Agenzia nazionale per le nuove tecnologie,
l'energia e lo sviluppo economico sostenibile

MINISTERO DELLO SVILUPPO ECONOMICO

Ricerca di Sistema elettrico

VITJEFF32.BOLIB - An ENEA-Bologna Fine-Group Coupled (199 n + 42 γ) Cross Section Library in AMPX Format Based on JEFF-3.2 Data

M. Pescarini, R. Orsi, M. Frisoni

Report RdS/PAR2014/125

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M. PESCARINI, R. ORSI, R. FRISONI - ENEA

Settembre 2015

Report Ricerca di Sistema Elettrico
Accordo di Programma Ministero dello Sviluppo Economico - ENEA
Piano Annuale di Realizzazione 2014
Area: Produzione di energia elettrica e protezione dell'ambiente
Progetto: Sviluppo competenze scientifiche nel campo della sicurezza nucleare e collaborazione ai programmi internazionali per il nucleare di IV Generazione
Linea: Sviluppo competenze scientifiche nel campo della sicurezza nucleare
Obiettivo:Studi ed analisi di sicurezza e sostenibilità
Responsabile del Progetto: Felice De Rosa, ENEA

Titolo

VITJEFF32.BOLIB - An ENEA-Bologna Fine-Group Coupled (199 n + 42 γ) Cross Section Library in AMPX Format Based on JEFF-3.2 Data

Descrittori

Tipologia del documento: Rapporto tecnico

Collocazione contrattuale: Accordo di programma ENEA-MSE su sicurezza nucleare e reattori di IV generazione

Argomenti trattati: Fisica nucleare, dati nucleari, fisica dei reattori nucleari

Sommario

The ENEA-Bologna Nuclear Data Group produced the VITJEFF32.BOLIB multi-group coupled (199 n + 42 γ) cross section library in AMPX format, based on the OECD-NEA Data Bank JEFF-3.2 evaluated nuclear data library. The generation of the VITJEFF32.BOLIB library for nuclear fission applications was conceived as an European counterpart of the ORNL VITAMIN-B7 library based on ENDF/B-VII.0 data. The present library has the same neutron/photon energy group structure and general features as the former ORNL VITAMIN-B6 reference library and was produced using similar data processing methodologies, based on the NJOY-2012.53 and SCAMPI nuclear data processing systems. VITJEFF32.BOLIB is a pseudo-problem-independent library based on the Bondarenko (f-factor) method for the treatment of neutron resonance self-shielding and temperature effects. The library contains 184 standard (not bound) nuclides singularly processed at 4 temperatures (300, 600, 1000 and 2100 K) and at 11 background cross sections. Thermal scattering cross sections were processed at all the temperatures available in the JEFF-3.2 thermal scattering law data file for 6 additional bound nuclides: H-1 in light water, H-1 in polyethylene, H-1 in zirconium hydride, H-2 in heavy water, C in graphite and Be in beryllium metal. From VITJEFF32.BOLIB it is possible to generate, through the ENEA-Bologna 2007 Revision of SCAMPI, collapsed working libraries of self-shielded cross sections in AMPX or FIDO-ANISN format for LWR applications.

Note

Authors: Massimo PESCARINI, Roberto ORSI, Manuela FRISONI

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Massimo PESCARINI, Roberto ORSI, Manuela FRISONI

July 2015

1 - INTRODUCTION

The ENEA-Bologna Nuclear Data Group produced a multi-group coupled neutron and photon cross section library in AMPX format for nuclear fission applications, based on the OECD-NEA Data Bank JEFF-3.2 /1/ /2/ /3/ /4/ /5/ evaluated nuclear data library. The result of this effort is the present VITJEFF32.BOLIB library, which has the same neutron and photon energy group structure (199 neutron groups + 42 photon groups) and general basic features as the former ORNL DLC-184/VITAMIN-B6 /6/ reference library in AMPX format, based on the US ENDF/B-VI Release 3 /7/ evaluated nuclear data library. The generation of the present library took into account the experience accumulated by the ENEA-Bologna Nuclear Data Group in the data processing and testing of the previously generated VITJEFF311.BOLIB /8/, VITENDF70.BOLIB /9/, VITJEFF31.BOLIB /10/ and VITJEF22.BOLIB /11/ similar libraries in AMPX format, respectively based on the JEFF-3.1.1 /12/, ENDF/B-VII.0 /13/, JEFF-3.1 /14/ and JEF-2.2 /15/ evaluated nuclear data libraries. The production of the VITJEFF32.BOLIB library intends to propose to the users of the JEFF-3.2 nuclear data a VITAMIN-B6-type library, i.e., a fine-group pseudo-problem-independent cross section library based on the Bondarenko /16/ (f-factor) method for the treatment of neutron resonance self-shielding and temperature effects. For "pseudo-problem-independent multi-group library" is understood that the library is prepared with enough detail in energy, temperatures and neutron resonance self-shielding so as to be applicable to a wide range of physical systems.

The VITJEFF32.BOLIB library was generated through an updated automatic calculation procedure based on the LANL NJOY-2012.53 /17/ nuclear data processing system, with the updating "upnea053", and the ENEA-Bologna 2007 Revision /18/ of the ORNL SCAMPI /19/ nuclear data processing system. In particular this automatic procedure, developed originally at the ENEA-Bologna Nuclear Data Group with the fundamental contribution of a former specialist of the State Scientific Center of the Russian Federation Institute for Physics and Power Engineering of Obninsk (SSC RF IPPE-Obninsk), permits to produce quickly large group-wise cross section libraries in AMPX format with the potential of generating, through further proper data processing with the ENEA-Bologna 2007 Revision of the SCAMPI system, broad-group working libraries of collapsed and self-shielded cross sections in AMPX or FIDO-ANISN format for different applications. Concerning this, the ENEA-Bologna Nuclear Data Group generated recently the BUGJEFF311.BOLIB /20/ and BUGENDF70.BOLIB /21/ broad-group coupled neutron and photon working cross section libraries in FIDO-ANISN /22/ format, through problem-dependent cross section collapsing of the VITJEFF311.BOLIB and VITENDF70.BOLIB libraries respectively. In particular

the BUGJEFF311.BOLIB and the BUGENDF70.BOLIB working libraries adopt the neutron and photon energy group structure (47 neutron groups + 20 photon groups) of the former ORNL DLC-0185/BUGLE-96 /6/ similar reference library derived from VITAMIN-B6 and they are specifically dedicated to LWR shielding and pressure vessel dosimetry applications.

Finally, the VITJEFF32.BOLIB library was extensively tested on many thermal, intermediate and fast neutron spectrum criticality safety benchmark experiments.

1.1 - Background

In recent years, the multi-dimensional deterministic transport codes using group-wise cross section libraries extended their practical simulation capability to an enlarged variety of nuclear systems, characterized by different neutron spectra and high geometrical complexity. In particular the three-dimensional (3D) discrete ordinates (S_N) codes, like for example TORT /23/ /24/, increased their competitiveness with respect to the corresponding 3D Monte Carlo stochastic codes, as for example MCNP /25/ /26/. Comparable or even more convenient performances in terms of CPU times were in fact obtained with the same calculation precision, similar description capability of complex geometries and suitable simulation of different neutron and photon spectral conditions. Various factors concurred, in particular, to determine the increased flexibility and convenience in the practical use of the 3D discrete ordinates codes: the impressive increased performance of modern computers, innovative general-purpose fine-group cross section libraries with upscatter cross sections and new ancillary pre/post-processor systems of programs, dedicated to simplify and to strengthen the preparation and the graphical verification of the input of the geometrical model.

About the availability of innovative fine-group libraries, for example, the interesting features of the VITAMIN-B6 /6/ library must be underlined. Unlike similar previous libraries as VITAMIN-E /27/, VITAMIN-C /28/ or VITAMIN-J /29/, VITAMIN-B6 introduced fine-group discretization (more than 30 neutron groups) in the thermal neutron energy region below about 5 eV, including upscatter cross sections. This has the potential of treating with precision, together with the present fast calculation performances, problems where a rigorous description of the thermal neutron spectrum is essential. This is specifically requested, for example, in the case of the boron neutron capture therapy (BNCT) medical applications /30/ or when it is necessary to calculate (see /31/) the thermal neutron and photon radiation damage, as emerged for some material testing reactors (MTRs) /32/ and light water reactors (LWRs) /33/ /34/. The ENEA-Bologna Nuclear Data Group contributed, in particular, in this sector with the following libraries, freely distributed by OECD-NEA Data Bank: VITJEFF311.BOLIB /8/, VITENDF70.BOLIB /9/ VITJEFF31.BOLIB /10/ and VITJEF22.BOLIB /11/ in AMPX format together with MATJEFF31.BOLIB /35/ and MATJEF22.BOLIB /36/ in MATXS format. The VITJEF311.BOLIB library is exclusively based on the on the OECD-NEA Data Bank JEFF-3.1.1 /12/ (see also /14/ and /37/) evaluated nuclear data library whereas VITENDF70.BOLIB is based on the US ENDF/B-VII.0 /13/ evaluated nuclear data library. VITJEFF31.BOLIB and MATJEFF31.BOLIB (see also /38/) are respectively based on the OECD-NEA Data Bank JEFF-3.1 /14/ evaluated nuclear data library (VITJEFF31.BOLIB) and on both the JEFF-3.1 and JEFF-3.1.1 evaluated nuclear data libraries (MATJEFF31.BOLIB). Finally VITJEF22.BOLIB and MATJEF22.BOLIB are based (see also /39/), in particular, on the OECD-NEA Data Bank JEF-2.2 /15/ evaluated nuclear data library.

At present, the availability of the VITJEFF32.BOLIB library permits to obtain derived working libraries of collapsed and self-shielded cross sections, through the ENEA-Bologna 2007 Revision /18/ of the SCAMPI /19/ nuclear data processing 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 converted into the AMPX or the FIDO-ANISN /22/ format. The cross sections in AMPX format can be used by the XSDRNPM one-dimensional (1D) discrete ordinates transport code, included in the SCAMPI system. The cross sections in FIDO-ANISN format can be used by the discrete ordinates transport codes included in the following US packages of deterministic codes: the ORNL DOORS-3.2 /24/ system (including the ANISN-ORNL 1D code, the DORT 2D code and the TORT 3D code), the LANL PARTISN-5.97 /40/ 3D parallel system and the ATTILA /41/ 3D commercial code with unstructured spatial grids (finite elements). Moreover the cross sections in FIDO-ANISN format can be read by the discrete ordinates transport codes of the Russian package CNCSN 2009 /42/, including the ROZ-6.6 1D code, the KASKAD-S-2.5 (serial) and KASKAD-S-3.0 (parallel multi-threaded) 2D codes and the KATRIN-2.0 (serial) and KATRIN-2.5 (parallel multi-threaded) 3D codes. Moreover the cross sections in FIDO-ANISN format are used by the ORNL MORSE /43/ 3D Monte Carlo code.

