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Assessment of Nuclear Data Needs for Broad-Group SCALE Library Related to VVER Spent Fuel Applications

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Report done under the IAEA Contract No. 10615/R0.

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Abstract

A preliminary study aimed at the issue of feasibility to generate a broad-group SCALE library related to VVER spent fuel applications was made. The SCALE code system has been installed and is being used in many countries operating VVER-type reactors for criticality and shielding analyses as well as spent fuel isotopic inventory calculations but still without an extensive validation and verification for the VVER environment. This study should be a contribution to QA connected with the SCALE code system application for the VVER calculations as a basis on which the generation of the specific VVER SCALE library can be prepared. Possible ways of the broad-group library development are described.

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Contents

1 Introduction

During the last two decades, a very large popularity all over the world achieved the SCALE code system developed by ORNL TN, U.S.A. at the request of the U.S. NRC. The code system can be used for criticality safety, radionuclide inventory, shielding and heat transfer calculations including an automated problem dependent group cross section data processing.

One of the most important features of the SCALE system is the capability to simplify the user knowledge and effort required to prepare material mixtures and to perform adequate problem-dependent cross-section processing.

During 1990’s, the SCALE code system has been also installed and is currently used for making analyses in all the countries operating VVER-type reactors: Bulgaria, Czechia, Germany, Slovakia, the Ukraine and Hungary. (In Romania, it is planned to be used for calculations related to CANDU reactor.)

All members of the Association of the State Nuclear Authorities of the countries operating VVER-type reactors focused on licensing process of dry spent fuel storage facilities. In 1996, they agreed on an urgent need for implementation of the SCALE code system to obtain serious calculational support for performing standard analyses concerning criticality safety, shielding, spent fuel isotopic inventory and heat transfer.

Because the SCALE code system was developed in USA, it was tailored above all to western type PWRs. It means that all the well-established computer codes, libraries and methods utilized within the SCALE system (except KENO VI code which has been incorporated into the SCALE code system only recently) was developed to describe prevalently above mentioned PWR. Especially, the 44-group library, which is the most preferred library in SCALE, was collapsed from the 238-group library using spectra typical for PWRs of the western type.

However, the VVER reactor cores and spent fuel facility arrays are in principle of hexagonal patterns and also of different level of undermoderation, which has an influence on spectra that should be used for processing the neutron data libraries. That is why only after joining KENO VI as a general geometry code, there has been a possibility of the full description of VVER core/storage unit array hexagonal patterns in part of criticality safety analyses.

As far as VVER applications are concerned, an additional verification and validation should be performed for the separate codes (hexagonal geometry) as well as for data libraries used within SCALE. For the code system to be licensed by the regulatory bodies for the VVERs, it seems that it is necessary to prepare a new broad-group library collapsed from a fine-group one by using a spectrum typical for the VVER fuel assembly. The goal to generate a broad-group library for VVER applications is appreciated very much within the whole Eastern and Central Europe nuclear research community because the SCALE code has to be approved by the regulatory bodies in compliance with QA. Thus, the assessment of the nuclear data, generation of a broad-group SCALE library for VVER applications and its extensive validation belong to fulfilment of QA for using the SCALE code system in the VVER environment.

2 SCALE overview

SCALE (Standardized Computer Analyses for Licensing Evaluation) [1] code system was developed in the Computational Physics and Engineering Division at Oak Ridge National Laboratory (ORNL), USA, and its development has been directed at safety analyses of spent fuel storage and transport casks. In 1976, the U.S. Nuclear Regulatory Commission (NRC) staff proposed the development of an easy-to-use analysis system that provided the technical capabilities of the individual modules with which they were familiar. With this proposal, the development of the SCALE code system started. The NRC staff provided ORNL with some general development criteria for SCALE:

(1) focus on applications related to nuclear fuel facilities and package designs,

(2) use well-established computer codes and data libraries,

(3) design an input format for the occasional or novice user,

(4) prepare "standard" analysis sequences (control modules) that will automate the use of multiple codes (functional modules) and data to perform a system analysis, and

(5) provide complete documentation and public availability.

As the system has grown in popularity over the years and additional options have been requested, the control modules have been improved, the system has been considerably enhanced and the current release is Version 4.4 [1].

SCALE is a modular system, which contains a series of codes that were used before only independently. It also uses some modules from the AMPX system [2]. Table 1 provides a summary of the major applications of each of **functional modules** in the current version of the SCALE code system. Two functional modules are of great importance for data processing because they prepare problem dependent data for modules carrying out the criticality or shielding calculations:

BONAMI performs resonance shielding through the application of the Bondarenko shielding factor method. As input, the program requires the presence of shielding factor data on the AMPX master library interface. As output, BONAMI produces a problem-dependent master library. Thus, in the SCALE sequences, it is always used in conjunction with NITAWL-II which, even if no resonance processing is done, converts the master library into an AMPX working library.

NITAWL-II applies the Nordheim Integral Technique to perform neutron cross-section processing in the resonance energy range. This technique involves a fine energy group calculation of the slowing-down flux across each resonance with subsequent flux weighting of the resonance cross sections. The major function of NITAWL-II is its conversion of cross-section libraries from a problem-independent to a problem-dependent form. However, NITAWL-II also assembles group-to-group transfer arrays from the elastic and inelastic scattering components and performs other tasks in producing the problem-dependent working library.

Table 1. SCALE functional modules

Module	Function
BONAMI	Resonance self-shielding of cross sections with Bondarenko factors
NITAWL-II	Resonance self-shielding of cross sections with resolved resonance data
XSDRNPM	General 1-D, discrete-ordinates code for: - zone-weighting of cross sections - eigenvalue calculations for neutron multiplication - fixed-source calculation for shielding analysis - adjoint calculation for determining importance functions
XSDOSE	Module for calculation of dose at a point based on the 1-D leakage flux from a finite shield
COUPLE	Interface module for preparation of cross-section and spectral data for ORIGEN-S
ORIGEN-S	General-purpose point-depletion and decay code to calculate isotopic, decay heat, radiation source terms, and curie levels
ICE	Cross-section utility module for mixing cross sections
MORSE-SGC	Monte Carlo code with combinatorial and array geometry features used to perform radiation shielding analysis
HEATING7.2	Finite-volume, multidimensional code for conduction and radiation heat transfer
KENO V.a	Monte Carlo code for calculation of neutron multiplication factors
KENO-VI	Monte Carlo code for calculation of neutron multiplication factors for complex geometries (e.g. hexagonal)
OCULAR	Calculation of radiation exchange factors
QAD-CGGP	3-D point-kernel gamma-ray shielding analysis

Table 2. SCALE control modules

Control module	Analysis function(s)	Functional modules executed
CSAS	1-D deterministic calculation of neutron multiplication 3-D Monte Carlo calculation of neutron multiplication Problem-dependent cross-section processing Multiplication search on geometry or material concentrations	BONAMI NITAWL-II XSDRNPM KENO V.a ICE
CSAS6	3-D Monte Carlo calculation of neutron multiplication for complex geometries (e.g. hexagonal)	BONAMI NITAWL-II XSDRNPM KENO-VI
SAS1	1-D deterministic calculation of radiation transport through shield and dose evaluation at a point Calculation of dose at detector based on leakage from critical volume	BONAMI NITAWL-II XSDRNPM XSDOSE
SAS2H	Point depletion/decay of nuclear fuel 1-D radial shielding analysis in cylindrical geometry	BONAMI NITAWL-II XSDRNPM COUPLE ORIGEN-S XSDOSE
SAS3	Dose evaluation using MORSE Monte Carlo code	BONAMI NITAWL-II XSDRNPM MORSE-SGC
SAS4	Calculation of dose outside of transportation package using MORSE code and automated biasing techniques	BONAMI NITAWL-II XSDRNPM MORSE-SGC
QADS	3-D point-kernel gamma-ray shielding analysis	QAD-CGGP
HTAS1	R-Z steady-state and transient analyses of a transportation package	OCULAR HEATING7.2

In order to use the system more efficiently, a number of **control modules** were developed which cover most of tasks for which the system can be used. A summary of the major applications of each of the control modules in the current version of the SCALE code system is given in Table 2 along with the functional modules that are executed. The SCALE control modules are designed to allow complex analyses using simple input descriptions. Each shielding or criticality control module (1) uses the Standard Composition Library (see [1], Sect. M8) for specifying the materials and mixtures used in a calculation and (2) provides automatic problem-dependent cross-section preparation prior to problem execution via the functional modules.

The SCALE control modules are designed to read **AMPX master format libraries** [2]. These libraries are very general and many include temperature-dependent cross-section data as well as resonance data. The master format libraries are used as a basis for creating an AMPX working format library that has problem-dependent (user-specified) temperature dependence and appropriate resonance processing. The SCALE control module sequences access BONAMI first to process nuclides with Bondarenko data. The master library output from BONAMI is input to NITAWL-II, where resonance data are processed via the Nordheim integral treatment and an AMPX working format library is produced. The SCALE criticality and shielding functional modules are all designed to use an AMPX working library format.

3 SCALE Libraries

A summary of all the libraries used within and distributed with the SCALE code system is given in Table 3. In this work, only the libraries used for criticality and shielding calculations are of interest. These libraries are in the AMPX master library format (Part A in Table 3).

3.1 Libraries used within SCALE code system

In the SCALE system there are nine cross-section libraries currently available and distributed with SCALE (see [1], Section M4), eight of which are automatically available in the SCALE system. **Six of these libraries were designed primarily for criticality analysis**:

The **218-group library** (218GROUPNDF4) is a fine-group library derived from ENDF/B-IV data. The library contains 140 fast groups and 78 thermal groups and includes explicit resonance data in the resolved resonance range. No unresolved resonance data are available in the library.

