an identical order of scattering for both neutrons and photons was adopted in the generation of the VITAMIN-B6, VITJEFF22.BOLIB /39/, MATJEF22.BOLIB /40/, VITJEFF31.BOLIB /42/, MATJEFF31.BOLIB /43/ and VITJEFF311.BOLIB cross sections.

2.6 - Convergence Parameters

The following numerical values of the fractional error tolerances were chosen as input parameters in NJOY to generate the libraries VITJEFF311.BOLIB, VITJEFF31.BOLIB /42/ and MATJEFF31.BOLIB /43/: 0.1% for resolved resonance reconstruction and for linearization in RECONR and 0.1% for thinning in BROADR. These data have reduced numerical values with respect to the 0.2% corresponding error tolerance values used to generate VITAMIN-B6 /9/, VITJEFF22.BOLIB /39/ and MATJEF22.BOLIB /40/, chosen on the basis of the ORNL experience with the VITAMIN libraries and the experience of the NJOY users.

2.7 - Processing Codes and Procedures

The NJOY-259 /18/ nuclear data processing system and the ENEA-Bologna 2007 Revision /20/ of the SCAMPI /19/ nuclear data processing system were used on a Personal Computer (CPU INTEL Pentium III, 448 MB of RAM; FSF-g77 version 0.5.26 FORTRAN compiler for NJOY and f77 Absoft version 5.0 FORTRAN 77 compiler for SCAMPI) with the Linux Red Hat 7.1 operating system to generate the VITJEFF311.BOLIB library. The following modules of NJOY were used to process neutron interaction (n-n), gamma ray production (n-γ) and gamma ray interaction (γ-γ) data into the GENDF format, from the JEFF-3.1.1 incident neutron and photo-atomic data in ENDF-6 format. Specifically, the MODER, RECONR, BROADR, THERMR, HEATR, GASPR, PURR, GROUPR modules were used for the incident neutron data while the MODER, RECONR and GAMINR modules were used for the photo-atomic data. Then the ENEA-Bologna revised version of the SMILER module, contained in the ENEA-Bologna 2007 Revision of SCAMPI, was used to translate the fine-group data from the GENDF format into the AMPX master library format of VITJEFF311.BOLIB. The RADE module of SCAMPI was used to check and screen the data for internal consistency and "sanity", i.e. the data values are physical and within expected bounds. Then the module AIM of SCAMPI was used to convert the master cross section libraries for the standard and bound nuclide cross section files from binary to BCD format.
A brief description of the function of the NJOY and SCAMPI modules is presented in TAB. 2.9. A schematic diagram illustrating the VITJEFF311.BOLIB processing procedure to produce the standard nuclide cross section files is given in FIG. 2.3 while the procedure to produce the bound nuclide cross section files is reported in FIG. 2.4.

TAB. 2.9

Modules from the NJOY-99.259 and SCAMPI
Nuclear Data Processing Systems Used to Process VITJEFF311.BOLIB.

NJOY-99.259 System

Module	Function
MODER	Converts between ENDF/B standard coded mode and the NJOY blocked binary mode.
RECONR	Reconstructs point-wise cross sections from JEFF resonance parameters and interpolation schemes.
BROADR	Doppler-broadens and thins point-wise cross sections.
THERMR	Produces cross sections and energy-to-energy matrices for free or bound scatterers in the thermal energy range.
HEATR	Generates heat production cross sections (KERMA factors) and damage-energy production.
GASPR	Computes gas production cross sections.
PURR	Computes probability tables and effective point-wise self-shielded cross sections in the unresolved energy range.
GROUPR	Generates self-shielded multi-group cross sections and group-to-group scattering and photon production matrices in GENDF format.
GAMINR	Computes multi-group photo-atomic cross sections, KERMA factors, group-to-group photon scattering matrices.

SCAMPI System (ENEA-Bologna 2007 Revision)

Module	Function
SMILER	Translates GENDF files produced by NJOY into AMPX master interface format.
RADE	Performs sanity and consistency tests on multi-group libraries.
AIM	Converts master cross section libraries from binary format to BCD (or vice-versa).

FIG. 2.3 Procedure for Generating the VITJEFF311.BOLIB Library in AMPX Format from JEFF-3.1.1.

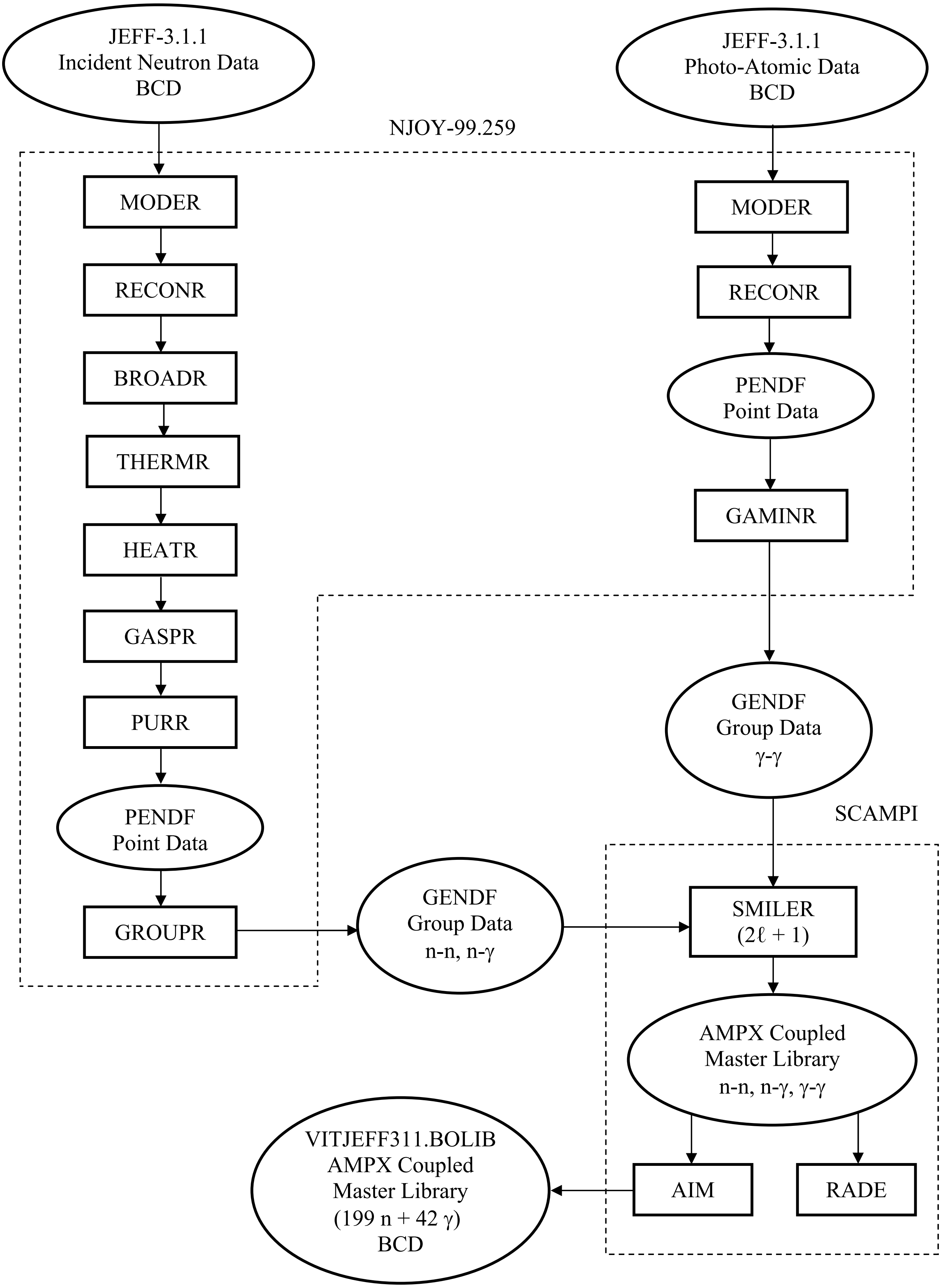
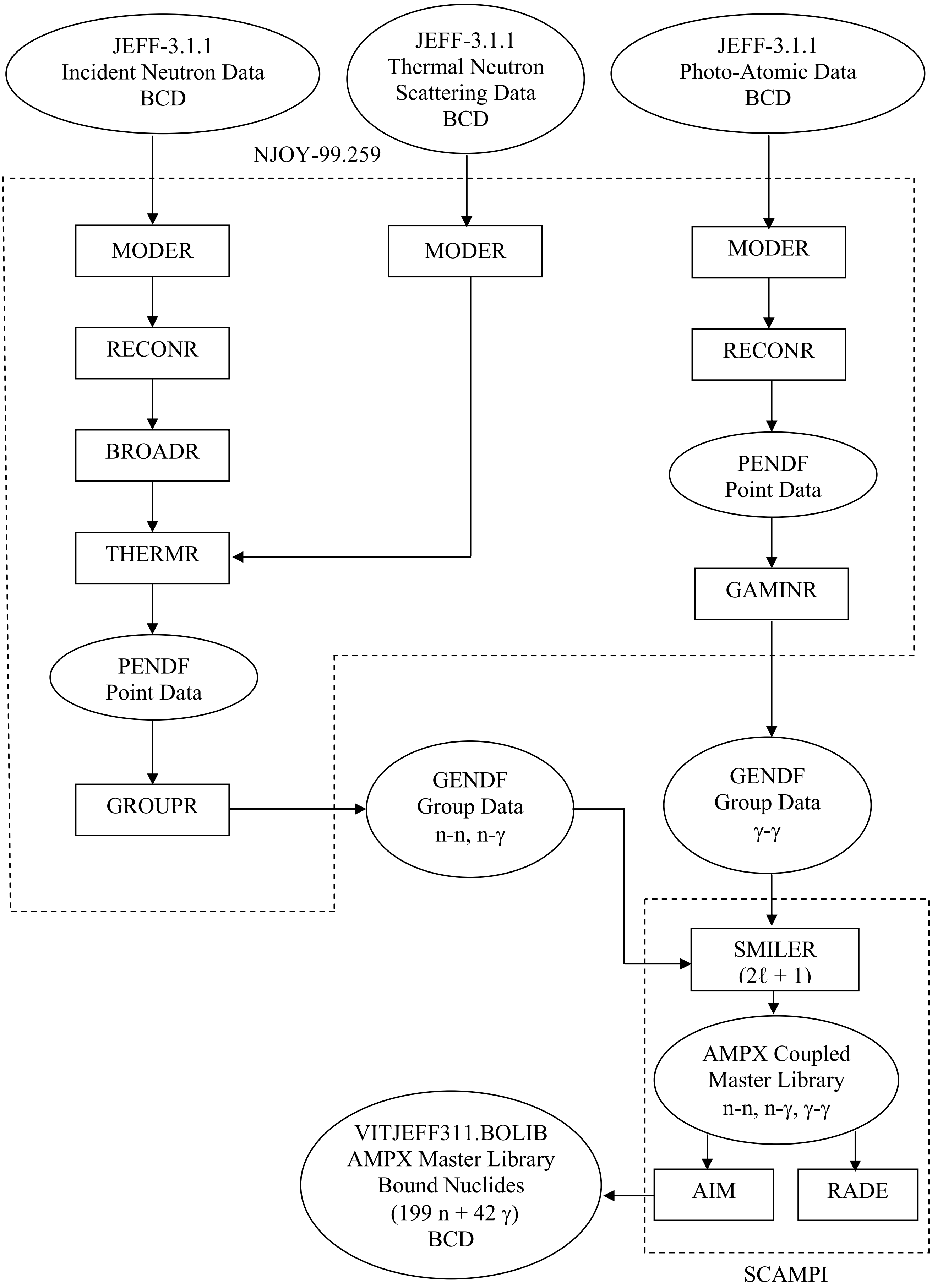


FIG. 2.4 Procedure for Generating the VITJEFF311.BOLIB Bound Nuclides in AMPX Format from JEFF-3.1.1.



2.8 - Response Functions

At present only the following "response" functions are included in tabulated form in the VITJEFF311.BOLIB library package: neutron and photon group energy boundaries, neutron and photon group energy widths, neutron and photon group lethargy boundaries, neutron and photon group lethargy widths, total (prompt + delayed) neutron fission spectra (χ) for the U-235, U-238 and Pu-239 nuclides.
The total neutron fission spectra (χ) were obtained through the ENEA-Bologna 2007 Revision /20/ of the SCAMPI /19/ system which allows processing of delayed neutron spectra. In particular the BONAMI and NITAWL modules were firstly used to generate an AMPX working file for each fissile nuclide, containing infinitely dilute cross sections (background cross section σ_0 = 1.0E+10 barns) at the temperature of 300 °K. Then the fine-group χ-vectors were calculated by the ICE module with the KOPT=4 option (nuclide-dependent spectrum option) in the 1$$ array, i.e. using the neutron flux spectrum derived from the weighting functions corresponding to the IWT=4 option in GROUPR (see 2.4), always provided in each nuclide data file of an AMPX working library.
Then the normalization of the total neutron fission spectra (χ) to one neutron per fission was performed since the ICE module with the KOPT=4 option does not ensure a proper normalization (see /19/).
The resulting total fission spectra for the U-235, U-238 and Pu-239 nuclides are reported in TAB. 2.10.
A 199 group representation of the U-235 total fission spectrum is shown in FIG. 2.5.

TAB. 2.10

VITJEFF311.BOLIB Library Total Neutron Fission Spectra for U-235, U-238 and Pu-239.

Group	Upper Energy [eV]	U-235 X	U-238 X	Pu-239 X
1	1.9640E+07	4.48634E-06	3.94788E-06	7.66615E-06
2	1.7332E+07	1.78079E-06	1.60138E-06	2.95963E-06
3	1.6905E+07	2.53131E-06	2.18954E-06	3.98909E-06
4	1.6487E+07	7.81960E-06	6.90577E-06	1.23082E-05
5	1.5683E+07	1.38064E-05	1.21619E-05	2.10980E-05
6	1.4918E+07	1.04157E-05	9.01790E-06	1.53522E-05
7	1.4550E+07	1.34932E-05	1.16883E-05	1.96454E-05
8	1.4191E+07	1.67545E-05	1.50734E-05	2.50188E-05
9	1.3840E+07	2.22685E-05	1.91597E-05	3.14141E-05
10	1.3499E+07	6.20526E-05	5.50109E-05	8.85352E-05
11	1.2840E+07	4.44331E-05	3.82734E-05	6.05660E-05
12	1.2523E+07	5.48144E-05	4.75153E-05	7.43261E-05
13	1.2214E+07	1.47663E-04	1.30673E-04	2.00851E-04
14	1.1618E+07	2.20852E-04	1.93610E-04	2.91131E-04
15	1.1052E+07	3.19940E-04	2.80900E-04	4.13668E-04
16	1.0513E+07	4.49965E-04	3.98708E-04	5.75562E-04
17	1.0000E+07	5.99347E-04	5.53062E-04	7.83175E-04
18	9.5123E+06	8.15864E-04	7.53669E-04	1.04731E-03
19	9.0484E+06	1.09025E-03	1.00782E-03	1.37538E-03
20	8.6071E+06	1.43111E-03	1.32404E-03	1.77577E-03
21	8.1873E+06	1.84619E-03	1.71003E-03	2.25512E-03
22	7.7880E+06	2.34196E-03	2.17232E-03	2.81865E-03
23	7.4082E+06	2.92300E-03	2.71586E-03	3.46956E-03
24	7.0469E+06	3.59107E-03	3.34234E-03	4.20754E-03
25	6.7032E+06	1.36032E-03	1.26761E-03	1.58118E-03
26	6.5924E+06	2.98395E-03	2.78344E-03	3.44828E-03
27	6.3763E+06	5.18124E-03	4.84220E-03	5.93333E-03
28	6.0653E+06	6.09379E-03	5.70925E-03	6.90957E-03
29	5.7695E+06	7.07732E-03	6.64938E-03	7.95391E-03
30	5.4881E+06	8.11953E-03	7.65120E-03	9.05134E-03
31	5.2205E+06	9.21733E-03	8.70945E-03	1.01952E-02
32	4.9659E+06	1.03581E-02	9.80805E-03	1.13679E-02
33	4.7237E+06	1.15305E-02	1.09448E-02	1.25648E-02
34	4.4933E+06	2.66507E-02	2.53788E-02	2.87301E-02
35	4.0657E+06	3.14387E-02	3.00347E-02	3.34139E-02
36	3.6788E+06	3.60389E-02	3.45405E-02	3.77900E-02
37	3.3287E+06	1.96127E-02	1.88410E-02	2.03681E-02
38	3.1664E+06	2.06003E-02	1.98246E-02	2.12646E-02
39	3.0119E+06	2.14575E-02	2.06917E-02	2.20251E-02
40	2.8651E+06	2.22640E-02	2.15152E-02	2.27310E-02
41	2.7253E+06	2.29178E-02	2.21992E-02	2.32859E-02
42	2.5924E+06	2.34630E-02	2.27850E-02	2.37343E-02
43	2.4660E+06	1.58803E-02	1.54561E-02	1.60097E-02
44	2.3852E+06	4.01882E-03	3.91614E-03	4.04520E-03
45	2.3653E+06	4.00035E-03	3.89954E-03	4.02398E-03
46	2.3457E+06	8.04248E-03	7.84671E-03	8.08335E-03
47	2.3069E+06	1.61455E-02	1.57754E-02	1.62007E-02
48	2.2313E+06	2.43510E-02	2.38530E-02	2.43721E-02
49	2.1225E+06	2.43972E-02	2.39736E-02	2.43506E-02

TAB. 2.10 Continued

VITJEFF311.BOLIB Library Total Neutron Fission Spectra for U-235, U-238 and Pu-239.

Group	Upper Energy [eV]	U-235 X	U-238 X	Pu-239 X
50	2.0190E+06	2.43373E-02	2.39899E-02	2.42303E-02
51	1.9205E+06	2.41570E-02	2.38867E-02	2.39984E-02
52	1.8268E+06	2.38688E-02	2.36694E-02	2.36653E-02
53	1.7377E+06	2.34896E-02	2.33652E-02	2.32459E-02
54	1.6530E+06	2.30563E-02	2.29963E-02	2.27777E-02
55	1.5724E+06	2.25625E-02	2.25670E-02	2.22532E-02
56	1.4957E+06	2.20254E-02	2.20962E-02	2.16849E-02
57	1.4227E+06	2.13875E-02	2.15035E-02	2.10207E-02
58	1.3534E+06	2.07795E-02	2.09350E-02	2.03925E-02
59	1.2874E+06	2.01309E-02	2.03243E-02	1.97221E-02
60	1.2246E+06	1.94995E-02	1.97386E-02	1.90615E-02
61	1.1648E+06	1.87936E-02	1.90647E-02	1.83393E-02
62	1.1080E+06	3.54692E-02	3.60894E-02	3.45371E-02
63	1.0026E+06	1.39890E-02	1.42825E-02	1.35780E-02
64	9.6164E+05	1.87407E-02	1.91761E-02	1.81573E-02
65	9.0718E+05	1.53174E-02	1.56990E-02	1.48162E-02
66	8.6294E+05	1.46587E-02	1.50698E-02	1.41464E-02
67	8.2085E+05	1.39844E-02	1.44136E-02	1.34682E-02
68	7.8082E+05	1.33529E-02	1.38066E-02	1.28256E-02
69	7.4274E+05	1.27052E-02	1.31593E-02	1.21860E-02
70	7.0651E+05	1.20692E-02	1.25259E-02	1.15595E-02
71	6.7206E+05	1.14648E-02	1.19202E-02	1.09617E-02
72	6.3928E+05	1.08856E-02	1.13527E-02	1.03819E-02
73	6.0810E+05	1.03334E-02	1.08166E-02	9.82693E-03
74	5.7844E+05	9.77173E-03	1.02396E-02	9.26605E-03
75	5.5023E+05	9.22275E-03	9.67864E-03	8.73353E-03
76	5.2340E+05	8.72070E-03	9.17890E-03	8.25128E-03
77	4.9787E+05	1.59519E-02	1.68286E-02	1.50676E-02
78	4.5049E+05	1.40749E-02	1.48626E-02	1.32738E-02
79	4.0762E+05	6.41478E-03	6.80173E-03	6.03474E-03
80	3.8774E+05	6.03571E-03	6.42696E-03	5.66134E-03
81	3.6883E+05	1.08968E-02	1.16218E-02	1.02371E-02
82	3.3373E+05	9.53176E-03	1.01784E-02	8.94473E-03
83	3.0197E+05	1.02318E-03	1.09402E-03	9.60899E-04
84	2.9849E+05	3.75444E-04	4.01535E-04	3.52413E-04
85	2.9721E+05	7.87118E-04	8.41727E-04	7.38664E-04
86	2.9452E+05	2.11554E-03	2.26292E-03	1.98357E-03
87	2.8725E+05	4.02992E-03	4.31547E-03	3.77173E-03
88	2.7324E+05	7.28865E-03	7.81679E-03	6.81516E-03
89	2.4724E+05	3.27959E-03	3.51652E-03	3.06538E-03
90	2.3518E+05	3.05510E-03	3.27803E-03	2.85379E-03
91	2.2371E+05	2.84805E-03	3.05869E-03	2.65982E-03
92	2.1280E+05	2.65307E-03	2.85222E-03	2.48060E-03
93	2.0242E+05	2.47137E-03	2.65741E-03	2.31141E-03
94	1.9255E+05	2.30820E-03	2.48433E-03	2.15161E-03
95	1.8316E+05	2.15475E-03	2.32160E-03	2.00460E-03
96	1.7422E+05	2.00338E-03	2.16015E-03	1.86326E-03
97	1.6573E+05	1.86824E-03	2.01579E-03	1.73866E-03
98	1.5764E+05	1.73602E-03	1.87426E-03	1.61744E-03

TAB. 2.10 Continued

VITJEFF311.BOLIB Library Total Neutron Fission Spectra for U-235, U-238 and Pu-239.

Group	Upper Energy [eV]	U-235 X	U-238 X	Pu-239 X
99	1.4996E+05	1.62100E-03	1.74717E-03	1.50793E-03
100	1.4264E+05	1.50719E-03	1.62267E-03	1.39752E-03
101	1.3569E+05	1.40544E-03	1.51266E-03	1.30014E-03
102	1.2907E+05	1.30900E-03	1.41037E-03	1.20914E-03
103	1.2277E+05	1.21423E-03	1.30842E-03	1.12171E-03
104	1.1679E+05	1.13086E-03	1.21988E-03	1.04564E-03
105	1.1109E+05	2.48766E-03	2.68860E-03	2.30789E-03
106	9.8037E+04	2.07834E-03	2.25651E-03	1.92853E-03
107	8.6517E+04	6.96572E-04	7.59306E-04	6.45577E-04
108	8.2503E+04	5.11391E-04	5.58464E-04	4.73812E-04
109	7.9499E+04	1.23807E-03	1.35848E-03	1.14576E-03
110	7.1998E+04	7.30083E-04	7.93764E-04	6.77181E-04
111	6.7379E+04	1.61274E-03	1.73743E-03	1.49681E-03
112	5.6562E+04	5.74620E-04	6.17295E-04	5.32070E-04
113	5.2475E+04	8.27758E-04	8.93520E-04	7.65796E-04
114	4.6309E+04	6.89198E-04	7.46958E-04	6.36047E-04
115	4.0868E+04	7.73059E-04	8.35209E-04	7.13264E-04
116	3.4307E+04	2.75165E-04	2.97730E-04	2.53259E-04
117	3.1828E+04	3.55949E-04	3.89019E-04	3.26245E-04
118	2.8501E+04	1.55695E-04	1.71657E-04	1.41477E-04
119	2.7000E+04	9.57272E-05	1.05607E-04	8.67927E-05
120	2.6058E+04	1.26578E-04	1.39790E-04	1.14577E-04
121	2.4788E+04	5.99585E-05	6.63017E-05	5.42148E-05
122	2.4176E+04	5.78285E-05	6.40114E-05	5.22600E-05
123	2.3579E+04	1.61386E-04	1.79092E-04	1.45764E-04
124	2.1875E+04	2.33884E-04	2.64614E-04	2.10532E-04
125	1.9305E+04	3.63276E-04	4.27517E-04	3.19686E-04
126	1.5034E+04	2.53425E-04	3.02326E-04	2.20052E-04
127	1.1709E+04	7.85115E-05	9.53192E-05	6.80818E-05
128	1.0595E+04	9.38298E-05	1.06459E-04	8.40772E-05
129	9.1188E+03	1.12985E-04	1.20666E-04	1.03061E-04
130	7.1017E+03	7.83891E-05	8.41517E-05	7.09374E-05
131	5.5308E+03	5.44406E-05	5.87428E-05	4.87847E-05
132	4.3074E+03	2.43355E-05	2.65728E-05	2.17985E-05
133	3.7074E+03	1.35173E-05	1.47549E-05	1.19892E-05
134	3.3546E+03	1.16936E-05	1.27690E-05	1.02945E-05
135	3.0354E+03	1.01218E-05	1.10814E-05	8.86445E-06
136	2.7465E+03	4.53598E-06	4.98280E-06	3.96259E-06
137	2.6126E+03	4.22137E-06	4.65081E-06	3.68442E-06
138	2.4852E+03	7.58396E-06	8.40061E-06	6.61777E-06
139	2.2487E+03	6.56777E-06	7.34044E-06	5.73968E-06
140	2.0347E+03	1.28311E-05	1.44365E-05	1.11171E-05
141	1.5846E+03	8.97493E-06	1.01691E-05	7.63463E-06
142	1.2341E+03	6.29102E-06	7.26677E-06	5.32361E-06
143	9.6112E+02	4.41967E-06	5.18909E-06	3.70017E-06
144	7.4852E+02	3.11174E-06	3.70669E-06	2.56509E-06
145	5.8295E+02	2.19649E-06	2.64935E-06	1.77240E-06
146	4.5400E+02	1.55463E-06	1.91310E-06	1.23770E-06
147	3.5357E+02	1.10342E-06	1.37540E-06	8.54833E-07

TAB. 2.10 Continued

VITJEFF311.BOLIB Library Total Neutron Fission Spectra for U-235, U-238 and Pu-239.