Concerning the possibility to describe very complicated geometries requiring 3D spatial analyses, it is underlined that, up to recent times, only 3D Monte Carlo codes could obtain satisfactory results with high calculation precision. At present, with the recent introduction and availability of new pre/post-processor systems (e.g., the ENEA-Bologna BOT3P /44/ /45/ /46/ /47/ and the Japanese TORTWARE /48/ systems) of ancillary programs dedicated to the multi-dimensional deterministic transport codes for the automatic generation and graphical verification of the spatial mesh grids of the geometrical model, the simulation capability of complex geometries with the multi-dimensional discrete ordinates transport codes increased dramatically. This induced, obviously, an increased interest to give more options in terms of updated and flexible group-wise cross section library availability. The performance of the three-dimensional discrete ordinates transport codes can be now highly competitive with that of the 3D Monte Carlo codes.

About the cited pre-post-processor ancillary programs, the ENEA-Bologna Nuclear Data Group originally developed the BOT3P system (freely distributed by OECD-NEA Data Bank and ORNL-RSICC), which was extensively tested on neutron shielding benchmark integral experiment calculations /49/ /50/ /51/ /52/ /53/ /54/ /55/ with the DORT 2D and TORT 3D codes. The BOT3P system, based on combinatorial geometry algorithms, was initially dedicated to the DORT and TORT discrete ordinates transport codes of the DOORS system but it is now easily possible to generate automatically detailed spatial mesh grids 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.
Two meaningful applications confirmed, in particular, the flexibility and the performance of BOT3P supporting the DORT and TORT codes: 1) 2D and 3D analyses /56/ in Cartesian geometry of PWR fuel assemblies, with a very fine approximated description of the cylindrical fuel pins and 2) heavy 3D (about 2.0×10^6 spatial cells) fixed source calculations /57/ in cylindrical geometry, addressed to obtain the heating rate distribution in the internals of a large Westinghouse AP1000 pressurized water reactor (PWR).

Concerning the deterministic codes, it is really an upsetting fact that the 3D deterministic transport codes currently cannot be fully used for the scarce free availability (see /58/) of broad-group working libraries (as for example /20/ and /21/) 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 /57/ or even in the development /59/ of the 3D deterministic codes. Moreover they directly generate /60/, for example, 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. It is underlined, in particular, that the 3D deterministic codes applied, for example, 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.

Taking into account the previous notes, it is considered important (see /58/), in general, to update and to extend further the availability of the fine-group multi-purpose cross section libraries dedicated to the simulations of nuclear fission systems with discrete ordinates codes. As already mentioned, starting from these libraries, derived broad-group working cross section libraries can be generated with parameterized sets of collapsed and self-shielded cross sections for the various applications, characterized by specific compositional, geometrical, spectral and temperature conditions. It is underlined that the generation of broad-group working libraries contributes to give, in particular, a strong impulse to promote the use of the 3D discrete ordinates transport codes, like TORT, which can have convergence problems when fine-group working libraries are used with hundreds of thousands of volumetric spatial meshes, possibly needed to describe accurately complex in-core and ex-core reactor geometrical models.
In particular, an increased generation of broad-group working libraries like BUGJEFF311.BOLIB /20/ and BUGENDF70.BOLIB /21/, respectively derived /61/ (see also /62/ as preliminary work) from the VITJEFF311.BOLIB and VITENDF70.BOLIB fine-group multi-purpose libraries, would permit to extend the field of application of the modern multi-dimensional discrete ordinates deterministic codes which can continue to offer important complementary information /31/ /49/ /50/ /51/ /52/ /53/ /54/ /55/ /56/ /57/ /63/ with respect to the results obtained with the Monte Carlo codes.

Moreover, 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 /58/ that a specific interest dedicated to the generation of broad-group working cross section libraries should be promoted.

It is expected, in particular, that the multi-purpose nature of VITJEFF32.BOLIB, like the former VITAMIN-B6 reference library, will make this library useful for shielding and, potentially, for reactor physics analyses with JEFF-3.2 /1/ /2/ /3/ /4/ /5/ nuclear data.

In conclusion, during the last years, the ENEA-Bologna Nuclear Data Group 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. Six fine-group cross section libraries /8/ /9/ /10/ /11/ /35/ /36/ and two broad-group working cross section libraries /20/ /21/ for nuclear fission applications were generated and are presently freely distributed by OECD-NEA Data Bank and/or ORNL-RSICC.

2. A pre/post-processor system /44/ /45/ /46/ /47/ 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 /49/ /50/ /51/ /52/ /53/ /54/ /55/ were performed also within the activities /53/ of the OECD-NEA Nuclear Science Committee TFRDD Task Force /31/ on nuclear fission reactor ageing problems.

4. The whole set of the IRDF-2002 /64/ dosimetry cross sections was processed /65/ in the 47 neutron group structure of the BUGLE-96 /6/ cross section library using a flat neutron spectrum and neutron 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 respectively included in the packages of the BUGJEFF311.BOLIB and BUGENDF70.BOLIB libraries.

1.2 - JEFF-3.2 Evaluated Nuclear Data Library

The VITJEFF32.BOLIB library is based on the OECD-NEA Data Bank JEFF-3.2 general purpose evaluated nuclear data library which was released on March 5, 2014. It contains incident neutron data for 472 nuclides or elements from 1-H-1 to 100-Fm-255. The JEFF project is a collaborative effort among the member countries of the OECD-NEA Data Bank to develop a reference evaluated 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. The JEFF-3.2 various libraries store all data in the internationally-accepted ENDF-6 /66/ format.

The JEFF-3.2 thermal scattering data, available for all important moderator and structural materials, remained unchanged with respect to the corresponding data in the JEFF-3.1.2, JEFF-3.1.1 and JEFF-3.1 previous evaluated nuclear data libraries. 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. 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 LANL NJOY /67/ nuclear data processing system to obtain thermal scattering data that are accurate over a wider range of energy and momentum transfer.

At present a dedicated document/report describing organically in detail the content, the features and the specific updatings of the various files is not yet available although it is foreseen to be published in 2016. On the other hand, for the moment, several OECD-NEADB JEF/DOCs /1/ /2/ /3/ /4/ /5/ are available on the matter and give partial information on the JEFF-3.2 evaluated data library and its performance.

1.3 - Cross Section Processing and Testing

The calculation approach used to produce the VITJEFF32.BOLIB fine-group library is consistent with the recommendations contained in 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) /68/). The previously cited ANS document recommends, in particular, the use of VITAMIN-B6 /6/ as a reference library of group-averaged data for radiation protection and shielding calculations dedicated to light water reactor plants. Following, in general, the same data processing methodology based on NJOY and SCAMPI, the VITJEFF32.BOLIB library adopts, in particular, the same neutron and photon fine-group structures and weighting spectra used to generate VITAMIN-B6.

The nuclear data processing methodology followed in ENEA-Bologna employs both the following modular nuclear data processing systems, i.e., the LANL NJOY-2012.53 /17/ system and the ENEA-Bologna 2007 Revision /18/ of the ORNL SCAMPI /19/ system. Several modules of NJOY were used to process the neutron interaction, the photon production and the photon interaction data from the JEFF-3.2 formats to a group-averaged format.
In order to process correctly modern evaluated nuclear data like the JEFF-3.2 data files, it was necessary to develop an updated and corrected version of the SCAMPI system, originally developed at ORNL from the AMPX-77 /69/ system and already employed at ORNL to generate the VITAMIN-B6 data in the AMPX format. In particular, the previously cited 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-2012.53 nuclear data processing system, to translate the intermediate NJOY file into the AMPX master format for the VITJEFF32.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.

A detailed description of the data processing performed for the generation of the VITJEFF32.BOLIB fine-group library is given in Chapter 2 while the results of a validation of the library on many thermal, intermediate and fast neutron spectrum criticality safety benchmark experiments are presented in Chapter 3.

2 - LIBRARY SPECIFICATIONS

The VITJEFF32.BOLIB library is a fine-group pseudo-problem-independent cross section library, based on the Bondarenko /16/ (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-3.2 /1/ /2/ /3/ /4/ /5/ evaluated nuclear data library. It has the same neutron and photon energy group structure (199 neutron groups + 42 photon groups) and general basic features as the ORNL DLC-184/VITAMIN-B6 /6/ American library in AMPX format, based on the ENDF/B-VI Release 3 /7/ US evaluated nuclear data library.

The VITJEFF32.BOLIB library was generated through an updated automatic calculation procedure based on the LANL NJOY-2012.53 /17/ nuclear data processing system, with the updating "upnea053", and the ENEA-Bologna 2007 Revision /18/ of the ORNL SCAMPI /19/ nuclear data processing system. VITJEFF32.BOLIB was extensively tested on many thermal, intermediate and fast neutron spectrum criticality safety 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 VITJEFF32.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 VITJEFF32.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 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 (see /19/), used to generate VITAMIN-B6 and VITJEF22.BOLIB /11/, it is possible to obtain only the prompt component of the fission neutron spectrum.

At present, the availability of the VITJEFF32.BOLIB library permits to obtain derived working libraries of collapsed and 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 /22/ 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 /69/ and SCAMPI nuclear data processing systems, or in the ORNL SCALE-6 /70/ 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 /24/ system, by the PARTISN /40/ 3D

parallel time-dependent discrete ordinates system and, finally, by the MORSE /43/ 3D Monte Carlo stochastic code.

2.1 - Name

The present fine-group pseudo-problem-independent library is designated as VITJEFF32.BOLIB.
"VIT" suggests that the main features of the library are similar to those of the ORNL VITAMIN-B6 /6/ library and to the ENEA fine-group libraries /8/ /9/ /10/ /11/ in AMPX format with the same neutron/photon energy group structure. The "JEFF32" designation conveniently reflects the origin of the evaluated data: the JEFF-3.2 evaluated nuclear data library /1/ /2/ /3/ /4/ /5/. 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 190 cross section files, derived from the JEFF-3.2 /1/ /2/ /3/ /4/ /5/ evaluated nuclear data library, was processed for the VITJEFF32.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-3.2 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 two data files (C-nat and V-nat) correspond to evaluated natural elements whereas the other ones correspond to single isotope evaluated data files.

The Bondarenko /16/ (f-factor) method was used for handling neutron resonance self-shielding and temperature effects. As for VITAMIN-B6 /6/, all the 184 standard (not bound) nuclides were processed at the same 4 values of temperature (300, 600, 1000 and 2100 K). Concerning the background cross section σ_0 values used, a conservative choice was performed with respect to both VITAMIN-B7 /71/ and VITAMIN-B6 ORNL libraries: 11 values of background cross section σ_0 (0.01, 1, 10, 50, 100, 300, 1000, 1.0E+04, 1.0E+05,1.0E+06 and 1.0E+10 barns) were used. This approach (the same background cross section set for each standard nuclide) was more similar to those employed in the VITAMIN-B7 generation but it was included, in addition to the values used for the data processing of VITAMIN-B7, the 0.01 barns value for σ_0. In consequence of this choice, it is underlined in particular that, with respect to the σ_0 values used in the generation of the Fe-56 processed files in the VITAMIN-B7 (AMPX format), VITAMIN-B6 (AMPX format), VITJEF22.BOLIB /11/ (AMPX format) and MATJEF22.BOLIB /36/ (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 VITJEFF32.BOLIB. The same additional σ_0 value was included in the data processing of the VITJEFF311.BOLIB /8/, VITENDF70.BOLIB /9/ and VITJEFF31.BOLIB /10/ similar libraries in AMPX format and in the MATJEFF31.BOLIB /35/ library in MATXS format. This additional σ_0 numerical value improves (see also /72/) 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 /6/, /20/ and /21/).