The **27-group library** (27GROUPNDF4) is the broad-group library collapsed from the 218-group library and has 14 fast and 13 thermal groups. This library has been extensively validated against critical experiments. The **27-group depletion library** (27BURNUPLIB) contains the same data as 27GROUPNDF4 plus pre-release ENDF/B-V data for a large number of fission products. This was the first library designed for use with the SAS2 depletion/decay sequence.

The **238-group library** (238GROUPNDF5) is the most complete library in SCALE. This library contains data for all ENDF/B-V nuclides and has 148 fast and 90 thermal groups. Most resonance nuclides in the 238-group library have resonance data in the resolved resonance region and Bondarenko factors in the unresolved resonance region.

The **44-group library** (44GROUPNDF5) is a broad-group version of 238GROUPNDF5 designed for analysis of light-water-reactor (LWR) fresh and spent fuel systems and has been extensively validated against LWR critical experiments. The 238- and 44-group libraries are the preferred criticality safety analysis libraries in SCALE and are described in more details below.

The **Hansen-Roach 16-group library** (HANSEN-ROACH) is based on the original Hansen and Roach data. Important nuclides not available in the library were added by collapsing the 218-group ENDF/B-IV library to the 16-group structure. Although the library was originally developed for fast systems, a modification to the σ_p data for ^{238}U has allowed it to be successfully used as a general-purpose library.

The other **three libraries were developed as shielding libraries:**

The SCALE **18-group gamma library** (18GROUPGAMMA) is based on data that were later approved as ENDF/B-IV data. The **Straker-Morrison 22-neutron and 18-gamma-group coupled library** (22N-18COUPLE) contains the same gamma data as

Table 3. SCALE Data Libraries

A. AMPX Master Format Libraries

The following SCALE libraries are **AMPX master format libraries** (Section M4 of the SCALE Manual). These libraries are read and processed by BONAMI, NITAWL, and/or the AMPX utilities (Section M16 of the SCALE Manual) before use by KENO, XSDRNPM, or MORSE.

Criticality cross-section libraries

File name	Library name	Unit	Description
scale.rev03.xn16	HANSEN-ROACH	81	Hansen-Roach 16 group library
scale.rev07.xn238	238GROUPNDF5	84	ENDF/B-V 238-group library
scale.rev09.xn44	44GROUPNDF5	83	ENDF/B-V 44-group library
scale.rev04.xn218	218GROUPNDF4	--	ENDF/B-IV 218-group library
scale.rev04.xn27	27GROUPNDF4	82	ENDF/B-IV 27-group library
scale.rev05.xn27burn	27BURNUPLIB	87	ENDF/B-IV, ENDF/B-V

Shielding cross-section libraries

File name	Library name	Unit	Description
scale.rev03.xn22g18	22N-18COUPLE	85	Straker-Morrison 22 neutron groups, 18 gamma groups
scale.rev04.xn27g18	27N-18COUPLE	88	ENDF/B-IV 27-group library/ 18GROUPGAMMA library
scale.rev05.xg18	18GROUPGAMMA	86	OGRE point-data 18-group gamma library

B. Standard Composition Library

The following library is the Standard Composition Library (Section M8).

scale.rev16.sclib

C. KENO libraries

Name	Description
albedos	KENO albedos
weights	KENO biasing weights

Table 3. (continued)

D. ORIGEN-S binary libraries

The following libraries are ORIGEN-S binary libraries (see Table M6.8.2).

Name	Description
baslmfbr	Basic LMFBR library
maphh2ob	Master photon library, bremsstrahlung in H2O
maphnobr	Master photon library, no bremsstrahlung
maphuo2b	Master photon library, bremsstrahlung in UO2
prlimlwr	Preliminary LWR library - default initial library for SAS2
pwr33f71.sas1inp	ORIGEN-S source term file generated by PWR, 3.2 wt%, 33 GWD/MTU SAS2 sample case. Used as input for SAS1 sample problems.

E. ORIGEN-S card-image (ASCII) libraries

The following libraries are ORIGEN-S card-image (ASCII) libraries and are stored in data/origen (see Table M6.8.1).

Name	Description
end6dec	ENDF/B-VI decay data base for light elements, actinides, fission products
mpbrh2om	Master photon data for bremsstrahlung from negatrons slowing down in H2O
mpbrh2op	Master photon data for bremsstrahlung from positrons slowing down in H2O
mpbruo2m	Master photon data for bremsstrahlung from negatrons slowing down in UO2
mpbruo2p	Master photon data for bremsstrahlung from positrons slowing down in UO2
mpdkxgam	Master photon decay X- and gamma-ray line data
mpsfangm	Master photon gamma ray spectra from spontaneous fission and (alpha,n) reactions
xsectpho	Cross-section and photon-yield libraries for light elements, actinides, fission products

F. Libraries Used by QADS and QAD-CGGP

Name	Description
attenuat	QAD-CGGP attenuation factors (ASCII file)
buildup	QAD-CGGP buildup factors (ASCII file)
scale.rev01.qadxslib	Dummy AMPX master format cross-section library (this file contains all the nuclides in the Std. Comp. Lib which are needed when MIPLIB checks the Std. Comp. input for valid compositions)

18GROUPGAMMA. The 22-neutron-group data were taken from ENDF/B-II and developed in conjunction with air-over-ground radiation transport studies done in the late 1960s. The group collapse of the cross sections was tailored for water-filled shipping cask calculations. The **27-neutron-group and 18-gamma-group coupled library** (27N-18COUPLE) contains neutron data from 27GROUPNDF4 and gamma data from 18GROUPGAMMA. This library has been widely used in LWR spent fuel shielding calculations and has been validated against experimental data.

3.1.1 The 238-group ENDF/B-V library (238GROUPNDF5)

The 238-group ENDF/B-V library is a general-purpose criticality analysis library and so far the most complete library available in SCALE. This library is also known as the LAW (Library to Analyze Radioactive Waste) Library.

The LAW library is based on ENDF/B-V evaluations. One of the major tenets of ENDF is to reject adjustments that make evaluations produce "correct" results. This approach is taken to ensure that evaluations improve because of advances in the evaluation art and not because of some fortuitous (and often misunderstood) change in an associated calculational procedure. In this spirit, the ENDF/B-derived libraries are never adjusted.

The library contains data for all nuclides (more than 300) available in ENDF/B-V processed by the AMPX-77 systems [2]. It also contains data for ^{14}N, ^{15}N, ^{16}O, ^{154}Eu, and ^{155}Eu from ENDF/B-VI. These five nuclides are included because the new evaluations are thought to be superior to those in Version V. A special nuclide set, identified by nuclide ID number 900, contains dose factors based on the ANSI standards.

The library has 148 fast groups and 90 thermal groups (below 3 eV). The group structure is listed in Table 4.

Most resonance nuclides in the 238 group and 44 group have resonance data (to be processed by NITAWL-II) in the resolved resonance range and Bondarenko factors (to be processed by BONAMI) for the unresolved range. Both libraries contain resolved resonance data for p-wave and d-wave resonances (l = 1 and l = 2, respectively) as shown in Table 5.

These data can have a significant effect on results for unmoderated, intermediate-energy problems. Resonance structures in several light-to-intermediate mass “nonresonance” ENDF nuclides (i.e., ^{7}Li, ^{19}F, ^{27}Al, and ^{28}Si) are accounted for using Bondarenko shielding factors. These structures can also be important in intermediate energy problems. Nuclides with thermal scattering data are listed in Table 6.

All nuclides in the 238-group LAW Library use the same weighting spectrum, consisting of

(1) Maxwellian spectrum (peak at 300 K) from 10^{-5} to 0.125 eV,

(2) a 1/E spectrum from 0.125 eV to 67.4 keV,

(3) a fission spectrum (effective temperature at 1.273 MeV) from 67.4 keV to 10 MeV,

(4) a 1/E spectrum from 10 to 20 MeV.

A plot of this spectrum is shown in Fig.1, below. All nuclides use a P_5 Legendre expansion to fit the elastic and discrete level inelastic scattering processes, thereby making the library