Group	Upper Energy [eV]	U-235 X	U-238 X	Pu-239 X
148	2.7536E+02	7.85624E-07	9.98676E-07	5.96637E-07
149	2.1445E+02	5.61097E-07	7.29894E-07	4.19010E-07
150	1.6702E+02	4.02281E-07	5.31605E-07	2.91008E-07
151	1.3007E+02	2.89281E-07	3.91127E-07	2.04772E-07
152	1.0130E+02	2.08874E-07	2.89126E-07	1.44637E-07
153	7.8893E+01	1.51370E-07	2.13896E-07	1.01824E-07
154	6.1442E+01	1.10117E-07	1.58499E-07	7.15353E-08
155	4.7851E+01	8.04209E-08	1.18339E-07	5.08100E-08
156	3.7266E+01	5.89565E-08	8.83326E-08	3.58919E-08
157	2.9023E+01	4.33948E-08	6.62723E-08	2.55252E-08
158	2.2603E+01	3.20561E-08	5.00089E-08	1.83412E-08
159	1.7604E+01	2.37784E-08	3.77009E-08	1.30798E-08
160	1.3710E+01	1.77013E-08	2.85686E-08	9.42107E-09
161	1.0677E+01	1.02584E-08	2.17288E-08	6.83841E-09
162	8.3153E+00	7.00407E-09	1.65386E-08	4.95594E-09
163	6.4760E+00	5.45498E-09	1.26059E-08	3.59495E-09
164	5.0435E+00	4.24822E-09	9.64013E-09	2.62909E-09
165	3.9279E+00	3.30878E-09	7.38146E-09	1.92535E-09
166	3.0590E+00	2.57650E-09	5.65931E-09	1.41392E-09
167	2.3824E+00	2.00682E-09	4.35364E-09	1.04883E-09
168	1.8554E+00	1.56281E-09	3.34837E-09	7.76228E-10
169	1.4450E+00	5.52162E-10	1.17331E-09	2.64959E-10
170	1.3000E+00	6.65259E-10	1.40701E-09	3.12785E-10
171	1.1253E+00	1.72503E-10	3.63616E-10	7.99556E-11
172	1.0800E+00	1.52320E-10	3.20643E-10	7.02072E-11
173	1.0400E+00	1.52320E-10	3.20262E-10	6.98380E-11
174	1.0000E+00	4.70556E-10	9.85567E-10	2.11945E-10
175	8.7643E-01	2.91046E-10	6.06230E-10	1.27856E-10
176	8.0000E-01	4.47213E-10	9.26529E-10	1.91640E-10
177	6.8256E-01	2.18961E-10	4.51400E-10	9.17001E-11
178	6.2506E-01	3.55973E-10	7.30810E-10	1.46093E-10
179	5.3158E-01	1.20257E-10	2.45946E-10	4.85182E-11
180	5.0000E-01	3.27527E-10	6.67844E-10	1.30001E-10
181	4.1399E-01	1.79700E-10	3.64975E-10	6.99958E-11
182	3.6680E-01	1.59175E-10	3.22478E-10	6.12136E-11
183	3.2500E-01	1.90401E-10	3.84739E-10	7.22505E-11
184	2.7500E-01	1.90401E-10	3.83650E-10	7.11922E-11
185	2.2500E-01	1.56128E-10	3.13761E-10	5.75879E-11
186	1.8400E-01	1.29472E-10	2.59617E-10	4.72161E-11
187	1.5000E-01	9.52003E-11	1.90555E-10	3.44055E-11
188	1.2500E-01	9.52003E-11	1.90286E-10	3.41410E-11
189	1.0000E-01	1.14240E-10	2.27567E-10	4.02080E-11
190	7.0000E-02	7.61602E-11	1.51013E-10	2.61360E-11
191	5.0000E-02	3.80801E-11	7.52512E-11	1.28672E-11
192	4.0000E-02	3.80801E-11	7.50970E-11	1.27334E-11
193	3.0000E-02	3.42721E-11	6.74309E-11	1.13456E-11
194	2.1000E-02	2.47521E-11	4.83001E-11	8.12658E-12
195	1.4500E-02	1.71360E-11	3.34194E-11	5.59297E-12
196	1.0000E-02	1.90401E-11	3.71324E-11	6.14635E-12

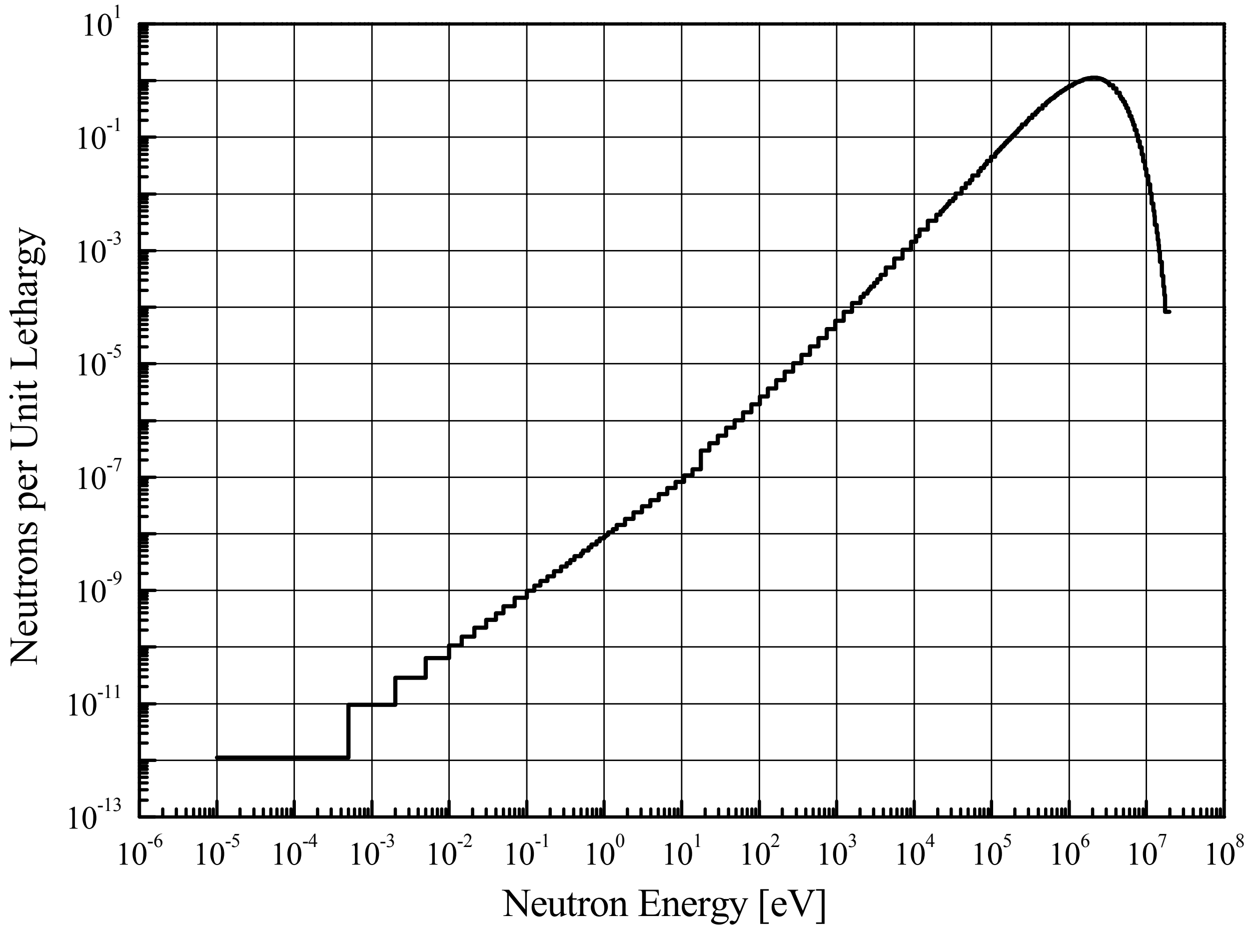
TAB. 2.10 Continued

VITJEFF311.BOLIB Library Total Neutron Fission Spectra for U-235, U-238 and Pu-239.

Group	Upper Energy [eV]	U-235 X	U-238 X	Pu-239 X
197	5.0000E-03	1.14240E-11	2.22794E-11	3.63687E-12
198	2.0000E-03	5.71202E-12	1.11397E-11	1.80304E-12
199	5.0000E-04	1.90400E-12	3.71321E-12	5.95697E-13
	Lower Energy 1.0000E-05			

FIG. 2.5

199 Group Representation of the Total (Prompt + Delayed) Neutron Fission Spectrum
for the U-235 Processed File Included in the VITJEFF311.BOLIB Library.
Spectrum Averaged on Incident Neutron Energies and Normalized to 1 Neutron per Fission.



2.9 - Library Validation

The VITJEFF311.BOLIB library was extensively tested on many thermal, intermediate and fast neutron spectrum criticality benchmark experiments, contained in the ICSBEP (2004 Edition) /59/ database.
The ENEA-Bologna 2007 Revision /20/ of the SCAMPI /19/ system was used to prepare the working libraries of self-shielded cross sections and to perform the one-dimensional (1D) criticality transport calculations. In particular, the XSDRNPM discrete ordinates module was used to perform 1D k-effective (k_{eff}) transport calculations using working library cross sections, properly self-shielded by the BONAMI module. The P_5-S_{16} approximation was adopted in the transport calculations whose results are presented in TAB. 2.11 and TAB. 2.12: P_5 corresponds to L=ℓ-max, the maximum order of the Legendre polynomial (P_ℓ) expansion of the scattering cross section matrices used in the calculations and S_{16} represents the order of the flux angular discretization.

In particular, the VITJEFF311.BOLIB library was specifically tested with particular attention on various Pu-239 criticality benchmark experiments.
The validation of the VITJEFF311.BOLIB library, including the processed cross sections of the revised JEFF-3.1.1 Pu-239 evaluated data file (see, in particular, 1.2 and 2.2), showed a significant correction (see TAB. 2.11) of the results of the transport calculations on the plutonium criticality experiments with thermal neutron spectrum with respect to the corresponding results obtained with the VITJEFF31.BOLIB /42/ library. For example, the systematic overestimation of the k-effective (k_{eff}) results, observed in the analysis of the plutonium solution experiments when the JEFF-3.1 Pu-239 cross sections of the VITJEFF31.BOLIB library were employed, was reduced by about 300-400 pcm in the VITJEFF311.BOLIB calculations, as shown in TAB. 2.11.
On the contrary the results obtained with the two libraries on the plutonium criticality experiments with fast neutron spectrum were nearly identical, as reported in TAB. 2.12.

TAB. 2.11

Comparison of the VITJEFF31.BOLIB and VITJEFF311.BOLIB Calculation Results on Plutonium Benchmark Experiments with Thermal and Intermediate Neutron Spectrum.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark-Model $k_{eff} \pm \Delta k_{eff}$(pcm)	Geometry/ P_L - S_N	VITJEFF31 k_{eff}	VITJEFF311 k_{eff}
Thermal Neutron Spectrum					
PU-SOL-THERM-006-001	H2O	1.00000 ± (350)	1D Sph./ P5-S16	1.00094	0.99716
PU-SOL-THERM-006-002	H2O	1.00000 ± (350)	1D Sph./ P5-S16	1.00217	0.99843
PU-SOL-THERM-006-003	H2O	1.00000 ± (350)	1D Sph./ P5-S16	1.00164	0.99800
PU-SOL-THERM-011-001	--	1.00000 ± (520)	1D Sph./ P5-S16	1.01069	1.00721
PU-SOL-THERM-011-002	--	1.00000 ± (520)	1D Sph./ P5-S16	1.01536	1.01190
PU-SOL-THERM-011-003	--	1.00000 ± (520)	1D Sph./ P5-S16	1.01735	1.01397
PU-SOL-THERM-011-004	--	1.00000 ± (520)	1D Sph./ P5-S16	1.00990	1.00656
PU-SOL-THERM-011-005 (PNL-5R)	--	1.00000 ± (520)	1D Sph./ P5-S16	1.00677	1.00364
PU-SOL-THERM-011-006 (PNL-3R)	--	1.00000 ± (520)	1D Sph./ P5-S16	0.99547	0.99165
PU-SOL-THERM-011-007	--	1.00000 ± (520)	1D Sph./ P5-S16	1.00140	0.99760
PU-SOL-THERM-011-008	--	1.00000 ± (520)	1D Sph./ P5-S16	0.99801	0.99421
PU-SOL-THERM-011-009	--	1.00000 ± (520)	1D Sph./ P5-S16	0.99461	0.99088
PU-SOL-THERM-011-010	--	1.00000 ± (520)	1D Sph./ P5-S16	1.00453	1.00083
PU-SOL-THERM-011-011 (PNL-4R)	--	1.00000 ± (520)	1D Sph./ P5-S16	1.00106	0.99752
PU-SOL-THERM-011-012	--	1.00000 ± (520)	1D Sph./ P5-S16	1.00077	0.99702
PU-SOL-THERM-021-007 (PNL-1)	--	1.00000 ± (320)	1D Sph./ P5-S16	1.00750	1.00412
PU-SOL-THERM-021-008 (PNL-2)	--	1.00000 ± (650)	1D Sph./ P5-S16	1.00378	1.00226
PU-SOL-THERM-021-009	--	1.00000 ± (320)	1D Sph./ P5-S16	1.00788	1.00461
Intermediate Neutron Spectrum					
ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark-Model $k_{eff} \pm \Delta k_{eff}$ (pcm)	Geometry/ P_L - S_N	VITJEFF31 k_{eff}	VITJFF311 k_{eff}
PU-COMP-INTER-001	--	1.00000 ± (1100)	Inf. Homo./ P5-S16	1.00124	1.00110

TAB. 2.12

Comparison of the VITJEFF31.BOLIB and VITJEFF311.BOLIB Calculation Results on Plutonium Benchmark Experiments with Fast Neutron Spectrum.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark-Model $k_{eff} \pm \Delta k_{eff}$ (pcm)	Geometry/ P_L - S_N	VITJEFF31 k_{eff}	VITJEFF311 k_{eff}
Fast Neutron Spectrum					
PU-MET-FAST-001-001 (JEZEBEL)	--	1.00000 ± (200)	1D Sph./ P5-S16	0.99889	0.99889
PU-MET-FAST-002-001 (JEZEBEL-240)	--	1.00000 ± (200)	1D Sph./ P5-S16	1.00277	1.00277
PU-MET-FAST-006-001 (FLATTOP-PU)	NU	1.00000 ± (300)	1D Sph./ P5-S16	1.00306	1.00305
PU-MET-FAST-008-001 (THOR)	Th	1.00000 ± (60)	1D Sph./ P5-S16	1.00124	1.00124
PU-MET-FAST-009-001	Al	1.00000 ± (270)	1D Sph./ P5-S16	1.00401	1.00401
PU-MET-FAST-010-001	NU	1.00000 ± (180)	1D Sph./ P5-S16	1.00091	1.00091
PU-MET-FAST-011-001	H2O	1.00000 ± (100)	1D Sph./ P5-S16	1.00185	0.99943
PU-MET-FAST-018-001	Be	1.00000 ± (300)	1D Sph./ P5-S16	1.00202	1.00200
PU-MET-FAST-023-001	Graphite	1.00000 ± (230)	1D Sph./ P5-S16	0.99850	0.99850
PU-MET-FAST-024-001	Polyethylene	1.00000 ± (200)	1D Sph./ P5-S16	0.99949	0.99948
PU-MET-FAST-030-001	Graphite	1.00000 ± (210)	1D Sph./ P5-S16	1.00396	1.00395
PU-MET-FAST-031-001	Polyethylene	1.00000 ± (210)	1D Sph./ P5-S16	1.00391	1.00385

3 - BUGJEFF311.BOLIB BROAD-GROUP LIBRARY SPECIFICATIONS

The ENEA-Bologna Nuclear Data Group generated the BUGJEFF311.BOLIB /4/ broad-group coupled neutron/photon working cross section library in FIDO-ANISN /3/ format, based on the OECD-NEA Data Bank JEFF-3.1.1 /5/ /6/ evaluated nuclear data library. This BUGLE-type library has features similar to the ORNL DLC-0185/BUGLE-96 /9/ broad-group working library and the same neutron and photon energy group structures (47 n + 20 γ) with the 47 neutron energy groups covering the energy range 1.0E-05 eV - 1.7332E+07 eV and the 20 photon groups included within the energy range 1.0E+04 - 1.4E+07 eV.

As previously performed at ORNL, where BUGLE-96 was obtained through proper cross section collapsing with the ORNL SCAMPI /19/ nuclear data processing system from the ORNL DLC-0184/VITAMIN-B6 /9/ (ENDF/B-VI.3 /10/) fine-group (199 n + 42 γ) library, the ENEA-Bologna BUGJEFF311.BOLIB library was generated with the same methodology and reactor models previously used to produce the BUGLE-96 library. It was obtained through cross section collapsing from the recently produced ENEA-Bologna VITJEFF311.BOLIB fine-group library (see Chapter 2), based on JEFF-3.1.1 data and characterized by the same neutron and photon energy group structure as VITAMIN-B6.

In order to perform this task an updating was required to the original SCAMPI, developed at ORNL from the AMPX-77 /22/ system and already employed to generate BUGLE-96. In particular, the so called "ENEA-Bologna 2007 Revision of SCAMPI" /20/ was developed (see 1.3) and released to the OECD-NEA Data Bank and ORNL-RSICC.

3.1 - Name

The present problem-dependent broad-group working cross section library, derived through proper cross section collapsing of the ENEA-Bologna VITJEFF311.BOLIB fine-group mother library, is designated as BUGJEFF311.BOLIB /4/.
"BUG" suggests that the main features of the library are similar to those of the BUGLE-96 library, generated at ORNL. The "JEFF311" designation in both ENEA-Bologna libraries conveniently reflects the origin of the evaluated data, i.e. the OECD-NEA Data Bank JEFF-3.1.1 /5/ /6/ evaluated nuclear data library (see 1.2). Finally, "BOLIB" means BOlogna LIBrary and so it is indicative of the place of production of the library.

3.2 - Materials, Legendre Order of Scattering and Energy Group Structure

The BUGJEFF311.BOLIB /4/ library contains all the 182 nuclides, based on the the OECD-NEA Data Bank JEFF-3.1.1 /5/ /6/ evaluated nuclear data library, available in the VITJEFF311.BOLIB fine-group mother library, as listed in TAB. 2.1. Some nuclides appear several times due to the inclusion of different resonance self-shielding and energy weighting options for key fuel and structural materials.

The Legendre order of scattering of the cross sections contained in BUGJEFF311.BOLIB is the same as available in the VITJEFF311.BOLIB library: P_7 for both neutrons and photons for nuclides with Z=l through Z=29 (copper) and P_5 for the remainder of the nuclides (see TAB. 2.2).

The BUGJEFF311.BOLIB library, as previously reported, has the same neutron and photon energy group structures (47 neutron groups + 20 photon groups) as the ORNL BUGLE-96 library with 47 neutron groups covering the energy range 1.0E-05 eV - 1.7332E+07 eV and 20 photon groups included within the energy range 1.0E+04 eV - 1.4E+07 eV. The energy boundaries for the 47 neutron groups are given in TAB. 3.1 along with the corresponding VITJEFF311.BOLIB group numbers which were collapsed to form the BUGJEFF311.BOLIB groups. Similarly, the 20 photon group structure is given in TAB. 3.2.
With respect to the neutron energy range covered by the VITJEFF311.BOLIB library, it is underlined that in the BUGJEFF311.BOLIB neutron energy group structure (see TAB. 3.1), the contribution of the highest neutron energy group (neutron fine-group No.1 = 1.7332E+07 eV - 1.9640E+07 eV; see TAB. 2.4) of the VITJEFF311.BOLIB neutron group structure is omitted. Concerning the photon energy range covered by the VITJEFF311.BOLIB library, the contributions of the two highest photon energy groups (photon fine-group No.1 = 2.0E+07 eV - 3.0E+07 eV and No. 2 = 1.4E+07 eV - 2.0E+07 eV; see TAB. 2.5) and that of the lowest photon energy group (photon fine-group No. 42 = 1.0E+03 eV - 1.0E+04 eV; see TAB. 2.5) of the VITJEFF311.BOLIB photon group structure are omitted in the BUGJEFF311.BOLIB photon energy group structure (see TAB. 3.2).
The BUGJEFF311.BOLIB thermal neutron energy range below 5.0435 eV, i.e. the energy range containing the neutron groups which include upscatter in the BUGJEFF311T.BOLIB version of the library (see also 3.5), has only five neutron groups (see TAB. 3.1) with respect to the 36 neutron groups of the VITJEFF311.BOLIB library in the same energy range (see TAB. 2.4).

TAB. 3.1

Neutron Group Energy Boundaries for the BUGJEFF311.BOLIB Library.

Broad Group	Upper Energy [eV]	Upper Lethargy	VITJEFF311 Groups
1	1.7332E+07	-5.4997E-01	2-7
2	1.4191E+07	-3.5002E-01	8-12
3	1.2214E+07	-2.0000E-01	13-16
4	1.0000E+07	0.0000E+00	17-19
5	8.6071E+06	1.5000E-01	20-22
6	7.4082E+06	3.0000E-01	23-27
7	6.0653E+06	5.0000E-01	28-31
8	4.9659E+06	7.0000E-01	32-35
9	3.6788E+06	1.0000E+00	36-38
10	3.0119E+06	1.2000E+00	39-40
11	2.7253E+06	1.3000E+00	41-42
12	2.4660E+06	1.4000E+00	43-44
13	2.3653E+06	1.4417E+00	45
14	2.3457E+06	1.4500E+00	46-47
15	2.2313E+06	1.5000E+00	48-50
16	1.9205E+06	1.6500E+00	51-53
17	1.6530E+06	1.8000E+00	54-57
18	1.3534E+06	2.0000E+00	58-62
19	1.0026E+06	2.3000E+00	63-66
20	8.2085E+05	2.5000E+00	67-68
21	7.4274E+05	2.6000E+00	69-72
22	6.0810E+05	2.8000E+00	73-76
23	4.9787E+05	3.0000E+00	77-80
24	3.6883E+05	3.3000E+00	81-84
25	2.9721E+05	3.5159E+00	85-94
26	1.8316E+05	4.0000E+00	95-104
27	1.1109E+05	4.5000E+00	105-110
28	6.7379E+04	5.0000E+00	111-114
29	4.0868E+04	5.5000E+00	115-116
30	3.1828E+04	5.7500E+00	117-119
31	2.6058E+04	5.9500E+00	120-121
32	2.4176E+04	6.0250E+00	122-123
33	2.1875E+04	6.1250E+00	124-125
34	1.5034E+04	6.5000E+00	126-129
35	7.1017E+03	7.2500E+00	130-133
36	3.3546E+03	8.0000E+00	134-140
37	1.5846E+03	8.7500E+00	141-145
38	4.5400E+02	1.0000E+01	146-148
39	2.1445E+02	1.0750E+01	149-151
40	1.0130E+02	1.1500E+01	152-155
41	3.7266E+01	1.2500E+01	156-160
42	1.0677E+01	1.3750E+01	161-163
43	5.0435E+00	1.4500E+01	164-167
44	1.8554E+00	1.5500E+01	168-174
45	8.7643E-01	1.6250E+01	175-180
46	4.1399E-01	1.7000E+01	181-188
47	1.0000E-01	1.8421E+01	189-199
	1.0000E-05	2.7631E+01	

TAB. 3.2

Photon Group Energy Boundaries for the BUGJEFF311.BOLIB Library.

Broad Group	Upper Energy [eV]	VITJEFF311 Groups
1	1.4000E+07	3-4
2	1.0000E+07	5
3	8.0000E+06	6-7
4	7.0000E+06	8-9
5	6.0000E+06	10-11
6	5.0000E+06	12-13
7	4.0000E+06	14-15
8	3.0000E+06	16-17
9	2.0000E+06	18-19
10	1.5000E+06	20-22
11	1.0000E+06	23
12	8.0000E+05	24
13	7.0000E+05	25
14	6.0000E+05	26-29
15	4.0000E+05	30-31
16	2.0000E+05	32-33
17	1.0000E+05	34-36
18	6.0000E+04	37-39
19	3.0000E+04	40
20	2.0000E+04	41
	1.0000E+04	

3.3 - Self-Shielding, Weighting Spectra and Collapsing

As reported in the BUGLE-96 /9/ library user's manual, the accuracy of the results from a radiation transport calculation which uses broad-group cross section data can be significantly affected by the energy-dependent weighting spectrum used to collapse the data from point-wise or fine-group data. It is important to use a weighting spectrum which is sufficiently prototypical to provide the desired accuracy. In general, a broad-group library is useful only for the range of problems represented by the specific weighting functions. For BUGJEFF311.BOLIB /4/, this range includes in-vessel and reactor cavity analyses for light-water-cooled reactors (PWR and BWR). For other applications, the validity of the BUGJEFF311.BOLIB data will need to be explicitly demonstrated. Even for LWR applications, it is important that the proper data sets be used for specific regions of the reactor geometry to insure sufficiently accurate results.

The cross section sets contained in the BUGJEFF311.BOLIB library were produced in two phases. The first phase was dedicated 1) to properly self-shield the cross sections and 2) to calculate problem-dependent BWR- and PWR-specific neutron/photon weighting spectra. In the second phase, infinitely dilute (not self-shielded) and self-shielded cross section sets, derived from the VITJEFF311.BOLIB fine-group library, were collapsed to generate the BUGJEFF311.BOLIB broad-group cross section sets, using the neutron/photon weighting spectra, pre-calculated in the first phase of the data processing. It is underlined that the BUGJEFF311.BOLIB broad-group cross sections were generated from the VITJEFF311.BOLIB fine-group cross sections with the same methodology and reactor models previously used to produce the ORNL BUGLE-96 library. All the compositional, geometrical and temperature data needed for the cross section self-shielding, the BWR and PWR neutron/photon weighting spectra calculation methodology and the cross section collapsing procedure were consistently taken from the BUGLE-96 library user's manual, respectively from the corresponding ORNL data processing inputs which generated BUGLE-96.

In particular in the first phase, five different neutron/photon weighting spectra in the VITJEFF311.BOLIB neutron and photon energy group structures were calculated with a one-dimensional transport code in order to permit, in the second phase, problem-dependent cross section collapsing from the VITJEFF311.BOLIB neutron and photon fine-group energy structures into the BUGJEFF311.BOLIB neutron and photon broad-group energy structures.

In order to determine the BWR- and PWR-specific neutron/photon weighting spectra, one-dimensional fixed source transport calculations were performed introducing the same compositional/geometrical reactor models used to obtain BUGLE-96: the former representing a typical BWR plant and the latter representing a typical PWR plant. These reactor models, which correspond exactly to those described in the BUGLE-96 library user's manual, are shown in FIG. 3.1. The atomic densities for the various reactor regions, used in the transport calculations to determine the neutron and photon weighting spectra, are given in TAB. 3.3.

The atomic densities used in the transport calculations (see in particular 3.4 for the calculation details) were always directly taken from the transport code input examples reported in the APPENDIX A of the BUGLE-96 library user's manual. On the other hand in certain cases, e.g., for the magnesium, silicium, potassium, calcium and zirconium isotopes, contained in

VITJEFF311.BOLIB and involved in the transport calculations, it was necessary to determine their atomic densities which are not available in the BUGLE-96 library user's manual. In fact these isotopes are constituents of the natural elements included as corresponding data files in the VITAMIN-B6 /9/ library since the relative component isotopes were not available in the ENDF/B-VI.3 /10/ evaluated data library. The atomic densities of these isotopes were calculated on the basis of the natural isotopic abundances (see TAB. 3.3), taken from the BNL-NNDC database /60/.

The 1D fixed source transport calculations were performed using as volumetric source spectra the same fine-group neutron source spectrum data set for both types of reactors. These data were taken from the BUGLE-96 library user's manual (see APPENDIX A, TAB. A.6 and TAB. A.7).

Neutron and photon flux spectra from five representative spatial locations within the previously cited BWR and PWR models (see FIG. 3.1) were then selected corresponding to: 1) off-center in the BWR core region (spatial mesh interval #57 in the BWR model), 2) off-center in the PWR core region (spatial mesh interval #37 in the PWR model), 3) the downcomer region (spatial mesh interval #69 in the PWR model), 4) within the pressure vessel at a depth of one-fourth of the total thickness (spatial mesh interval #82 in the PWR model) and 5) within the concrete shield surrounding the reactor pressure vessel (spatial mesh interval #106 in the PWR model).
The midpoints of the one-dimensional spatial mesh intervals, where the selected neutron and photon flux spectra were calculated, are located at the following distances, respectively from the BWR and PWR core centers (see FIG. 3.1): at about 217.50 cm in the interval #57 in the BWR core region, at about 140.58 cm in the interval #37 in the PWR core region, at about 203.52 cm in the interval #69 in the PWR downcomer, at about 226.28 cm in the interval #82 at a depth of one-fourth of the total thickness of the PWR pressure vessel and at about 270.83 cm in the interval #106 within the concrete shield surrounding the PWR pressure vessel.
The calculated neutron flux spectra are compared graphically in FIG. 3.2 and listed in TAB. 3.4 while the corresponding photon flux spectra are compared in FIG. 3.3 and reported in TAB. 3.5.

The cross sections used in the transport calculations, dedicated to the determination of the five different neutron/photon weighting spectra, were previously separately self-shielded using the BWR and PWR compositional/geometrical models and the specific operating temperatures of the nuclides involved in the calculations. In particular, the proper cross section self-shielding factors were determined on the basis of the specific background cross sections and temperatures of the single nuclides constituting the various material mixtures of the reactor model spatial regions.

In the BWR and PWR core regions, the cross sections of the nuclides involved were self-shielded using the corresponding fuel-clad-moderator pin models. The key compositional, geometrical and temperature parameters for the BWR and PWR pin cell models are given in TAB. 3.6.

In the steel regions, the cross sections of the nuclides that are constituents of steels were separately self-shielded for carbon steel (A533-B), used for the BWR and PWR pressure vessels, and for stainless steel (SS-304), employed for the BWR and PWR core barrels, using

the atomic densities given in TAB. 3.7. As in the case of the BUGLE-96 library, the cross sections of the constituents of carbon steel and stainless steel were self-shielded at the temperature of 600 °K.
It is underlined that, as performed for BUGLE-96, the self-shielding of the cross sections of the nuclides constituting steel was performed following an approach that contained only steel instead of a 50%-50% mixture of water and stainless steel, which was the approach previously followed for similar ORNL working cross section libraries. The present choice using only steel constituents, adopted originally for BUGLE-96, permitted to obtain a significant improvement in the agreement of the results coming from one-dimensional transport calculations using ENDF/B-VI.3 nuclear data and the dosimeter experimental data relative to the ANO-1 (Arkansas Nuclear One) commercial nuclear power reactor, as reported in the BUGLE-96 library user's manual.

The cross section self-shielding for the nuclides of the iron-water mixture representing the PWR downcomer was calculated at the temperature of 590 °K.

Finally, concerning the nuclides constituting the concrete shields, their cross section self-shielding was performed at the temperature of 300 °K.