Thermal scattering cross sections were produced for six additional bound nuclides which were processed at all the temperatures (see TAB. 2.2) available in the JEFF-3.2 thermal scattering law data file which is the same included in the JEFF-3.1.2, JEFF-3.1.1 and JEFF-3.1 evaluated nuclear data libraries: 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.

Finally 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-ray production data in some JEFF-3.2 evaluated data files. Concerning this, it is recommended to verify carefully if the JEFF-3.2 data files of the nuclides involved in the calculations include gamma-ray production data (see TAB. 2.1).

TAB. 2.1

JEFF-3.2 Nuclides Processed for the VITJEFF32.BOLIB Library.

Z	Nuclide	JEFF-3.2 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	YES
	O-18	831	8018	YES
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

TAB. 2.1 Continued

JEFF-3.2 Nuclides Processed for the VITJEFF32.BOLIB Library.

Z	Nuclide	JEFF-3.2 MAT	AMPX Identifier	Gamma-Ray Production
	Ti-50	2237	22050	YES
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
30	Zn-64	3025	30064	YES
	Zn-66	3031	30066	YES
	Zn-67	3034	30067	YES
	Zn-68	3037	30068	YES
	Zn-70	3043	30070	YES
31	Ga-69	3125	31069	YES
	Ga-71	3131	31071	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	YES
	Ag-109	4731	47109	YES
48	Cd-106	4825	48106	NO
	Cd-108	4831	48108	NO
	Cd-110	4837	48110	YES
	Cd-111	4840	48111	YES
	Cd-112	4843	48112	NO
	Cd-113	4846	48113	YES
	Cd-114	4849	48114	NO

TAB. 2.1 Continued

JEFF-3.2 Nuclides Processed for the VITJEFF32.BOLIB Library.

Z	Nuclide	JEFF-3.2 MAT	AMPX Identifier	Gamma-Ray Production
	Cd-115m	4853	48115	YES
	Cd-116	4855	48116	NO
49	In-113	4925	49113	YES
	In-115	4931	49115	YES
50	Sn-112	5025	50112	NO
	Sn-114	5031	50114	NO
	Sn-115	5034	50115	NO
	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	YES
	Sn-123	5058	50123	NO
	Sn-124	5061	50124	YES
	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	YES
	Eu-154	6334	63154	YES
	Eu-155	6337	63155	YES
64	Gd-152	6425	64152	YES
	Gd-154	6431	64154	YES
	Gd-155	6434	64155	YES
	Gd-156	6437	64156	YES
	Gd-157	6440	64157	YES
	Gd-158	6443	64158	YES
	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-180	7425	74180	YES
	W-182	7431	74182	YES
	W-183	7434	74183	YES
	W-184	7437	74184	YES
	W-186	7443	74186	YES

TAB. 2.1 Continued

JEFF-3.2 Nuclides Processed for the VITJEFF32.BOLIB Library.

Z	Nuclide	JEFF-3.2 MAT	AMPX Identifier	Gamma-Ray Production
75	Re-185	7525	75185	YES
	Re-187	7531	75187	YES
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
90	Th-230	9034	90230	NO
	Th-232	9040	90232	YES
91	Pa-231	9131	91231	YES
	Pa-233	9137	91233	YES
92	U-232	9219	92232	YES
	U-233	9222	92233	YES
	U-234	9225	92234	YES
	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	YES
	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	YES
	Am-242	9546	95242	NO
	Am-242m	9547	95601	NO
	Am-243	9549	95243	NO
96	Cm-241	9628	96241	YES
	Cm-242	9631	96242	YES
	Cm-243	9634	96243	YES
	Cm-244	9637	96244	YES
	Cm-245	9640	96245	YES
	Cm-246	9643	96246	YES
	Cm-247	9646	96247	YES
	Cm-248	9649	96248	YES

TAB. 2.2

Processed Thermal Scattering Data in the VITJEFF32.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-3.2 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 VITJEFF32.BOLIB library adopts the same neutron and photon energy group structures as the VITAMIN-B6 /6/ library with 199 neutron energy groups (see TAB. 2.3) and 42 photon energy groups (see TAB. 2.4). 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 /27/ 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 /70/ 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 VITJEFF32.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. 2.5. 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 VITJEFF32.BOLIB, through the ENEA-Bologna 2007 Revision /18/ of the SCAMPI /19/ data processing system, without having to repeat the multi-group averaging directly from the JEFF-3.2 files.

The full VITJEFF32.BOLIB library neutron energy group structure given in TAB. 2.3 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 /29/ (an OECD-NEA Data Bank library based on the VITAMIN-C /28/ 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 VITJEFF32.BOLIB library photon energy group structure given in TAB. 2.4 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. 2.3

Neutron Group Energy Boundaries for the VITJEFF32.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. 2.3 Continued

Neutron Group Energy Boundaries for the VITJEFF32.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. 2.3 Continued

Neutron Group Energy Boundaries for the VITJEFF32.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. 2.3 Continued

Neutron Group Energy Boundaries for the VITJEFF32.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. 2.3 Continued

Neutron Group Energy Boundaries for the VITJEFF32.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. 2.4

Photon Group Energy Boundaries for the VITJEFF32.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. 2.5

VITJEFF32.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 VITJEFF32.BOLIB library cross sections are the same as those employed in the generation of the VITAMIN-B6 /6/ 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 /17/ system. The breakpoint energies for the 3-region spectrum are similar to those used in VITAMIN-C /28/. 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)		
$W_1(E) = C_1 E e^{-E/kT}$	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)		
$W_3(E) = C_3 E^{1/2} e^{-E/\theta}$	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. 2.6 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 photon weighting function is shown in FIG. 2.2 and listed in TAB. 2.7 in a 42 group representation.

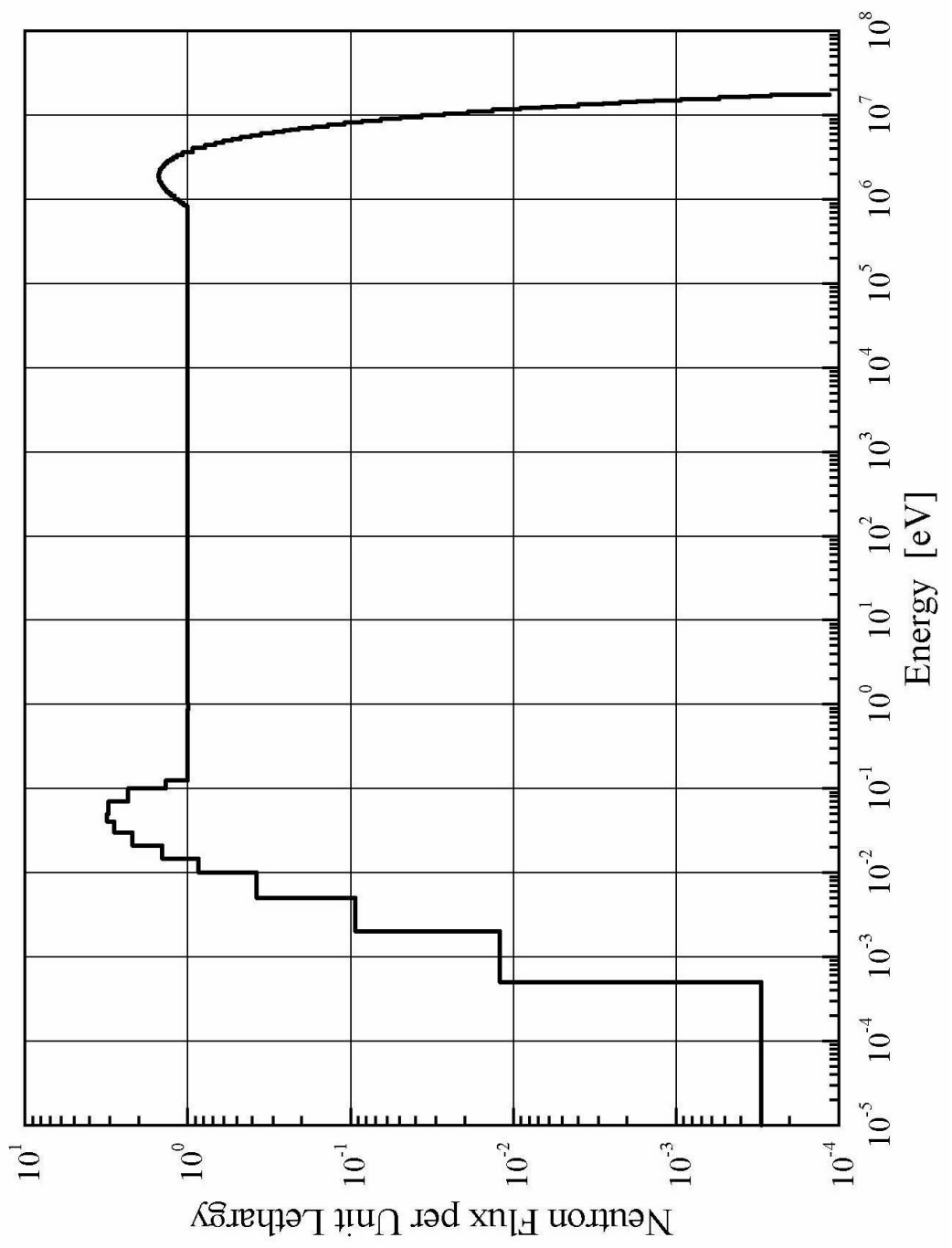


FIG. 2.1 199 Group Representation of Standard Weighting Spectrum Used to Create VITJEFF32.BOLIB Neutron Cross Sections from JEFF-3.2 Pointwise Data.