Table 4. Neutron energy group structure for SCALE ENDF/B-V libraries

238 group	44 group	Upper Energy (eV)	238 group	44 group	Upper Energy (eV)	238 group	44 group	Upper Energy (eV)	238 group	44 group	Upper Energy (eV)
1	1	2.0000E+07	61		3.9000E+03	121		2.0000E+01	181		1.0900E+00
2		1.7333E+07	62		3.7400E+03	122		1.9000E+01	182		1.0800E+00
3		1.5683E+07	63	15	3.0000E+03	123		1.8500E+01	183		1.0700E+00
4		1.4550E+07	64		2.5800E+03	124		1.7000E+01	184		1.0600E+00
5		1.3840E+07	65		2.2900E+03	125		1.6000E+01	185		1.0500E+00
6		1.2840E+07	66		2.2000E+03	126		1.5100E+01	186		1.0400E+00
7		1.0000E+07	67		1.8000E+03	127		1.4400E+01	187		1.0300E+00
8	2	8.1873E+06	68		1.5500E+03	128		1.3750E+01	188		1.0200E+00
9	3	6.4340E+06	69		1.5000E+03	129		1.2900E+01	189		1.0100E+00
10	4	4.8000E+06	70		1.1500E+03	130		1.1900E+01	190	25	1.0000E+00
11		4.3040E+06	71		9.5000E+02	131		1.1500E+01	191		9.7500E-01
12	5	3.0000E+06	72		6.8300E+02	132	19	1.0000E+01	192		9.5000E-01
13	6	2.4790E+06	73		6.7000E+02	133		9.1000E+00	193		9.2500E-01
14	7	2.3540E+06	74	16	5.5000E+02	134	20	8.1000E+00	194		9.0000E-01
15	8	1.8500E+06	75		3.0500E+02	135		7.1500E+00	195		8.5000E-01
16		1.5000E+06	76		2.8500E+02	136		7.0000E+00	196		8.0000E-01
17	9	1.4000E+06	77		2.4000E+02	137		6.7500E+00	197		7.5000E-01
18		1.3560E+06	78		2.1000E+02	138		6.5000E+00	198		7.0000E-01
19		1.3170E+06	79		2.0750E+02	139		6.2500E+00	199		6.5000E-01
20		1.2500E+06	80		1.9250E+02	140	21	6.0000E+00	200	26	6.2500E-01
21		1.2000E+06	81		1.8600E+02	141		5.4000E+00	201		6.0000E-01
22		1.1000E+06	82		1.2200E+02	142		5.0000E+00	202		5.5000E-01
23		1.0100E+06	83		1.1900E+02	143	22	4.7500E+00	203		5.0000E-01
24		9.2000E+05	84		1.1500E+02	144		4.0000E+00	204		4.5000E-01
25	10	9.0000E+05	85		1.0800E+02	145		3.7300E+00	205	27	4.0000E-01
26		8.7500E+05	86	17	1.0000E+02	146		3.5000E+00	206	28	3.7500E-01
27		8.6110E+05	87		9.0000E+01	147		3.1500E+00	207	29	3.5000E-01
28		8.2000E+05	88		8.2000E+01	148		3.0500E+00	208	30	3.2500E-01
29		7.5000E+05	89		8.0000E+01	149	23	3.0000E+00	209		3.0000E-01
30		6.7900E+05	90		7.6000E+01	150		2.9700E+00	210	31	2.7500E-01
31		6.7000E+05	91		7.2000E+01	151		2.8700E+00	211	32	2.5000E-01
32		6.0000E+05	92		6.7500E+01	152		2.7700E+00	212	33	2.2500E-01
33		5.7300E+05	93		6.5000E+01	153		2.6700E+00	213	34	2.0000E-01
34		5.5000E+05	94		6.1000E+01	154		2.5700E+00	214		1.7500E-01
35		4.9952E+05	95		5.9000E+01	155		2.4700E+00	215	35	1.5000E-01
36		4.7000E+05	96		5.3400E+01	156		2.3800E+00	216		1.2500E-01
37		4.4000E+05	97		5.2000E+01	157		2.3000E+00	217	36	1.0000E-01
38		4.2000E+05	98		5.0600E+01	158		2.2100E+00	218		9.0000E-02
39	11	4.0000E+05	99		4.9200E+01	159		2.1200E+00	219		8.0000E-02
40		3.3000E+05	100		4.8300E+01	160		2.0000E+00	220	37	7.0000E-02
41		2.7000E+05	101		4.7000E+01	161		1.9400E+00	221		6.0000E-02
42		2.0000E+05	102		4.5200E+01	162		1.8600E+00	222	38	5.0000E-02
43		1.5000E+05	103		4.4000E+01	163	24	1.7700E+00	223	39	4.0000E-02
44		1.2830E+05	104		4.2400E+01	164		1.6800E+00	224	40	3.0000E-02
45	12	1.0000E+05	105		4.1000E+01	165		1.5900E+00	225	41	2.5300E-02
46		8.5000E+04	106		3.9600E+01	166		1.5000E+00	226	42	1.0000E-02
47		8.2000E+04	107		3.9100E+01	167		1.4500E+00	227	43	7.5000E-03
48		7.5000E+04	108		3.8000E+01	168		1.4000E+00	228		5.0000E-03
49		7.3000E+04	109		3.7000E+01	169		1.3500E+00	229		4.0000E-03
50		6.0000E+04	110		3.5500E+01	170		1.3000E+00	230	44	3.0000E-03
51		5.2000E+04	111		3.4600E+01	171		1.2500E+00	231		2.5000E-03
52		5.0000E+04	112		3.3750E+01	172		1.2250E+00	232		2.0000E-03
53		4.5000E+04	113		3.3250E+01	173		1.2000E+00	233		1.5000E-03
54		3.0000E+04	114		3.1750E+01	174		1.1750E+00	234		1.2000E-03
55	13	2.5000E+04	115		3.1250E+01	175		1.1500E+00	235		1.0000E-03
56	14	1.7000E+04	116	18	3.0000E+01	176		1.1400E+00	236		7.5000E-04
57		1.3000E+04	117		2.7500E+01	177		1.1300E+00	237		5.0000E-04
58		9.5000E+03	118		2.5000E+01	178		1.1200E+00	238		1.0000E-04
59		8.0300E+03	119		2.2500E+01	179		1.1100E+00			1.0000E-05
60		6.0000E+03	120		2.1000E+01	180		1.1000E+00			

Table 5. Resonance nuclides in the ENDF/B-V libraries

Std. comp. alphanumeric name	Nuclide ID No.	Highest order resonance (l- value)
NA	11023	0
S	16000	0
CR	24000	0
CR (1/EsigT)	24301	0
CRSS	24304	0
MN	25055	0
FE	26000	1
FE (1/EsigT)	26301	0
FESS	26304	0
CO-59	27059	1
NI	28000	0
NI (1/EsigT)	28301	0
NISS	28304	0
CU	29000	1
GE-72	32072	1
GE-73	32073	1
GE-74	32074	1
GE-76	32076	0
AS-75	33075	1
SE-74	34074	1
SE-76	34076	2
SE-77	34077	1
SE-78	34078	1
SE-80	34080	1
SE-82	34082	1
BR-79	35079	1
BR-81	35081	1
KR-78	36078	1
KR-80	36080	1
KR-82	36082	2
KR-83	36083	1
KR-84	36084	1
KR-86	36086	0
RB-85	37085	0
RB-87	37087	0
SR-84	38084	0
SR-86	38086	0
SR-87	38087	0
SR-88	38088	0
Y-89	39089	0
ZR	40000	0
ZR-90	40090	0
ZR-91	40091	0
ZR-92	40092	0
ZR-94	40094	0
ZR-96	40096	0
NB-93	41093	0
NB-94	41094	0
MO	42000	0
MO-92	42092	0
MO-94	42094	0
MO-95	42095	0

Std. comp. alphanumeric name	Nuclide ID No.	Highest order resonance (l- value)
MO-96	42096	0
MO-97	42097	0
MO-98	42098	0
MO-100	42100	0
TC-99	43099	0
RU-99	44099	0
RU-100	44100	0
RU-101	44101	0
RU-102	44102	0
RU-104	44104	0
RH-103	45103	0
PD-104	46104	0
PD-105	46105	0
PD-106	46106	0
PD-108	46108	0
AG-107	47107	0
AG-109	47109	0
CD-110	48110	0
CD-111	48111	0
CD-112	48112	0
CD-113	48113	0
CD-114	48114	0
CD-116	48116	0
IN-113	49113	0
IN-115	49115	0
SN-112	50112	0
SN-114	50114	0
SN-115	50115	0
SN-116	50116	0
SN-117	50117	0
SN-118	50118	0
SN-119	50119	0
SN-120	50120	0
SN-122	50122	0
SN-124	50124	0
SB-121	51121	0
SB-123	51123	0
TE-122	52122	0
TE-123	52123	0
TE-124	52124	0
TE-125	52125	0
TE-126	52126	0
TE-128	52128	0
TE-130	52130	0
I-127	53127	0
I-129	53129	0
XE-124	54124	0
XE-126	54126	0
XE-128	54128	0
XE-129	54129	0
XE-130	54130	0
XE-131	54131	0

Table 5. (continued)

Std. comp. alphanumeric name	Nuclide ID No.	Highest order resonance (l- value)
XE-132	54132	0
XE-134	54134	0
CS-133	55133	0
CS-136	55136	0
BA-134	56134	0
BA-135	56135	0
BA-136	56136	0
BA-137	56137	0
LA-139	57139	0
PR-141	59141	0
ND-142	60142	0
ND-143	60143	0
ND-144	60144	0
ND-145	60145	0
ND-146	60146	0
ND-148	60148	0
ND-150	60150	0
PM-147	61147	0
PM-148M	61601	0
SM-147	62147	0
SM-149	62149	0
SM-150	62150	0
SM-151	62151	0
SM-152	62152	0
SM-154	62154	0
EU	63000	0
EU-151	63151	0
EU-152	63152	0
EU-153	63153	0
EU-154 (ENDF/B-VI)	63154	0
EU-155 (ENDF/B-VI)	63155	0
GD-152	64152	0
GD-154	64154	0
GD-155	64155	0
GD-156	64156	0
GD-157	64157	0
GD-158	64158	0
GD-160	64160	0
TB-159	65159	0
DY-160	66160	0
DY-161	66161	0
DY-162	66162	0
DY-163	66163	0
DY-164	66164	0
HO-165	67165	0
ER-166	68166	0
ER-167	68167	0
LU-175	71175	0
LU-176	71176	0
HF	72000	0
HF-174	72174	0
HF-176	72176	0
HF-177	72177	0
HF-179	72179	0
HF-178	72178	0
HF-180	72180	0
TA-181	73181	0
TA-182	73182	0
W	74000	0
W-182	74182	0
W-183	74183	0
W-184	74184	0
W-186	74186	0
RE-185	75185	0
RE-187	75187	0
AU	79197	0
TH-230	90230	0
TH-232	90232	0
PA-231	91231	0
PA-233	91233	0
U-232	92232	0
U-234	92234	0
U-235	92235	0
U-236	92236	0
U-237	92237	0
U-238	92238	0
NP-237	93237	0
NP-238	93238	0
PU-236	94236	0
PU-238	94238	0
PU-239	94239	0
PU-240	94240	0
PU-242	94242	0
PU-243	94243	0
PU-244	94244	0
AM-241	95241	0
AM-242	95242	0
AM-243	95243	0
AM-242M	95601	0
CM-242	96242	0
CM-243	96243	0
CM-244	96244	0
CM-245	96245	0
CM-246	96246	0
CM-247	96247	0
CM-248	96248	0
BK-249	97249	0
CF-249	98249	0
CF-250	98250	0
CF-251	98251	0
CF-252	98252	0
CF-253	98253	0
ES-253	99253	0
EU-154 (ENDF/B-V)	631541	0
EU-155 (ENDF/B-V)	631551	0