Although it was decided to use, as much as possible, the input data given in the BUGLE-96 library user's manual, it seems proper to make a few remarks.
The atomic densities of the concrete constituents used in the cross section self-shielding and spectrum calculations, except that of carbon, present different values in TAB. 3.3 (spectrum calculations) and in TAB. 3.7 (self-shielding calculations). The different numerical values reported were respectively taken from the BUGLE-96 /9/ library user's manual (respectively from page 31, TAB. 3.3 and from page A.8 of APPENDIX A, TAB. A.5), although both concrete compositions are labelled with "Type 04".
The atomic densities of the iron isotopes used in the cross section self-shielding calculations for the carbon and stainless steel components were calculated with a different set of natural atomic abundances with respect to the set of atomic abundances of the iron isotopes reported in TAB. 3.3. In particular, in this case, the following atomic abundances were used to determine the atomic densities of the iron isotopes: 5.8% for Fe-54, 91.8% for Fe-56, 2.1% for Fe-57 (identical to the numerical value reported in TAB. 3.3) and 0.3% for Fe-58.
Silicon is present in the carbon and stainless steel nuclide compositions (see TAB. 3.3) used in the spectrum calculations whilst it is not included, as steel constituent, in the corresponding nuclide compositions employed in the cross section self-shielding calculations.

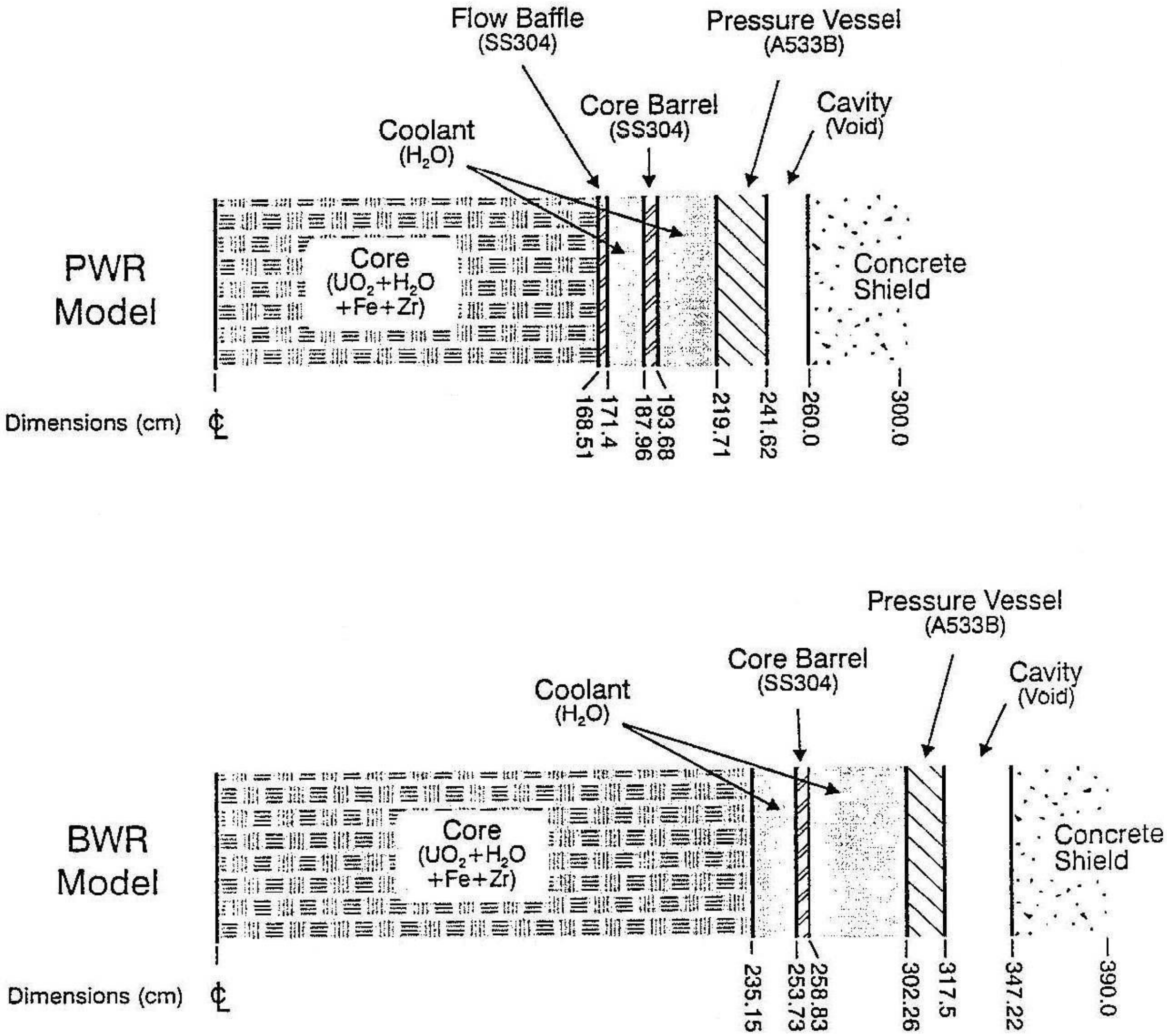
The second phase of the data processing was dedicated, as previously reported, to the cross section collapsing of infinitely dilute (not-self-shielded) and self-shielded cross sections, using the neutron/photon weighted spectra, pre-calculated in the first phase of the data processing.

Concerning the self-shielded cross sections, six sets of collapsed and self-shielded cross sections were generated using the five pre-calculated neutron/photon weighted spectra: in particular there is 1) a set of cross sections for the PWR core materials collapsed with the PWR core flux spectra using a fuel-clad-moderator pin model, 2) a set of cross sections for an iron-water mixture of structural and coolant materials collapsed with the PWR downcomer flux spectra, 3) a set of cross sections for the carbon steel pressure vessel materials collapsed with the PWR flux spectra at the one-quarter thickness (T) position in the pressure vessel (1/4 T PV), 4) a set of cross sections for the biological shield concrete materials collapsed with the PWR flux spectra in the concrete biological shield, 5) a set of cross sections for the carbon and stainless steel materials collapsed with the PWR pressure vessel flux spectra at the one quarter thickness (T) position in the pressure vessel (1/4 T PV) and, finally, 6) a set of cross sections for the BWR core materials collapsed with the BWR core flux spectra using a fuel-clad-moderator pin model.

Finally, a cross section set of collapsed and infinitely dilute (not self-shielded) cross sections was generated for all the 182 materials contained in the VITJEFF311.BOLIB fine-group library. In particular the VITJEFF311.BOLIB fine-group cross sections, processed at the infinite dilution background cross section (σ_0 = 1.0E+10 barns) and at the temperature of 300 °K, were collapsed using the neutron/photon weighting spectrum, pre-calculated in the concrete PWR biological shield during the first phase of the data processing.

FIG. 3.1

One-Dimensional PWR and BWR Radial Geometry and Composition Models[a] Adopted to Calculate the Specific Flux Spectra for Collapsing the VITJEFF311.BOLIB Library Fine-Group Cross Sections into the BUGJEFF311.BOLIB Broad-Group Library.



([a]) Figure taken from reference /9/.

TAB. 3.3

Atomic Densities[a] and Natural Isotopic Abundances Used in BWR and PWR Models for Spectrum Calculations.

	HOMOGENEOUS CORES		COOLANT	
	BWR	PWR	BWR	PWR
Hydrogen	1.5354-2[b]	2.768-2	4.950-2	4.714-2
Oxygen	7.6770-3	1.384-2	2.475-2	2.357-2
Boron-10	0.0	2.466-6	0.0	4.200-6
Zirconium	5.7645-3	4.257-3		
Iron	2.0030-5	1.444-5		
U-235	1.2125-4	1.903-4		
U-238	5.3220-3	6.515-3		
Fuel Oxygen	1.0884-2	1.343-2		

	STEELS		CONCRETE	
	SS-304	A533-B		Type 04
Carbon	2.37-4	9.81-4	Hydrogen	7.77-3
Silicon	8.93-4	3.71-4	Carbon	1.15-4
Chromium	1.74-2	1.27-4	Oxygen	4.38-2
Manganese	1.52-3	1.12-3	Sodium	1.05-3
Iron	5.83-2	8.19-2	Magnesium	1.48-4
Nickel	8.55-3	4.44-4	Aluminum	2.39-3
			Silicon	1.58-2
			Potassium	6.93-4
			Calcium	2.92-3
			Iron	3.13-4

NATURAL ISOTOPIC ABUNDANCES (%)

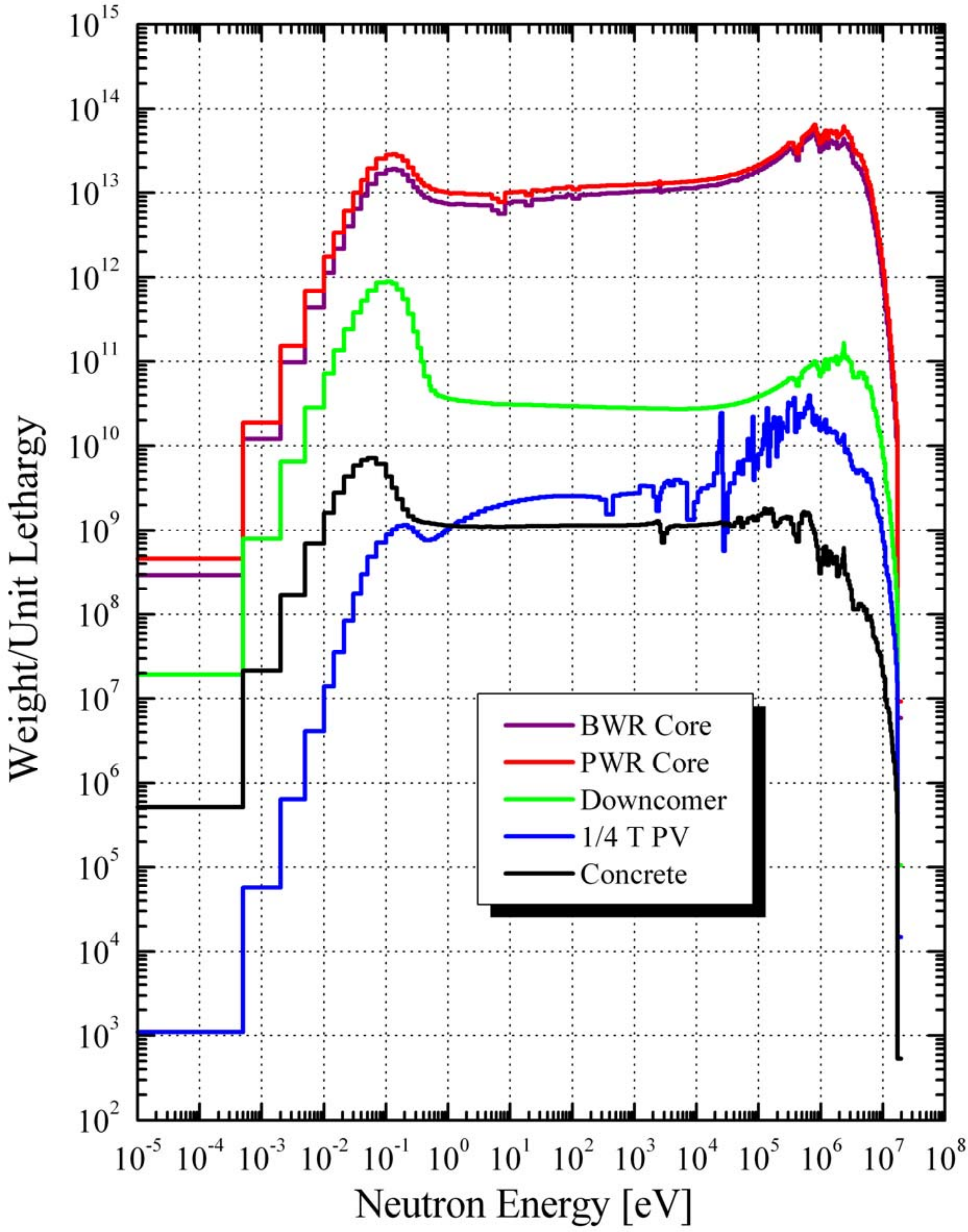
Mg-24	78.99	Ca-40	96.941	Fe-54	5.90	Zr-90	51.45
Mg-25	10.00	Ca-42	0.647	Fe-56	91.72	Zr-91	11.22
Mg-26	11.01	Ca-43	0.135	Fe-57	2.10	Zr-92	17.15
		Ca-44	2.086	Fe-58	0.28	Zr-94	17.38
Si-28	92.23	Ca-46	0.004			Zr-96	2.80
Si-29	4.67	Ca-48	0.187	Ni-58	68.27		
Si-30	3.10			Ni-60	26.10		
		Cr-50	4.345	Ni-61	1.13		
K-39	93.2581	Cr-52	83.790	Ni-62	3.59		
K-40	0.0117	Cr-53	9.500	Ni-64	0.91		
K-41	6.7302	Cr-54	2.365				

([a]) In units of [Atoms·b^{-1}·cm^{-1}].

([b]) Read as 1.535×10^{-2}.

FIG. 3.2

Comparison of Five BWR- and PWR-Specific Neutron Flux Spectra Calculated with VITJEFF311.BOLIB and Used to Generate BUGJEFF311.BOLIB.



TAB. 3.4

Neutron Weighting Spectra from BWR/PWR Models for BUGJEFF311.BOLIB.

Fine Group	BWR Core (Int#57)[a]	PWR Core (Int#37)	Downcomer (Int#69)	1/4T PV (Int#82)	Concrete (Int#106)
1	7.3239E+05	1.1519E+06	1.3145E+04	1.8576E+03	6.7235E+01
2	2.7971E+08	4.3187E+08	3.3781E+06	3.9239E+05	1.0951E+04
3	3.1613E+08	4.9326E+08	4.9624E+06	6.4382E+05	2.0702E+04
4	1.0491E+09	1.6250E+09	1.5205E+07	1.9552E+06	6.3359E+04
5	1.7307E+09	2.6654E+09	2.3234E+07	2.8671E+06	8.9397E+04
6	1.2295E+09	1.8879E+09	1.5710E+07	1.8762E+06	5.7131E+04
7	1.5756E+09	2.4228E+09	2.0189E+07	2.3799E+06	7.0998E+04
8	1.9932E+09	3.0640E+09	2.5266E+07	2.9492E+06	8.7456E+04
9	2.4663E+09	3.7839E+09	3.0245E+07	3.4740E+06	1.0201E+05
10	6.7993E+09	1.0400E+10	7.9281E+07	8.8949E+06	2.5227E+05
11	5.0381E+09	7.6875E+09	5.5873E+07	6.1052E+06	1.7028E+05
12	5.1999E+09	7.9394E+09	6.0411E+07	6.6990E+06	1.8849E+05
13	1.4308E+10	2.1628E+10	1.4028E+08	1.4754E+07	3.8883E+05
14	2.0244E+10	3.0477E+10	1.8447E+08	1.8584E+07	4.7463E+05
15	3.0467E+10	4.6379E+10	3.1205E+08	3.2133E+07	8.6159E+05
16	3.9849E+10	6.0012E+10	3.5891E+08	3.6742E+07	9.2776E+05
17	5.4393E+10	8.1985E+10	4.8028E+08	4.8096E+07	1.2112E+06
18	7.3727E+10	1.1135E+11	6.4701E+08	6.3280E+07	1.6156E+06
19	9.3545E+10	1.4032E+11	7.4821E+08	7.1699E+07	1.7851E+06
20	1.1729E+11	1.7492E+11	8.4572E+08	7.7768E+07	1.8563E+06
21	1.5247E+11	2.2815E+11	1.1012E+09	9.8012E+07	2.3170E+06
22	1.8869E+11	2.8148E+11	1.2893E+09	1.1226E+08	2.5848E+06
23	2.2636E+11	3.3565E+11	1.4030E+09	1.1871E+08	2.7062E+06
24	2.8755E+11	4.2866E+11	1.8333E+09	1.5173E+08	3.5227E+06
25	1.0908E+11	1.6256E+11	6.8208E+08	5.6149E+07	1.3371E+06
26	2.4167E+11	3.6058E+11	1.4893E+09	1.2031E+08	2.8385E+06
27	4.1699E+11	6.2094E+11	2.5071E+09	2.0333E+08	4.7830E+06
28	4.6445E+11	6.8539E+11	2.4388E+09	1.9238E+08	4.4221E+06
29	5.2446E+11	7.7032E+11	2.5139E+09	1.8988E+08	4.3510E+06
30	6.3855E+11	9.4461E+11	3.2182E+09	2.3320E+08	5.7554E+06
31	6.9703E+11	1.0224E+12	3.1259E+09	2.2233E+08	5.5129E+06
32	8.0366E+11	1.1819E+12	3.6506E+09	2.5156E+08	6.2452E+06
33	8.4826E+11	1.2384E+12	3.6106E+09	2.6093E+08	6.2597E+06
34	1.9180E+12	2.7866E+12	7.3764E+09	5.1540E+08	1.3279E+07
35	2.0504E+12	2.9348E+12	6.4976E+09	4.7523E+08	1.1445E+07
36	2.2748E+12	3.2183E+12	6.4604E+09	5.2109E+08	1.1491E+07
37	1.3510E+12	1.9110E+12	3.8129E+09	2.8673E+08	7.4119E+06
38	1.5987E+12	2.2737E+12	4.8797E+09	3.3368E+08	9.9052E+06
39	1.6131E+12	2.2760E+12	5.0203E+09	3.9504E+08	1.1122E+07
40	1.7375E+12	2.4450E+12	5.2259E+09	4.0813E+08	1.2582E+07
41	1.9038E+12	2.6720E+12	5.6906E+09	4.5331E+08	1.5069E+07
42	1.9175E+12	2.6768E+12	5.5402E+09	4.2093E+08	1.5023E+07
43	1.3282E+12	1.8540E+12	4.1250E+09	3.2773E+08	1.3242E+07
44	3.5999E+11	5.0513E+11	1.3109E+09	1.1037E+08	4.2290E+06
45	3.6730E+11	5.1532E+11	1.3853E+09	1.1306E+08	5.1460E+06
46	7.2170E+11	1.0057E+12	2.4102E+09	1.9010E+08	8.7466E+06
47	1.3143E+12	1.8063E+12	4.2484E+09	4.2106E+08	1.5447E+07
48	1.8500E+12	2.5214E+12	5.5940E+09	5.7634E+08	1.9367E+07
49	1.8000E+12	2.4388E+12	5.2604E+09	5.6436E+08	1.8037E+07

TAB. 3.4 Continued

Neutron Weighting Spectra from BWR/PWR Models for BUGJEFF311.BOLIB.

Fine Group	BWR Core (Int#57)	PWR Core (Int#37)	Downcomer (Int#69)	1/4T PV (Int#82)	Concrete (Int#106)
50	1.7562E+12	2.3671E+12	5.0691E+09	5.4219E+08	1.5255E+07
51	1.6917E+12	2.2643E+12	4.6533E+09	5.7728E+08	1.4187E+07
52	2.0018E+12	2.6777E+12	5.7465E+09	7.1152E+08	2.4364E+07
53	1.9555E+12	2.5867E+12	5.4217E+09	7.3470E+08	2.1592E+07
54	1.9091E+12	2.5114E+12	5.1001E+09	7.1522E+08	2.0036E+07
55	1.9987E+12	2.6203E+12	5.3005E+09	7.1302E+08	2.3917E+07
56	2.0937E+12	2.7275E+12	5.3509E+09	7.3258E+08	2.6672E+07
57	2.0442E+12	2.6438E+12	5.2440E+09	7.9296E+08	2.7870E+07
58	1.7082E+12	2.1967E+12	4.0884E+09	7.9294E+08	1.9273E+07
59	2.1270E+12	2.7375E+12	5.1791E+09	7.2167E+08	2.8238E+07
60	2.1328E+12	2.7154E+12	5.2900E+09	1.0144E+09	3.2172E+07
61	1.9885E+12	2.5164E+12	4.7785E+09	9.3606E+08	3.1375E+07
62	3.2802E+12	4.1426E+12	7.4718E+09	1.5656E+09	3.9120E+07
63	1.2822E+12	1.6166E+12	2.8231E+09	6.3644E+08	1.2760E+07
64	2.1474E+12	2.6847E+12	4.7444E+09	1.2357E+09	2.5809E+07
65	2.0789E+12	2.5650E+12	4.3877E+09	9.3054E+08	3.2270E+07
66	2.4045E+12	2.9309E+12	4.8731E+09	1.1290E+09	3.8297E+07
67	2.6712E+12	3.2165E+12	5.0539E+09	8.8682E+08	4.5843E+07
68	2.5645E+12	3.0499E+12	4.7574E+09	9.3792E+08	5.1914E+07
69	2.3914E+12	2.8268E+12	4.5789E+09	1.3921E+09	5.7971E+07
70	2.3065E+12	2.7189E+12	4.4356E+09	1.4915E+09	6.3819E+07
71	2.2483E+12	2.6424E+12	4.3804E+09	1.9857E+09	7.5439E+07
72	2.1889E+12	2.5660E+12	4.2351E+09	1.6678E+09	8.0729E+07
73	2.1286E+12	2.4910E+12	4.1594E+09	1.3725E+09	8.0898E+07
74	2.0697E+12	2.4194E+12	4.0481E+09	1.4140E+09	7.4864E+07
75	2.0087E+12	2.3462E+12	3.9110E+09	1.1691E+09	8.2656E+07
76	1.9270E+12	2.2507E+12	3.7573E+09	1.0891E+09	7.8501E+07
77	3.2101E+12	3.7814E+12	6.4210E+09	2.3833E+09	1.2234E+08
78	2.4602E+12	2.9455E+12	5.1722E+09	1.6396E+09	7.2997E+07
79	1.4428E+12	1.7298E+12	3.0108E+09	7.2722E+08	4.2888E+07
80	1.4510E+12	1.7287E+12	3.0103E+09	1.8434E+09	4.5104E+07
81	3.3084E+12	3.8850E+12	6.4215E+09	3.0278E+09	1.1868E+08
82	3.3689E+12	3.9075E+12	6.3181E+09	3.1850E+09	1.4250E+08
83	3.7631E+11	4.3374E+11	7.0191E+08	3.8014E+08	1.6521E+07
84	1.3837E+11	1.5948E+11	2.5869E+08	1.1714E+08	6.2043E+06
85	2.9094E+11	3.3541E+11	5.4458E+08	1.8898E+08	1.2724E+07
86	7.9006E+11	9.1129E+11	1.4812E+09	3.6723E+08	3.4505E+07
87	1.5436E+12	1.7801E+12	2.9013E+09	8.2864E+08	7.2098E+07
88	2.9422E+12	3.3905E+12	5.5789E+09	1.6458E+09	1.4039E+08
89	1.4053E+12	1.6185E+12	2.6873E+09	9.3147E+08	6.9155E+07
90	1.3580E+12	1.5664E+12	2.6215E+09	6.0206E+08	6.8949E+07
91	1.3185E+12	1.5223E+12	2.5652E+09	1.0651E+09	6.2252E+07
92	1.2830E+12	1.4825E+12	2.5083E+09	5.6567E+08	6.0760E+07
93	1.2475E+12	1.4429E+12	2.4525E+09	3.7407E+08	5.7625E+07
94	1.2138E+12	1.4053E+12	2.4045E+09	8.7033E+08	5.5261E+07
95	1.1841E+12	1.3721E+12	2.3609E+09	1.0827E+09	6.3661E+07
96	1.1420E+12	1.3312E+12	2.3096E+09	9.0576E+08	7.8863E+07
97	1.1493E+12	1.3203E+12	2.2682E+09	7.9655E+08	8.9970E+07
98	1.0913E+12	1.2712E+12	2.2209E+09	4.8873E+08	8.6617E+07

TAB. 3.4 Continued

Neutron Weighting Spectra from BWR/PWR Models for BUGJEFF311.BOLIB.

Fine Group	BWR Core (Int#57)	PWR Core (Int#37)	Downcomer (Int#69)	1/4T PV (Int#82)	Concrete (Int#106)
99	1.0890E+12	1.2573E+12	2.1821E+09	2.8973E+08	7.9435E+07
100	1.0518E+12	1.2214E+12	2.1420E+09	1.4058E+09	8.8034E+07
101	1.0204E+12	1.1921E+12	2.1086E+09	5.1416E+08	7.9893E+07
102	1.0137E+12	1.1761E+12	2.0737E+09	9.0157E+08	9.0544E+07
103	9.8132E+11	1.1447E+12	2.0336E+09	6.0226E+08	7.9210E+07
104	9.6005E+11	1.1230E+12	2.0029E+09	4.5503E+08	7.9817E+07
105	2.3364E+12	2.7218E+12	4.8586E+09	9.9374E+08	1.8917E+08
106	2.2145E+12	2.5925E+12	4.6801E+09	6.7793E+08	1.6432E+08
107	8.2202E+11	9.6022E+11	1.7354E+09	1.8806E+08	6.2423E+07
108	6.3016E+11	7.3754E+11	1.3454E+09	8.1564E+08	5.4291E+07
109	1.6204E+12	1.9152E+12	3.5141E+09	6.7259E+08	1.4024E+08
110	1.1092E+12	1.2777E+12	2.3052E+09	7.9553E+08	9.1559E+07
111	2.7308E+12	3.2050E+12	5.9040E+09	1.1849E+09	2.1480E+08
112	1.1309E+12	1.3298E+12	2.4628E+09	3.4735E+08	8.2378E+07
113	1.8238E+12	2.1553E+12	4.0287E+09	8.0119E+08	1.7619E+08
114	1.7450E+12	2.0814E+12	3.9350E+09	5.8978E+08	1.5482E+08
115	2.4639E+12	2.8761E+12	5.3747E+09	6.2721E+08	1.9617E+08
116	1.0177E+12	1.1973E+12	2.2636E+09	2.1053E+08	9.0450E+07
117	1.4724E+12	1.7336E+12	3.2856E+09	1.0434E+08	1.3481E+08
118	7.0584E+11	8.3571E+11	1.5962E+09	3.0815E+07	6.2801E+07
119	4.6164E+11	5.4529E+11	1.0508E+09	1.6573E+08	4.3437E+07
120	6.4703E+11	7.6342E+11	1.4750E+09	1.2164E+09	6.1607E+07
121	3.1482E+11	3.7613E+11	7.3485E+08	5.7214E+08	3.1330E+07
122	3.1674E+11	3.7683E+11	7.3022E+08	2.8860E+08	3.0885E+07
123	9.5805E+11	1.1303E+12	2.1765E+09	6.3446E+08	9.1577E+07
124	1.5375E+12	1.8387E+12	3.5806E+09	5.9270E+08	1.4984E+08
125	3.0830E+12	3.6409E+12	7.0731E+09	8.4455E+08	2.9524E+08
126	2.9813E+12	3.5439E+12	6.9968E+09	7.8338E+08	2.9152E+08
127	1.1694E+12	1.3940E+12	2.7754E+09	2.8481E+08	1.1546E+08
128	1.7226E+12	2.0627E+12	4.1365E+09	3.2490E+08	1.7004E+08
129	2.8182E+12	3.3914E+12	6.8645E+09	3.3412E+08	2.8536E+08
130	2.8214E+12	3.3662E+12	6.8486E+09	9.0725E+08	2.8074E+08
131	2.7555E+12	3.3100E+12	6.8338E+09	9.7831E+08	2.8314E+08
132	1.6377E+12	1.9721E+12	4.1090E+09	5.0829E+08	1.6632E+08
133	1.0929E+12	1.3153E+12	2.7458E+09	3.8065E+08	1.0599E+08
134	1.0776E+12	1.3033E+12	2.7492E+09	3.6174E+08	9.1679E+07
135	1.0508E+12	1.2870E+12	2.7522E+09	3.2124E+08	7.1571E+07
136	5.1014E+11	6.3259E+11	1.3758E+09	1.4096E+08	4.7266E+07
137	5.8315E+11	6.7766E+11	1.3760E+09	1.1597E+08	5.9188E+07
138	1.0518E+12	1.2770E+12	2.7537E+09	1.6872E+08	1.2840E+08
139	1.0811E+12	1.3030E+12	2.7635E+09	2.4932E+08	1.2288E+08
140	2.6117E+12	3.1810E+12	6.9277E+09	8.2684E+08	3.0127E+08
141	2.5992E+12	3.1663E+12	6.9431E+09	8.4127E+08	2.9183E+08
142	2.5893E+12	3.1565E+12	6.9566E+09	6.8673E+08	2.8759E+08
143	2.5398E+12	3.1118E+12	6.9937E+09	6.7854E+08	2.8645E+08
144	2.5081E+12	3.0834E+12	7.0366E+09	6.6962E+08	2.8622E+08
145	2.4818E+12	3.0611E+12	7.0790E+09	6.4427E+08	2.8620E+08
146	2.4609E+12	3.0450E+12	7.1125E+09	3.8570E+08	2.8567E+08
147	2.4372E+12	3.0264E+12	7.1683E+09	5.7508E+08	2.8563E+08

TAB. 3.4 Continued

Neutron Weighting Spectra from BWR/PWR Models for BUGJEFF311.BOLIB.