TAB. 2.6

Neutron Energy Weighting Spectrum for the VITJEFF32.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. 2.6 Continued

Neutron Energy Weighting Spectrum for the VITJEFF32.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		

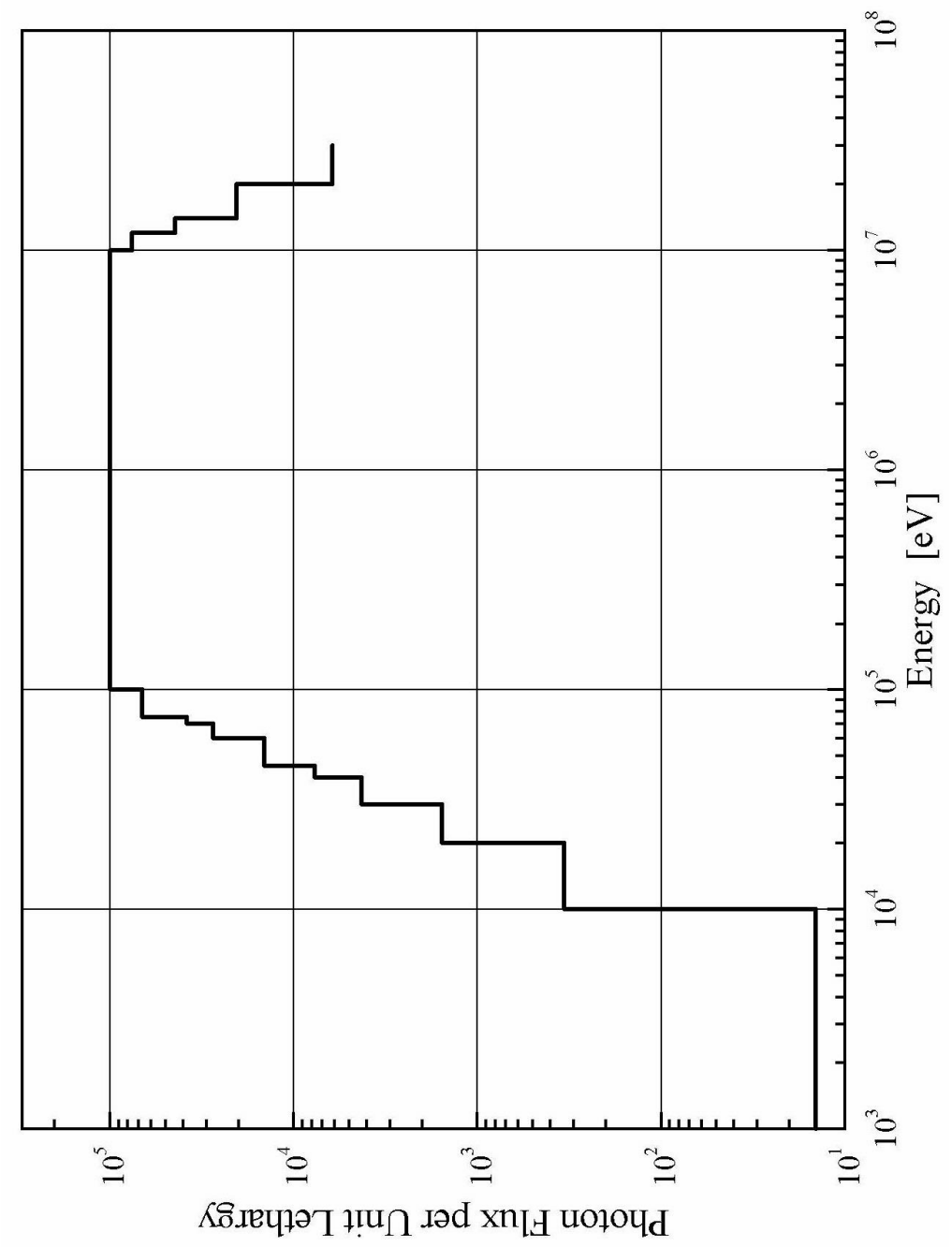


FIG. 2.2 42 Group Representation of Standard Weighting Spectrum Used to Create VITJEFF32.BOLIB Photon Cross Sections from JEFF-3.2 Pointwise Data.

TAB. 2.7

Photon Energy Weighting Spectrum for the VITJEFF32.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=30 (zinc) and P_5 for the remainder of the nuclides. In particular, the previous values corresponding to L=ℓ-max are the maximum order of the Legendre polynomial (P_ℓ) expansion of the scattering cross section matrix, available for the specific nuclide.
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 /6/ library user's manual. For the same nuclide, an identical order of scattering for both neutrons and photons was originally adopted in the generation of the VITAMIN-B6 cross sections and similarly was done in the processing of the ENEA libraries VITJEFF32.BOLIB, VITJEFF311.BOLIB /8/, VITENDF70.BOLIB /9/, VITJEFF31.BOLIB /10/, VITJEFF22.BOLIB /11/, MATJEFF31.BOLIB /35/ and MATJEF22.BOLIB /36/.

2.6 - Convergence Parameters

The following numerical values of the fractional error tolerances were chosen as input parameters in NJOY /17/ to generate the libraries VITJEFF32.BOLIB, VITJEFF311.BOLIB /8/, VITENDF70.BOLIB /9/, VITJEFF31.BOLIB /10/ and MATJEFF31.BOLIB /35/: 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 /6/, VITJEFF22.BOLIB /11/ and MATJEF22.BOLIB /36/, 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-2012-53 /17/ nuclear data processing system and the ENEA-Bologna 2007 Revision /18/ 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 VITJEFF32.BOLIB library. The following modules of NJOY were used to process neutron interaction (n-n), photon production (n-γ) and photon interaction (γ-γ) data into the GENDF format, from the JEFF-3.2 incident neutron and photo-atomic data in ENDF-6 /66/ 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 VITJEFF32.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. 2.8. A schematic diagram illustrating the VITJEFF32.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. 2.8

Modules from the NJOY-2012.53 and SCAMPI
Nuclear Data Processing Systems Used to Process VITJEFF32.BOLIB.

NJOY-2012.53 System

Module	Function
MODER	Converts between ENDF 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 VITJEFF32.BOLIB Library in AMPX Format from JEFF-3.2.

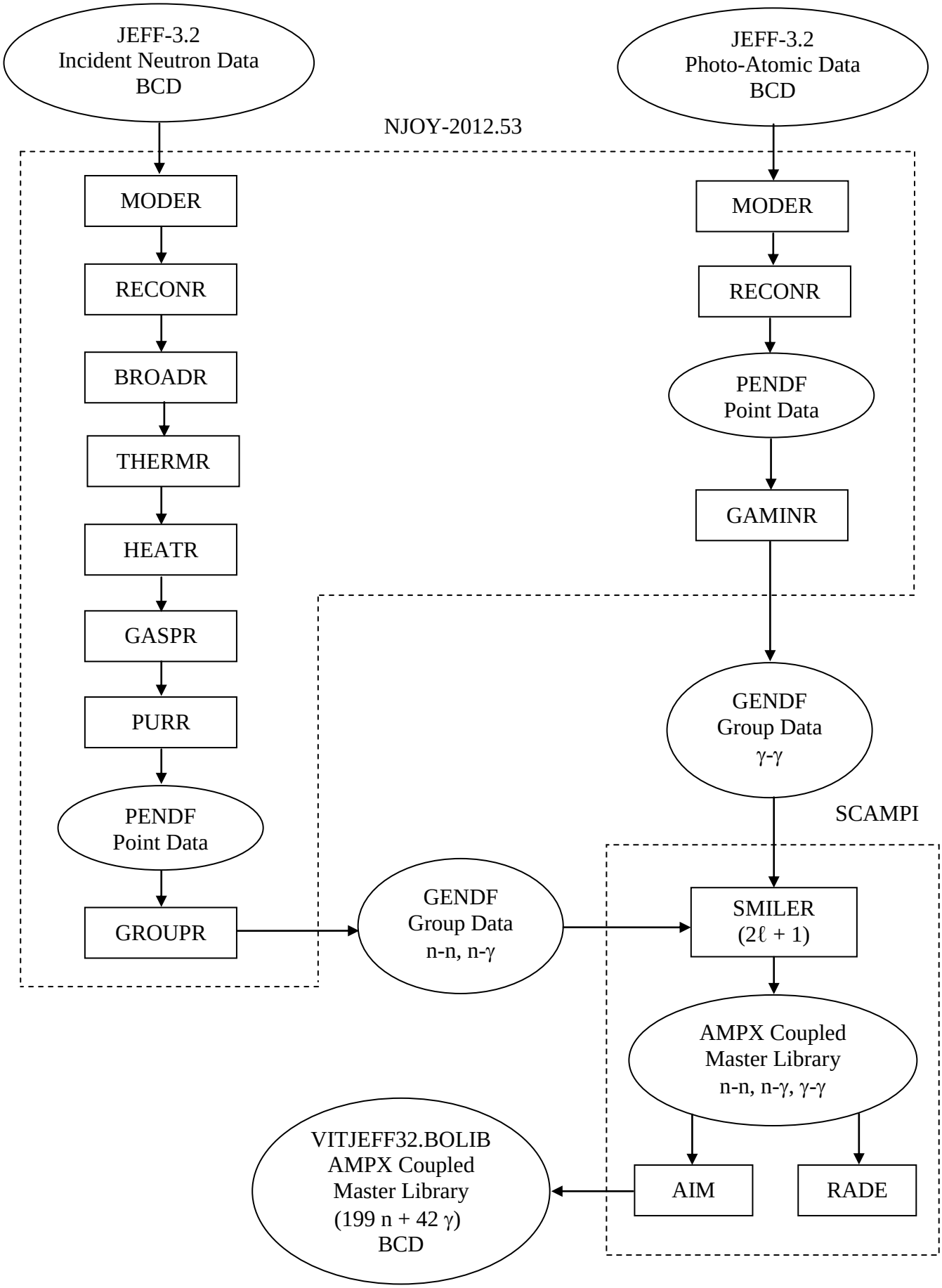
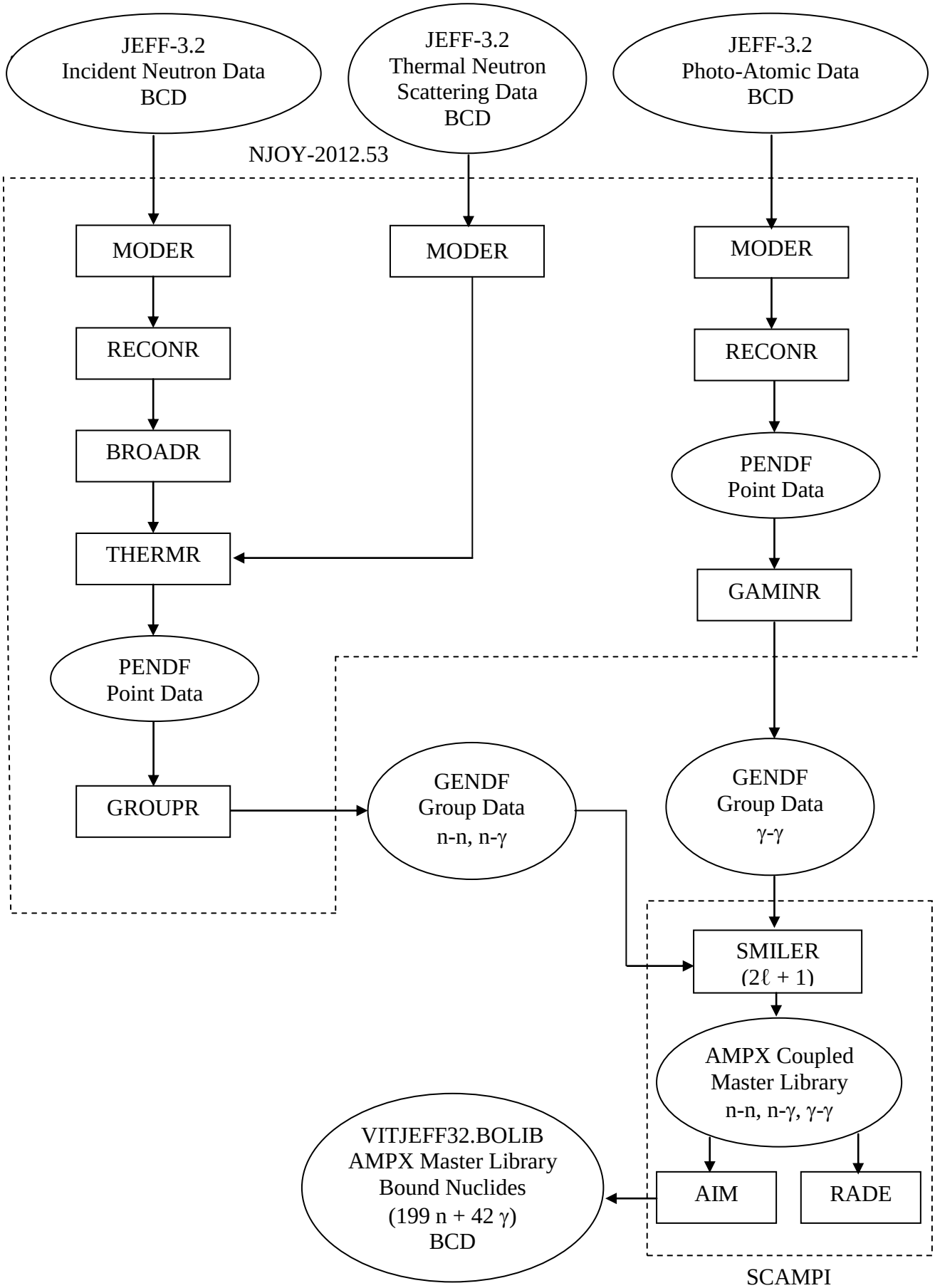


FIG. 2.4 Procedure for Generating the VITJEFF32.BOLIB Bound Nuclides in AMPX Format from JEFF-3.2.