Table 6. Nuclides in ENDF/B-V libraries with multiple sets of thermal-scattering data

Std. comp. alphanumeric name	Nuclide ID No.	Temperatures (K) for which thermal-scattering cross-section data are available
H	1001	296, 500, 900
D	1002	296, 500, 900
H-3	1003	296, 500, 900
HFREEGAS	1801	296, 500, 900
DFREEGAS	1802	296, 500, 900
H-POLY	1901	296, 500, 900
HE-3	2003	296, 400, 500, 600, 700, 800, 1000, 1200
HE	2004	296, 400, 500, 600, 700, 800, 1000, 1200
LI-6	3006	296, 500, 900
LI-7	3007	296, 500, 900
BE	4009	296, 500, 900
BEBOUND	4309	296, 500, 900
B-10	5010	296, 500, 900
B-11	5011	296, 500, 900
C-12	6012	296, 500, 900
C-GRAPHITE	6312	296, 500, 900
N-14	7014	96, 500, 900
N-15	7015	296, 500, 900
O-16 (ENDF/B-VI)	8016	296, 500, 900
O-17	8017	296, 500, 900
F	9019	296, 500, 900
NA	11023	300, 500, 900
MG	12000	296, 500, 900
AL	13027	296, 500, 900
SI	14000	296, 500, 900
P	15031	296, 500, 900
S	16000	296, 500, 900
S-32	16032	296, 500, 900
CL	17000	300, 500, 900, 2100.1
K	19000	300, 500, 900, 2100.1
CA	20000	296, 500, 900
TI	22000	296, 500, 900
V	23000	296, 500, 900
CR	24000	296, 500, 900
CR (1/EsigT)	24301	296, 500, 900
CRSS	24304	296, 500, 900
MN	25055	296, 500, 900
FE	26000	296, 500, 900
FE (1/EsigT)	26301	296, 500, 900
FESS	26304	296, 500, 900
CO-59	27059	296, 500, 900
NI	28000	296, 500, 900
NI (1/EsigT)	28301	296, 500, 900
NISS	28304	296, 500, 900
CU	29000	296, 500, 900
GA	31000	296, 500, 900
GE-72	32072	296, 500, 900
GE-73	32073	296, 500, 900
GE-74	32074	296, 500, 900
GE-76	32076	296, 500, 900
AS-75	33075	296, 500, 900
SE-74	34074	296, 400, 500, 600, 700, 800, 1000, 1200,1600, 2000
SE-76	34076	296, 500, 900
SE-77	34077	296, 500, 900
SE-78	34078	296, 350
SE-80	34080	296, 350, 400, 450, 500, 600, 800, 1000
SE-82	34082	296, 350, 400, 450, 500, 600, 800, 1000
BR-79	35079	296, 500, 900
BR-81	35081	296, 500, 900
KR-78	36078	296, 500, 900
KR-80	36080	296, 500, 900
KR-82	36082	296, 500, 900
KR-83	36083	296, 500, 900
KR-84	36084	296, 500, 900
KR-85	36085	296, 500, 900
KR-86	36086	296, 500, 900
RB-85	37085	296, 500, 900
RB-86	37086	296, 500, 900
RB-87	37087	296, 500, 900
SR-84	38084	296, 500, 900
SR-86	38086	296, 500, 900
SR-87	38087	296, 500, 900
SR-88	38088	296, 500, 900
SR-89	38089	296, 500, 900
SR-90	38090	296, 500, 900
Y-89	39089	296, 500, 900
Y-90	39090	296, 500, 900
Y-91	39091	296, 500, 900
ZR	40000	296, 500, 900
ZR-90	40090	296, 500, 900
ZR-91	40091	296, 500, 900
ZR-92	40092	296, 500, 900
ZR-93	40093	296, 500, 900
ZR-94	40094	296, 500, 900
ZR-95	40095	296, 500, 900
ZR-96	40096	296, 500, 900
NB-93	41093	296, 500, 900
NB-94	41094	296, 500, 900
NB-95	41095	296, 500, 900
MO	42000	296, 500, 900
MO-92	42092	296, 500, 900
MO-94	42094	296, 500, 900
MO-95	42095	296, 500, 900
MO-96	42096	296, 500, 900
MO-97	42097	296, 500, 900
MO-98	42098	296, 500, 900
MO-99	42099	296, 500, 900
MO-100	42100	296, 500, 900
TC-99	43099	296, 500, 900
RU-96	44096	296, 500, 900
RU-98	44098	296, 500, 900
RU-99	44099	296, 500, 900
RU-100	44100	296, 500, 900
RU-101	44101	296, 500, 900
RU-102	44102	296, 500, 900
RU-103	44103	295, 500, 900
RU-104	44104	296, 500, 900
RU-105	44105	296, 500, 900
RU-106	44106	296, 500, 900
RH-103	45103	296, 500, 900
RH-105	45105	296, 500, 900
PD-102	46102	296, 500, 900
PD-104	46104	296, 500, 900
PD-105	46105	296, 500, 900
PD-106	46106	296, 500, 900
PD-107	46107	296, 500, 900
PD-108	46108	296, 500, 900
PD-110	46110	296, 500, 900
AG-107	47107	296, 500, 900
AG-109	47109	296, 500, 900
AG-111	47111	296, 500, 900
CD	48000	296, 500, 900
CD-106	48106	296, 500, 900
CD-108	48108	296, 500, 900
CD-110	48110	296, 500, 900
CD-111	48111	296, 500, 900
CD-112	48112	296, 500, 900

Table 6. (continued)

Std. comp. alphanumeric name	Nuclide ID No.	Temperatures (K) for which thermal-scattering cross-section data are available
CD-113	48113	296, 500, 900
CD-114	48114	296, 500, 900
CD-116	48116	296, 500, 900
CD-115M	48601	296, 500, 900
IN-113	49113	296, 500, 900
IN-115	49115	296, 500, 900
SN-112	50112	296, 500, 900
SN-114	50114	296, 500, 900
SN-115	50115	296, 500, 900
SN-116	50116	296, 500, 900
SN-117	50117	296, 500, 900
SN-118	50118	296, 500, 900
SN-119	50119	296, 500, 900
SN-120	50120	296, 500, 900
SN-122	50122	296, 500, 900
SN-123	50123	296, 500, 900
SN-124	50124	296, 500, 900
SN-125	50125	296, 500, 900
SN-126	50126	296, 500, 900
SB-121	51121	296, 500, 900
SB-123	51123	296, 500, 900
SB-124	51124	296, 500, 900
SB-125	51125	296, 500, 900
SB-126	51126	296, 500, 900
TE-120	52120	296, 500, 900
TE-122	52122	296, 500, 900
TE-123	52123	296, 500, 900
TE-124	52124	296, 500, 900
TE-125	52125	296, 500, 900
TE-126	52126	296, 500, 900
TE-128	52128	296, 500, 900
TE-130	52130	296, 500, 900
TE-132	52132	296, 500, 900
TE-127M	52601	296, 500, 900
TE-129M	52611	296, 500, 900
I-127	53127	296, 500, 900
I-129	53129	296, 500, 900
I-130	53130	296, 500, 900
I-131	53131	296, 500, 900
I-135	53135	296, 500, 900
XE-124	54124	296, 500, 900
XE-126	54126	296, 500, 900
XE-128	54128	296, 500, 900
XE-129	54129	296, 500, 900
XE-130	54130	296, 500, 900
XE-131	54131	296, 500, 900
XE-132	54132	296, 500, 900
XE-133	54133	296, 500, 900
XE-134	54134	296, 500, 900
XE-135	54135	296, 500, 900
XE-136	54136	296, 500, 900
CS-133	55133	296, 500, 900
CS-134	55134	296, 500, 900
CS-135	55135	296, 500, 900
CS-136	55136	296, 500, 900
CS-137	55137	296, 500, 900
BA-134	56134	296, 500, 900
BA-135	56135	296, 500, 900
BA-136	56136	296, 500, 900
BA-137	56137	296, 500, 900
BA-138	56138	296, 500, 900
BA-140	56140	296, 500, 900
LA-139	57139	296, 500, 900
LA-140	57140	296, 500, 900
CE-140	58140	296, 500, 900
CE-141	58141	296, 500, 900
CE-142	58142	296, 500, 900
CE-143	58143	296, 500, 900
CE-144	58144	296, 500, 900
PR-141	59141	296, 500, 900
PR-142	59142	296, 500, 900
PR-143	59143	296, 500, 900
ND-142	60142	296, 500, 900
ND-143	60143	296, 500, 900
ND-144	60144	296, 500, 900
ND-145	60145	296, 500, 900
ND-146	60146	296, 500, 900
ND-147	60147	296, 500, 900
ND-148	60148	296, 500, 900
ND-150	60150	296, 500, 900
PM-147	61147	296, 500, 900
PM-148	61148	296, 500, 900
PM-149	61149	296, 500, 900
PM-151	61151	296, 500, 900
PM-148M	61601	296, 500, 900
SM-144	62144	296, 500, 900
SM-147	62147	296, 500, 900
SM-148	62148	296, 500, 900
SM-149	62149	296, 500, 900
SM-150	62150	296, 500, 900
SM-151	62151	296, 500, 900
SM-152	62152	296, 500, 900
SM-153	62153	296, 500, 900
SM-154	62154	296, 500, 900
EU	63000	296, 500, 900
EU-151	63151	296, 500, 900
EU-152	63152	296, 500, 900
EU-153	63153	296, 500, 900
EU-154(ENDF/B-VI)	63154	296, 500, 900
EU-155(ENDF/B-VI)	63155	296, 500, 900
EU-156	63156	296, 500, 900
EU-157	63157	296, 500, 900
GD-152	64152	296, 500, 900
GD-154	64154	296, 500, 900
GD-155	64155	296, 500, 900
GD-156	64156	296, 500, 900
GD-157	64157	296, 500, 900
GD-158	64158	296, 500, 900
GD-160	64160	296, 500, 900
TB-159	65159	296, 500, 900
TB-160	65160	296, 500, 900
DY-160	66160	296, 500, 900
DY-161	66161	296, 500, 900
DY-162	66162	296, 500, 900
DY-163	66163	296, 500, 900
DY-164	66164	296, 500, 900
HO-165	67165	296, 500, 900
ER-166	68166	296, 500, 900
ER-167	68167	296, 500, 900
LU-175	71175	296, 500, 900
LU-176	71176	296, 500, 900
HF	72000	296, 500, 900
HF-174	72174	296, 500, 900
HF-176	72176	296, 500, 900
HF-177	72177	296, 500, 900
HF-178	72178	296, 500, 900
HF-179	72179	296, 500, 900
HF-180	72180	296, 500, 900
TA-181	73181	296, 500, 900
TA-182	73182	296, 500, 900
W	74000	296, 500, 900
W-182	74182	296, 500, 900