Fine Group	BWR Core (Int#57)	PWR Core (Int#37)	Downcomer (Int#69)	1/4T PV (Int#82)	Concrete (Int#106)
148	2.3881E+12	2.9768E+12	7.2097E+09	6.1278E+08	2.8543E+08
149	2.3775E+12	2.9682E+12	7.2488E+09	6.2756E+08	2.8508E+08
150	2.3362E+12	2.9315E+12	7.2911E+09	6.3452E+08	2.8475E+08
151	2.1412E+12	2.7369E+12	7.3294E+09	6.3726E+08	2.8417E+08
152	2.3367E+12	2.9312E+12	7.3713E+09	6.3745E+08	2.8361E+08
153	2.2176E+12	2.8101E+12	7.4153E+09	6.3529E+08	2.8302E+08
154	2.2155E+12	2.8116E+12	7.4590E+09	6.3086E+08	2.8237E+08
155	2.1165E+12	2.7201E+12	7.5024E+09	6.2406E+08	2.8165E+08
156	2.0737E+12	2.6587E+12	7.5446E+09	6.1471E+08	2.8081E+08
157	2.0944E+12	2.6948E+12	7.5870E+09	6.0278E+08	2.7992E+08
158	1.7705E+12	2.3404E+12	7.6270E+09	5.8795E+08	2.7886E+08
159	1.9840E+12	2.5839E+12	7.6691E+09	5.7051E+08	2.7782E+08
160	1.9605E+12	2.5517E+12	7.7101E+09	5.5019E+08	2.7667E+08
161	1.9034E+12	2.4911E+12	7.7481E+09	5.2690E+08	2.7533E+08
162	1.4191E+12	1.9487E+12	7.7863E+09	5.0098E+08	2.7392E+08
163	1.5615E+12	2.1408E+12	7.8239E+09	4.7256E+08	2.7240E+08
164	1.7646E+12	2.3661E+12	8.0364E+09	4.5086E+08	2.7688E+08
165	1.7634E+12	2.3624E+12	8.1155E+09	4.1904E+08	2.7438E+08
166	1.7967E+12	2.4062E+12	8.2485E+09	3.8546E+08	2.7545E+08
167	1.8078E+12	2.4247E+12	8.4037E+09	3.5198E+08	2.7670E+08
168	1.8356E+12	2.4652E+12	8.5945E+09	3.1992E+08	2.7856E+08
169	7.8240E+11	1.0524E+12	3.7029E+09	1.2799E+08	1.1851E+08
170	1.0578E+12	1.4264E+12	5.1331E+09	1.6418E+08	1.6266E+08
171	2.9898E+11	4.0386E+11	1.4792E+09	4.4995E+07	4.6511E+07
172	2.7682E+11	3.7403E+11	1.3667E+09	4.0418E+07	4.2827E+07
173	2.8997E+11	3.9184E+11	1.4285E+09	4.0952E+07	4.4590E+07
174	9.8882E+11	1.3365E+12	4.8730E+09	1.3096E+08	1.5081E+08
175	6.9493E+11	9.3992E+11	3.4446E+09	8.5246E+07	1.0519E+08
176	1.2323E+12	1.6684E+12	6.1952E+09	1.3827E+08	1.8512E+08
177	6.9782E+11	9.4611E+11	3.6058E+09	7.2289E+07	1.0389E+08
178	1.3207E+12	1.7942E+12	7.2891E+09	1.2640E+08	1.9409E+08
179	5.1487E+11	7.0119E+11	3.1512E+09	4.6633E+07	7.4356E+07
180	1.6629E+12	2.2757E+12	1.2548E+10	1.4382E+08	2.3259E+08
181	1.1507E+12	1.5893E+12	1.2095E+10	9.6747E+07	1.5179E+08
182	1.2486E+12	1.7416E+12	1.7621E+10	1.0469E+08	1.5476E+08
183	1.9446E+12	2.7502E+12	3.7807E+10	1.6088E+08	2.2231E+08
184	2.7853E+12	4.0075E+12	7.3480E+10	2.1608E+08	2.9411E+08
185	3.3189E+12	4.8530E+12	1.0981E+11	2.3050E+08	3.5738E+08
186	3.7818E+12	5.6051E+12	1.4674E+11	2.3018E+08	4.8081E+08
187	3.5109E+12	5.2614E+12	1.5228E+11	1.8672E+08	5.7898E+08
188	4.2059E+12	6.3541E+12	1.9852E+11	1.9900E+08	9.6792E+08
189	5.9865E+12	9.0997E+12	3.0596E+11	2.5613E+08	2.1661E+09
190	4.3008E+12	6.5747E+12	2.3522E+11	1.6304E+08	2.4015E+09
191	2.0632E+12	3.1692E+12	1.1805E+11	6.6806E+07	1.5263E+09
192	1.8682E+12	2.8806E+12	1.1046E+11	5.0345E+07	1.6879E+09
193	1.4194E+12	2.1958E+12	8.6576E+10	3.0138E+07	1.5501E+09
194	8.0526E+11	1.2493E+12	5.0426E+10	1.3069E+07	1.0279E+09
195	4.1826E+11	6.5041E+11	2.6716E+10	5.2096E+06	5.9779E+08
196	3.0404E+11	4.7382E+11	1.9757E+10	2.8160E+06	4.7866E+08

TAB. 3.4 Continued

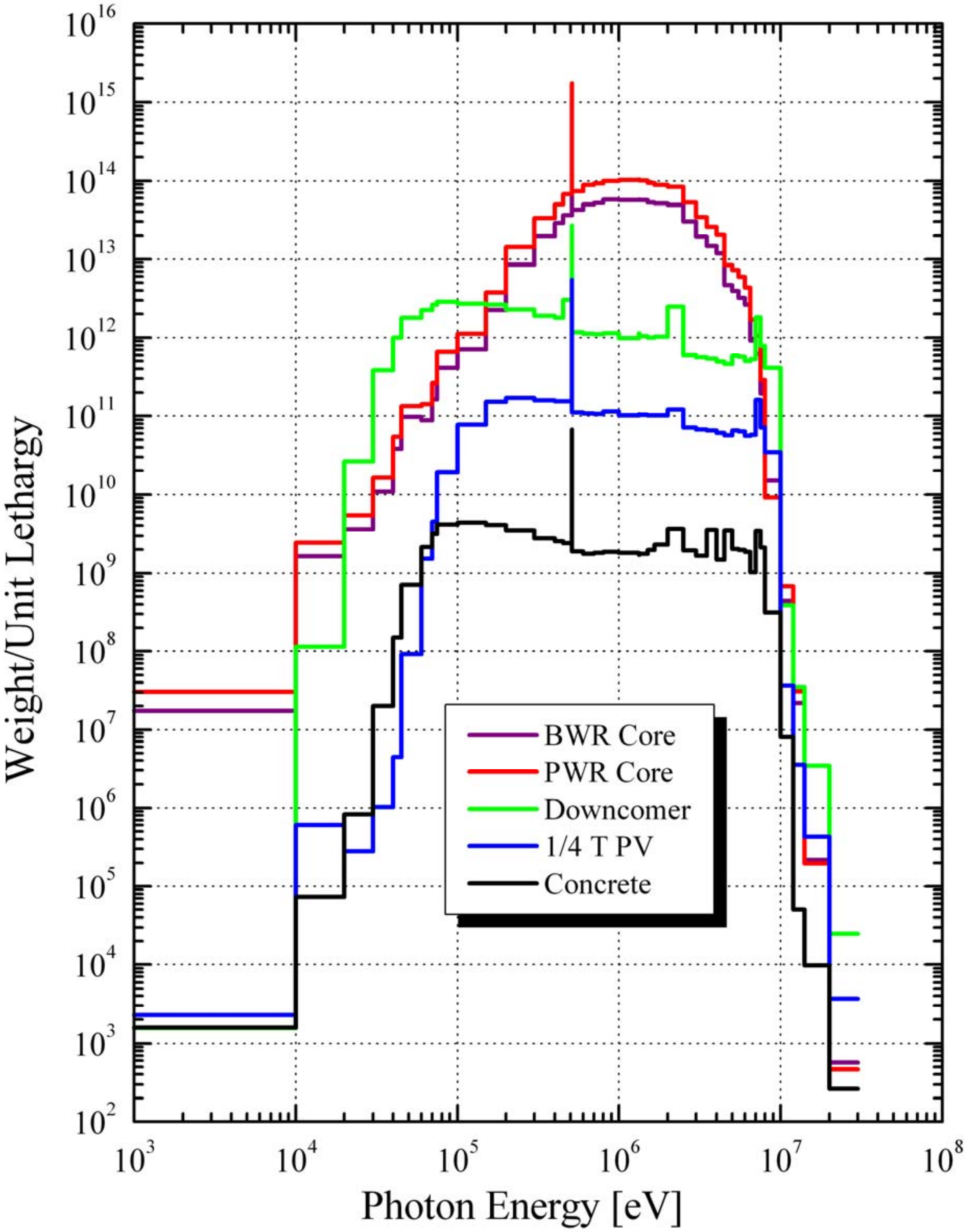
Neutron Weighting Spectra from BWR/PWR Models for BUGJEFF311.BOLIB.

Fine Group	BWR Core (Int#57)	PWR Core (Int#37)	Downcomer (Int#69)	1/4T PV (Int#82)	Concrete (Int#106)
197	9.0206E+10	1.4091E+11	5.9482E+09	5.8310E+05	1.5424E+08
198	1.6634E+10	2.6035E+10	1.1023E+09	7.8990E+04	2.9649E+07
199	1.1412E+09	1.7860E+09	7.4705E+07	4.3337E+03	2.0276E+06

([a]) Spatial mesh interval number from BWR or PWR model.

FIG. 3.3

Comparison of Five BWR- and PWR-Specific Photon Flux Spectra Calculated with VITJEFF311.BOLIB and Used to Generate BUGJEFF311.BOLIB.



TAB. 3.5

Photon Weighting Spectra from BWR/PWR Models for BUGJEFF311.BOLIB.

Fine Group	BWR Core (Int#57)[a]	PWR Core (Int#37)	Downcomer (Int#69)	1/4T PV (Int#82)	Concrete (Int#106)
1	2.3028E+02	1.8872E+02	1.0064E+04	1.4942E+03	1.0674E+02
2	7.6550E+04	7.0694E+04	1.2166E+06	1.5332E+05	3.5060E+03
3	3.3591E+06	4.7585E+06	5.3966E+06	5.4642E+05	7.7858E+03
4	8.0108E+07	1.2411E+08	7.0717E+07	6.6592E+06	1.4689E+06
5	3.3551E+09	2.0459E+09	9.1594E+10	7.8019E+09	7.0153E+07
6	1.2607E+10	1.8405E+10	5.0809E+10	4.6017E+09	1.3615E+08
7	4.3189E+10	7.3141E+10	1.2395E+11	1.1154E+10	2.3849E+08
8	6.7706E+10	1.2374E+11	3.9317E+10	4.2429E+09	7.6755E+07
9	2.1000E+11	3.4765E+11	4.0438E+10	4.4972E+09	1.4872E+08
10	2.7910E+11	5.2115E+11	4.9719E+10	5.4938E+09	1.7186E+08
11	3.7428E+11	6.9264E+11	5.5743E+10	6.2119E+09	1.9288E+08
12	4.9253E+11	8.8986E+11	4.8780E+10	6.0072E+09	3.6803E+08
13	1.4000E+12	2.4001E+12	5.8168E+10	7.1794E+09	1.7301E+08
14	1.9616E+12	3.4313E+12	7.2125E+10	8.7337E+09	4.7478E+08
15	2.9837E+12	5.2677E+12	8.6694E+10	1.0411E+10	2.5605E+08
16	5.4768E+12	9.6192E+12	1.0966E+11	1.2982E+10	3.5095E+08
17	1.0909E+13	1.8796E+13	5.5653E+11	2.6907E+10	8.1310E+08
18	9.5626E+12	1.6490E+13	1.9102E+11	1.9134E+10	4.2603E+08
19	5.3355E+12	9.4519E+12	1.0199E+11	1.0283E+10	1.9872E+08
20	6.3749E+12	1.1354E+13	1.1848E+11	1.1634E+10	1.9816E+08
21	4.3433E+11	7.8020E+11	8.5560E+09	7.8398E+08	1.2681E+07
22	1.6289E+13	2.9142E+13	2.8367E+11	2.9022E+10	5.1405E+08
23	1.2797E+13	2.2337E+13	2.5562E+11	2.5616E+10	4.1223E+08
24	6.9108E+12	1.2308E+13	1.4839E+11	1.4266E+10	2.4146E+08
25	7.7086E+12	1.3563E+13	1.7330E+11	1.6735E+10	2.7145E+08
26	6.7557E+12	1.1707E+13	1.8513E+11	1.7555E+10	3.0013E+08
27	3.9373E+12	6.7837E+12	1.0469E+11	2.1387E+10	2.6336E+08
28	4.5242E+12	8.4083E+12	3.8024E+11	1.9255E+10	3.0005E+08
29	3.4093E+12	5.9076E+12	2.1023E+11	1.8283E+10	3.0006E+08
30	5.6292E+12	9.6626E+12	5.4558E+11	4.6009E+10	7.9440E+08
31	3.4601E+12	5.8311E+12	9.2477E+11	6.9643E+10	1.4196E+09
32	6.4370E+11	1.0746E+12	7.5205E+11	4.4079E+10	1.1682E+09
33	2.8737E+11	4.5506E+11	1.0978E+12	3.1402E+10	1.7803E+09
34	1.1859E+11	1.8964E+11	8.1847E+11	5.5233E+09	1.1912E+09
35	1.1307E+10	1.8152E+10	1.8098E+11	3.1377E+08	2.1680E+08
36	1.3620E+10	2.1978E+10	3.4537E+11	2.3425E+08	3.3018E+08
37	2.8269E+10	3.8854E+10	5.1335E+11	2.6333E+07	2.0363E+08
38	4.5416E+09	6.4354E+09	1.1841E+11	5.2414E+05	1.7707E+07
39	3.1356E+09	4.7629E+09	1.0948E+11	2.9737E+05	5.7803E+06
40	1.4591E+09	2.2093E+09	1.0791E+10	1.1307E+05	3.3657E+05
41	1.1286E+09	1.6877E+09	7.9677E+07	4.1664E+05	5.0593E+04
42	4.0359E+07	6.9783E+07	3.5773E+03	5.2632E+03	3.6363E+03

([a]) Spatial mesh interval number from BWR or PWR model.

TAB. 3.6

Key Parameters for BWR and PWR Pin Cells in Self-Shielding Calculations.

	BWR	PWR
Inner radius clad [cm]	0.53213	0.41783
Outer radius clad [cm]	0.6134	0.47498
Outer radius cell [cm]	0.9174	0.71079
Region temperature [°K]		
Pellet	921	921
Clad	672	672
Moderator	551	583
Pellet nuclear density [Atoms$\cdot$b$^{-1}\cdot$cm^{-1}]		
U-235	4.959-4[a]	6.325-4
U-238	2.177-2	2.166-2
Oxygen	4.455-2	4.465-2
Moderator density [Atoms$\cdot$b$^{-1}\cdot$cm^{-1}]		
Hydrogen	2.475-2	4.714-2
Oxygen	1.2375-2	2.357-2
Boron-10	0.0	4.200-6
Zircaloy-4 density [Atoms$\cdot$b$^{-1}\cdot$cm^{-1}]		
Cromium	7.64-5	7.64-5
Iron	1.45-4	1.45-4
Nickel	8.77-4	8.77-4
Zirconium	4.27-2	4.27-2

([a]) Read as 4.959×10^{-4}.

TAB. 3.7

Atomic Densities[a] Used for Steel and Concrete Constituents in Self-Shielding Calculations.

	STEELS		CONCRETE	
	Stainless Steel	Carbon Steel		Type 04
Carbon	2.37-4[b]	9.81-4	Hydrogen	8.60-3
Chromium	1.74-2	1.27-4	Carbon	1.15-4
Manganese	1.52-3	1.12-3	Oxygen	4.33-2
Iron	5.83-2	8.19-2	Sodium	9.64-4
Nickel	8.55-3	4.44-4	Magnesium	1.24-4
			Aluminum	1.74-4
			Silicon	1.66-3
			Potassium	4.60-4
			Calcium	1.50-3
			Iron	3.45-4

([a]) In units of [Atoms·b^{-1}·cm^{-1}].
([b]) Read as 2.37×10^{-4}.

3.4 - Processing Codes and Procedures

All the computational tools used to self-shield, temperature correct, and collapse the VITJEFF311.BOLIB fine-group cross sections into the BUGJEFF311.BOLIB /4/ broad-group cross sections were modules of the ENEA-Bologna 2007 Revision /20/ of the SCAMPI /19/ nuclear data processing system which was used on a Personal Computer (CPU INTEL Pentium III, 448 MB of RAM; f77 Absoft version 5.0 FORTRAN 77 compiler) with the Linux Red Hat 7.1 operating system. The names and a brief description of the primary SCAMPI modules used are given in TAB. 3.8.

The first part of the data processing procedure, dedicated to the generation of the BUGJEFF311.BOLIB library, is given in FIG. 3.4 which diagrams the sequence of steps needed to select and self-shield specific sets of cross sections and to perform the BWR and PWR one-dimensional transport calculations addressed to obtain five neutron/photon flux weighting spectra, employed in the second part of the data processing procedure for a proper cross section collapsing.

Starting from the VITJEFF311.BOLIB binary AMPX master library, it was necessary to perform one-dimensional transport calculations with the XSDRNPM module of SCAMPI, using proper fine-group working cross sections self-shielded with the BONAMI module, to obtain BWR- and PWR-specific neutron/photon flux weighting spectra to collapse the fine-group cross sections of the VITJEFF311.BOLIB mother library. In particular, five different fine-group neutron/photon flux weighting spectra in the VITJEFF311.BOLIB (or VITAMIN-B6 /9/) neutron and photon energy group structures were calculated (see also 3.3) with two XSDRNPM fixed source transport calculations simulating the simplified in-vessel and ex-vessel one-dimensional radial geometries and compositions at the reactor core midplanes, typical of the BWR and PWR models. The same fine-group neutron source spectrum data set was introduced in both BWR and PWR spectrum calculations in the 31** volumetric source spectra array of XSDRNPM. These data, taken from the BUGLE-96 library user's manual (see APPENDIX A, TAB. A.6 and TAB. A.7), are normalized to the unity. The XNF normalization factor numerical value, in the 5** array of XSDRNPM, permits respectively to obtain the BWR and the PWR total neutron source (XNF = 7.46419E+17 in the BWR case and XNF = 7.2676E+17 in the PWR case). The calculation of these BWR- and PWR-specific neutron/photon flux weighting spectra permitted the problem-dependent collapsing of the VITJEFF311.BOLIB cross sections in the second part of the data processing procedure. The complete detailed listings of the 199 group values of the neutron flux weighting spectra is reported in TAB. 3.4 and graphically represented in FIG. 3.2 while the corresponding 42 group photon spectra are respectively inserted in TAB. 3.5 and shown in FIG. 3.3.

The second part of the data processing procedure is diagrammed in FIG. 3.5. The starting point of this sequence is represented by the AMPX master library of fine-group self-shielded cross sections, previously calculated during the first part of the data processing procedure. Then the MALOCS module was used to perform the collapsing of the self-shielded cross sections from the VITJEFF311.BOLIB fine-group neutron and photon energy structures into the respective broad-group energy structures of the BUGJEFF311.BOLIB (or BUGLE-96 /9/) library.

In particular the five neutron/photon flux weighting spectra, previously calculated with the XSDRNPM module in the first part of the data processing procedure, were inserted in the MALOCS module to obtain six cross section sets of self-shielded cross sections which were included in the BUGJEFF311.BOLIB library.

The ANISN /3/ code methodology was selected in the MALOCS module for removal of the upscatter transfer matrix in the thermal energy range.
As reported in the BUGLE-96 library user's manual, removing upscatter is done for purposes of economy, since it eliminates the need to perform outer (source) iterations during flux convergence. However, removing the upscatter terms does require a non-physical adjustment to the cross sections, since in reality, low-energy neutrons can increase their kinetic energy by scattering off low-Z nuclei such as hydrogen. For most shielding problems, this is an acceptable approximation because the leading shielding issues are frequently dominated by the transport of higher-energy neutrons and an accurate transport of the thermal neutrons is relatively unimportant.
The approach used for removing the upscatter terms in BUGJEFF311.BOLIB and BUGLE-96 is the same as implemented in the ANISN code. Conceptually, the upscatter between two groups is set to zero and the downscatter is reduced by an equivalent amount to preserve the net transfer reaction rate between the two groups. The within-group scatter terms of both groups are increased by a corresponding amount to preserve the total scatter reaction rate.
While this yields an acceptable solution in most circumstances, it can cause the generation of negative downscatter terms if the upscatter is greater than the downscatter between two groups. This highlights the importance of using a particular cross section set only for the type of application for which it was intended.

A final collapsing sequence within the second part of the data processing procedure is diagrammed in FIG. 3.6.
In particular, starting from the VITJEFF311.BOLIB binary AMPX master library, a set of infinitely dilute cross sections at 300 °K, for the whole set of 182 materials contained in the VITJEFF311.BOLIB fine-group library, were collapsed with the MALOCS module introducing in input the neutron/photon weighting spectrum for concrete, previously calculated during the first part of the data processing procedure. A set of infinitely dilute (not self-shielded) broad-group cross sections was generated and included in the BUGJEFF311.BOLIB library. These data can be used for general purposes and for cases where the problem-specific self-shielded/weighted data sets are not appropriate.

In both the collapsing procedures, for self-shielded (see FIG. 3.5) and infinitely dilute (not self-shielded) (see FIG. 3.6) cross sections, the NITAWL and ALPO modules were used for format conversion, respectively from the AMPX master to the AMPX working format and from the AMPX working to the FIDO-ANISN /3/ format.

The complete BUGJEFF311.BOLIB library actually contains three distinct types of data: 1) the infinitely dilute (not self-shielded) cross section set for all the 182 materials contained in the VITJEFF311.BOLIB library, 2) six sets of self-shielded and energy weighted cross sections for nuclides specific to BWR and PWR models, and 3) a set of response functions and KERMA factors.

TAB. 3.8

Modules of the SCAMPI Nuclear Data Processing System (ENEA-Bologna 2007 Revision) Used to Produce the BUGJEFF311.BOLIB Library.

Module	Function
AIM	Converts master libraries from binary-to-BCD (or vice-versa).
ALPO	Produces ANISN library from AMPX working library format.
AJAX	Merges and deletes nuclides from master libraries.
BONAMI	Performs interpolation on Bondarenko factors to self-shield reaction cross sections.
MALOCS	Collapses energy group structure of master library.
NITAWL	Converts master library to working library format.
XSDRNPM	Performs a one-dimensional discrete ordinates or diffusion theory calculation using cross sections in an AMPX working library. Performs spatial cross section weighting.

FIG. 3.4 Procedure for Calculating BWR- and PWR-Specific Flux Spectra Using the VITJEFF311.BOLIB Library.

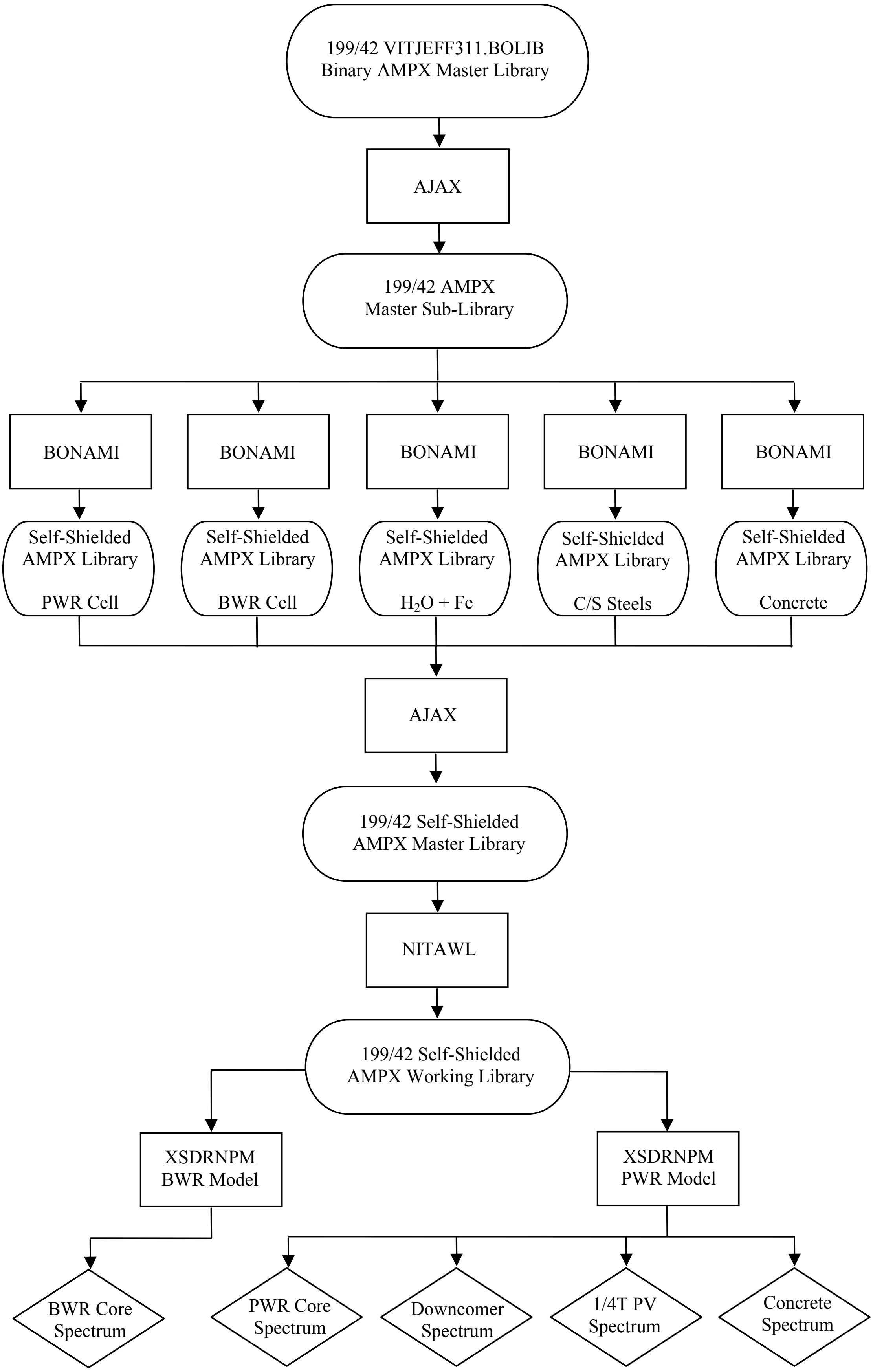


FIG. 3.5 Procedure for Generating the BUGJEFF311.BOLIB Library Self-Shielded and Collapsed Cross Sections Using BWR- and PWR-Specific Flux Spectra.