2.8 - Response Functions

At present only the following "response" functions are included in tabulated form in the VITJEFF32.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 /18/ 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 neutron fission spectra for the U-235, U-238 and Pu-239 nuclides are reported in TAB. 2.9.

A 199 group representation of the U-235, U-238 and Pu-239 total neutron fission spectra are shown in FIG. 2.5.

TAB. 2.9

VITJEFF32.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	4.20898E-06	3.61717E-06	7.84742E-06
2	1.7332E+07	1.71773E-06	1.47693E-06	3.01501E-06
3	1.6905E+07	2.35267E-06	2.02453E-06	4.06127E-06
4	1.6487E+07	7.43665E-06	6.41025E-06	1.25197E-05
5	1.5683E+07	1.31245E-05	1.13432E-05	2.14373E-05
6	1.4918E+07	9.74240E-06	8.43858E-06	1.55874E-05
7	1.4550E+07	1.26345E-05	1.09619E-05	1.99355E-05
8	1.4191E+07	1.63007E-05	1.41676E-05	2.53743E-05
9	1.3840E+07	2.07262E-05	1.80468E-05	3.18429E-05
10	1.3499E+07	5.95332E-05	5.19830E-05	8.96663E-05
11	1.2840E+07	4.14361E-05	3.62718E-05	6.12915E-05
12	1.2523E+07	5.14489E-05	4.51184E-05	7.51761E-05
13	1.2214E+07	1.41493E-04	1.24444E-04	2.02992E-04
14	1.1618E+07	2.09587E-04	1.85044E-04	2.93991E-04
15	1.1052E+07	3.03902E-04	2.69390E-04	4.17355E-04
16	1.0513E+07	4.31111E-04	3.83615E-04	5.80062E-04
17	1.0000E+07	5.97669E-04	5.33760E-04	7.88494E-04
18	9.5123E+06	8.13778E-04	7.29486E-04	1.05356E-03
19	9.0484E+06	1.08729E-03	9.78181E-04	1.38269E-03
20	8.6071E+06	1.42701E-03	1.28846E-03	1.78426E-03
21	8.1873E+06	1.84061E-03	1.66819E-03	2.26485E-03
22	7.7880E+06	2.33457E-03	2.12408E-03	2.82967E-03
23	7.4082E+06	2.91330E-03	2.66132E-03	3.48185E-03
24	7.0469E+06	3.57810E-03	3.28186E-03	4.22104E-03
25	6.7032E+06	1.35520E-03	1.24625E-03	1.58593E-03
26	6.5924E+06	2.97257E-03	2.73908E-03	3.45811E-03
27	6.3763E+06	5.16198E-03	4.77214E-03	5.94882E-03
28	6.0653E+06	6.07320E-03	5.63605E-03	6.92553E-03
29	5.7695E+06	7.05806E-03	6.57441E-03	7.96866E-03
30	5.4881E+06	8.10432E-03	7.57599E-03	9.06257E-03
31	5.2205E+06	9.20618E-03	8.63551E-03	1.02018E-02
32	4.9659E+06	1.03498E-02	9.73712E-03	1.13709E-02
33	4.7237E+06	1.15313E-02	1.08787E-02	1.25654E-02
34	4.4933E+06	2.66681E-02	2.52669E-02	2.87275E-02
35	4.0657E+06	3.14593E-02	2.99591E-02	3.34082E-02
36	3.6788E+06	3.60594E-02	3.45086E-02	3.77881E-02
37	3.3287E+06	1.96183E-02	1.88422E-02	2.03719E-02
38	3.1664E+06	2.06024E-02	1.98371E-02	2.12708E-02
39	3.0119E+06	2.14577E-02	2.07146E-02	2.20331E-02
40	2.8651E+06	2.22614E-02	2.15481E-02	2.27402E-02
41	2.7253E+06	2.29146E-02	2.22407E-02	2.32957E-02
42	2.5924E+06	2.34585E-02	2.28339E-02	2.37444E-02
43	2.4660E+06	1.58767E-02	1.54922E-02	1.60164E-02
44	2.3852E+06	4.01794E-03	3.92555E-03	4.04686E-03
45	2.3653E+06	3.99931E-03	3.90900E-03	4.02561E-03
46	2.3457E+06	8.04088E-03	7.86607E-03	8.08652E-03
47	2.3069E+06	1.61424E-02	1.58153E-02	1.62066E-02
48	2.2313E+06	2.43482E-02	2.39149E-02	2.43794E-02
49	2.1225E+06	2.43966E-02	2.40367E-02	2.43555E-02

TAB. 2.9 Continued

VITJEFF32.BOLIB Library Total Neutron Fission Spectra for U-235, U-238 and Pu-239.

Group	Upper Energy [eV]	U-235 χ	U-238 χ	Pu-239 χ
50	2.0190E+06	2.43381E-02	2.40529E-02	2.42325E-02
51	1.9205E+06	2.41593E-02	2.39483E-02	2.39973E-02
52	1.8268E+06	2.38722E-02	2.37284E-02	2.36607E-02
53	1.7377E+06	2.34946E-02	2.34214E-02	2.32379E-02
54	1.6530E+06	2.30625E-02	2.30490E-02	2.27664E-02
55	1.5724E+06	2.25705E-02	2.26163E-02	2.22390E-02
56	1.4957E+06	2.20354E-02	2.21425E-02	2.16684E-02
57	1.4227E+06	2.13998E-02	2.15463E-02	2.10023E-02
58	1.3534E+06	2.07926E-02	2.09743E-02	2.03727E-02
59	1.2874E+06	2.01454E-02	2.03596E-02	1.97015E-02
60	1.2246E+06	1.95133E-02	1.97712E-02	1.90408E-02
61	1.1648E+06	1.88089E-02	1.90938E-02	1.83191E-02
62	1.1080E+06	3.55024E-02	3.61359E-02	3.44994E-02
63	1.0026E+06	1.39977E-02	1.42984E-02	1.35643E-02
64	9.6164E+05	1.87535E-02	1.91945E-02	1.81409E-02
65	9.0718E+05	1.53283E-02	1.57109E-02	1.48045E-02
66	8.6294E+05	1.46683E-02	1.50800E-02	1.41370E-02
67	8.2085E+05	1.39925E-02	1.44215E-02	1.34611E-02
68	7.8082E+05	1.33611E-02	1.38133E-02	1.28207E-02
69	7.4274E+05	1.27116E-02	1.31635E-02	1.21831E-02
70	7.0651E+05	1.20751E-02	1.25281E-02	1.15583E-02
71	6.7206E+05	1.14707E-02	1.19209E-02	1.09619E-02
72	6.3928E+05	1.08896E-02	1.13529E-02	1.03832E-02
73	6.0810E+05	1.03371E-02	1.08169E-02	9.83262E-03
74	5.7844E+05	9.77175E-03	1.02388E-02	9.28390E-03
75	5.5023E+05	9.22235E-03	9.67666E-03	8.75125E-03
76	5.2340E+05	8.72229E-03	9.17685E-03	8.25807E-03
77	4.9787E+05	1.59518E-02	1.68228E-02	1.50724E-02
78	4.5049E+05	1.40713E-02	1.48541E-02	1.32775E-02
79	4.0762E+05	6.41611E-03	6.79819E-03	6.03593E-03
80	3.8774E+05	6.03408E-03	6.42484E-03	5.66206E-03
81	3.6883E+05	1.08992E-02	1.16162E-02	1.02373E-02
82	3.3373E+05	9.52990E-03	1.01736E-02	8.94358E-03
83	3.0197E+05	1.02388E-03	1.09349E-03	9.60691E-04
84	2.9849E+05	3.75655E-04	4.01354E-04	3.52334E-04
85	2.9721E+05	7.87409E-04	8.41356E-04	7.38491E-04
86	2.9452E+05	2.11536E-03	2.26205E-03	1.98306E-03
87	2.8725E+05	4.02744E-03	4.31445E-03	3.77056E-03
88	2.7324E+05	7.28808E-03	7.81626E-03	6.81237E-03
89	2.4724E+05	3.27894E-03	3.51657E-03	3.06384E-03
90	2.3518E+05	3.05194E-03	3.27843E-03	2.85220E-03
91	2.2371E+05	2.84524E-03	3.05943E-03	2.65819E-03
92	2.1280E+05	2.65286E-03	2.85313E-03	2.47895E-03
93	2.0242E+05	2.47252E-03	2.65852E-03	2.30976E-03
94	1.9255E+05	2.30576E-03	2.48604E-03	2.14998E-03
95	1.8316E+05	2.15069E-03	2.32373E-03	2.00299E-03
96	1.7422E+05	1.99954E-03	2.16247E-03	1.86168E-03
97	1.6573E+05	1.86608E-03	2.01822E-03	1.73712E-03
98	1.5764E+05	1.73670E-03	1.87674E-03	1.61593E-03

TAB. 2.9 Continued

VITJEFF32.BOLIB Library Total Neutron Fission Spectra for U-235, U-238 and Pu-239.