Table 6. (continued)

Std. comp. alphanumeric name	Nuclide ID No.	Temperatures (K) for which thermal-scattering cross-section data are available
W-183	74183	296, 500, 900
W-184	74184	296, 500, 900
W-186	74186	296, 500, 900
RE-185	75185	296, 500, 900
RE-187	75187	296, 500, 900
AU	79197	296, 500, 900
PB	82000	296, 500, 900
BI-209	83209	296, 500, 900
TH-230	90230	296, 500, 900
TH-232	90232	296, 500, 900
PA-231	91231	296, 500, 900
PA-233	91233	296, 500, 900
U-232	92232	296, 500, 900
U-233	92233	296, 500, 900
U-234	92234	296, 500, 900
U-235	92235	296, 500, 900
U-236	92236	296, 500, 900
U-237	92237	296, 500, 900
U-238	92238	296, 500, 900
NP-237	93237	296, 500, 900
NP-238	93238	296, 500, 900
PU-236	94236	296, 500, 900
PU-237	94237	296, 500, 900
PU-238	94238	296, 500, 900
PU-239	94239	296, 500, 900
PU-240	94240	296, 500, 900
PU-241	94241	296, 500, 900
PU-242	94242	296, 500, 900
PU-243	94243	296, 500, 900
PU-244	94244	296, 500, 900
AM-241	95241	296, 500, 900
AM-242M	95242	296, 500, 900
AM-243	95243	296, 500, 900
AM-242	95601	296, 500, 900
CM-241	96241	296, 500, 900
CM-242	96242	296, 500, 900
CM-243	96243	296, 500, 900
CM-244	96244	296, 500, 900
CM-245	96245	296, 500, 900
CM-246	96246	296, 500, 900
CM-247	96247	296, 500, 900
CM-248	96248	296, 500, 900
BK-249	97249	296, 500, 900
CF-249	98249	296, 500, 900
CF-250	98250	296, 500, 900
CF-251	98251	296, 500, 900
CF-252	98252	296, 500, 900
CF-253	98253	296, 500, 900
ES-253	99253	296, 500, 900
EU-154(ENDF/B-V)	631541	296, 500, 900
EU-155(ENDF/B-V)	631551	296, 500, 900
N-14 (ENDF/B-VI)	701401	296, 500, 900
N-15 (ENDF/B-VI)	701501	296, 500, 900
O-16 (ENDF/B-V)	801601	296, 500, 900

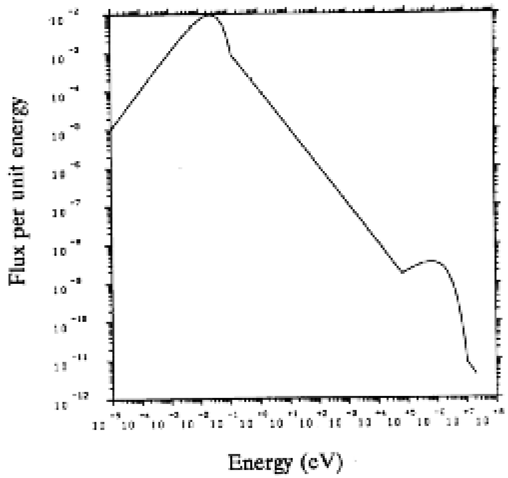

Fig.1 Weighting function for 238-group LAW Library

A special material is included in the library with an identifier of 99, which contains 238-group weighting spectra for collapsing the 238-group library using the MALOCS module to produce an application-specific collapsed library. Several spectra are included, as listed below:

1. spectrum based on a fuel cell from a 17 × 17 Westinghouse LWR assembly and identified by 9001,
2. spectrum designed for use with the Molten Salt Reactor Experiment (MSRE) fuel storage tanks at ORNL and identified by 9002,
3. average spectrum in a 27-cm carbon steel shield for use in cask shielding studies and identified by 9003,
4. average spectrum in the lead region of an 18.6-cm lead/13-cm resin shield for use in shielding cask studies and identified by 9004,
5. average spectrum in the resin region of an 18.6-cm lead/13-cm resin shield for use in shielding cask studies and identified by 9005,
6. average spectrum in a 50-cm concrete shield for cask shielding studies and identified by 9006, and
7. spectrum in an infinite medium of hydrogen and U with H/X = 300.

In cases 3 through 6, the spent fuel source was a 15 × 15 Westinghouse LWR assembly with initial enrichment of 3.0 wt % and burned to 30 GWd/MTU and cooled for 5 years.

Data testing has been performed for 33 benchmarks, including 28 Cross Section Evaluation Working Group (CSEWG) benchmarks. Results obtained for these benchmarks are very close to those obtained by other data testers using different ENDF/B-V-based cross-section libraries. There is considerable improvement in the trend of k_{eff} vs leakage obtained with the use of the ENDF/B-VI oxygen evaluation. The LAW-238 library appears to be acceptable for general use in criticality and reactor physics applications. The library has had minimal testing for shielding applications and should be evaluated by the user for applicability.

3.1.2 The 44-group ENDF/B-V library (44GROUPNDF5)

The 44-group ENDF/B-V library has been developed for use in the analysis of fresh and spent fuel and radioactive waste systems. Collapsed from the fine-group 238GROUPNDF5 cross-section library, this broad-group library contains all nuclides (more than 300) from the ENDF/B-V data files. Broad-group boundaries were chosen as a subset of the parent 238GROUPNDF5 boundaries, emphasizing the key spectral aspects of a typical LWR fuel package. Specifically, the broad-group structure was designed to accommodate the following features:

- two windows in the oxygen cross-section spectrum; a window in the cross section of iron;
- the Maxwellian peak in the thermal range; and
- the 0.3-eV resonance in ^{239}Pu (which, due to its low energy, cannot be properly modelled via the SCALE Nordheim Integral Treatment module NITAWL-II).

The resulting boundaries represent 22 fast and 22 thermal energy groups (below 3 eV); the full group structure is compared to that of the 238-group library in Table 4. The fine-group 238GROUPNDF5 cross sections were collapsed into this broad-group structure **using a fuel cell spectrum calculated based on a 17 × 17 Westinghouse pressurized-water reactor (PWR) assembly**.

Because of the significantly improved and conservative behaviour of the ENDF/B-VI ^{16}O evaluation under conditions where higher-order scattering terms are important (e.g., high leakage geometries), this cross section has been included in the 238-group and 44-group libraries as the default for ^{16}O. Similarly, ENDF/B-VI evaluations of ^{14}N and ^{15}N are included in the library; however, ENDF/B-V versions remain the default for these isotopes. The ENDF/B-VI nitrogen data were processed using the same methods used for ^{16}O, and, like oxygen, were tested to see if significant differences between ENDF/B-V and ENDF/B-VI could be identified. No significant differences have been identified; however, because they had already been processed into AMPX master library format and were readily available, ENDF/B-VI ^{14}N and ^{15}N cross sections are included in the library. Finally, ENDF/B-VI evaluations of ^{154}Eu and ^{155}Eu are also included in the library because the more recent ENDF/B-VI evaluations include resonance parameters not included in previous evaluations and yield energy-dependent cross sections significantly different from those obtained using ENDF/B-V cross sections. Comparisons of depletion/decay calculations to experimental isotopic measurements have indicated that the ENDF/B-VI europium evaluations are more accurate than those available in ENDF/B-V. However, as with ^{16}O, ENDF/B-V cross sections are also available within the library.