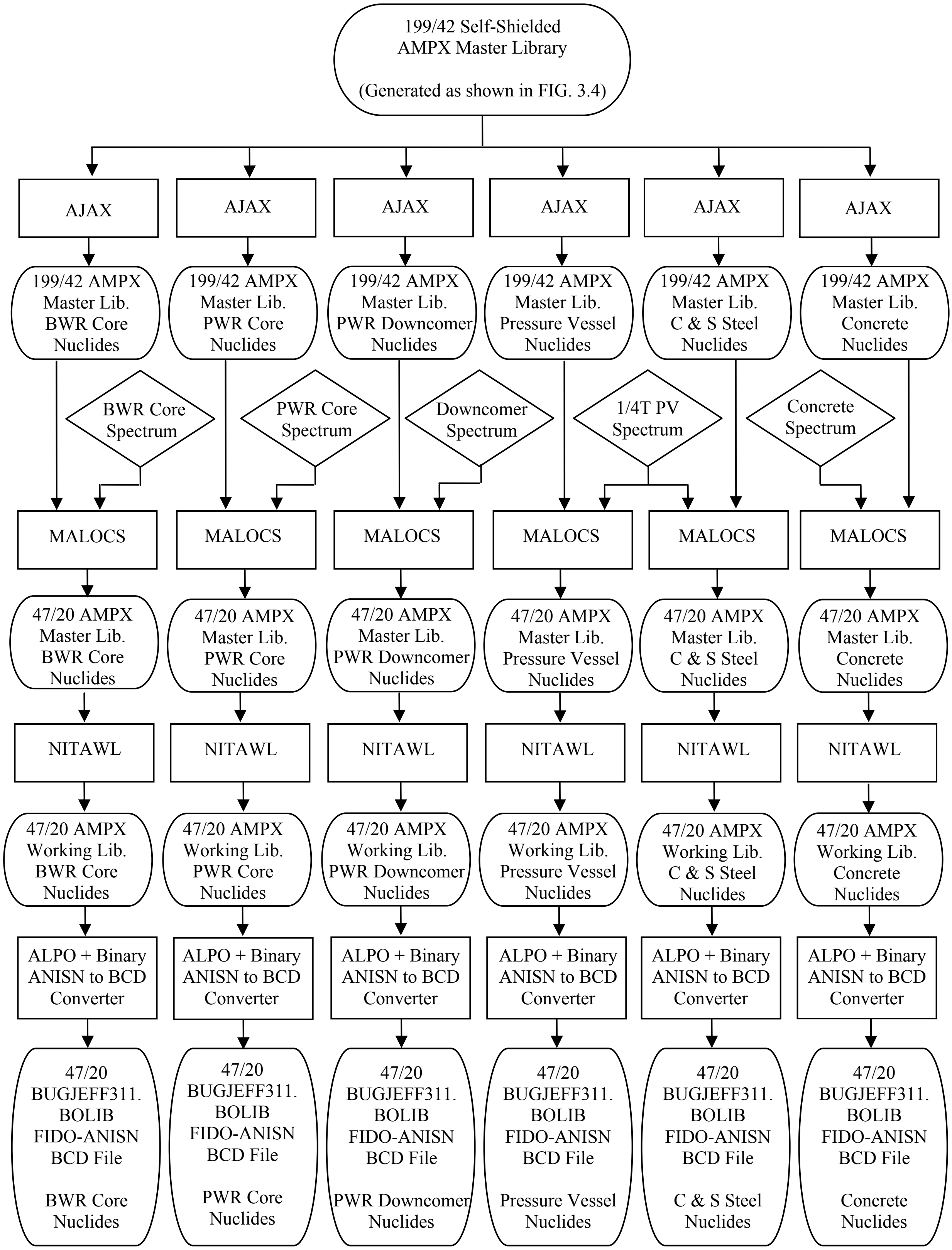
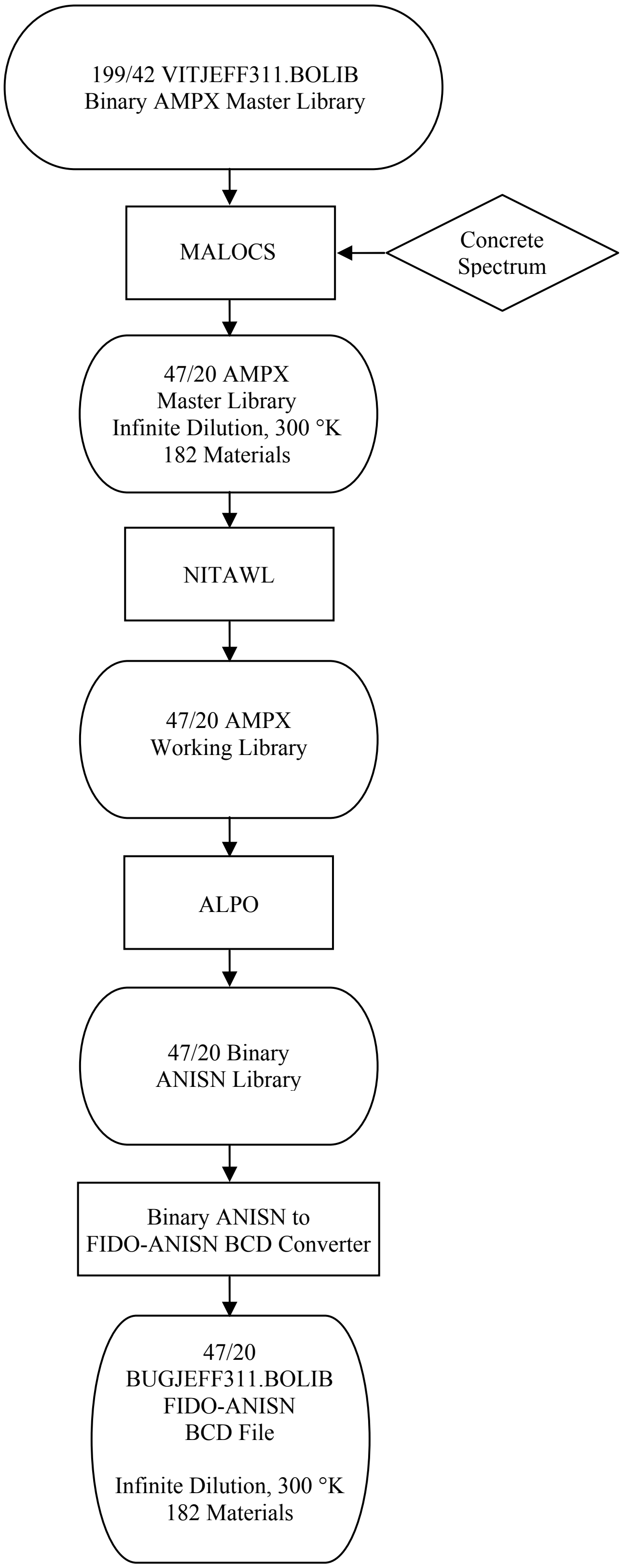


FIG. 3.6 Procedure for Generating the BUGJEFF311.BOLIB Library Infinitely Dilute and Collapsed Cross Sections at 300 °K Using Concrete Flux Spectrum.



3.5 - Library Format and Content

The BUGJEFF311.BOLIB /4/ library package consists of two major parts:

BUGJEFF311.BOLIB - including the self-shielded and infinitely dilute cross section sets;

BUGJEFF311T.BOLIB - including the same cross sections as BUGJEFF311.BOLIB with the thermal neutron upscattering cross sections retained in the thermal neutron energy region below 5.0435 eV.

The BUGJEFF311.BOLIB broad-group data library package is available in ANISN /3/ card image format for direct use, e.g., in the ORNL deterministic radiation transport codes ANISN (1D), DORT (2D) and TORT (3D) included in the DOORS /31/ system or in the ORNL Monte Carlo code MORSE (3D) /55/.

For BUGJEFF311.BOLIB, the Carlson table width is 67 (total number of 47 neutron + 20 photon groups) and the table length is 70 (total number of groups plus 3). For BUGJEFF311T.BOLIB, the Carlson table width is 67 (total number of groups) and the table length is 74 (total number of groups plus 3 plus 4 upscatter groups).

In the BUGJEFF311.BOLIB library, the cross section table positions 1 through 4 are defined as:

1. absorption cross section (σ_a);
2. fission cross section times the number of neutrons produced per fission ($\nu\sigma_f$);
3. total cross section (σ_t);
4. within-group scattering cross section ($\sigma_{g\rightarrow g}$).

These positions are followed by the standard downscatter transfer matrix. As mentioned in 3.4, the upscatter transfer matrix was removed using the ANISN methodology option in MALOCS for the BUGJEFF311.BOLIB library.
In the case of the BUGJEFF311T.BOLIB library, the upscatter cross sections for the four lower energy neutron groups in each cross section matrix occupy the cross section table positions from 4 to 7 and consequently, in this case, the within-group scattering cross section ($\sigma_{g\rightarrow g}$) takes up the position 8.

Each cross section matrix (67×70 cross section data in BUGJEFF311.BOLIB without upscatter and 67×74 in BUGJEFF311T.BOLIB with upscatter) is preceded by a title card containing four integer parameters and an alpha/numeric descriptor. The integer parameters (4I6 format) include: 1) the number of columns in the cross section table (total number of energy groups), 2) the number of rows in the table (normally equals the number of columns plus 3), 3) a control code which is generally not used and 4) a unique identification (ANISN identifier or ANISN-ID) number. The 36-character descriptor field (36H format) can contain any pertinent information, but usually includes the order of the Legendre polynomial (P_ℓ) expansion of the scattering cross section matrix, the specific isotope or element and special processing treatments such as self-shielding or energy weighting in the specific BWR or PWR spatial region.

On the first step, the collapsing procedure outlined in FIG. 3.5 generated the self-shielded cross sections without thermal upscattering data for the BUGJEFF311.BOLIB library. The collapsing procedure was then repeated for the six MALOCS cases to produce self-shielded cross sections with upscattering data. On this second step a new library with upscattering data, designated as BUGJEFF311T.BOLIB, was created. The difference between the production of the collapsed data for BUGJEFF311.BOLIB and BUGJEFF311T.BOLIB depends on a single parameter (IOPT7) of the 3$$ array in the MALOCS module input: IOPT7=0 (no upscatter) for BUGJEFF311.BOLIB or IOPT7=2 (with upscatter, according to the “ANISN” scheme) for BUGJEFF311T.BOLIB.

Listings of the library contents for BUGJEFF311.BOLIB are given in the TABs. 3.9 and 3.10. TAB. 3.9 lists all the 182 materials included in the “standard weighted” library, i.e. the collection of materials which were processed as infinitely dilute and collapsed using the neutron and photon flux spectra for concrete. TAB. 3.10 lists the “special weighted” library, i.e. the collection of materials which were processed with specific self-shielding compositions and collapsed using the BWR and PWR neutron and photon flux spectra. As in the case of the corresponding BUGLE-96 special weighted library, the self-shielded cross sections of the carbon steel constituents in the “Carbon & Stainless Steel” cross section set are the same as those included in the pressure vessel cross section set, designated as “PWR 1/4 T in Pressure Vessel”.
In both TABs. 3.9 and 3.10, the range of the ANISN identifiers (ANISN-IDs) for each nuclide are for the P_0 through P_L components, where L=ℓ-max is either 5 or 7 (see 3.2).

TAB. 3.9

Nuclides in the BUGJEFF311.BOLIB Library which are Infinitely Dilute
and Weighted with a Concrete Flux Spectrum.

Entry	Nuclide	ANISN-ID	Entry	Nuclide	ANISN-ID
1	Ag-107	1-6	49	Er-162	333-338
2	Ag-109	7-12	50	Er-164	339-344
3	Al-27	13-20	51	Er-166	345-350
4	Am-241	21-26	52	Er-167	351-356
5	Am-242	27-32	53	Er-168	357-362
6	Am-242m	33-38	54	Er-170	363-368
7	Am-243	39-44	55	Eu-151	369-374
8	Au-197	45-50	56	Eu-152	375-380
9	B-10	51-58	57	Eu-153	381-386
10	B-11	59-66	58	Eu-154	387-392
11	Ba-138	67-72	59	Eu-155	393-398
12	Be-9	73-80	60	F-19	399-406
13	Be-9 (Thermal)	81-88	61	Fe-54	407-414
14	Bi-209	89-94	62	Fe-56	415-422
15	C-nat	95-102	63	Fe-57	423-430
16	C-nat(Graphite)	103-110	64	Fe-58	431-438
17	Ca-40	111-118	65	Ga-nat	439-444
18	Ca-42	119-126	66	Gd-152	445-450
19	Ca-43	127-134	67	Gd-154	451-456
20	Ca-44	135-142	68	Gd-155	457-462
21	Ca-46	143-150	69	Gd-156	463-468
22	Ca-48	151-158	70	Gd-157	469-474
23	Cd-106	159-164	71	Gd-158	475-480
24	Cd-108	165-170	72	Gd-160	481-486
25	Cd-110	171-176	73	H-1(H_2O)	487-494
26	Cd-111	177-182	74	H-1(CH_2)	495-502
27	Cd-112	183-188	75	H-1(ZrH)	503-510
28	Cd-113	189-194	76	H-2(D_2O)	511-518
29	Cd-114	195-200	77	H-3	519-526
30	Cd-115m	201-206	78	He-3	527-534
31	Cd-116	207-212	79	He-4	535-542
32	Cl-35	213-220	80	Hf-174	543-548
33	Cl-37	221-228	81	Hf-176	549-554
34	Cm-241	229-234	82	Hf-177	555-560
35	Cm-242	235-240	83	Hf-178	561-566
36	Cm-243	241-246	84	Hf-179	567-572
37	Cm-244	247-252	85	Hf-180	573-578
38	Cm-245	253-258	86	In-113	579-584
39	Cm-246	259-264	87	In-115	585-590
40	Cm-247	265-270	88	K-39	591-598
41	Cm-248	271-276	89	K-40	599-606
42	Co-59	277-284	90	K-41	607-614
43	Cr-50	285-292	91	Li-6	615-622
44	Cr-52	293-300	92	Li-7	623-630
45	Cr-53	301-308	93	Mg-24	631-638
46	Cr-54	309-316	94	Mg-25	639-646
47	Cu-63	317-324	95	Mg-26	647-654
48	Cu-65	325-332	96	Mn-55	655-662

TAB. 3.9 Continued

Nuclides in the BUGJEFF311.BOLIB Library which are Infinitely Dilute
and Weighted with a Concrete Flux Spectrum.

Entry	Nuclide	ANISN-ID	Entry	Nuclide	ANISN-ID
97	Mo-92	663-668	140	Si-28	951-958
98	Mo-94	669-674	141	Si-29	959-966
99	Mo-95	675-680	142	Si-30	967-974
100	Mo-96	681-686	143	Sn-112	975-980
101	Mo-97	687-692	144	Sn-114	981-986
102	Mo-98	693-698	145	Sn-115	987-992
103	Mo-100	699-704	146	Sn-116	993-998
104	N-14	705-712	147	Sn-117	999-1004
105	N-15	713-720	148	Sn-118	1005-1010
106	Na-23	721-728	149	Sn-119	1011-1016
107	Nb-93	729-734	150	Sn-120	1017-1022
108	Ni-58	735-742	151	Sn-122	1023-1028
109	Ni-60	743-750	152	Sn-123	1029-1034
110	Ni-61	751-758	153	Sn-124	1035-1040
111	Ni-62	759-766	154	Sn_125	1041-1046
112	Ni-64	767-774	155	Sn-126	1047-1052
113	Np-237	775-780	156	Ta-181	1053-1058
114	Np-238	781-786	157	Ta-182	1059-1064
115	Np-239	787-792	158	Th-230	1065-1070
116	O-16	793-800	159	Th-232	1071-1076
117	O-17	801-808	160	Ti-46	1077-1084
118	P-31	809-816	161	Ti-47	1085-1092
119	Pa-231	817-822	162	Ti-48	1093-1100
120	Pa-233	823-828	163	Ti-49	1101-1108
121	Pb-204	829-834	164	Ti-50	1109-1116
122	Pb-206	835-840	165	U-232	1117-1122
123	Pb-207	841-846	166	U-233	1123-1128
124	Pb-208	847-852	167	U-234	1129-1134
125	Pu-236	853-858	168	U-235	1135-1140
126	Pu-237	859-864	169	U-236	1141-1146
127	Pu-238	865-870	170	U-237	1147-1152
128	Pu-239	871-876	171	U-238	1153-1158
129	Pu-240	877-882	172	V-nat	1159-1166
130	Pu-241	883-888	173	W-182	1167-1172
131	Pu-242	889-894	174	W-183	1173-1178
132	Pu-243	895-900	175	W-184	1179-1184
133	Pu-244	901-906	176	W-186	1185-1190
134	Re-185	907-912	177	Y-89	1191-1196
135	Re-187	913-918	178	Zr-90	1197-1202
136	S-32	919-926	179	Zr-91	1203-1208
137	S-33	927-934	180	Zr-92	1209-1214
138	S-34	935-942	181	Zr-94	1215-1220
139	S-36	943-950	182	Zr-96	1221-1226

TAB. 3.10

Nuclides in the BUGJEFF311.BOLIB Library which are Self-Shielded and Weighted with BWR- and PWR-Specific Flux Spectra.

Nuclide	ANISN-ID	Description
B-10	2001-2008	PWR Core Coolant
Cr-50	2009-2016	PWR Core Clad
Cr-52	2017-2024	PWR Core Clad
Cr-53	2025-2032	PWR Core Clad
Cr-54	2033-2040	PWR Core Clad
Fe-54	2041-2048	PWR Core Clad
Fe-56	2049-2056	PWR Core Clad
Fe-57	2057-2064	PWR Core Clad
Fe-58	2065-2072	PWR Core Clad
H-1 (H_2O)	2073-2080	PWR Core Coolant
Ni-58	2081-2088	PWR Core Clad
Ni-60	2089-2096	PWR Core Clad
Ni-61	2097-2104	PWR Core Clad
Ni-62	2105-2112	PWR Core Clad
Ni-64	2113-2120	PWR Core Clad
O-16	2121-2128	PWR Core Coolant
O-16	2129-2136	PWR Core Fuel
U-235	2137-2142	PWR Core Fuel
U-238	2143-2148	PWR Core Fuel
Zr-90	2149-2154	PWR Core Clad
Zr-91	2155-2160	PWR Core Clad
Zr-92	2161-2166	PWR Core Clad
Zr-94	2167-2172	PWR Core Clad
Zr-96	2173-2178	PWR Core Clad
H-1 (H_2O)	3001-3008	PWR Downcomer
O-16	3009-3016	PWR Downcomer
C-nat	3017-3024	PWR Downcomer
Cr-50	3025-3032	PWR Downcomer
Cr-52	3033-3040	PWR Downcomer
Cr-53	3041-3048	PWR Downcomer
Cr-54	3049-3056	PWR Downcomer
Fe-54	3057-3064	PWR Downcomer
Fe-56	3065-3072	PWR Downcomer
Fe-57	3073-3080	PWR Downcomer
Fe-58	3081-3088	PWR Downcomer
Mn-55	3089-3096	PWR Downcomer
Ni-58	3097-3104	PWR Downcomer
Ni-60	3105-3112	PWR Downcomer
Ni-61	3113-3120	PWR Downcomer
Ni-62	3121-3128	PWR Downcomer
Ni-64	3129-3136	PWR Downcomer

TAB. 3.10 Continued

Nuclides in the BUGJEFF311.BOLIB Library which are Self-Shielded and Weighted with BWR- and PWR-Specific Flux Spectra.

Nuclide	ANISN-ID	Description
C-nat	4001-4008	PWR 1/4 T in Pressure Vessel
Cr-50	4009-4016	PWR 1/4 T in Pressure Vessel
Cr-52	4017-4024	PWR 1/4 T in Pressure Vessel
Cr-53	4025-4032	PWR 1/4 T in Pressure Vessel
Cr-54	4033-4040	PWR 1/4 T in Pressure Vessel
Fe-54	4041-4048	PWR 1/4 T in Pressure Vessel
Fe-56	4049-4056	PWR 1/4 T in Pressure Vessel
Fe-57	4057-4064	PWR 1/4 T in Pressure Vessel
Fe-58	4065-4072	PWR 1/4 T in Pressure Vessel
Mn-55	4073-4080	PWR 1/4 T in Pressure Vessel
Ni-58	4081-4088	PWR 1/4 T in Pressure Vessel
Ni-60	4089-4096	PWR 1/4 T in Pressure Vessel
Ni-61	4097-4104	PWR 1/4 T in Pressure Vessel
Ni-62	4105-4112	PWR 1/4 T in Pressure Vessel
Ni-64	4113-4120	PWR 1/4 T in Pressure Vessel
Al-27	5001-5008	Concrete Type 04
C-nat	5009-5016	Concrete Type 04
Ca-40	5017-5024	Concrete Type 04
Ca-42	5025-5032	Concrete Type 04
Ca-43	5033-5040	Concrete Type 04
Ca-44	5041-5048	Concrete Type 04
Ca-46	5049-5056	Concrete Type 04
Ca-48	5057-5064	Concrete Type 04
Fe-54	5065-5072	Concrete Type 04
Fe-56	5073-5080	Concrete Type 04
Fe-57	5081-5088	Concrete Type 04
Fe-58	5089-5096	Concrete Type 04
H-1 (H_2O)	5097-5104	Concrete Type 04
K-39	5105-5112	Concrete Type 04
K-40	5113-5120	Concrete Type 04
K-41	5121-5128	Concrete Type 04
Mg-24	5129-5136	Concrete Type 04
Mg-25	5137-5144	Concrete Type 04
Mg-26	5145-5152	Concrete Type 04
Na-23	5153-5160	Concrete Type 04
O-16	5161-5168	Concrete Type 04
Si-28	5169-5176	Concrete Type 04
Si-29	5177-5184	Concrete Type 04
Si-30	5185-5192	Concrete Type 04

TAB. 3.10 Continued

Nuclides in the BUGJEFF311.BOLIB Library which are Self-Shielded and Weighted with BWR- and PWR-Specific Flux Spectra.

Nuclide	ANISN-ID	Description
C-nat	6001-6008	Carbon Steel
C-nat	6009-6016	Stainless Steel
Cr-50	6017-6024	Carbon Steel
Cr-50	6025-6032	Stainless Steel
Cr-52	6033-6040	Carbon Steel
Cr-52	6041-6048	Stainless Steel
Cr-53	6049-6056	Carbon Steel
Cr-53	6057-6064	Stainless Steel
Cr-54	6065-6072	Carbon Steel
Cr-54	6073-6080	Stainless Steel
Fe-54	6081-6088	Carbon Steel
Fe-54	6089-6096	Stainless Steel
Fe-56	6097-6104	Carbon Steel
Fe-56	6105-6112	Stainless Steel
Fe-57	6113-6120	Carbon Steel
Fe-57	6121-6128	Stainless Steel
Fe-58	6129-6136	Carbon Steel
Fe-58	6137-6144	Stainless Steel
Mn-55	6145-6152	Carbon Steel
Mn-55	6153-6160	Stainless Steel
Ni-58	6161-6168	Carbon Steel
Ni-58	6169-6176	Stainless Steel
Ni-60	6177-6184	Carbon Steel
Ni-60	6185-6192	Stainless Steel
Ni-61	6193-6200	Carbon Steel
Ni-61	6201-6208	Stainless Steel
Ni-62	6209-6216	Carbon Steel
Ni-62	6217-6224	Stainless Steel
Ni-64	6225-6232	Carbon Steel
Ni-64	6233-6240	Stainless Steel
Fe-54	7001-7008	BWR Core Clad
Fe-56	7009-7016	BWR Core Clad
Fe-57	7017-7024	BWR Core Clad
Fe-58	7025-7032	BWR Core Clad
H-1 (H_2O)	7033-7040	BWR Core Coolant
O-16	7041-7048	BWR Core Coolant
O-16	7049-7056	BWR Core Fuel
U-235	7057-7062	BWR Core Fuel
U-238	7063-7068	BWR Core Fuel
Zr-90	7069-7074	BWR Core Clad
Zr-91	7075-7080	BWR Core Clad
Zr-92	7081-7086	BWR Core Clad
Zr-94	7087-7092	BWR Core Clad
Zr-96	7093-7098	BWR Core Clad

3.6 - Response Functions

The package of the BUGJEFF311.BOLIB /4/ library contains many response functions in the neutron and photon energy group structures of the library. Following the designation adopted also in the BUGLE-96 /9/ library package, it is underlined that, for the sake of simplicity, the term “response functions” is intended here not only for the group dosimeter cross sections or the group KERMA factors available in the package, which can be properly considered in a strict physical sense as “response functions”. This denomination is in fact also extended to the group total neutron fission spectra and to the group total neutrons per fission as well as to useful general neutron data as, for example, the neutron group energy boundaries, the midpoint values of the energy groups, etc.. In particular the following four types of broad-group response functions are included in the package.

1. General neutron response functions in the BUGJEFF311.BOLIB 47 neutron energy group structure (see TAB. 3.11): group energy boundaries, group energy intervals (widths), group lethargy intervals (widths), midpoint values of the energy groups (E-mid), square-roots of the E-mid values and, finally, the multiplicative factors of the group neutron fluxes to obtain the total neutron flux, the neutron fluxes above 1.0 MeV and 0.1 MeV and the neutron flux below 0.414 eV.

2. Total (prompt + delayed) neutron fission spectra (χ) and total (prompt + delayed) neutrons per fission (ν) for 35 fissionable nuclides in the BUGJEFF311.BOLIB 47 neutron energy group structure.

3. Dosimetry cross sections for 71 nuclear reactions, processed (see /51/) from the IAEA International Reactor Dosimetry File /50/ (IRDF-2002) in the BUGJEFF311.BOLIB 47 neutron energy group structure.

4. Total neutron and photon KERMA factors for 182 materials (all the materials available in the library) in the BUGJEFF311.BOLIB 47 neutron and 20 photon energy group structures (see respectively TAB. 3.1 and TAB. 3.2).

The list of the available general neutron response functions is reported in TAB. 3.11 together with the list of the total (prompt + delayed) neutron fission spectra for 35 fissionable nuclides.

Concerning the total neutron fission spectra, it is underlined that the ENEA-Bologna Revision 2007 /20/ of the SCAMPI /19/ nuclear data processing system permitted to process (see the procedure described in 2.8) delayed neutron fission spectra to obtain the total (prompt + delayed) neutron fission spectra (χ) in the VITJEFF311.BOLIB 199 neutron fine-group energy structure (see TAB. 2.4) for all the 35 fissionable nuclides included in TAB. 3.11. In particular the 35 sets of normalized fine-group total neutron fission spectra (χ) were calculated with the procedure described in 2.8, using the BONAMI, NITAWL and ICE modules. For example, a 199 group graphical representation of the U-235 total neutron fission spectrum is shown in FIG. 2.5 while the total neutron fission spectrum fine-group χ values for U-235, U-238 and Pu-239 are listed in TAB. 2.10.
Then the fine-group χ values were summed up to obtain the corresponding broad-group χ value and this operation was obviously repeated for each broad-group.

In this procedure the small contribution of the first fine-group between 17.332 MeV and 19.640 MeV (see TAB. 2.4 and TAB. 3.1) was neglected and so a new normalization to one neutron per fission of the broad-group χ values was needed.
It is worth of note that the fissionable nuclides included in the BUGLE-96 library contain only the prompt neutron fission spectrum. Differently from the previous case, the total neutron fission spectrum is available for all the 35 fissionable nuclides included in the BUGJEFF311.BOLIB library, i.e. the neutron fission spectrum contains both the prompt and the delayed components.

Total (prompt + delayed) neutrons per fission (ν) data are available for the same 35 fissionable nuclides (TAB. 3.12) for which the previous total neutron fission spectra are given. These data were obtained through collapsing of the corresponding data contained in the VITJEFF311.BOLIB library, processed at the infinite dilution background cross section and at the temperature of 300 °K. The data collapsing was performed with the MALOCS module of the ENEA-Bologna Revision 2007 of the SCAMPI nuclear data processing system, using alternatively the "flat weighting" neutron spectrum and the "1/4 T PV weighting" neutron spectrum.

The whole set of point-wise dosimetry cross sections for 71 nuclear reactions (see TAB. 3.13), included in IRDF-2002, was processed through the GROUPIE program of the PREPRO 2007 /61/ nuclear data processing system into the BUGJEFF311.BOLIB 47 neutron energy group structure.

The collapsed group values of these detector cross sections were obtained using the flat weighting neutron spectrum and the 1/4 T PV weighting neutron spectrum in the VITJEFF311.BOLIB 199 neutron fine-group energy structure.

The KERMA factors for neutrons and photons were originally generated respectively with the HEATR and GAMINR modules of the NJOY-99.259 /18/ system in the VITJEFF311.BOLIB neutron and photon fine-group energy structures with 199 neutron groups and 42 photon groups. These data, contained in the VITJEFF311.BOLIB library and processed at the infinite dilution background cross section and at the temperature of 300 °K, were then collapsed with the MALOCS module of the ENEA-Bologna Revision 2007 of the SCAMPI system, into the 47 neutron and 20 photon broad-group energy structures of the BUGJEFF311.BOLIB library.
The neutron and photon weighting spectra for concrete (see respectively TAB. 3.4 and TAB. 3.5), calculated in a PWR biological shield, were used to perform the collapsing of the neutron and photon KERMA factors.
The neutron KERMA factors were obtained for all the 182 nuclides (see TAB. 3.14) contained in the VITJEFF311.BOLIB library (see TAB. 2.1) and in the infinite dilution cross section set of the BUGJEFF311.BOLIB library (see TAB. 3.9).
In TAB. 3.14, 27 nuclides (labelled with *) with negative group values of the neutron KERMA factors and 64 nuclides (labelled with #) without gamma production data (see also TAB. 2.1) are indicated. If the processed files of JEFF-3.1.1 nuclides presented one or more negative neutron KERMA factor group values, all the corresponding 47 neutron KERMA factor group values were set to zero, following the same procedure adopted for the BUGLE-96 library.