Group	Upper Energy [eV]	U-235 χ	U-238 χ	Pu-239 χ
99	1.4996E+05	1.62111E-03	1.74973E-03	1.50648E-03
100	1.4264E+05	1.50396E-03	1.62540E-03	1.39615E-03
101	1.3569E+05	1.40044E-03	1.51552E-03	1.29883E-03
102	1.2907E+05	1.30351E-03	1.41335E-03	1.20789E-03
103	1.2277E+05	1.20907E-03	1.31137E-03	1.12052E-03
104	1.1679E+05	1.12699E-03	1.22281E-03	1.04451E-03
105	1.1109E+05	2.48626E-03	2.69563E-03	2.30530E-03
106	9.8037E+04	2.08100E-03	2.26356E-03	1.92632E-03
107	8.6517E+04	6.97378E-04	7.61979E-04	6.44834E-04
108	8.2503E+04	5.12125E-04	5.60523E-04	4.73266E-04
109	7.9499E+04	1.23954E-03	1.36392E-03	1.14444E-03
110	7.1998E+04	7.31123E-04	7.96878E-04	6.76405E-04
111	6.7379E+04	1.61469E-03	1.74431E-03	1.49511E-03
112	5.6562E+04	5.75092E-04	6.19926E-04	5.31475E-04
113	5.2475E+04	8.28718E-04	8.97649E-04	7.64949E-04
114	4.6309E+04	6.89567E-04	7.50722E-04	6.35357E-04
115	4.0868E+04	7.73353E-04	8.39595E-04	7.12510E-04
116	3.4307E+04	2.75090E-04	2.99392E-04	2.52998E-04
117	3.1828E+04	3.56294E-04	3.91393E-04	3.25916E-04
118	2.8501E+04	1.55538E-04	1.72798E-04	1.41337E-04
119	2.7000E+04	9.55276E-05	1.06323E-04	8.67074E-05
120	2.6058E+04	1.26244E-04	1.40754E-04	1.14466E-04
121	2.4788E+04	5.97923E-05	6.67658E-05	5.41624E-05
122	2.4176E+04	5.76728E-05	6.44638E-05	5.22098E-05
123	2.3579E+04	1.61061E-04	1.80382E-04	1.45625E-04
124	2.1875E+04	2.33988E-04	2.66686E-04	2.10336E-04
125	1.9305E+04	3.60892E-04	4.31490E-04	3.19396E-04
126	1.5034E+04	2.50820E-04	3.05360E-04	2.19857E-04
127	1.1709E+04	7.81338E-05	9.63239E-05	6.80227E-05
128	1.0595E+04	9.53609E-05	1.10356E-04	8.44980E-05
129	9.1188E+03	1.15839E-04	1.27262E-04	1.04028E-04
130	7.1017E+03	7.95059E-05	8.72401E-05	7.14581E-05
131	5.5308E+03	5.45786E-05	5.99328E-05	4.90157E-05
132	4.3074E+03	2.42058E-05	2.65561E-05	2.17508E-05
133	3.7074E+03	1.32902E-05	1.45908E-05	1.19346E-05
134	3.3546E+03	1.14011E-05	1.25265E-05	1.02313E-05
135	3.0354E+03	9.78460E-06	1.07373E-05	8.78866E-06
136	2.7465E+03	4.37476E-06	4.80704E-06	3.92517E-06
137	2.6126E+03	4.06908E-06	4.47582E-06	3.64775E-06
138	2.4852E+03	7.27017E-06	7.97110E-06	6.53379E-06
139	2.2487E+03	6.30358E-06	6.91996E-06	5.65912E-06
140	2.0347E+03	1.21523E-05	1.33312E-05	1.09148E-05
141	1.5846E+03	8.30066E-06	9.11471E-06	7.44869E-06
142	1.2341E+03	5.73999E-06	6.29328E-06	5.15632E-06
143	9.6112E+02	3.96903E-06	4.35105E-06	3.56411E-06
144	7.4852E+02	2.72300E-06	2.98006E-06	2.44697E-06
145	5.8295E+02	1.86936E-06	2.04617E-06	1.67881E-06
146	4.5400E+02	1.28493E-06	1.40494E-06	1.15444E-06
147	3.5357E+02	8.75676E-07	9.57810E-07	7.86260E-07

TAB. 2.9 Continued

VITJEFF32.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	6.02569E-07	6.58781E-07	5.41060E-07
149	2.1445E+02	4.16391E-07	4.54637E-07	3.74161E-07
150	1.6702E+02	2.84168E-07	3.10564E-07	2.55101E-07
151	1.3007E+02	1.95890E-07	2.13750E-07	1.76031E-07
152	1.0130E+02	1.35801E-07	1.48178E-07	1.22013E-07
153	7.8893E+01	9.31592E-08	1.01546E-07	8.37544E-08
154	6.1442E+01	6.40068E-08	6.98063E-08	5.75136E-08
155	4.7851E+01	4.37837E-08	4.75553E-08	3.94633E-08
156	3.7266E+01	2.92518E-08	3.12175E-08	2.67193E-08
157	2.9023E+01	2.02456E-08	2.17738E-08	1.83832E-08
158	2.2603E+01	1.41619E-08	1.53504E-08	1.27813E-08
159	1.7604E+01	9.77068E-09	1.06958E-08	8.74986E-09
160	1.3710E+01	6.80961E-09	7.52979E-09	6.04917E-09
161	1.0677E+01	4.78720E-09	5.34772E-09	4.21737E-09
162	8.3153E+00	3.34153E-09	3.77782E-09	2.91448E-09
163	6.4760E+00	2.33525E-09	2.67498E-09	2.01420E-09
164	5.0435E+00	1.63449E-09	1.89914E-09	1.39241E-09
165	3.9279E+00	1.14293E-09	1.34910E-09	9.60004E-10
166	3.0590E+00	8.00879E-10	9.61474E-10	6.62287E-10
167	2.3824E+00	5.69015E-10	6.94135E-10	4.63432E-10
168	1.8554E+00	4.00779E-10	4.98265E-10	3.20385E-10
169	1.4450E+00	1.31896E-10	1.66315E-10	1.03911E-10
170	1.3000E+00	1.52182E-10	1.93664E-10	1.18755E-10
171	1.1253E+00	3.82600E-11	4.89846E-11	2.96444E-11
172	1.0800E+00	3.33726E-11	4.28436E-11	2.57827E-11
173	1.0400E+00	3.29870E-11	4.24593E-11	2.54136E-11
174	1.0000E+00	9.89644E-11	1.28307E-10	7.56957E-11
175	8.7643E-01	5.88636E-11	7.70040E-11	4.45728E-11
176	8.0000E-01	8.66655E-11	1.14570E-10	6.48701E-11
177	6.8256E-01	4.06791E-11	5.43188E-11	3.00835E-11
178	6.2506E-01	6.35216E-11	8.57325E-11	4.64088E-11
179	5.3158E-01	2.06496E-11	2.80856E-11	1.49034E-11
180	5.0000E-01	5.41492E-11	7.45976E-11	3.85894E-11
181	4.1399E-01	2.83406E-11	3.94729E-11	1.98628E-11
182	3.6680E-01	2.41121E-11	3.39812E-11	1.66454E-11
183	3.2500E-01	2.76055E-11	3.94207E-11	1.87273E-11
184	2.7500E-01	2.62581E-11	3.80846E-11	1.74383E-11
185	2.2500E-01	2.04978E-11	3.02041E-11	1.33101E-11
186	1.8400E-01	1.60843E-11	2.40761E-11	1.01632E-11
187	1.5000E-01	1.12646E-11	1.71502E-11	6.93517E-12
188	1.2500E-01	1.07883E-11	1.66568E-11	6.47939E-12
189	1.0000E-01	1.22165E-11	1.92746E-11	7.07735E-12
190	7.0000E-02	7.60034E-12	1.23176E-11	4.19776E-12
191	5.0000E-02	3.60915E-12	5.91386E-12	1.91611E-12
192	4.0000E-02	3.45856E-12	5.77365E-12	1.77201E-12
193	3.0000E-02	2.96700E-12	5.01281E-12	1.45540E-12
194	2.1000E-02	2.04631E-12	3.13696E-12	9.58764E-13
195	1.4500E-02	1.35686E-12	2.14689E-12	6.06921E-13
196	1.0000E-02	1.43997E-12	2.38516E-12	6.09581E-13

TAB. 2.9 Continued

VITJEFF32.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	8.15365E-13	1.43098E-12	3.19114E-13
198	2.0000E-03	3.87036E-13	7.15470E-13	1.39778E-13
199	5.0000E-04	1.23282E-13	2.38484E-13	4.11032E-14
	Lower Energy 1.0000E-05			

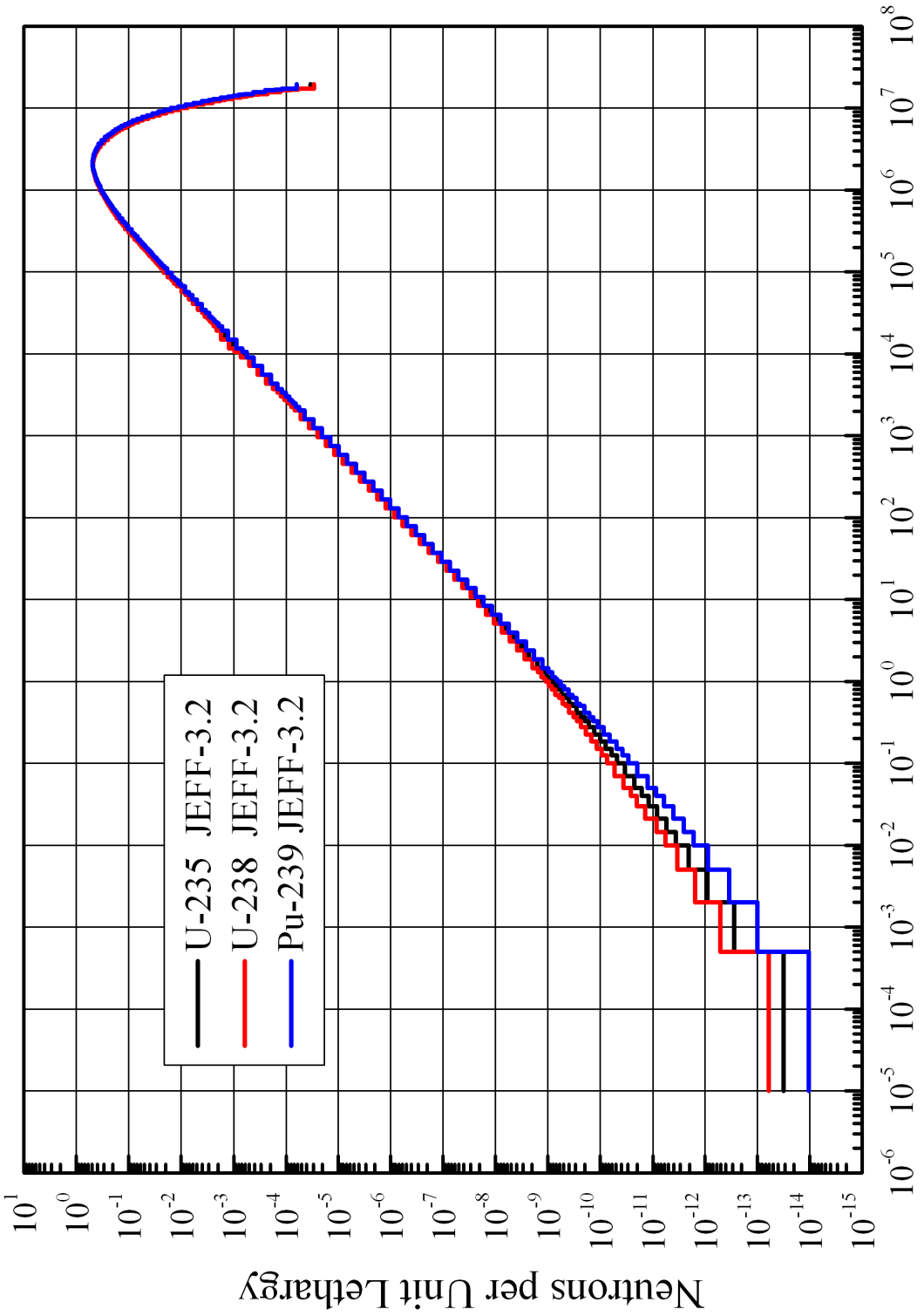


FIG. 2.5 199 Group Representation of the Total (Prompt + Delayed) Neutron Fission Spectrum for the U-235, U-238 and Pu-239 Processed Files Included in the VITJEFF32.BOLIB Library. Spectra Averaged on Incident Neutron Energies and Normalized to 1 Neutron per Fission.