The 44GROUPNDF5 library was tested against its parent library using a set of 33 benchmark problems in order to demonstrate that the collapsed set was an acceptable representation of 238GROUPNDF5, **except for intermediate energy systems**. Validation of the library within the SCALE system was based on a comparison of calculated values of k_{eff} with that of 93 experiments: 92 critical and 1 subcritical experiments.

The experiments primarily consisted of various configurations of light-water-reactor-type fuel representative of transportation and storage conditions. Additional experiments were included to allow comparison with results obtained in earlier validation of the 27GROUPNDF4 library.

Results show that **the broad 44-group structure is an acceptable representation of its parent 238-group library for thermal as well as hard fast spectrum systems**. Accurate broad-group analyses of intermediate spectrum systems will require either a more detailed group structure in this energy range or a more appropriate collapsing spectrum. Further, validation calculations indicate that the 44-group library is an accurate tool in the prediction of criticality for arrays of light-water-reactor-type fuel assemblies, as would be encountered in fresh or spent fuel transportation or storage environments. **Validation results for LWR-type UO_2 fuel show virtually no bias**. A positive bias of 0.5 to 1% has been observed for very thermal mixed-oxide systems. The bias is caused by inadequate representation of plutonium cross sections, possibly in the ENDF/B-V data. These validation results are consistently better than those seen for the same cases using the 27GROUPNDF4 library and make **the 44GROUPNDF5 library the recommended library for thermal and many hard fast spectrum systems**. For intermediate energy systems, the parent 238GROUPNDF5 library is recommended.

3.2 Other fine-group libraries for SCALE

3.2.1 EJ2-XMAS and EIJ2-XMAS libraries

Besides ENF/B-V and ENF/B-VI libraries, one of the best basic nuclear data libraries is the Joint Evaluated File version 2,2 (JEF2.2) which has been developed and benchmarked in Europe. That is why two fine-group libraries for SCALE system have been prepared at ECN-Petten, the Netherlands [6].

The first library, EJ2-XMAS (ECN JEF2), is a JEF2.2 based AMPX-Master library in the XMAS 172-group structure (see Table 7 for comparison with 238- and 44-group structures) for reactor calculations with the AMPX/SCALE-4 system. The group cross-section data were generated with NJOY89.62 and NJOY91.91 [3]. The library contains all the JEF2.2 nuclides which were successfully processed by NJOY.

The second library, EIJ2-XMAS library (ECN/IRI JEF2) has been developed in collaboration with IRI, Delft University of Technology. It differs from EJ2-XMAS library in that it was generated with NJOY91.118 and NSLINK4.2 [7] and contains only data of the 133 most important nuclides for reactivity, burnup and criticality calculations (see Table 8). The data of all other 181 nuclides available on JEF2.2 which are considered to be less important for reactor calculations, are copied from the previously compiled EJ2-XMAS library and put in a supplement to the EIJ2-XMAS library (see Table 9).

The data on the EJ2- and EIJ2-XMAS libraries allow Nordheim resolved-resonance treatment by the module SCALE/NITAWL and Bondarenko treatment of unresolved-resonances by SCALE/BONAMI. However, neither the Bondarenko method nor the Nordheim method is valid for very low-energy resonance self-shielding calculations (E_{res} < 1 eV). But in this energy range each resonance is covered by quite a number of groups. Cross

Table 7. Group structure for EIJ2-XMAS library

(compared with 238- and 44-group libraries)

238 group	44 group	172 group	Upper Energy (eV)
1	1		2.0000E+07
		1	1,9640E+07
2		2	1.7333E+07
3			1.5683E+07
		3	1.4918E+07
4			1.4550E+07
5		4	1.3840E+07
6			1.2840E+07
		5	1.1618E+07
7		6	1.0000E+07
8	2	7	8.1873E+06
		8	6.7032E+06
9	3		6.4340E+06
		9	6.0653E+06
		10	5.4881E+06
10	4		4.8000E+06
		11	4.4933E+06
11			4.3040E+06
		12	3.6788E+06
		13	3.0119E+06
12	5		3.0000E+06
13	6		2.4790E+06
		14	2.4660E+06
14	7		2.3540E+06
		15	2.2313E+06
		16	2.0190E+06
15	8		1.8500E+06
		17	1.6530E+06
16			1.5000E+06
17	9		1.4000E+06
18			1.3560E+06
		18	1.3534E+06
19			1.3170E+06
20			1.2500E+06
		19	1.2246E+06
21			1.2000E+06
		20	1.1080E+06
		21	1.0026E+06
22			1.1000E+06
23			1.0100E+06
24			9.2000E+05
		22	9.0718E+05
25	10		9.0000E+05
26			8.7500E+05
27			8.6110E+05
		23	8.2085E+05
28			8.2000E+05
29			7.5000E+05
30			6.7900E+05
31			6.7000E+05
		24	6.0810E+05
32			6.0000E+05
33			5.7300E+05
		25	5.5023E+05
34			5.5000E+05
35			4.9952E+05
		26	4.9787E+05
36			4.7000E+05
		27	4.5049E+05
37			4.4000E+05
38			4.2000E+05
		28	4.0762E+05
39	11		4.0000E+05
40			3.3000E+05
		29	3.0197E+05
		30	2.7324E+05
41			2.7000E+05
		31	2.4724E+05
42			2.0000E+05
		32	1.8316E+05
43			1.5000E+05
44			1.2830E+05
		33	1.2277E+05
		34	1.1109E+05
45	12		1.0000E+05
46			8.5000E+04
		35	8.2298E+04
47			8.2000E+04
48			7.5000E+04
49			7.3000E+04
		36	6.7380E+04
50			6.0000E+04
		37	5.5166E+04
51			5.2000E+04
52			5.0000E+04
53			4.5000E+04
		38	4.0868E+04
		39	3.6979E+04
54			3.0000E+04
		40	2.9283E+04
		41	2.7394E+04
55	13		2.5000E+04
		42	2.4788E+04
56	14		1.7000E+04
		43	1.6616E+04
		44	1.5034E+04
57			1.3000E+04

238 group	44 group	172 group	Upper Energy (eV)
		45	1.1138E+04
58			9.5000E+03
		46	9.1188E+03
59			8.0300E+03
		47	7.4659E+03
60			6.0000E+03
		48	5.5308E+03
		49	5.0045E+03
61			3.9000E+03
62			3.7400E+03
		50	3.5266E+03
		51	3.3546E+03
63	15		3.0000E+03
64			2.5800E+03
		52	2.2487E+03
65			2.2900E+03
66			2.2000E+03
		53	2.0347E+03
67			1.8000E+03
68			1.5500E+03
69			1.5000E+03
		54	1.5073E+03
		55	1.4338E+03
		56	1.2341E+03
70			1.1500E+03
		57	1.0104E+03
71			9.5000E+02
		58	9.1424E+02
		59	7.4852E+02
72			6.8300E+02
		60	6.7729E+02
73			6.7000E+02
74	16		5.5000E+02
		61	4.5400E+02
		62	3.7170E+02
75			3.0500E+02
		63	3.0433E+02
76			2.8500E+02
77			2.4000E+02
78			2.1000E+02
79			2.0750E+02
		64	2.0400E+02
80			1.9250E+02
81			1.8600E+02
		65	1.4863E+02
		66	1.3674E+02
82			1.2200E+02
83			1.1900E+02
84			1.1500E+02
85			1.0800E+02
86	17		1.0000E+02
		67	9.1661E+01
87			9.0000E+01
88			8.2000E+01
89			8.0000E+01
90			7.6000E+01
		68	7.5674E+01
91			7.2000E+01
		69	6.7904E+01
92			6.7500E+01
93			6.5000E+01
94			6.1000E+01
95			5.9000E+01
		70	5.5595E+01
96			5.3400E+01
97			5.2000E+01
		71	5.1578E+01
98			5.0600E+01
99			4.9200E+01
100			4.8300E+01
		72	4.8252E+01
101			4.7000E+01
		73	4.5517E+01
102			4.5200E+01
103			4.4000E+01
104			4.2400E+01
105			4.1000E+01
		74	4.0169re+01
106			3.9600E+01
107			3.9100E+01
108			3.8000E+01
		75	3.7267E+01
109			3.7000E+01
110			3.5500E+01
111			3.4600E+01
112			3.3750E+01
		76	3.3720E+01
113			3.3250E+01
114			3.1750E+01
115			3.1250E+01
		77	3.0511E+01
116	18		3.0000E+01
		78	2.7608e+01
117			2.7500E+01
118			2.5000E+01
		79	2.4981E+01
		80	2.2603E+01