Anyway, the generation of negative group values for the neutron KERMA factors of the 27 previously cited isotopes is almost certainly due to problems in the corresponding JEFF-3.1.1 evaluated data files rather than in their data processing.
Moreover it is important to note that, in total reactor power and heating calculations, the results can be heavily affected by the lack of gamma production data in some important JEFF-3.1.1 evaluated data files. Concerning this, it is recommended to check carefully if the JEFF-3.1.1 data files of the nuclides involved in the specific calculations include gamma production data, as it is easily possible to verify in TAB. 3.14.
The elements for which the photon KERMA factors are available are listed in TAB. 3.15: the photon KERMA factors are the same for all the isotopes of each element.

TAB. 3.11

Response Functions Included with BUGJEFF311.BOLIB.
General Neutron Responses and Total (Prompt + Delayed) Neutron Fission Spectra (χ).

	General Neutron Response		General Neutron Response
1	Group upper energy [MeV]	6	Total neutron flux
2	Group energy width [MeV]	7	E > 1.0 MeV neutron flux
3	Group lethargy width	8	E > 0.1 MeV neutron flux
4	Midpoint energy (E-mid) [MeV]	9	E < 0.414 eV neutron flux
5	Square-root (E-mid) [MeV$^{1/2}$]		

	Total Fission Spectrum (χ)		Total Fission Spectrum (χ)
1	Th-230 Fission spectrum (χ)	19	Pu-240 Fission spectrum (χ)
2	Th-232 Fission spectrum (χ)	20	Pu-241 Fission spectrum (χ)
3	Pa-231 Fission spectrum (χ)	21	Pu-242 Fission spectrum (χ)
4	Pa-233 Fission spectrum (χ)	22	Pu-243 Fission spectrum (χ)
5	U-232 Fission spectrum (χ)	23	Pu-244 Fission spectrum (χ)
6	U-233 Fission spectrum (χ)	24	Am-241 Fission spectrum (χ)
7	U-234 Fission spectrum (χ)	25	Am-242 Fission spectrum (χ)
8	U-235 Fission spectrum (χ)	26	Am-242m Fission spectrum (χ)
9	U-236 Fission spectrum (χ)	27	Am-243 Fission spectrum (χ)
10	U-237 Fission spectrum (χ)	28	Cm-241 Fission spectrum (χ)
11	U-238 Fission spectrum (χ)	29	Cm-242 Fission spectrum (χ)
12	Np-237 Fission spectrum (χ)	30	Cm-243 Fission spectrum (χ)
13	Np-238 Fission spectrum (χ)	31	Cm-244 Fission spectrum (χ)
14	Np-239 Fission spectrum (χ)	32	Cm-245 Fission spectrum (χ)
15	Pu-236 Fission spectrum (χ)	33	Cm-246 Fission spectrum (χ)
16	Pu-237 Fission spectrum (χ)	34	Cm-247 Fission spectrum (χ)
17	Pu-238 Fission spectrum (χ)	35	Cm-248 Fission spectrum (χ)
18	Pu-239 Fission spectrum (χ)		

TAB. 3.12

Response Functions Included with BUGJEFF311.BOLIB.
Total (Prompt + Delayed) Neutrons per Fission (ν) Collapsed Using
Flat Weighting and 1/4 T PV Weighting.

Neutrons per Fission (ν)			Neutrons per Fission (ν)		
1	Th-230	Neutrons per fission (ν)	19	Pu-240	Neutrons per fission (ν)
2	Th-232	Neutrons per fission (ν)	20	Pu-241	Neutrons per fission (ν)
3	Pa-231	Neutrons per fission (ν)	21	Pu-242	Neutrons per fission (ν)
4	Pa-233	Neutrons per fission (ν)	22	Pu-243	Neutrons per fission (ν)
5	U-232	Neutrons per fission (ν)	23	Pu-244	Neutrons per fission (ν)
6	U-233	Neutrons per fission (ν)	24	Am-241	Neutrons per fission (ν)
7	U-234	Neutrons per fission (ν)	25	Am-242	Neutrons per fission (ν)
8	U-235	Neutrons per fission (ν)	26	Am-242m	Neutrons per fission (ν)
9	U-236	Neutrons per fission (ν)	27	Am-243	Neutrons per fission (ν)
10	U-237	Neutrons per fission (ν)	28	Cm-241	Neutrons per fission (ν)
11	U-238	Neutrons per fission (ν)	29	Cm-242	Neutrons per fission (ν)
12	Np-237	Neutrons per fission (ν)	30	Cm-243	Neutrons per fission (ν)
13	Np-238	Neutrons per fission (ν)	31	Cm-244	Neutrons per fission (ν)
14	Np-239	Neutrons per fission (ν)	32	Cm-245	Neutrons per fission (ν)
15	Pu-236	Neutrons per fission (ν)	33	Cm-246	Neutrons per fission (ν)
16	Pu-237	Neutrons per fission (ν)	34	Cm-247	Neutrons per fission (ν)
17	Pu-238	Neutrons per fission (ν)	35	Cm-248	Neutrons per fission (ν)
18	Pu-239	Neutrons per fission (ν)			

TAB. 3.13

Response Functions Included with BUGJEFF311.BOLIB.
IRDF-2002 Neutron Dosimeter Cross Sections [barns] Collapsed Using
Flat Weighting and 1/4 T PV Weighting.

	Dosimeter			Dosimeter	
1	Li-6	(n,t)	37	Zn-64	(n,p)
2	B-10	(n,α)	38	As-75	(n,2n)
3	F-19	(n,2n)	39	Y-89	(n,2n)
4	Na-23	(n,γ)	40	Zr-90	(n,2n)
5	Na-23	(n,2n)	41	Nb-93	(n,2n)
6	Mg-24	(n,p)	42	Nb-93	(n,n')
7	Al-27	(n,p)	43	Nb-93	(n,γ)
8	Al-27	(n,α)	44	Rh-103	(n,n')
9	P-31	(n,p)	45	Ag-109	(n,γ)
10	S-32	(n,p)	46	In-115	(n,2n)
11	Sc-45	(n,γ)	47	In-115	(n,n')
12	Ti-46	(n,2n)	48	In-115	(n,γ)
13	Ti-46	(n,p)	49	I-127	(n,2n)
14	Ti-47	(n,x)	50	La-139	(n,γ)
15	Ti-47	(n,p)	51	Pr-141	(n,2n)
16	Ti-48	(n,x)	52	Tm-169	(n,2n)
17	Ti-48	(n,p)	53	Ta-181	(n,γ)
18	Ti-49	(n,x)	54	W-186	(n,γ)
19	V-51	(n,α)	55	Au-197	(n,2n)
20	Cr-52	(n,2n)	56	Au-197	(n,γ)
21	Mn-55	(n,γ)	57	Hg-199	(n,n')
22	Fe-54	(n,2n)	58	Pb-204	(n,n')
23	Fe-54	(n,α)	59	Th-232	(n,γ)
24	Fe-54	(n,p)	60	Th-232	(n,f)
25	Fe-56	(n,p)	61	U-235	(n,f)
26	Fe-58	(n,γ)	62	U-238	(n,f)
27	Co-59	(n,2n)	63	U-238	(n,γ)
28	Co-59	(n,α)	64	Np-237	(n,f)
29	Co-59	(n,γ)	65	Pu-239	(n,f)
30	Ni-58	(n,2n)	66	Am-241	(n,f)
31	Ni-58	(n,p)	67	B-nat	(n,disap)
32	Ni-60	(n,p)	68	B-nat	(n,γ)
33	Cu-63	(n,2n)	69	B-nat	(n,α)
34	Cu-63	(n,γ)	70	Cd-nat	(n,γ)
35	Cu-63	(n,α)	71	Gd-nat	(n,γ)
36	Cu-65	(n,2n)			

TAB. 3.14

Response Functions Included with BUGJEFF311.BOLIB.
Neutron KERMA Factor Data [eV·b] Collapsed Using Concrete Weighting Spectrum.

	Nuclide		Nuclide		Nuclide		Nuclide
1	Ag-107#	47	Cu-63	93	Mg-24	139	S-36*
2	Ag-109#	48	Cu-65	94	Mg-25	140	Si-28
3	Al-27	49	Er-162	95	Mg-26	141	Si-29
4	Am-241#	50	Er-164	96	Mn-55	142	Si-30
5	Am-242#	51	Er-166*	97	Mo-92*	143	Sn-112#
6	Am-242m#	52	Er-167	98	Mo-94*	144	Sn-114#
7	Am-243#	53	Er-168	99	Mo-95*	145	Sn-115#
8	Au-197*	54	Er-170	100	Mo-96*	146	Sn-116#
9	B-10	55	Eu-151*	101	Mo-97*	147	Sn-117#
10	B-11	56	Eu-152#	102	Mo-98*	148	Sn-118#
11	Ba-138#	57	Eu-153#	103	Mo-100*	149	Sn-119#
12	Be-9	58	Eu-154#	104	N-14	150	Sn-120#
13	Be-9 (Thermal)	59	Eu-155#	105	N-15	151	Sn-122#
14	Bi-209	60	F-19	106	Na-23*	152	Sn-123#
15	C-nat	61	Fe-54	107	Nb-93*	153	Sn-124#
16	C (Graphite)	62	Fe-56	108	Ni-58	154	Sn-125#
17	Ca-40	63	Fe-57	109	Ni-60	155	Sn-126#
18	Ca-42	64	Fe-58	110	Ni-61	156	Ta-181*
19	Ca-43	65	Ga-nat*	111	Ni-62	157	Ta-182#
20	Ca-44	66	Gd-152#	112	Ni-64	158	Th-230#
21	Ca-46	67	Gd-154#	113	Np-237	159	Th-232
22	Ca-48	68	Gd-155#	114	Np-238#	160	Ti-46
23	Cd-106#	69	Gd-156#	115	Np-239#	161	Ti-47
24	Cd-108#	70	Gd-157#	116	O-16	162	Ti-48
25	Cd-110#	71	Gd-158#	117	O-17#	163	Ti-49
26	Cd-111#	72	Gd-160#	118	P-31	164	Ti-50
27	Cd-112#	73	H-1 (H2O)	119	Pa-231#	165	U-232#
28	Cd-113#	74	H-1 (CH2)	120	Pa-233#	166	U-233
29	Cd-114#	75	H-1 (ZrH)	121	Pb-204	167	U-234#
30	Cd-115m#	76	H-2 (D2O)	122	Pb-206	168	U-235
31	Cd-116#	77	H-3#	123	Pb-207	169	U-236
32	Cl-35	78	He-3#	124	Pb-208	170	U-237
33	Cl-37	79	He-4#	125	Pu-236#	171	U-238
34	Cm-241#	80	Hf-174*	126	Pu-237#	172	V-nat*
35	Cm-242	81	Hf-176*	127	Pu-238#	173	W-182*
36	Cm-243	82	Hf-177*	128	Pu-239#	174	W-183*
37	Cm-244	83	Hf-178*	129	Pu-240	175	W-184*
38	Cm-245#	84	Hf-179*	130	Pu-241#	176	W-186*
39	Cm-246	85	Hf-180*	131	Pu-242	177	Y-89
40	Cm-247	86	In-113#	132	Pu-243	178	Zr-90
41	Cm-248	87	In-115#	133	Pu-244#	179	Zr-91
42	Co-59	88	K-39	134	Re-185#	180	Zr-92
43	Cr-50	89	K-40	135	Re-187#	181	Zr-94
44	Cr-52	90	K-41	136	S-32	182	Zr-96*
45	Cr-53	91	Li-6	137	S-33		
46	Cr-54	92	Li-7	138	S-34		

TAB. 3.14 Continued

Response Functions Included with BUGJEFF311.BOLIB.
Neutron KERMA Factor Data [eV·b] Collapsed Using Concrete Weighting Spectrum.

(*) The KERMA factors of this nuclide are set to zero in all the neutron groups.
(#) The photon production data of this nuclide are not available. All photon energy is deposited locally and this is consistent with the fact that there will be no contribution to the photon transport source from this nuclide.

TAB. 3.15

Response Functions Included with BUGJEFF311.BOLIB.
Photon KERMA Factor Data[a] [eV·b] Collapsed Using Concrete Weighting Spectrum.

	Z	Element		Z	Element		Z	Element
1	1	H	19	22	Ti	37	63	Eu
2	2	He	20	23	V	38	64	Gd
3	3	Li	21	24	Cr	39	68	Er
4	4	Be	22	25	Mn	40	72	Hf
5	5	B	23	26	Fe	41	73	Ta
6	6	C	24	27	Co	42	74	W
7	7	N	25	28	Ni	43	75	Re
8	8	O	26	29	Cu	44	79	Au
9	9	F	27	31	Ga	45	82	Pb
10	11	Na	28	39	Y	46	83	Bi
11	12	Mg	29	40	Zr	47	90	Th
12	13	Al	30	41	Nb	48	91	Pa
13	14	Si	31	42	Mo	49	92	U
14	15	P	32	47	Ag	50	93	Np
15	16	S	33	48	Cd	51	94	Pu
16	17	Cl	34	49	In	52	95	Am
17	19	K	35	50	Sn	53	96	Cm
18	20	Ca	36	56	Ba			

([a]) The photon KERMA factors are the same for all the isotopes of each element.

4 - BUGJEFF311.BOLIB PRELIMINARY VALIDATION

The BUGJEFF311.BOLIB /4/ library was preliminarily tested on two engineering neutron shielding benchmark experiments, specifically dedicated to improve the accuracy of the neutron fluence calculations in the structural components of the pressurized light water reactors (PWRs), whose geometrical and compositional specifications were contained in the SINBAD /27/ (see also /28/) international database of fission reactor neutron shielding benchmark experiments.
The PCA-Replica 12/13 /24/ (see also /25/) (Winfrith, United Kingdom) and the VENUS-3 /26/ (Mol, Belgium) neutron shielding benchmark experiments were simulated with three-dimensional fixed source transport calculations using the ORNL TORT-3.2 /11/ discrete ordinates deterministic code and the ENEA-Bologna systems of programs ADEFTA-4.1 /62/ and BOT3P-5.3 /13/ (see APPENDIX), respectively dedicated to the atomic density calculations and to the preparation and graphical verification of the geometrical models. The BUGJEFF311.BOLIB library was alternatively used in the transport calculations with the BUGLE-96 /9/ library, which was specifically employed to obtain corresponding reference dosimetric results. The IRDF-2002 /50/ flat weighting dosimeter cross sections /51/ in the 47 neutron energy group structure (see TAB. 3.1) were used in both the calculations for the PCA-Replica 12/13 and VENUS-3 benchmark experiments with the BUGJEFF311.BOLIB and BUGLE-96 libraries.

4.1 - PCA-Replica 12/13 Neutron Shielding Benchmark

4.1.1 - PCA-Replica 12/13 Experimental Details

The PCA-Replica neutron shielding benchmark experiment /24/ is a water/iron benchmark experiment including PWR thermal shield and pressure vessel simulators. The source of neutrons is a thin fission plate (whose dimensions are 63.5 cm × 40.2 cm × 0.6 cm) of highly enriched uranium (93.0 w% in U-235), irradiated by the NESTOR low-power experimental reactor through a graphite thermal column (total thickness 43.91 cm). Beyond the fission plate, the PCA-Replica shielding array (12/13 experimental configuration with two water gaps of about 12 cm and 13 cm) was arranged in a large parallelepiped steel tank (square section; side 180.0 cm) filled with water. After a first water gap (12.1 cm), there was the stainless steel thermal shield simulator (5.9 cm), the second water gap (12.7 cm), the mild steel pressure vessel simulator (thickness T = 22.5 cm) and a wide box made of a thin layer of aluminium simulating the air cavity between the pressure vessel and the biological shield in a real PWR.
The fission plate, the thermal shield, the pressure vessel and the void box were perfectly orthogonally aligned and centred along an imaginary line Z (horizontal or nuclear axis) passing through the centre of the fission plate. Along this nuclear axis three types of threshold detectors were located in ten positions and gave the integral measurements.

The Rh-103(n,n')Rh-103m, In-115(n,n')In-115m and S-32(n,p)P-32 threshold dosimeters were employed in the PCA-Replica experiment. The corresponding typical parameters in a light water material testing reactor (MTR) spectrum (see /63/), similar to that of PCA-Replica, are reported in TAB. 4.1 to help in the analysis of the calculated results.
In practice the results coming from Rh-103(n,n') and In-115(n,n') are comparable with neutron fluxes above about 1.0 MeV and the results from S-32(n,p) with neutron fluxes above about 3.0 MeV.

Moreover spectral measurements were performed in two positions: in the one-quarter thickness (T) of the reactor pressure vessel (RPV 1/4 T) simulator and in the void box. Two kinds of spectrometer were used. The spherical hydrogen-filled proportional counters employed were of type SP-2 of internal diameter 40.0 mm. Individual counters with gas fillings of approximately 0.5, 1.0, 3.0 and 10.0 atmospheres were used in combination, to cover the energy range from 50.0 keV to 1.2 MeV. The neutron fluxes between 1.0 and 10.0 MeV were determined with a spherical 3.5 ml organic liquid (NE213) scintillator.

TAB. 4.1

PCA-Replica - Dosimeter Parameters in a Light Water MTR Neutron Spectrum.

Dosimeter	Effective Energy Threshold [MeV]	90% Response Energy Range [MeV]	Median Energy [MeV]
Rh-103(n,n’)	0.69	0.53 – 5.4	1.9
In-115(n,n’)	1.30	1.0 – 5.6	2.4
S-32(n,p)	2.70	2.2 – 7.4	3.9

4.1.2 - PCA-Replica 12/13 Analysis and Results

The BUGJEFF311.BOLIB /4/ and the BUGLE-96 /9/ libraries were alternatively used to simulate the PCA-Replica 12/13 /24/ engineering neutron shielding benchmark experiment. The whole PCA-Replica 12/13 experimental array was reproduced with the TORT-3.2 /11/ code, using the BOT3P-5.3 /13/ system for the preparation of the input of the geometrical model and the ADEFTA-4.1 /62/ program for the calculation of the atomic densities of the isotopes involved, on the basis of the atomic abundances reported in the BNL-NNDC database /64/. In fact the atomic densities indicated in the official description /24/ of the PCA-Replica experiment are given for natural element except for two uranium isotopes, i.e. U-235 and U-238. All the calculations were performed only with the 29 neutron groups (see TAB. 3.1) above 3.1828E+04 eV since all the energy thresholds of the employed dosimeters are above this energy value.

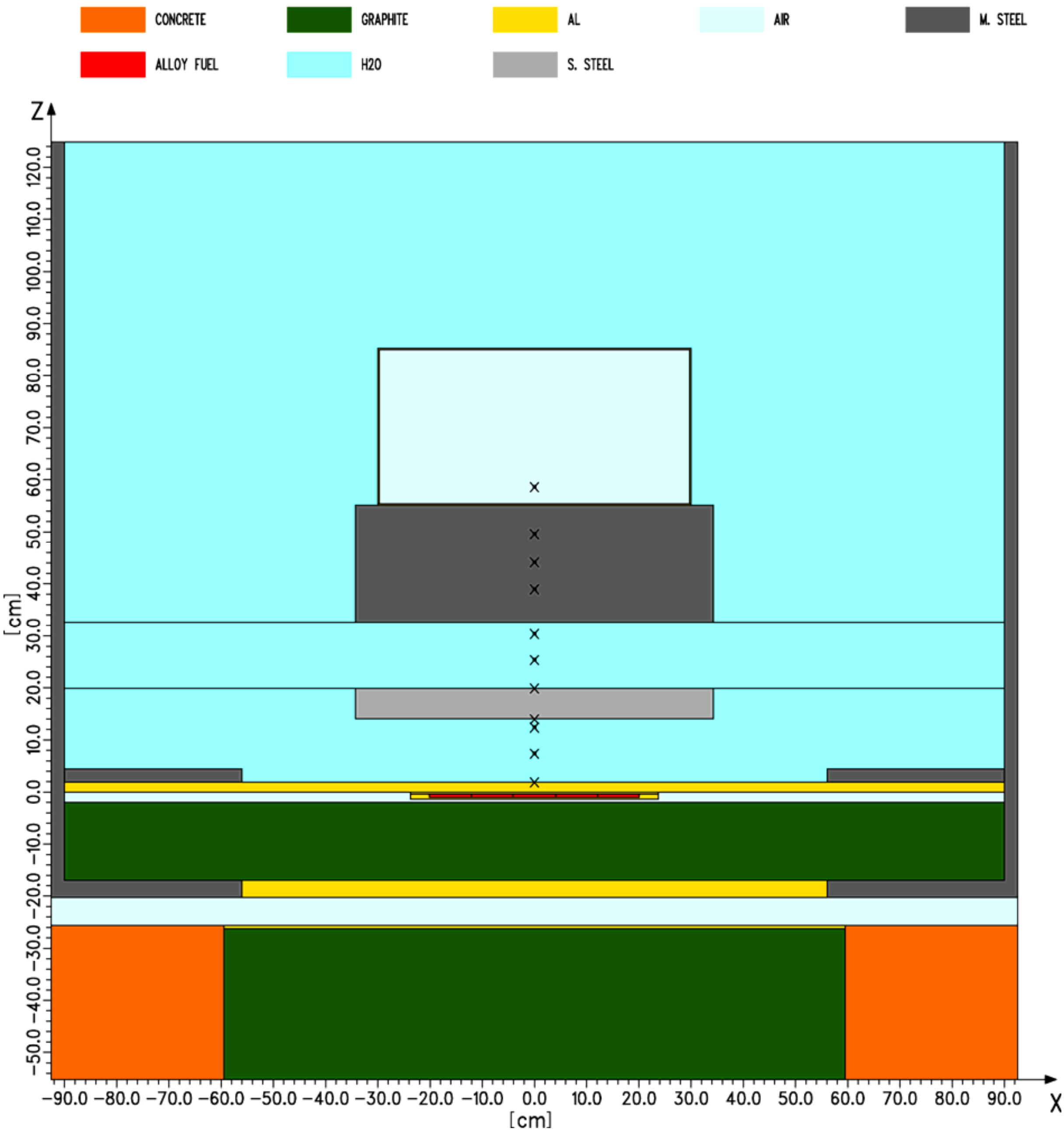
It was decided to reproduce the whole three-dimensional PCA-Replica experimental array in the (X,Y,Z) cartesian geometry in order to assure a detailed description of the spatial heterogeneity of the neutron source emitted by the fission plate. The origin of the cartesian co-ordinate system was taken in the centre of the fission plate.
In particular a parallelepiped geometry (whose dimensions were 185.08 cm × 180.0 cm × 180.0 cm, respectively along the X, Y and Z axis) was described with a 65X×63Y×182Z fine spatial mesh grid (see the horizontal section at the height Y=0.0 cm in FIG. 4.1), where Z is the horizontal nuclear axis on which the detector positions are located. Along this axis, in order to obtain the best accuracy in the calculations, volumetric meshes with sides always inferior to 0.5 cm were described. Both infinitely dilute and self-shielded cross sections were selected. Self-shielded cross sections from the library package were used when available: in particular it is underlined that the thermal shield (stainless steel) and the pressure vessel (mild steel) components of the PCA-Replica experiment were characterized by atomic densities

quite similar to those used to determine the background cross sections employed in the self-shielding of the BUGJEFF311.BOLIB /4/ cross sections.
Fixed source transport calculations with one source (outer) iteration were performed using fully symmetrical quadrature sets. The P_3-S_8 approximation was adopted: P_3 corresponds to the order of the expansion in Legendre polynomials of the scattering cross section matrix and S_8 represents the order of the flux angular discretization. Further calculations in the P_5-S_{16} approximation did not give significant differences in the integral dosimetric results.
The theta-weighted difference approximation was selected for the flux extrapolation model. In all the calculations the same numerical value (1.0E-03) for the point-wise flux convergence criterion was employed. The vacuum boundary condition was selected at the left, right, inside, outside, bottom and top geometrical boundaries.
As previously reported, a precise heterogeneous fission neutron source distribution in the fission plate was adopted, following the recommended official specifications (see /24/, page 55, TAB. A6 and page 57, FIG. A1).
The distributed (or volumetric) fission neutron sources used in the calculations with the BUGJEFF311.BOLIB library and the BUGLE-96 /9/ library were obtained using, respectively, the BUGJEFF311.BOLIB U-235 total (prompt + delayed) neutron fission spectrum (χ) data and the BUGLE-96 U-235 prompt neutron fission spectrum (χ) data (see /9/, page 58, TAB. 3.14), since the total neutron fission spectrum data are not available in the BUGLE-96 library. In order to determine the volumetric neutron source, the value of $\overline{\nu}$ (U-235) = 2.437 was used for the average number of neutrons produced per U-235 thermal fission, as suggested in the official description (see /24/, page 49) of the PCA-Replica experiment.

The IRDF-2002 /50/ flat weighting dosimeter cross sections /51/ in the 47 neutron energy group structure (see TAB. 3.1) for the Rh-103(n,n')Rh-103m, In-115(n,n')In-115m and S-32(n,p)P-32 nuclear reactions were used in the calculations with the BUGJEFF311.BOLIB and BUGLE-96 libraries to determine the detector activities in both water and steel locations. The use of the IRDF-2002 1/4T PV weighting dosimeter cross sections, to be used more properly in measurement positions located in steel, gave negligible differences in the pressure vessel simulator reaction rate results with respect to the corresponding results obtained with the IRDF-2002 flat weighting dosimeter cross sections. The reaction rate integral results obtained with the flat weighting dosimeter cross sections are reported in TAB. 4.2 and FIG. 4.2 for Rh-103(n,n')Rh-103m, in TAB. 4.3 and FIG. 4.3 for In-115(n,n')In-115m and in TAB. 4.4 and FIG. 4.4 for S-32(n,p)P-32. It is underlined that the calculated reaction rates for both the libraries are practically within the desired target accuracy of ±10%.
The spectral results are reported in FIGs. 4.5-6 and FIGs. 4.7-8, respectively for the 1/4 T reactor pressure vessel (RPV 1/4 T) position and for the void box position.

FIG. 4.1

PCA-Replica Model with TORT-3.2 (X,Y,Z), Horizontal Section at Y=0.0 cm.
Dosimeter Locations “×”, 65X×63Y×182Z Spatial Meshes.



TAB. 4.2

PCA-Replica - Summary of Experimental (E) and Calculated (C) Rh-103(n,n') Reaction Rates[a] per NESTOR Reactor Watt along the Z Horizontal Axis.

Detec. Pos.	Distance from Fission Plate [cm]	Experimental. Reaction Rates ± Random Error (1σ) (E) Systematic Error ± 3.0%	BUGJEFF311.BOLIB Calculation		BUGLE-96 Calculation		Reference Location
			Calculated Reaction Rates (C)	C/E[b]	Calculated Reaction Rates (C)	C/E[b]	
1	1.91	1.69E-20 ± 3.0%	1.80E-20	1.09	1.82E-20	1.10	12 cm Water Gap
2	7.41	3.78E-21 ± 3.0%	3.42E-21	0.92	3.43E-21	0.93	
3	12.41	1.40E-21 ± 3.0%	1.30E-21	0.95	1.30E-21	0.95	
4	14.01	1.27E-21 ± 3.0%	1.15E-21	0.92	1.15E-21	0.92	
5	19.91	4.23E-22 ± 3.0%	4.18E-22	1.01	4.11E-22	0.99	13 cm Water Gap
6	25.41	1.15E-22 ± 4.0%	1.02E-22	0.91	1.01E-22	0.89	
7	30.41	4.73E-23 ± 4.0%	4.11E-23	0.89	4.05E-23	0.87	
8	39.01	2.07E-23 ± 1.0%	2.02E-23	1.02	1.98E-23	1.00	RPV (1/4 T)
9	49.61	5.53E-24 ± 1.9%	5.61E-24	1.06	5.45E-24	1.03	RPV (3/4 T)
10	58.61	1.80E-24 ± 1.6%	1.65E-24	0.96	1.59E-24	0.92	Void Box

Note: The total experimental error (1σ level) should be calculated as the square root of the quadratic sum of the random error listed with each measurement and the systematic error indicated at the head of the column of the experimental results, as indicated on page 12 of reference /24/.

([a]) Reaction rates are in units of reactions/(s·atom·NESTOR Watt).

([b]) Experimental results contain a contribution from the NESTOR core background. Calculated results refer only to the neutrons produced in the fission plate for 1 Watt of NESTOR power. As indicated on page 10 of reference /24/, the E values, in the C/E ratios, are reduced by 4% in the RPV and Void Box and by 2% in the Water Gaps.