3 - LIBRARY VALIDATION

3.1 - Reactor Physics Benchmarks

The VITJEFF32.BOLIB library was extensively tested on about 80 thermal, intermediate and fast neutron spectrum criticality safety benchmark experiments, taking the compositional and geometrical data for the transport calculations exclusively from the ICSBEP handbook (2004 Edition) /73/ of benchmark specifications.
The k-effective (k_{eff}) results obtained with VITJEFF32.BOLIB were compared with the results previously obtained (see /8/) in ENEA-Bologna with the VITJEFF311.BOLIB /8/ library.
The ENEA-Bologna 2007 Revision /18/ of the SCAMPI /19/ system was used to prepare, through the BONAMI module, the working libraries of neutron self-shielded cross sections for the one-dimensional (1D) and two-dimensional (2D) transport calculations, respectively performed with the XSDRNPM 1D discrete ordinates transport code of the SCAMPI system and the DORT 2D discrete ordinates transport code, included in the DOORS-3.2 /24/ system.

Following the denominations reported in the ICSBEP handbook, the k-effective (k_{eff}) results obtained in the 1D and 2D transport calculations with the VITJEFF32.BOLIB library refer to HEU (Highly Enriched Uranium) benchmark experiments (TAB. 3.1), to IEU (Intermediate Enrichement Uranium) benchmark experiments (TAB. 3.2), to LEU (Low Enriched Uranium) benchmark experiments (TAB. 3.3), to a MIX (MIXed Plutonium-Uranium) benchmark experiment (TAB. 3.4), to U-233 benchmark experiments (TAB. 3.5) and to Pu-239 benchmark experiments (TAB. 3.6). The following acronyms are used in the cited tables: NU (natural uranium), DU (depleted uranium) and WC (wolfram carbide or tungsten carbide).
It is underlined that in the ICSBEP Handbook it is considered usually reasonable the assumption of a normal probability distribution for the k_{eff} values of the "experimental or benchmark-model" configurations. Consequently the k_{eff} values reported in TABs. 3.1÷3.6 are the mean values of the assumed normal distributions and their associated uncertainties correspond to one standard deviation (± 1sigma) which represents a 68% confidence level.

The k-effective (k_{eff}) results obtained with the VITJEFF32.BOLIB library are compared in the cited tables with the corresponding results obtained with the older VITJEFF311.BOLIB library. In the comparison of the k_{eff} calculated results obtained with the VITJEFF32.BOLIB library and the VITJEFF311.BOLIB older library one should take into account that, differently from VITJEFF311.BOLIB which was processed (see /8/) through NJOY-99.259 /67/, VITJEFF32.BOLIB was generated using NJOY-2012.53 /17/. The one-dimensional transport calculations in spherical geometry were performed with the XSDRNPM code, module of the SCAMPI system, in the P_5-S_{16} approximation: P_5 corresponds to L=ℓ-max, the maximum order of the Legendre polynomial (P_ℓ) expansion of the scattering cross section matrices and S_{16} represents the order of the flux angular discretization. The DORT 2D discrete ordinates code, included in the DOORS-3.2 system, was exclusively employed in the simulation of the IEU-MET-FAST-007 (BIG TEN) (see TAB. 3.2) fast neutron spectrum benchmark experiment with a 2D (R,Z) cylindrical geometry calculation in the P_3-S_8 approximation. The most relevant differences in the k_{eff} calculated results obtained using VITJEFF32.BOLIB with respect to the corresponding results obtained with VITJEFF311.BOLIB are reported herewith.

The VITJEFF32.BOLIB HEU-MET-FAST k_{eff} results present a systematic increase ranging from about 100 to about 700 pcm and are in general less adherent to the experimental results with respect to the corresponding results obtained with VITJEFF311.BOLIB.

The VITJEFF32.BOLIB k_{eff} results obtained for the IEU-MET-FAST-007 benchmark experiment (BIG TEN) are strongly overestimated with respect to the corresponding VITJEFF311.BOLIB k_{eff} values and are not statistically consistent with the experimental data.

The U-233-MET-FAST k_{eff} results using VITJEFF32.BOLIB appear systematically lower of about 200-400 pcm and more adherent to the experimental results with respect to the corresponding results obtained with VITJEFF311.BOLIB.

The PU-MET-FAST k_{eff} results using VITJEFF32.BOLIB appear systematically higher of about 100-300 pcm and in general less adherent to the experimental results with respect to the corresponding results obtained with VITJEFF311.BOLIB.

3.2 - Shielding Benchmarks

At present no testing of the VITJEFF32.BOLIB library was performed on integral neutron shielding benchmark experiments.

TAB. 3.1

VITJEFF32.BOLIB and VITJEFF311.BOLIB Criticality Calculation Results
for Highly Enriched Uranium (HEU) Benchmark Experiments.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark-Model $k_{eff} \pm \Delta k_{eff}$ (pcm)	Geometry/ P_L - S_N	VITJEFF32 k_{eff}	VITJEFF311 k_{eff}
Thermal Neutron Spectrum					
HEU-SOL-THERM-009-001	H2O	0.99900 ± (430)	1D Sph./ P5-S16	1.00189	1.00189
HEU-SOL-THERM-009-002	H2O	1.00000 ± (390)	1D Sph./ P5-S16	1.00203	1.00236
HEU-SOL-THERM-009-003	H2O	1.00000 ± (360)	1D Sph./ P5-S16	1.00101	1.00166
HEU-SOL-THERM-009-004	H2O	0.99860 ± (350)	1D Sph./ P5-S16	0.99511	0.99591
HEU-SOL-THERM-010-001	H2O	1.00000 ± (290)	1D Sph./ P5-S16	1.00035	1.00123
HEU-SOL-THERM-010-002	H2O	1.00000 ± (290)	1D Sph./ P5-S16	1.00096	1.00185
HEU-SOL-THERM-010-003	H2O	1.00000 ± (290)	1D Sph./ P5-S16	0.99956	1.00044
HEU-SOL-THERM-010-004	H2O	0.99920 ± (290)	1D Sph./ P5-S16	0.99819	0.99906
HEU-SOL-THERM-011-001	H2O	1.00000 ± (230)	1D Sph./ P5-S16	1.00438	1.00523
HEU-SOL-THERM-011-002	H2O	1.00000 ± (230)	1D Sph./ P5-S16	1.00052	1.00137
HEU-SOL-THERM-012-001	H2O	0.99990 ± (580)	1D Sph./ P5-S16	1.00053	1.00111
HEU-SOL-THERM-013-001 (ORNL-1)	--	1.00120 ± (260)	1D Sph./ P5-S16	0.99837	0.99892
HEU-SOL-THERM-013-002 (ORNL-2)	--	1.00070 ± (360)	1D Sph./ P5-S16	0.99739	0.99797
HEU-SOL-THERM-013-003 (ORNL-3)	--	1.00090 ± (360)	1D Sph./ P5-S16	0.99382	0.99442
HEU-SOL-THERM-013-004 (ORNL-4)	--	1.00030 ± (360)	1D Sph./ P5-S16	0.99539	0.99599
HEU-SOL-THERM-032 (ORNL-10)	--	1.00150 ± (260)	1D Sph./ P5-S16	0.99851	0.99878
Intermediate Neutron Spectrum					
ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark-Model $k_{inf} \pm \Delta k_{inf}$ (pcm)	Geometry/ P_L - S_N	VITJEFF32 k_{inf}	VITJEFF311 k_{inf}
HEU-COMP-INTER-004	--	1.00000 ± (400)	Inf. Homogeneous/ P5-S16	1.01070	1.00807

TAB. 3.1 Continued

VITJEFF32.BOLIB and VITJEFF311.BOLIB Criticality Calculation Results
for Highly Enriched Uranium (HEU) Benchmark Experiments.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark-Model $k_{eff} \pm \Delta k_{eff}$ (pcm)	Geometry/ P_L - S_N	VITJEFF32 k_{eff}	VITJEFF311 k_{eff}
Fast Neutron Spectrum					
HEU-MET-FAST-001-001 (GODIVA)	--	1.00000 ± (100)	1D Sph./ P5-S16	1.00051	0.99533
HEU-MET-FAST-002-001 (TOPSY)	NU	1.00000 ± (300)	1D Sph./ P5-S16	1.00779	1.00095
HEU-MET-FAST-003-001	NU (2in)	1.00000 ± (500)	1D Sph./ P5-S16	0.99865	0.99373
HEU-MET-FAST-003-002	NU (3in)	1.00000 ± (500)	1D Sph./ P5-S16	0.99887	0.99345
HEU-MET-FAST-003-003	NU (4in)	1.00000 ± (500)	1D Sph./ P5-S16	1.00415	0.99825
HEU-MET-FAST-003-004	NU (5in)	1.00000 ± (300)	1D Sph./ P5-S16	1.00269	0.99643
HEU-MET-FAST-003-005	NU (7in)	1.00000 ± (300)	1D Sph./ P5-S16	1.00742	1.00071
HEU-MET-FAST-003-006	NU (8in)	1.00000 ± (300)	1D Sph./ P5-S16	1.00776	1.00092
HEU-MET-FAST-003-007	NU (11in)	1.00000 ± (300)	1D Sph./ P5-S16	1.00849	1.00148
HEU-MET-FAST-003-008	WC (1.9in)	1.00000 ± (500)	1D Sph./ P5-S16	1.00461	1.00146
HEU-MET-FAST-003-009	WC (2.9in)	1.00000 ± (500)	1D Sph./ P5-S16	1.00613	1.00364
HEU-MET-FAST-003-010	WC (4.5in)	1.00000 ± (500)	1D Sph./ P5-S16	1.01029	1.00897
HEU-MET-FAST-003-011	WC (6.5in)	1.00000 ± (500)	1D Sph./ P5-S16	1.01479	1.01416
HEU-MET-FAST-003-012	Ni (8in)	1.00000 ± (500)	1D Sph./ P5-S16	1.01172	1.00922
HEU-MET-FAST-022-001	Al	1.00000 ± (190)	1D Sph./ P5-S16	1.00005	0.99527
HEU-MET-FAST-027-001	Pb	1.00000 ± (250)	1D Sph./ P5-S16	1.00458	1.00052
HEU-MET-FAST-028-001 (FLATTOP-25)	NU	1.00000 ± (300)	1D Sph./ P5-S16	1.00895	1.00218
HEU-MET-FAST-057-001	Pb	1.00000 ± (200)	1D Sph./ P5-S16	0.99684	0.99425
HEU-MET-FAST-057-002	Pb	1.00000 ± (230)	1D Sph./ P5-S16	1.00437	1.00122