238 group	44 group	172 group	Upper Energy (eV)
119			2.2500E+01
120			2.1000E+01
121			2.0000E+01
		81	1.9455E+01
122			1.9000E+01
123			1.8500E+01
124			1.7000E+01
125			1.6000E+01
		82	1.5928E+01
126			1.5100E+01
127			1.4400E+01
128			1.3750E+01
		83	1.3710E+01
129			1.2900E+01
130			1.1900E+01
131			1.1500E+01
		84	1.1225E+01
132	19		1.0000E+01
		85	9.9056E+00
		86	9.1898E+00
133			9.1000E+00
		87	8.3153E+00
134	20		8.1000E+00
		88	7.5240E+00
135			7.1500E+00
136			7.0000E+00
137			6.7500E+00
138			6.5000E+00
139			6.2500E+00
		89	6.1601E+00
140	21		6.0000E+00
141			5.4000E+00
		90	5.3464E+00
		91	5.0435E+00
142			5.0000E+00
143	22		4.7500E+00
		92	4.1293e+00
144		93	4.0000E+00
145			3.7300E+00
146			3.5000E+00
		94	3.3808e+00
		95	3.3000E+00
147			3.1500E+00
148			3.0500E+00
149	23		3.0000E+00
150			2.9700E+00
151			2.8700E+00
152			2.7700E+00
		96	2.7679E+00
		97	2.7200E+00
153			2.6700E+00
		98	2.6000E+00
154			2.5700E+00
		99	2.5500E+00
155			2.4700E+00
156			2.3800E+00
		100	2.3600E+00
157			2.3000E+00
158			2.2100E+00
		101	2.1300E+00
159			2.1200E+00
		102	2.1000E+00
		103	2.0200E+00
160			2.0000E+00
161			1.9400E+00
		104	1.9300E+00
162			1.8600E+00
		105	1.8400E+00
163	24		1.7700E+00
		106	1.7550E+00
164			1.6800E+00
		107	1.6700E+00
165		108	1.5900E+00
166		109	1.5000E+00
		110	1.4750E+00
167			1.4500E+00
		111	1.4450E+00
168			1.4000E+00
		112	1.3700E+00
169			1.3500E+00
		113	1.3375E+00
170		114	1.3000E+00
171			1.2500E+00
		115	1.2350E+00
172			1.2250E+00
173			1.2000E+00
174			1.1750E+00
		116	1.1700E+00
175		117	1.1500E+00
176			1.1400E+00
177			1.1300E+00
		118	1.1254E+00
178			1.1200E+00
179		119	1.1100E+00
180			1.1000E+00
		120	1.0970E+00
181			1.0900E+00

238 group	44 group	172 group	Upper Energy (eV)
182			1.0800E+00
		121	1.0710E+00
183			1.0700E+00
184			1.0600E+00
185			1.0500E+00
		122	1.0450E+00
186			1.0400E+00
		123	1.0350E+00
187			1.0300E+00
188		124	1.0200E+00
189			1.0100E+00
190	25		1.0000E+00
		125	9.9600E-01
		126	9.8600E-01
191			9.7500E-01
		127	9.7200E-01
192		128	9.5000E-01
		129	9.3000E-01
193			9.2500E-01
		130	9.1000E-01
194			9.0000E-01
		131	8.6000E-01
195		132	8.5000E-01
196			8.0000E-01
		133	7.9000E-01
		134	7.8000E-01
197			7.5000E-01
		135	7.0500E-01
198			7.0000E-01
199			6.5000E-01
200	26	136	6.2500E-01
201			6.0000E-01
202			5.5000E-01
		137	5.4000E-01
203		138	5.0000E-01
		139	4.8500E-01
204			4.5000E-01
		140	4.3300E-01
205	27	141	4.0000E-01
		142	3.9100E-01
206	28		3.7500E-01
207	29	143	3.5000E-01
208	30		3.2500E-01
		144	3.2000E-01
		145	3.1450E-01
209		146	3.0000E-01
		147	2.8000E-01
210	31		2.7500E-01
211	32		2.5000E-01
		148	2.4800E-01
212	33		2.2500E-01
		149	2.2000E-01
213	34		2.0000E-01
		150	1.8900E-01
		151	1.8000E-01
214			1.7500E-01
		152	1.6000E-01
215	35		1.5000E-01
		153	1.4000E-01
		154	1.3400E-01
216			1.2500E-01
		155	1.1500E-01
217	36	156	1.0000E-01
		157	9.5000E-02
218			9.0000E-02
219		158	8.0000E-02
		159	7.7000E-02
220	37		7.0000E-02
		160	6.7000E-02
221			6.0000E-02
		161	5.8000E-02
222	38	162	5.0000E-02
		163	4.2000E-02
223	39		4.0000E-02
		164	3.5000E-02
224	40	165	3.0000E-02
225	41		2.5300E-02
		166	2.5000E-02
		167	2.0000E-02
		168	1.5000E-02
226	42	169	1.0000E-02
227	43		7.5000E-03
		170	6.9000E-03
228		171	5.0000E-03
229			4.0000E-03
230	44	172	3.0000E-03
231			2.5000E-03
232			2.0000E-03
233			1.5000E-03
234			1.2000E-03
235			1.0000E-03
236			7.5000E-04
237			5.0000E-04
238			1.0000E-04
			1.0000E-05

sections of nuclides with resonances below 1 eV should only be collapsed after the flux is determined in a full fine-group (172) transport calculation (XSDRN [1]).

There are some other features of the EIJ2-XMAS library:

Thermal scattering treatment

In general the free gas assumption is used in the calculation of the thermal scattering matrix. For all nuclides marked with „T“ in column 7 of Table 8, the thermal scattering matrix is given at temperatures T = 293.6, 600, 900, 1000, 1200, 1500, 2000, 2500 K. All other nuclides have a thermal scattering matrix at T=293.6 K.

The nuclides H in H_2O, D in D_2O, Be in Beryllium and C in graphite are given a special thermal scattering treatment which accounts not only for upscattering but also for molecular, crystalline and solid state effects.

The thermal range defined for thermal scattering treatment extends from 10^{-5} eV to 3.30 eV.

Bondarenko treatment

The Bondarenko treatment in the (un)resolved-resonance range is applied to σ_t, σ_{sc}, σ_f and $\sigma_{n,\gamma}$ for several values of σ_0 and temperatures.

The Bondarenko treatment is applied to all nuclides marked with „B“ in column 6 of Table 8 at $\sigma_0 = 10^{10}, 10^4, 10^3, 300, 100, 30, 10, 10^{-3}$ b.

The Bondarenko treatment is applied to all nuclides marked with „b“ in column 6 of Table 8 at $\sigma_0 = 10^{10}, 10^3, 100, 10$ b.

For some nuclides the Bondarenko treatment is also applied in the resolved-resonance range (structural materials with Reich-Moore resolved-resonance parameters and some fission products). These nuclides are marked with „b“ in column 5.

The temperatures for the Bondarenko treatment are:

T = 293.6, 600, 900, 1000, 1200, 1500, 2000, 2500 K.

It should be noted that the Bondarenko factors in the thermal range (E < 3.3 eV) account only for temperature effects at low energies.

Nordheim treatment

A Nordheim treatment of resolved-resonances is possible for all the nuclides marked with „N“ in column 5 of Table 8.

Weighting spectrum.

The weighting spectrum used in the group averaging in NJOY is

Maxwellian + 1/E + Fission

With the following characteristic energies:

E_{th} = 0.025 eV the „temperature“ of the Maxwellian distribution (in eV),

$E_{th,br}$ = 0.4 eV thermal break, (0.102 eV in case of EJ-XMAS),

$E_{f,br}$ = 0.8 MeV fission break, (0.82 MeV in case of EJ-XMAS),

E_f = 1.4 MeV the „temperature“ of the fission distribution (in eV).

Legendre order

The Legendre order used for all scattering matrices (elastic and inelastic scattering and (n,2n), (n,3n), etc.) is P_3.

Conversion of Reich-Moore to MLBW parameters

For several nuclides on the JEF2.2 library, Reich-Moore (RM) resolved-resonance parameters are given. The Nordheim resolved-resonance treatment module of the SCALE system, NITAWL, cannot treat RM parameters. It can handle only Single-Level Breit-Wigner parameters (SLBW). Multi-Level Breit-Wigner parameters (MLBW) are also treated as SLBW parameters by NITAWL. This means that for some *actinides*, the RM parameters had to be converted to MLBW parameters. It is emphasized that in NITAWL these converted (approximate) resolved-resonance parameters are used only for the calculation of the self shielding and the Doppler effect as a correction on the infinite diluted cross section at the base temperature of T=293.6 K. The infinite diluted cross sections themselves (at temperature T=293.6 K) are calculated by NJOY from the original unchanged JEF2.2 evaluation with the RM parameters.

The energy upper limits up to which the RM parameters are converted to MLBW and up to which the RM parameters are put on the AMPX-M (E_h) are as follows:

Nuclide	E_h AMPX-M(eV)	$E_{h,orig}$ in JEF2.2(eV)
U235	454	2250
U238	5100	10000
Pu239	454	1000
Pu241	304	300
Cm243	25	26
Cm245	55.6	61

The remaining part of the resolved-resonance region, ranging from E_h to $E_{n,orig}$, can be treated with the Bondarenko method by BONAMI. The value of E_h was chosen to be close to a group boundary. At energies above E_h the Bondarenko method yields a reasonably good description of self-shielding and Doppler broadening.

There are also some *structural materials* for which RM parameters were used in JEF2.2. In these cases the Bondarenko method has to be applied to account for the resolved-resonance self shielding.

For details of the conversion to MLBW parameters see [8, 9].

Natural elements

The natural elements do not have Nordheim or Bondarenko data necessary to calculate the self shielding, even if the JEF2 evaluation contains (un)resolved-resonance parameters. The reason for this is that CSAS can not always handle elemental evaluations (multi-isotopic evaluations) to create correct input decks for BONAMI and NITAWL.

Except for special reasons the elemental evaluations should be used rather than combining isotopic evaluations. However, in fission product poisoning, burnup calculations (burnable poisons like Gd isotopes), or when large self-shielding effects are expected (Cd isotopes in control rods) the isotopic evaluations should be used. Note that isotopic evaluations are not necessarily consistent with elemental evaluations.

Contents of the EIJ2-XMAS library is given in Table 8.