TAB. 4.3

PCA-Replica - Summary of Experimental (E) and Calculated (C) In-115(n,n') Reaction Rates[a] per NESTOR Reactor Watt along the Z Horizontal Axis.

Detec. Pos.	Distance from Fission Plate [cm]	Experimental. Reaction Rates ± Random Error (1σ) (E) Systematic Error ± 2.0%	BUGJEFF311.BOLIB Calculation		BUGLE-96 Calculation		Reference Location
			Calculated Reaction Rates (C)	C/E[b]	Calculated Reaction Rates (C)	C/E[b]	
1	1.91	--	--	--	--	--	12 cm Water Gap
2	7.41	--	--	--	--	--	
3	12.41	--	--	--	--	--	
4	14.01	--	--	--	--	--	
5	19.91	--	--	--	--	--	13 cm Water Gap
6	25.41	--	--	--	--	--	
7	30.41	--	--	--	--	--	
8	39.01	3.93E-24 ± 0.9%	3.89E-24	1.03	3.80E-24	1.01	RPV (1/4 T)
9	49.61	8.23E-25 ± 1.4%	7.79E-25	0.99	7.57E-25	0.96	RPV (3/4 T)
10	58.61	2.31E-25 ± 1.5%	2.15E-25	0.97	2.09E-25	0.94	Void Box

Note: The total experimental error (1σ level) should be calculated as the square root of the quadratic sum of the random error listed with each measurement and the systematic error indicated at the head of the column of the experimental results, as indicated on page 12 of reference /24/.

([a]) Reaction rates are in units of reactions/(s·atom·NESTOR Watt).

([b]) Experimental results contain a contribution from the NESTOR core background. Calculated results refer only to the neutrons produced in the fission plate for 1 Watt of NESTOR power. As indicated on page 10 of reference /24/, the E values, in the C/E ratios, are reduced by 4% in the RPV and Void Box and by 2% in the Water Gaps.

TAB. 4.4

PCA-Replica - Summary of Experimental (E) and Calculated (C) S-32(n,p) Reaction Rates[a] per NESTOR Reactor Watt along the Z Horizontal Axis.

Detec. Pos.	Distance from Fission Plate [cm]	Experimental. Reaction Rates ± Random Error (1σ) (E) Systematic Error ± 4.0%	BUGJEFF311.BOLIB Calculation		BUGLE-96 Calculation		Reference Location
			Calculated Reaction Rates (C)	C/E[b]	Calculated Reaction Rates (C)	C/E[b]	
1	1.91	--	--	--	--	--	12 cm Water Gap
2	7.41	--	--	--	--	--	
3	12.41	--	--	--	--	--	
4	14.01	--	--	--	--	--	
5	19.91	--	--	--	--	--	13 cm Water Gap
6	25.41	--	--	--	--	--	
7	30.41	--	--	--	--	--	
8	39.01	1.08E-24 ± 1.5%	9.85E-25	0.95	9.66E-25	0.93	RPV (1/4 T)
9	49.61	1.46E-25 ± 1.9%	1.38E-25	0.98	1.34E-25	0.95	RPV (3/4 T)
10	58.61	3.73E-26 ± 1.3%	3.63E-26	1.01	3.52E-26	0.98	Void Box

Note: The total experimental error (1σ level) should be calculated as the square root of the quadratic sum of the random error listed with each measurement and the systematic error indicated at the head of the column of the experimental results, as indicated on page 12 of reference /24/.

([a]) Reaction rates are in units of reactions/(s·atom·NESTOR Watt).

([b]) Experimental results contain a contribution from the NESTOR core background. Calculated results refer only to the neutrons produced in the fission plate for 1 Watt of NESTOR power. As indicated on page 10 of reference /24/, the E values, in the C/E ratios, are reduced by 4% in the RPV and Void Box and by 2% in the Water Gaps.

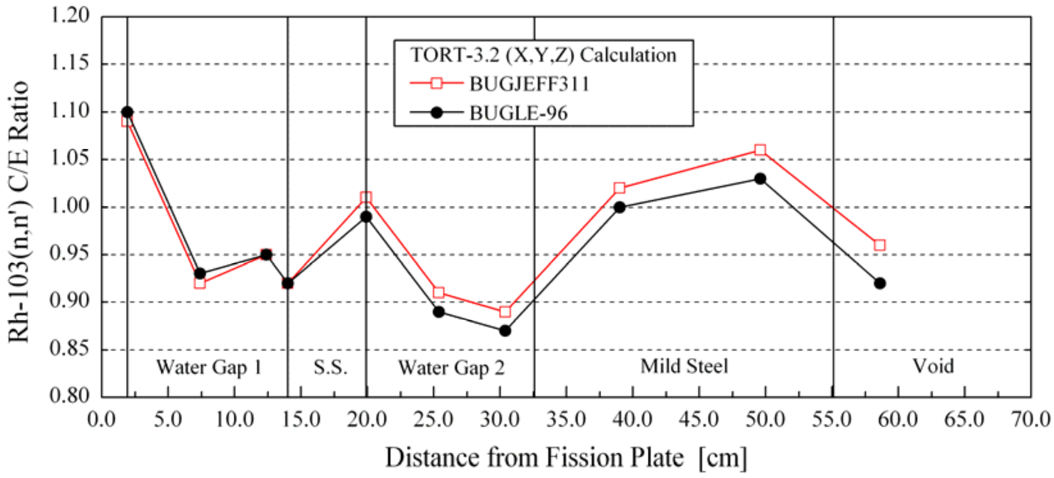


FIG. 4.2 PCA-Replica - Rh-103(n,n') Reaction Rates Ratios (Calculated/Experimental).

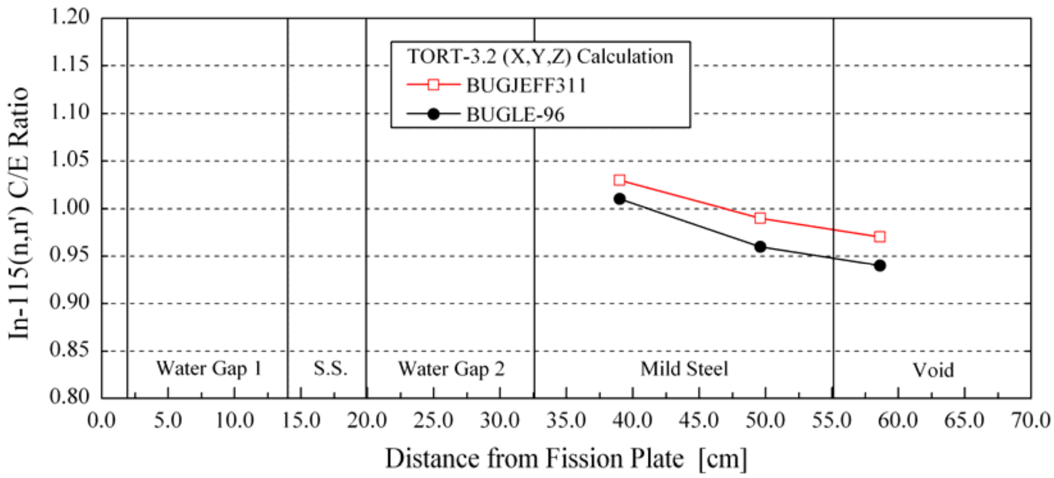


FIG. 4.3 PCA-Replica - In-115(n,n') Reaction Rates Ratios (Calculated/Experimental).

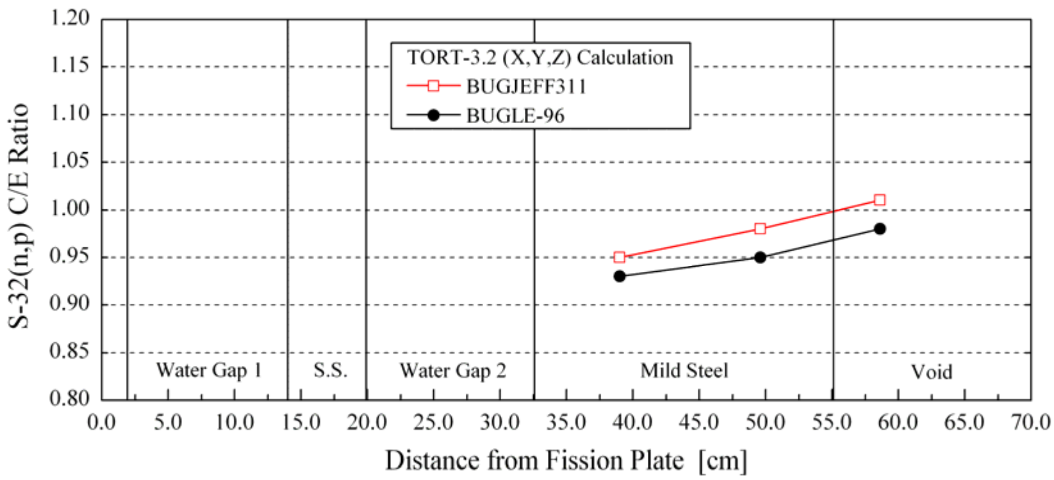


FIG. 4.4 PCA-Replica - S-32(n,p) Reaction Rates Ratios (Calculated/Experimental).

FIG. 4.5

PCA-Replica - Comparison of Experimental and Calculated Neutron Fluxes
in the RPV 1/4 T Position (Mild Steel).

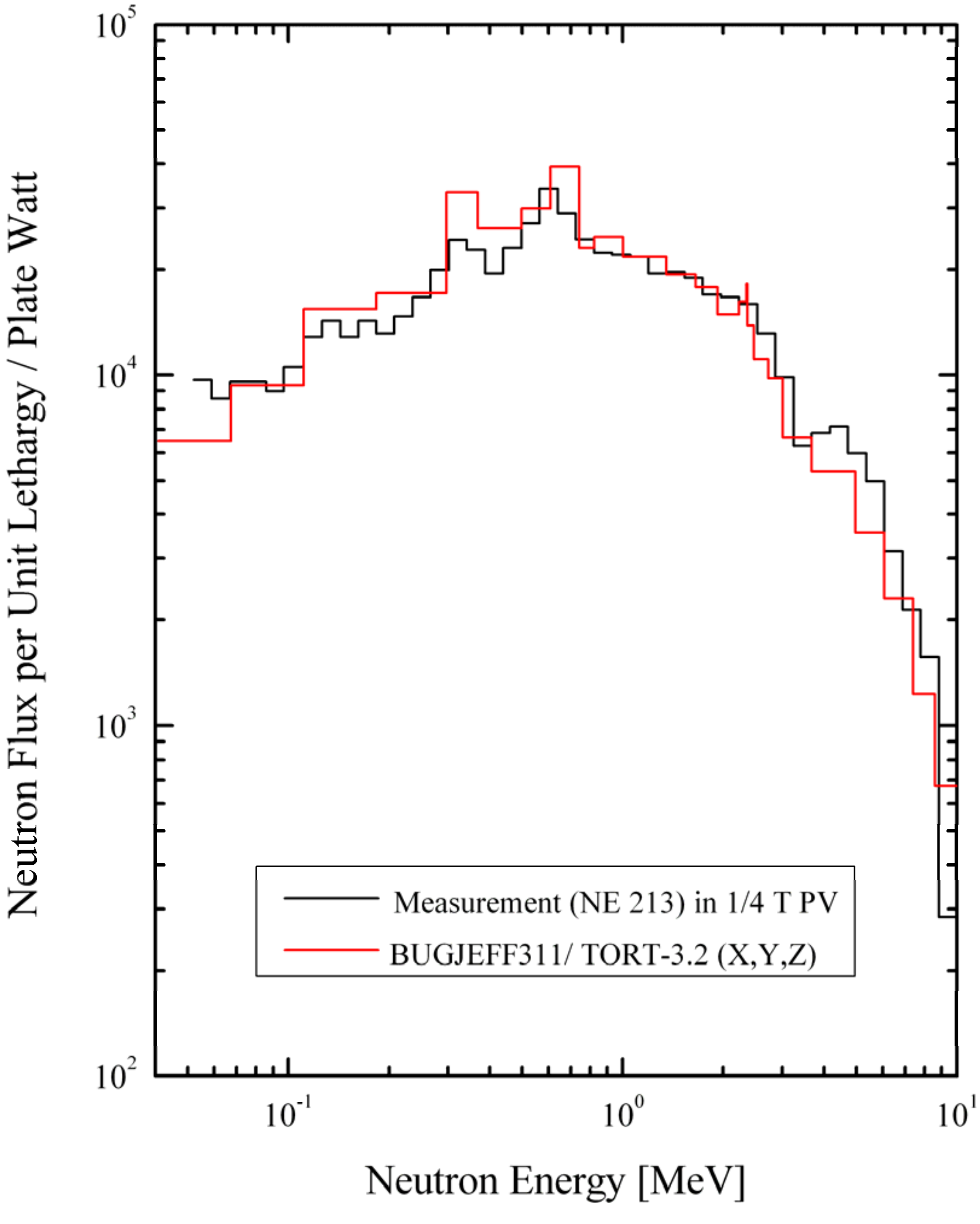


FIG. 4.6

PCA-Replica - Comparison of Experimental and Calculated Neutron Fluxes in the RPV 1/4 T Position (Mild Steel).

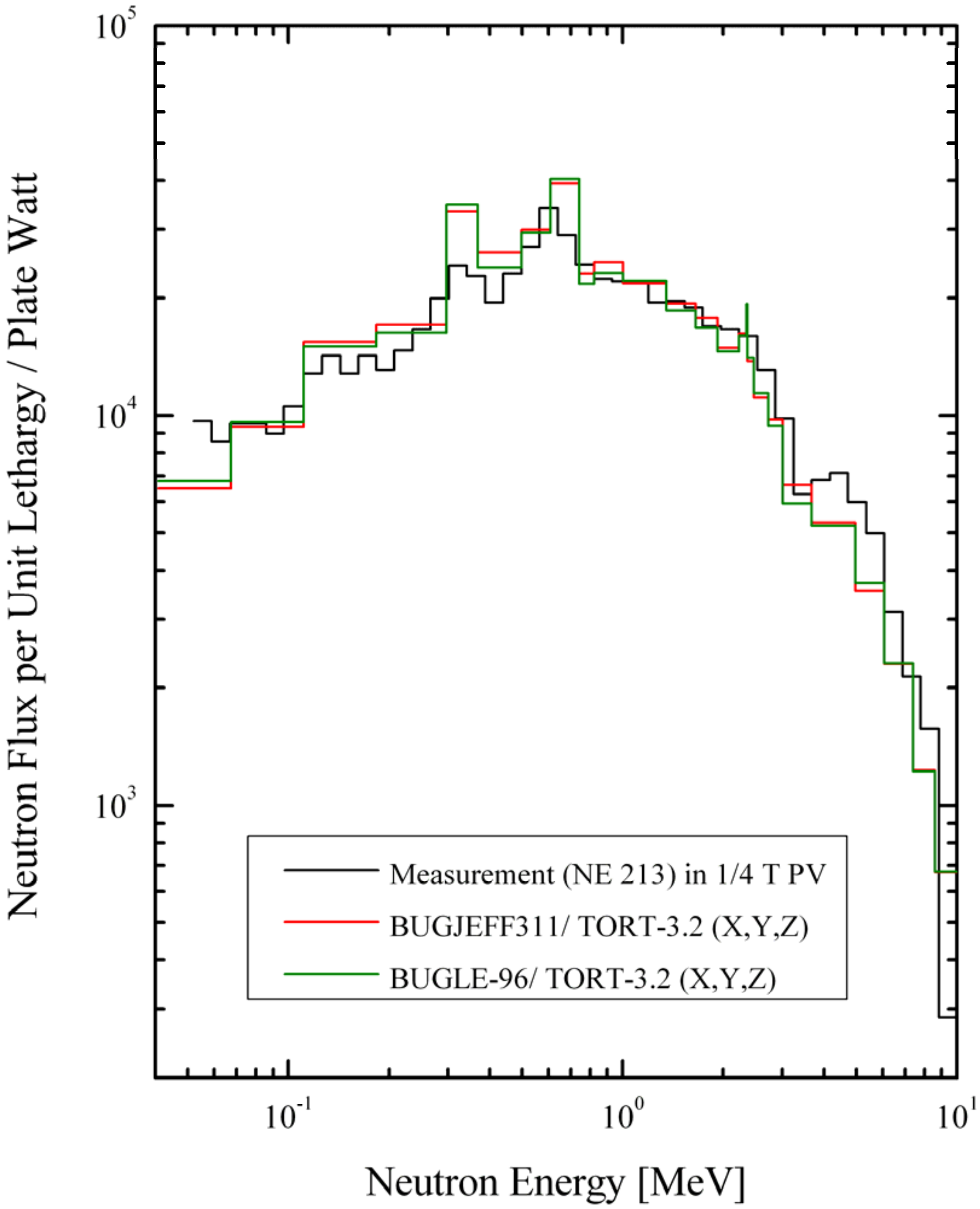


FIG. 4.7

PCA-Replica - Comparison of Experimental and Calculated Neutron Fluxes
in the Void Box Position (Air).

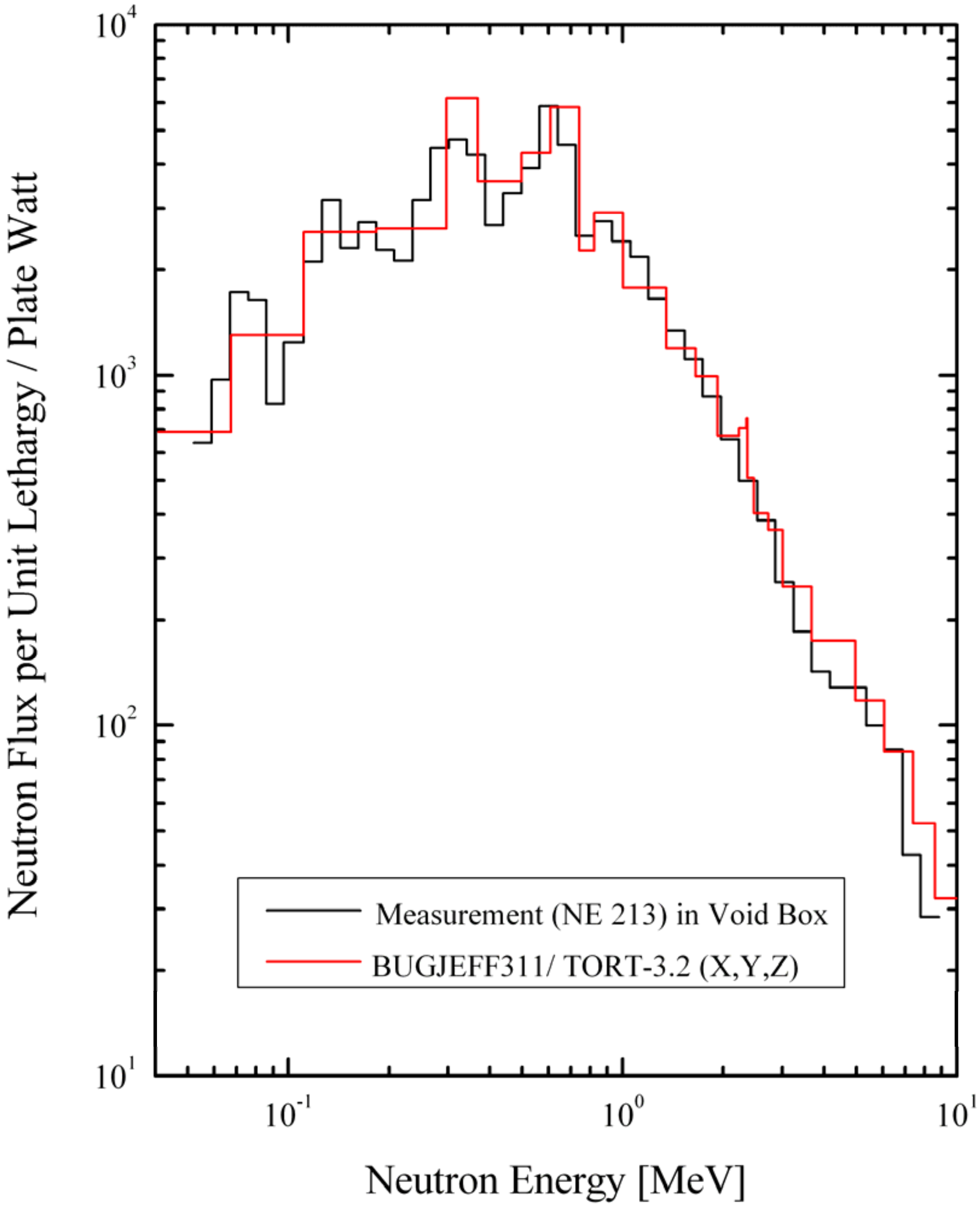
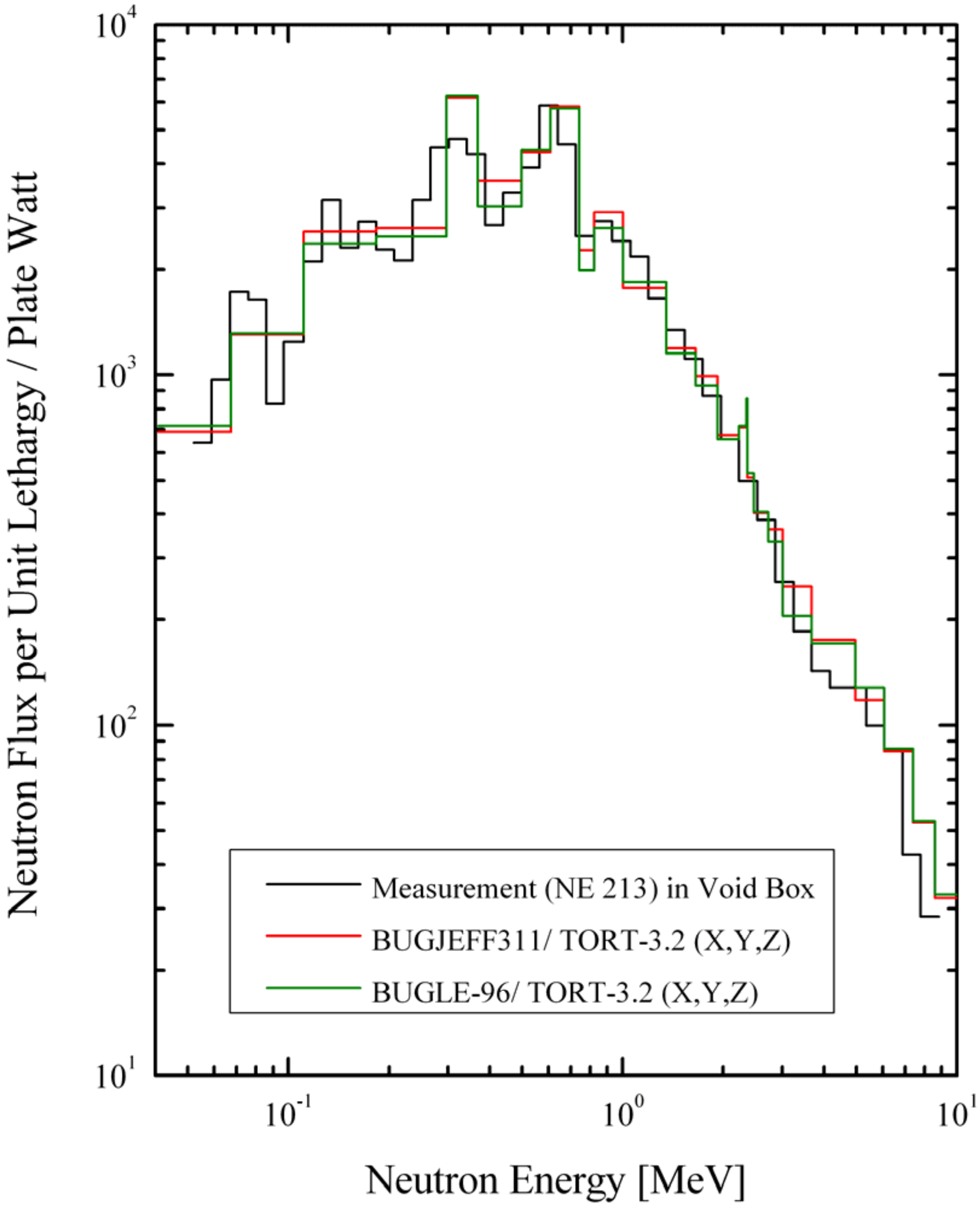


FIG. 4.8

PCA-Replica - Comparison of Experimental and Calculated Neutron Fluxes
in the Void Box Position (Air).



4.2 - VENUS-3 Neutron Shielding Benchmark

4.2.1 - VENUS-3 Experimental Details

The VENUS-3 /26/ low-flux neutron shielding benchmark experiment (Mol, Belgium) is closely related to LWR-PV safety. It was designed to test the accuracy of the nuclear data and transport codes in the calculation of the neutron radiation damage parameters in stainless steel reactor components, in a context of great precision of the experimental results. Among the available experiments, the VENUS-3 configuration offers the exceptional advantage of exhibiting a realistic radial core shape and a typical PWR neutron spectrum. Typical “17x17” PWR fuel assemblies were employed and a mock-up of the pressure vessel internals, representative of a three-loop Westinghouse power plant, was prepared. VENUS-3 was conceived taking into account that, for some early built reactors, it was proposed to reduce the lead factor at the level of the PV horizontal welding by loading Partial Length Shielded Assemblies (PLSA) at the most critical corners of the core periphery (the shielded part was obtained by replacing part of the fuel length by a stainless steel rod). VENUS-3 was addressed to test this improvement, introducing a PLSA region in the core, and to permit the validation of the analytical methods needed to predict the azimuthal variation of the fluence in the pressure vessel. The VENUS-3 core was designed, in particular, with the following objectives.

1. It had to be representative of typical irradiation conditions of a modern PWR pressure vessel.

2. It had to fit the grid and the vessel geometries of the VENUS facility. This led to a limitation of the core size and of the amount of simulated internals. In particular the second water gap and the pressure vessel of a typical PWR were not simulated.

3. The core loading was projected to obtain a radial power shape factor as low as possible, in order to reach, in the different stainless steel components, fast flux levels high enough to perform accurate measurements. Secondly, the core loading was planned to achieve azimuthal flux variations as high as possible to allow a valuable test of the analytical methods. Finally a quadrangular geometry symmetry was preferred, with two quadrants including both the PLSA fuel region and the unperturbed reference fuel region.

All these objectives were attained with a cruciform-shaped core configuration. The core consists of three types of fuel pins: 1) stainless-steel-clad UO_2 rods (typical of a “15x15” lattice of the early Generation I reactors of Westinghouse plants) containing 4% enriched U-235, 2) zircaloy-clad UO_2 rods containing 3.3% enriched U-235 and 3) zircaloy-clad UO_2 rods containing 3.3% enriched U-235 over the upper half of their height and zircaloy-clad steel rods over the lower half. The first two types of fuel pins are of uniform composition over their complete height. The 4% enriched rods are positioned in the inner part of the core while the 3.3% enriched rods are located in the arms of the cross configuration together with the PLSA-modified rods. The pin-to-pin pitch for all fuel types is 1.26 cm, typical value of the “17x17” lattices in existing PWR fuel assemblies. In one quadrant of the configuration between 0° and 90° (see the horizontal section in FIG. 4.9 and the vertical section in FIG. 4.10), a mock-up of PWR pressure vessel internals is placed with a total of 639 fuel pins (including those in the PLSA) and 11 control rods. The other quadrants are loaded with fuel pins "quasi" identical to the fuel pins of the first previous quadrant (due to fuel inventory limitations) and with some absorbing rods for criticality balance adjustment. Starting from the centre, the core quadrant between 0° and 90° may be divided in the following 10 horizontal radial regions:

- the CENTRAL HOLE (water);
- the INNER BAFFLE (stainless steel thickness: 2.858 cm);
- the 4/0 FUEL REGION: 4% enriched uranium fuel rods and 11 pyrex control rods, typical of PWR poison clusters;
- the 3/0 FUEL REGION: 3.3% enriched uranium fuel rods and PLSA rods;
- the OUTER BAFFLE (stainless steel thickness. 2.858 cm);
- the REFLECTOR (water minimum thickness: 2.169 cm);
- the BARREL (stainless steel thickness: 4.99 cm);
- the WATER GAP (water thickness: 5.80 cm);
- the NEUTRON PAD (stainless steel average thickness: 6.72 cm);
- the VENUS environment, i.e., the jacket (air filled), the reactor vessel (stainless steel) and the reactor room (air).