TAB. 3.2

VITJEFF32.BOLIB and VITJEFF311.BOLIB Criticality Calculation Results
for Intermediate Enrichment Uranium (IEU) Benchmark Experiments.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark-Model $k_{eff} \pm \Delta k_{eff}$ (pcm)	Geometry/ $P_L - S_N$	VITJEFF32 k_{eff}	VITJEFF311 k_{eff}
Fast Neutron Spectrum					
IEU-MET-FAST-007 (BIG TEN) Simplified Model	DU	1.00450 ± (70)	2D Cyl./ P3-S8	1.01503	0.99714
IEU-MET-FAST-007 (BIG TEN) Two Zone Model	DU	0.99480 ± (130)	2D Cyl./ P3-S8	1.00810	0.99039

TAB. 3.3

VITJEFF32.BOLIB and VITJEFF311.BOLIB Criticality Calculation Results
for Low Enriched Uranium (LEU) Benchmark Experiments.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark-Model $k_{eff} \pm \Delta k_{eff}$ (pcm)	Geometry/ $P_L - S_N$	VITJEFF32 k_{eff}	VITJEFF311 k_{eff}
Thermal Neutron Spectrum					
LEU-SOL-THERM-003-003	--	0.99950 ± (420)	1D Sph./ P5-S16	1.00258	1.00358
LEU-SOL-THERM-003-006	--	0.99990 ± (490)	1D Sph./ P5-S16	0.99949	1.00088
LEU-SOL-THERM-003-009	--	0.99960 ± (520)	1D Sph./ P5-S16	0.99811	0.99942

TAB. 3.4

VITJEFF32.BOLIB and VITJEFF311.BOLIB Criticality Calculation Results
for Mixed Plutonium-Uranium (MIX) Benchmark Experiments.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark-Model $k_{eff} \pm \Delta k_{eff}$ (pcm)	Geometry/ $P_L - S_N$	VITJEFF32 k_{eff}	VITJEFF311 k_{eff}
Fast Neutron Spectrum					
MIX-MET-FAST-001-001	--	1.00000 ± (160)	1D Sph./ P5-S16	0.99948	0.99740

TAB. 3.5

VITJEFF32.BOLIB and VITJEFF311.BOLIB Criticality Calculation Results
for U-233 Benchmark Experiments.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark-Model $k_{eff} \pm \Delta k_{eff}$ (pcm)	Geometry/ $P_L - S_N$	VITJEFF32 k_{eff}	VITJEFF311 k_{eff}
Fast Neutron Spectrum					
U233-MET-FAST-001-001 (JEZEBEL-233)	--	1.00000 ± (100)	1D Sph./.P5-S16	1.00083	1.00383
U233-MET-FAST-002-001	HEU	1.00000 ± (100)	1D Sph./.P5-S16	1.00011	1.00257
U233-MET-FAST-002-002	HEU	1.00000 ± (110)	1D Sph./.P5-S16	1.00166	1.00342
U233-MET-FAST-003-001	NU	1.00000 ± (100)	1D Sph./.P5-S16	1.00189	1.00575
U233-MET-FAST-003-002	NU	1.00000 ± (100)	1D Sph./.P5-S16	1.00363	1.00719
U233-MET-FAST-006-001 (FLATTOP-23)	NU	1.00000 ± (140)	1D Sph./.P5-S16	1.00472	1.00665

TAB. 3.6

VITJEFF32.BOLIB and VITJEFF311.BOLIB Criticality Calculation Results
for Plutonium Benchmark Experiments.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark-Model $k_{eff} \pm \Delta k_{eff}$ (pcm)	Geometry/ P_L - S_N	VITJEFF32 k_{eff}	VITJEFF311 k_{eff}
Thermal Neutron Spectrum					
PU-SOL-THERM-006-001	H2O	1.00000 ± (350)	1D Sph./ P5-S16	0.99726	0.99716
PU-SOL-THERM-006-002	H2O	1.00000 ± (350)	1D Sph./ P5-S16	0.99849	0.99843
PU-SOL-THERM-006-003	H2O	1.00000 ± (350)	1D Sph./ P5-S16	0.99798	0.99800
PU-SOL-THERM-011-001	--	1.00000 ± (520)	1D Sph./ P5-S16	1.00690	1.00721
PU-SOL-THERM-011-002	--	1.00000 ± (520)	1D Sph./ P5-S16	1.01156	1.01190
PU-SOL-THERM-011-003	--	1.00000 ± (520)	1D Sph./ P5-S16	1.01357	1.01397
PU-SOL-THERM-011-004	--	1.00000 ± (520)	1D Sph./ P5-S16	1.00614	1.00656
PU-SOL-THERM-011-005 (PNL-5R)	--	1.00000 ± (520)	1D Sph./ P5-S16	1.00306	1.00364
PU-SOL-THERM-011-006 (PNL-3R)	--	1.00000 ± (520)	1D Sph./ P5-S16	0.99174	0.99165
PU-SOL-THERM-011-007	--	1.00000 ± (520)	1D Sph./ P5-S16	0.99765	0.99760
PU-SOL-THERM-011-008	--	1.00000 ± (520)	1D Sph./ P5-S16	0.99427	0.99421
PU-SOL-THERM-011-009	--	1.00000 ± (520)	1D Sph./ P5-S16	0.99088	0.99088
PU-SOL-THERM-011-010	--	1.00000 ± (520)	1D Sph./ P5-S16	1.00079	1.00083
PU-SOL-THERM-011-011 (PNL-4R)	--	1.00000 ± (520)	1D Sph./ P5-S16	0.99733	0.99752
PU-SOL-THERM-011-012	--	1.00000 ± (520)	1D Sph./ P5-S16	0.99702	0.99702
PU-SOL-THERM-021-007 (PNL-1)	--	1.00000 ± (320)	1D Sph./ P5-S16	1.00375	1.00412
PU-SOL-THERM-021-008 (PNL-2)	--	1.00000 ± (650)	1D Sph./ P5-S16	1.00148	1.00226
PU-SOL-THERM-021-009	--	1.00000 ± (320)	1D Sph./ P5-S16	1.00421	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	VITJEFF32 k_{eff}	VITJFF311 k_{eff}
PU-COMP-INTER-001	--	1.00000 ± (1100)	Inf. Homogeneous/ P5-S16	1.00103	1.00110

TAB. 3.6 Continued

VITJEFF32.BOLIB and VITJEFF311.BOLIB Criticality Calculation Results
for Plutonium Benchmark Experiments.

ICSBEP Handbook Benchmark Name	Reflector	Experimental or Benchmark-Model $k_{eff} \pm \Delta k_{eff}$ (pcm)	Geometry/ P_L - S_N	VITJEFF32 k_{eff}	VITJEFF311 k_{eff}
Fast Neutron Spectrum					
PU-MET-FAST-001-001 (JEZEBEL)	--	1.00000 ± (200)	1D Sph./ P5-S16	1.00044	0.99889
PU-MET-FAST-002-001 (JEZEBEL-240)	--	1.00000 ± (200)	1D Sph./ P5-S16	1.00267	1.00277
PU-MET-FAST-006-001 (FLATTOP-PU)	NU	1.00000 ± (300)	1D Sph./ P5-S16	1.00642	1.00305
PU-MET-FAST-008-001 (THOR)	Th	1.00000 ± (60)	1D Sph./ P5-S16	0.99861	1.00124
PU-MET-FAST-009-001	Al	1.00000 ± (270)	1D Sph./ P5-S16	1.00468	1.00401
PU-MET-FAST-010-001	NU	1.00000 ± (180)	1D Sph./ P5-S16	1.00257	1.00091
PU-MET-FAST-011-001	H2O	1.00000 ± (100)	1D Sph./ P5-S16	1.00242	0.99943
PU-MET-FAST-018-001	Be	1.00000 ± (300)	1D Sph./ P5-S16	1.00290	1.00200
PU-MET-FAST-023-001	Graphite	1.00000 ± (230)	1D Sph./ P5-S16	1.00027	0.99850
PU-MET-FAST-024-001	Polyethylene	1.00000 ± (200)	1D Sph./ P5-S16	1.00227	0.99948
PU-MET-FAST-030-001	Graphite	1.00000 ± (210)	1D Sph./ P5-S16	1.00439	1.00395
PU-MET-FAST-031-001	Polyethylene	1.00000 ± (210)	1D Sph./ P5-S16	1.00607	1.00385

4 - CONCLUSION

The ENEA-Bologna Nuclear Data Group generated the VITJEFF32.BOLIB fine-group coupled cross section library in AMPX format in the same neutron and photon energy group structure (199 n + 42 γ) of the ORNL DLC-0184/VITAMIN-B6 library. This pseudo-problem-independent library is based on the Bondarenko (f-factor) method for the treatment of neutron resonance self-shielding and temperature effects.

The VITJEFF32.BOLIB library contains processed data derived from the OECD-NEA Data Bank JEFF-3.2 evaluated nuclear data library. It was produced using the NJOY-2012.53 nuclear data processing system through an ENEA-Bologna automatic procedure and it was tested on several thermal, intermediate and fast neutron spectrum criticality safety benchmark experiments.

It is underlined that it is foreseen to generate the BUGJEFF32.BOLIB broad-group working library in FIDO-ANISN format, dedicated to LWR shielding and pressure vessel dosimetry applications. BUGJEFF32.BOLIB will be obtained from VITJEFF32.BOLIB, through problem-dependent cross section collapsing and neutron self-shielding calculations performed by the ENEA-Bologna 2007 Revision of the SCAMPI nuclear data processing system. In particular, BUGJEFF32.BOLIB will have the same neutron and photon group structure (47 n + 20 γ) of the ORNL DLC-0185/BUGLE-96 library, derived from VITAMIN-B6 through problem-dependent cross section collapsing.

Further testing of the VITJEFF32.BOLIB library will continue in future and it is not excluded that new response functions or additional nuclides can be added, also on the basis of possible specific requests.

An analogous data processing activity will be performed also using the US ENDF/B-VII.1 nuclear data files.

It is believed, in general, that it should be very important to further promote, at the international level (UNO-IAEA, OECD-NEA, industrial organizations, R&D institutions, etc.), not only the development of fine-group general-purpose cross section libraries like VITJEFF32.BOLIB but also the generation of new working cross section libraries for radiation shielding applications, like BUGJEFF32.BOLIB, dedicated to various types of Generation III and IV nuclear fission reactors with different compositional, geometrical and spectral specifications. In fact the availability of these working libraries, derived through problem-dependent cross section collapsing from the previously cited general-purpose libraries, could promote, in particular, the use of the three-dimensional deterministic codes in radiation shielding and radiation damage calculations for nuclear safety. This is increasingly requested, due to the fact that these transport codes (TORT, PARTISN, KATRIN, etc.) reached in the last years an effective capability of complex geometry description, through modern dedicated pre/post-processor systems (BOT3P, TORTWARE, etc.) for the automatic generation of the spatial meshes.

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