The In-115(n,n')In-115m, Ni-58(n,p)Co-58 and Al-27(n,α)Na-24 threshold dosimeters were employed in the VENUS-3 experiment. The corresponding typical parameters in a light water material testing reactor (MTR) spectrum (see /63/), similar to that of VENUS-3, are reported in TAB. 4.5 to help in the analysis of the obtained calculated results.

TAB. 4.5

VENUS-3 - Dosimeter Parameters in a Light Water MTR Neutron Spectrum.

Dosimeter	Effective Energy Threshold [MeV]	90% Response Energy Range [MeV]	Median Energy [MeV]
In-115(n,n')	1.30	1.0 – 5.6	2.4
Ni-58(n,p)	2.60	1.9 – 7.5	3.9
Al-27(n,α)	7.30	6.5 – 12.0	8.6

In practice (see also /65/) the results coming from In-115(n,n') are comparable with neutron fluxes above about 1.0 MeV, the results from Ni-58(n,p) with neutron fluxes above about 3.0 MeV and the results from Al-27(n,α) with neutron fluxes above about 8.0 MeV.
In the VENUS-3 experiment the total number of the dosimeters is 386: the In-115(n,n') dosimeters are in 104 positions, the Ni-58(n,p) dosimeters are in 244 positions and the Al-27(n,α) dosimeters are in 38 positions. In other words, each set of dosimeters is placed in a part of the 268 total different spatial locations. Axially, the dosimeters are located at 14 different axial levels between 105.0 cm and 155.0 cm, respectively the lower height and the upper height of the active core region (see FIG. 4.10). The maximum total uncertainty of the

VENUS-3 experimental equivalent fission fluxes corresponding to each of the three dosimeters is ±5% (see /47/, page 31).

FIG. 4.9

VENUS-3 Model with TORT-3.2 (R,Θ,Z), Horizontal Section at Z=114.50 cm.
Dosimeter Locations “×“, 111R×113Θ×71Z Spatial Meshes.

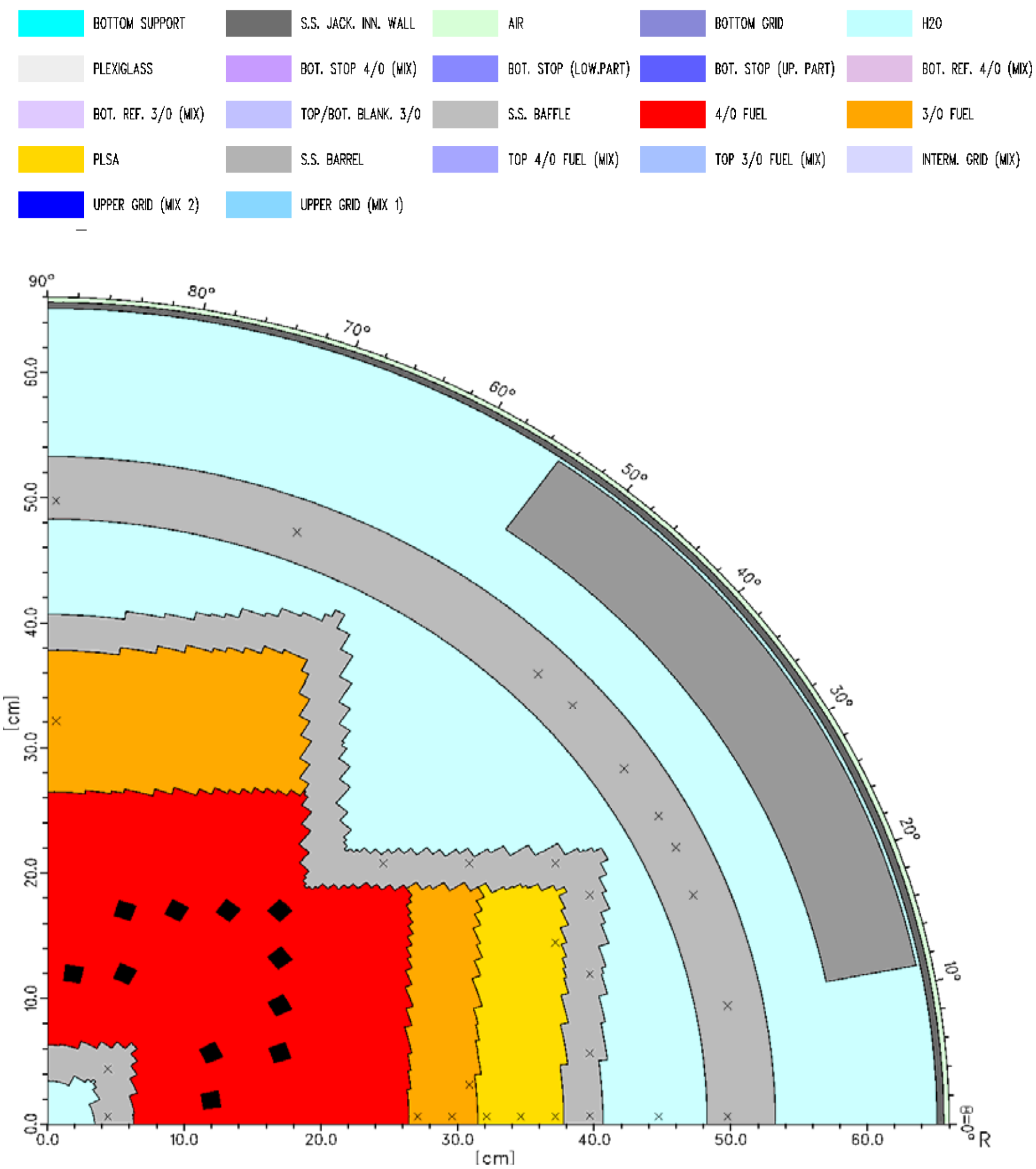
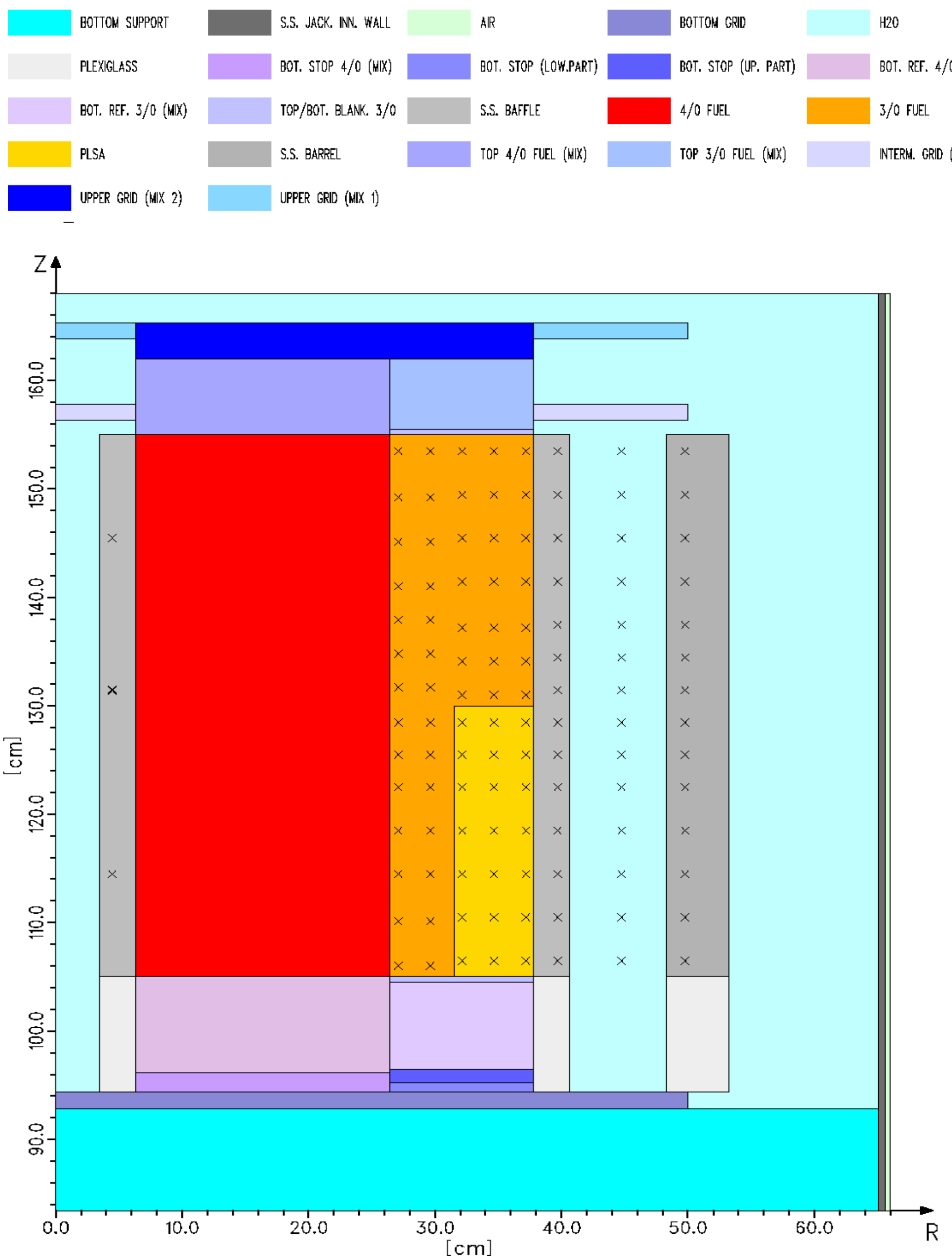


FIG. 4.10

VENUS-3 Model with TORT-3.2 (R,Θ,Z), Vertical Section at Θ=0°.
Dosimeter Locations “×”, 111R×113Θ×71Z Spatial Meshes.



4.2.2 - VENUS-3 Analysis and Results

The BUGJEFF311.BOLIB /4/ and the BUGLE-96 /9/ libraries were alternatively used to simulate the VENUS-3 /26/ (see also /45/ /46/ and /47/) engineering neutron shielding benchmark experiment. Both infinitely dilute and self-shielded cross sections were selected. In the case, e.g., of Fe-56, in the material mixtures of stainless steel components, the self-shielded cross sections were used. All the calculations were performed only with the 26 neutron groups (see TAB. 3.1) above 1.1109E+05 eV since all the energy thresholds of the employed dosimeters are above this energy value. Three-dimensional calculations in cylindrical (R,Θ,Z) geometry were performed through the TORT-3.2 /11/ discrete ordinates (S_N) transport code, included in the ORNL DOORS-3.2 /31/ modular system, using both the previously cited libraries. Fixed source calculations with one source (outer) iteration were performed in the P_3-S_8 approximation: P_3 corresponds to the order of the expansion in Legendre polynomials of the scattering cross section matrix and S_8 represents the order of the flux angular discretization. Fully symmetrical quadrature sets were introduced. The theta-weighted difference approximation was selected for the flux extrapolation model. In all the calculations the same numerical value (1.0E-04) for the point-wise flux convergence criterion was employed. The BOT3P-5.3 /13/ system of pre/post-processor programs was used to prepare the automatic generation of the input data for the neutron source and for the geometrical models together with the graphical visualizations. The (R,Θ,Z) geometrical model is shown in FIG. 4.9 and FIG. 4.10, reproducing respectively the horizontal and the vertical sections. It is underlined that the (R,Θ,Z) model is also usually adopted for the LWR-PV radiation damage transport analyses. In particular a horizontal plane section between 0° and 90° was described (i.e. the first quadrant up to a radius of 66.0 cm, reported in FIG. 4.9) containing the barrel, the neutron pad and the jacket inner wall with a 111R×113Θ×71Z fine spatial mesh grid. The jacket outer wall and the external regions beyond the jacket outer wall were not included since it was considered that they could only slightly affect the results. The following boundary conditions were selected: reflection at the left, inside and outside boundaries and vacuum at the right, bottom and top boundaries.

The distributed (or volumetric) fission neutron sources used in the BUGJEFF311.BOLIB and BUGLE-96 calculations and the calculated results in terms of equivalent fission fluxes for the three threshold detectors were obtained using respectively, the BUGJEFF311.BOLIB U-235 total (prompt + delayed) neutron fission spectrum (χ) data and the BUGLE-96 U-235 prompt neutron fission spectrum (χ) data (see /9/, page 58, TAB. 3.14), since the total neutron fission spectrum data are not available in the BUGLE-96 library. To determine the volumetric neutron source, the value of $\bar{\nu}$ (U-235) = 2.432 for the average number of neutrons produced per U-235 thermal fission was used, as proposed value (see /66/, page 7) for the ENDF/B-VI U-235 processed data file, contained in the BUGLE-96 library.

The calculated dosimeter reaction rates (activities) were divided by the corresponding value of the flat weighting dosimeter cross section, averaged on the specific U-235 fission spectrum. The following flat weighting corresponding values (see TAB. 4.6) were used in all the calculations in order to treat simultaneously both water and steel dosimeter locations.

TAB. 4.6

VENUS-3 - IRDF-2002 Dosimeter Cross Sections Averaged on the U-235 Neutron Fission Spectra Respectively Taken from the BUGJEFF311.BOLIB and BUGLE-96 Libraries.

Library	In115(n,n') [barns]	Ni-58(n,p) [barns]	Al-27(n,α) [barns]
BUGJEFF311	1.8742E-01	1.0835E-01	7.8148E-04
BUGLE-96	1.8853E-01	1.0906E-01	7.8671E-04

A synthesis of the Calculated/Experimental (C/E) results for the In-115(n,n')In-115m, Ni-58(n,p)Co-58 and Al-27(n,α)Na-24 threshold dosimeters, in terms of equivalent fission flux ratios, are respectively reported in FIG. 4.11, FIG. 4.12 and FIG. 4.13.
Deviations contained within ±5% from the 386 dosimeter experimental data were obtained in about 83% of the calculated results with BUGJEFF311.BOLIB and in about 88% of the results with BUGLE-96. The calculated equivalent fission fluxes for both the libraries were practically within the desired target accuracy of ±10% (see TAB. 4.7), recommended by OECD-NEA.

TAB. 4.7

VENUS-3 - Percentages[a] of the Calculated (C) Equivalent Fission Fluxes with Deviations Exceeding 5% and 10% the Corresponding Experimental (E) Fluxes.

Library	In115(n,n')	Ni-58(n,p)	Al-27(n,α)
	|C-E| / E > 5%		
BUGJEFF311	4.8%	19.7%	28.9%
BUGLE-96	3.8%	12.3%	28.9%
Library	In115(n,n')	Ni-58(n,p)	Al-27(n,α)
	|C-E| / E > 10%		
BUGJEFF311	0.0%	1.2%	0.0%
BUGLE-96	0.0%	1.6%	2.6%

([a]) Percentages calculated on the total number of each dosimeter type: 104 for In, 244 for Ni and 38 for Al.

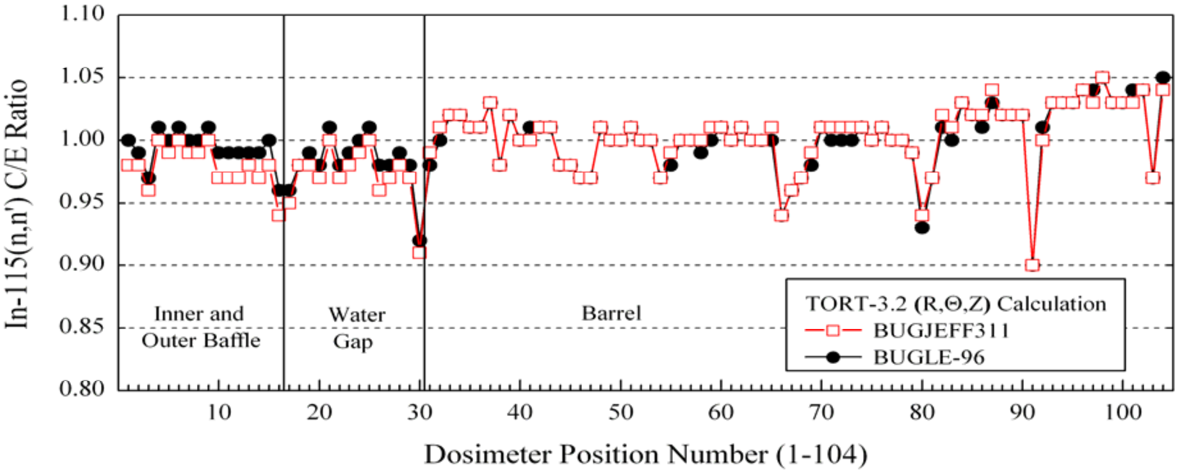


FIG. 4.11 VENUS-3 - In-115(n,n’) Equivalent Fission Flux Ratios (Calculated/Experimental).

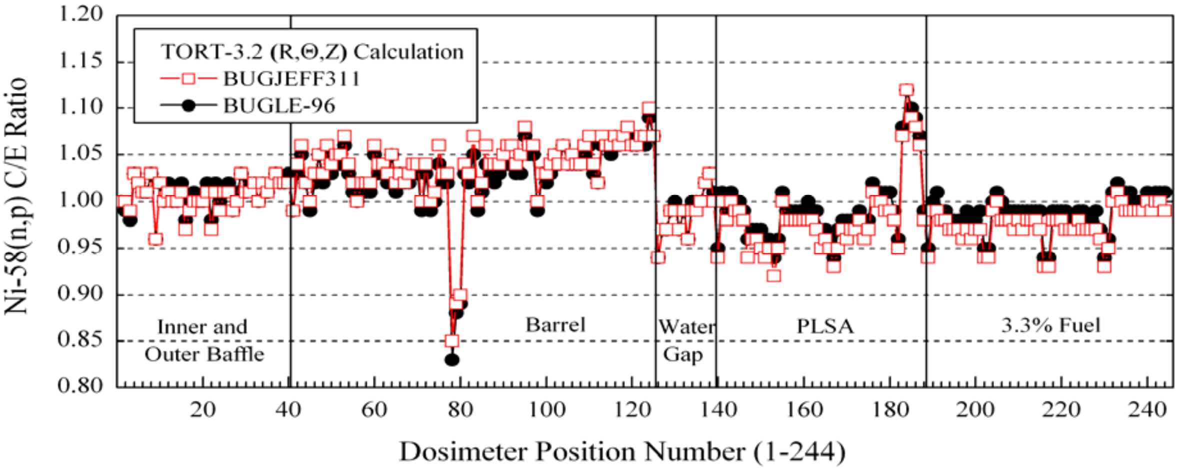


FIG. 4.12 VENUS-3 - Ni-58(n,p) Equivalent Fission Flux Ratios (Calculated/Experimental).

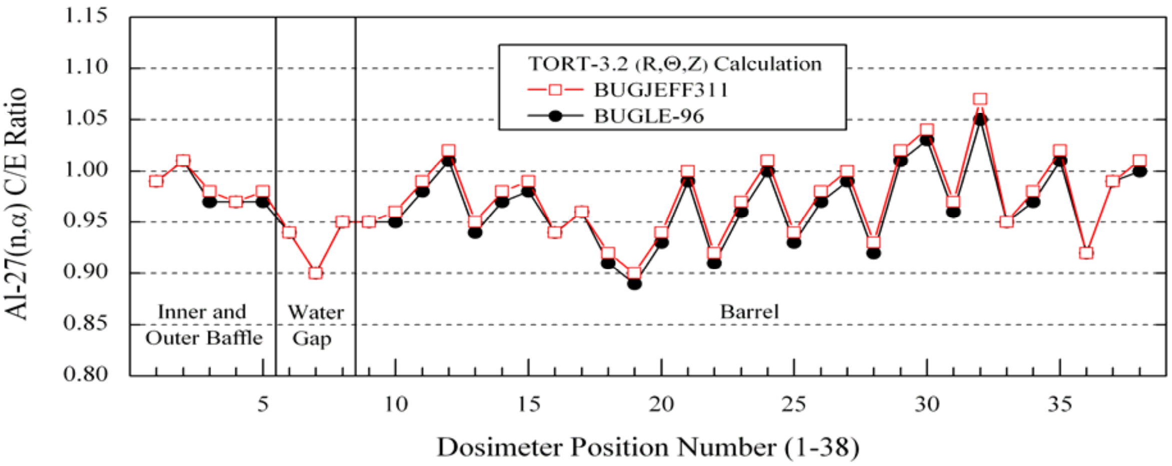


FIG. 4.13 VENUS-3 - Al-27(n,α) Equivalent Fission Flux Ratios (Calculated/Experimental).

5 - CONCLUSION

The ENEA-Bologna Nuclear Data Group produced two multi-group cross section libraries for nuclear fission applications, named VITJEFF311.BOLIB and BUGJEFF311.BOLIB.

VITJEFF311.BOLIB is a fine-group general-purpose library in AMPX format, based on the JEFF-3.1.1 evaluated nuclear data library, which was generated in the neutron and photon energy group structures (199 n + 42 γ) of the DLC-0184 ZZ-VITAMIN-B6 similar library produced at ORNL. From the VITJEFF311.BOLIB library, specifically conceived for a variety of nuclear fission applications, broad-group coupled neutron/photon working cross section libraries for LWR shielding and pressure vessel dosimetry applications can be derived through problem-dependent cross section collapsing. The VITJEFF311.BOLIB library will be transferred to OECD-NEA Data Bank and will be freely distributed.

The BUGJEFF311.BOLIB broad-group coupled neutron/photon working cross section library in FIDO-ANISN format is specifically dedicated to LWR shielding and pressure vessel dosimetry applications. It was generated following the previously cited problem-dependent collapsing methodology, recommended by the American National Standard ANSI/ANS-6.1.2-1999 (R2009) "Neutron and Gamma-Ray Cross Sections for Nuclear Radiation Protection Calculations for Nuclear Power Plants". The BUGJEFF311.BOLIB library was recently transferred to OECD-NEA Data Bank and is freely distributed with the designation NEA-1866/01 ZZ-BUGJEFF311.BOLIB. The relative "Abstract" in the OECD-NEA internet site is at the following address:

http://www.oecd-nea.org/tools/abstract/detail/nea-1866/

The BUGJEFF311.BOLIB library has the same neutron and photon energy group structures (47 n + 20 γ) of the DLC-185 ZZ-BUGLE-96 similar library, generated at ORNL for the same applications, which has had a good success all over the world since its release in 1996. The BUGJEFF311.BOLIB library is available in two versions in the dedicated package: BUGJEFF311.BOLIB, without upscattering cross sections in the thermal neutron energy region, and BUGJEFF311T.BOLIB, including the upscattering cross sections. The BUGJEFF311.BOLIB library was processed with an updated and corrected version of the ORNL SCAMPI data processing system, the ENEA-Bologna 2007 Revision, already transferred to OECD-NEA Data Bank for free distribution with the designation PSR-0352/05 SCAMPI. The library was preliminarily validated on two engineering neutron shielding benchmark experiments (PCA-Replica 12/13 and VENUS-3) included in the SINBAD international database of shielding benchmark experiments. The two cited benchmark experiments were specifically designed for the improvement of the accuracy of the LWR radiation shielding and radiation damage calculations. The accuracy of the calculated results for both the integral experiments is practically within the desired target value of ±10%. Further validation of the BUGJEFF311.BOLIB library will be performed on other integral neutron shielding benchmark experiments.

Similar data processing and validation activities will be continued using the ENDF/B-VII.0 evaluated nuclear data library. The possibility is being studied to increase, in particular, the number of the thermal neutron energy groups with respect to the BUGLE-96 neutron energy group structure to permit more accurate analyses of the thermal neutron and photon radiation damage in applications where these contributions to the total damage are not negligible.

It is believed that it should be very important to further promote, at the international level (UNO-IAEA, OECD-NEA, industrial organizations, R&D institutions, etc.), the generation of new working cross section libraries for radiation shielding applications, dedicated to various types of Generation III and IV nuclear fission reactors with different spectral, geometrical and compositional specifications. In fact the availability of these libraries could promote, in particular, the use of the three-dimensional deterministic codes in radiation shielding and radiation damage applications for nuclear safety. This is increasingly requested, due to the fact that these transport codes (TORT, PARTISN, KATRIN, etc.) have now sophisticated possibilities of complex geometry description, through modern dedicated pre/post-processor systems (BOT3P, TORTWARE, etc.) for the automatic generation of the spatial meshes.

In general, the severe nuclear accidents to the PWR unit No. 2 of the Three Mile Island (Harrisburg, US, March 28, 1979) nuclear power plant and, just recently, to the BWR units No. 1, 2 and 3 of the Fukushima Dai-ichi (Japan, March 11, 2011) nuclear power plant, emphasized and confirmed that the structural integrity of the LWR pressure vessel is one of the most relevant key factors within the defence-in-depth approach of the LWR nuclear safety. The RPV structural integrity is particularly important for PWR long term operations, especially when approaching the End-of-Life (EoL) neutron fluence values in the pressure vessel. The monitoring and the evaluation of the degradation of the RPV materials require not only suitable experimental techniques (reactor dosimetry, thermo-mechanical tests on RPV steels, etc.) but also proven calculation tools as, e.g., group working cross section libraries like BUGLE-96 or BUGJEFF311.BOLIB which can play a crucial role to quantify accurately the neutron and photon radiation damage to the pressure vessel, during the whole LWR lifetime.

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APPENDIX

Development and Testing of the ENEA-Bologna BOT3P Pre/Post-Processor Code System

Development and Testing of the ENEA-Bologna BOT3P Pre/Post-Processor Code System

The pre/post-processor code system BOT3P /13/ /14/ /15/ /16/ was updated and improved by adding new options, according to the users' feedback, leading to the BOT3P Version 5.5.
BOT3P is a set of standard FORTRAN 77 language codes developed at the ENEA-Bologna Nuclear Data Group and is designed to run on Linux/UNIX platforms. BOT3P Version 1.0 was originally conceived as a set of standard FORTRAN 77 language programs in order to give to the users of the two-dimensional (2D) DORT and three-dimensional (3D) TORT discrete ordinates transport codes of the ORNL DOORS /31/ system of deterministic codes (distributed by OECD-NEA Data Bank) some useful calculation tools to prepare and check their input data files. In particular BOT3P contains modules that automatically generate the spatial mesh grids for both Cartesian and cylindrical geometries in two-dimensions and three-dimensions, using a combinatorial geometry methodology to describe complicated 2D and 3D input geometries. Moreover BOT3P allows the check of the input geometrical models and the visualization of the results through graphical modules that perform 2D cuts and 3D views.

Later versions of BOT3P extended the possibility to produce geometrical, material distribution and neutron fixed source data to other deterministic transport codes such as TWODANT and THREEDANT (both included in the LANL DANTSYS package of deterministic codes), PARTISN /32/ (the LANL updated parallel version of DANTSYS distributed by OECD-NEA Data Bank), the sensitivity code SUSD3D (distributed by OECD-NEA Data Bank) and potentially to any transport code, through BOT3P binary output files that can be very easily interfaced. See, for example, the Westinghouse Electric Co. parallel discrete ordinates transport code RAPTOR-M3G /36/ (RApid Parallel Transport Of Radiation-Multiple 3D Geometries) and the Russian two and three-dimensional neutron, photon and charged particle discrete ordinates transport codes KASKAD-S-2.5 and KATRIN-2.0, included in the CNCSN 2009 /33/ system of deterministic codes (distributed by OECD-NEA Data Bank).

BOT3P allows users to model (X,Y), (X,Z), (Y,Z), (R,Θ) and (R,Z) geometries in two dimensions and (X,Y,Z) and (R,Θ,Z) geometries in three dimensions.
BOT3P was systematically and successfully used to prepare the geometrical models in deterministic transport calculations dedicated to the analysis of complex neutron shielding and criticality benchmarks. Moreover BOT3P was properly employed to generate the (R,Θ,Z) geometrical models in power reactor applications, such as for example in the Westinghouse AP1000 internals heating rate distribution calculations with the TORT code, performed by Ansaldo Nucleare, and in the Westinghouse IRIS (International Reactor Innovative and Secure) shielding and pressure vessel dosimetry calculations with the TORT code, performed by ENEA.

The importance to update the methodologies and modeling options implemented in this code system is due to the fact that BOT3P has got world-wide diffusion and is currently used both in many foreign research institutes and in important industrial organizations such as, for example, Westinghouse Electric Co. and Ansaldo Nucleare. BOT3P Version 5.3 /13/ is currently available from both OECD-NEA Data Bank and ORNL-RSICC with the following designations:

- NEA-1678 BOT3P-5.3: BOT3P-5.3, 3D Mesh Generator and Graphical Display of Geometry for Radiation Transport Codes, Display of Results.

- RSICC CODE PACKAGE PSR-530: BOT3P-5.3: Code System for 2D and 3D Mesh Generation and Graphical Display of Geometry and Results for Radiation Transport Codes.