Legend to Table 8:

Column 1: nuclide; mass number A='nat' indicates the natural element
Column 2: material ID in JEF2.2 file. This is not equal to ID number on AMPX-M
Column 3: presence and format of the resolved-resonance parameters in JEF2.2 library
Column 4: presence of the unresolved-resonance parameters in JEF2.2 library
Column 5: 'N' means that Nordheim treatment with NITAWL is possible
Col 5 & 6: 'B' or 'b' means that Bondarenko treatment with BONAMI is possible:
'B' means Bondarenko treatment for $\sigma_0 = 10^{10}, 10^4, 10^3, 300, 100, 30, 10, 10^{-3}$ b
'b' means Bondarenko treatment for $\sigma_0 = 10^{10}, 10^3, 100, 10$ b
The temperatures for the Bondarenko treatment are: 293.6, 600, 900, 1000, 1200, 1500, 2000, 2500 K.
Column 7: 'T' means that a temperature dependent thermal scattering matrix is included
Column 8: remarks

Contents of the Supplement to the EIJ2-XMAS library is given in Table 9.

The data of all nuclides not included in EIJ2-XMAS library are copied from the previous compiled EJ2-XMAS library and are put in the Supplement to the EIJ2-XMAS library.

Legend to Table 9:

Col 1 - 3: the same as in Table 8
Column 4: + means that Nordheim treatment with NITAWL is possible
Column 5: + means that Bondarenko treatment with BONAMI is possible
Column 6: shows the thermal capture cross section
Column 7: gives the clasification of the nuclide according to the following table:

Class	σ_0 and T_0 specifications	Nordheim
1	T_{H2O}, T_{D2O}=293.6, 323.6, 373.6, 423.6, 473.6, 523.6, 573.6, 623.6 K σ_0 =10 b	-
2	T_0 =293.6 K σ_0 =10 b	-
3	T_0 =293.6 K σ_0 =10 b	+
4	T_0 =293.6, 600, 900, 1000, 1200, 1500, 2000, 2500 K $\sigma_0 = 10^{10}, 10^3, 100, 10$ b	-
5	T_0 =293.6, 600, 900, 1000, 1200, 1500, 2000, 2500 K $\sigma_0 = 10^{10}, 10^3, 100, 10$ b	+
6	T_0 =293.6, 600, 900, 1000, 1200, 1500, 2000, 2500 K $\sigma_0 = 10^{10}, 10^4, 10^3, 300, 100, 30, 10, 10^{-3}$ b	-
7	T_0 =293.6, 600, 900, 1000, 1200, 1500, 2000, 2500 K $\sigma_0 = 10^{10}, 10^4, 10^3, 300, 100, 30, 10, 10^{-3}$ b	+
8	T_0 =293.6, 600, 900, 1000, 1200, 1500, 2000, 2500 K σ_0 =10 b	-
9	T_0 =293.6, 600, 900, 1000, 1200, 1500, 2000, 2500 K σ_0 =10 b	+

Table 8. Contents of the EIJ2-XMAS library

Isotope	ID	RRP	URP	Treatment			Remark
	JEF2.2	JEF2.2	JEF2.2	R	U	T	
H in H_2O	125/1					T	
D in D_2O	128/11					T	
1-T-3	131					T	
2-He-3	225					T	
2-He-4	228					T	
3-Li-6	325					T	
3-Li-7	328					T	
4-Be-9	425/26					T	in Be
5-B-10	525					T	
5-B-11	528					T	
C-nat	xxx					T	free
C-nat	600/31					T	in graphite
7-N-14	725					T	
8-O-16	825					T	
8-O-17	828					T	
9-F-19	925					T	
13-Al-27	1325					T	
14-Si-nat	1400					T	
18-Ar-36	1825	MLBW	+	N	B	T	from EFF2
18-Ar-38	1831	MLBW	+	N	B	T	from EFF2
18-Ar-40	1837	MLBW		N		T	from EFF2
24-Cr-50	2425	RM		B		T	
24-Cr-52	2431	RM		B		T	
24-Cr-53	2434	RM		B		T	
24-Cr-54	2437	RM		B		T	
25-Mn-55	2525	MLBW		N		T	
26-Fe-54	2625	RM		B		T	
26-Fe-56	2631	RM	+	B	B	T	
26-Fe-57	2634	RM		B		T	
26-Fe-58	2637	RM	+	B	B	T	
28-Ni-58	2825	RM		B		T	
28-Ni-60	2831	RM		B		T	bf.gt. 3
28-Ni-61	2834	RM		B		T	
28-Ni-62	2837	RM		B		T	
28-Ni-64	2843	RM		B		T	
29-Cu-nat	2900	MLBW				T	
31-Ga-nat	3100					T	
36-Kr-83	3640	MLBW		b		T	
40-Zr-nat	4000	MLBW				T	
40-Zr-90	4025	MLBW				T	
40-Zr-91	4028	MLBW	+	N	B	T	
40-Zr-92	4031	MLBW		N		T	
40-Zr-93	4034	MLBW	+	N	B	T	
40-Zr-94	4037	MLBW		N		T	
40-Zr-95	4040	MLBW	+	N	B	T	
40-Zr-96	4043	MLBW	+	N	B	T	
41-Nb-95	4131	MLBW	+	b	b		
42-Mo-95	4234	MLBW		b			
43-Tc-99	4331	MLBW	+	N			
44-Ru-101	4440	MLBW	+	b			
44-Ru-103	4446	MLBW	+	b	b		
45-Rh-103	4525	MLBW	+	b			
45-Rh-105	4531						
46-Pd-105	4634	MLBW	+	b	b		
46-Pd-107	4640	MLBW	+	b			
46-Pd-108	4643	MLBW	+	b			bf.gt. 3
47-Ag-107	4725	MLBW		N			
47-Ag-109	4731	MLBW	+	N			
47-Ag-111	4737						
51-Sb-121	5125	MLBW					
51-Sb-123	5131	MLBW					
53-I-127	5325	MLBW	+	b			
53-I-129	5331	MLBW	+	N			
53-I-135	5349						
54-Xe-131	5446	MLBW		N			
54-Xe-135	5458						
55-Cs-133	5525	MLBW	+	b	b		
55-Cs-134	5528	MLBW		b			
55-Cs-135	5531	MLBW	+	b	b		
57-La-139	5728	MLBW	+	b			
59-Pr-141	5925	MLBW	+	b			
60-Nd-143	6028	MLBW	+	b	b		
60-Nd-144	6031	MLBW	+	b			
60-Nd-145	6034	MLBW	+	b			
60-Nd-146	6037	MLBW	+	b			
61-Pm-147	6149	MLBW	+	b	b		
61-Pm-148	6152						
61-Pm-148m	6153	MLBW		b			
61-Pm-149	6155						
62-Sm-147	6234	MLBW	+	b	b		
62-Sm-149	6240	MLBW	+	N	B		
62-Sm-150	6243	MLBW		b			
62-Sm-151	6246	MLBW	+	b	b		
62-Sm-152	6249	MLBW	+	b	b		
63-Eu-153	6331	MLBW	+	N	B		
63-Eu-154	6334	MLBW	+	N	B		
63-Eu-155	6337	MLBW	+	N	B		
64-Gd-154	6431	MLBW		b			
64-Gd-155	6434	MLBW	+	N	B		
64-Gd-156	6437	MLBW	+	b	b		
64-Gd-157	6440	MLBW		N			
64-Gd-158	6443	MLBW		b			
66-Dy-160	6637	MLBW		b			
66-Dy-161	6640	MLBW		b			
66-Dy-162	6643	MLBW		b			
66-Dy-163	6646	MLBW		N			
66-Dy-164	6649	MLBW	+	N	B		
67-Ho-165	6725	MLBW		N			
72-Hf-174	7225	MLBW		N			
72-Hf-176	7231	MLBW		N			
72-Hf-177	7234	MLBW		N			
72-Hf-178	7237	MLBW		N			
72-Hf-179	7240	MLBW		N			
72-Hf-180	7243	MLBW		N			
73-Ta-181	7328	MLBW	+				
79-Au-197	7925	MLBW		N			
83-Bi-209	8325						
92-U-233	9222	MLBW		N			
92-U-234	9225	MLBW	+	N	B		
92-U-235	9228	RM$\rightarrow$ML	+	N	B	T	
92-U-236	9231	MLBW	+	N	B		
92-U-238	9237	RM$\rightarrow$ML	+	N	B	T	
93-Np-237	9346	MLBW		N			
93-Np-238	9349	MLBW	+	N			
93-Np-239	9352	MLBW		N			
94-Pu-238	9434	MLBW		N			
94-Pu-239	9437	RM$\rightarrow$ML	+	N	B	T	
94-Pu-240	9440	MLBW	+	N	B	T	
94-Pu-241	9443	RM$\rightarrow$ML	+	N	B	T	
94-Pu-242	9446	MLBW		N		T	
95-Am-241	9543	MLBW		N			
95-Am-242m	9547	MLBW	+	N			
95-Am-243	9549	MLBW	+	N	B		
96-Cm-242	9631	MLBW	+	N			
96-Cm-243	9634	RM$\rightarrow$ML	+	N	B		
96-Cm-244	9637	MLBW	+	N			
96-Cm-245	9640	RM$\rightarrow$ML	+	N	B		
96-Cm-247	9646	MLBW	+	N			
97-Bk-249	9752	MLBW	+	N			
98-Cf-249	9852	MLBW	+	N			
98-Cf-250	9855	MLBW	+	N			
98-Cf-252	9861	MLBW	+	N			
98-Cf-253	9864	MLBW	+	N			
99-Es-253	9917	MLBW	+	N			

Table 9. Contents of the EJ2-XMAS library (as supplement to EIJ-XMAS library)

Isotop	ID JEF2.2	RRP JEF2.2	RRP EJ2	BON	$\sigma_{n,\gamma}^{th}$ (b)	Class
1-H-1	125				0.33	8
1-D-2	128				0.000506	8
7-A-15	728	MLBW	+		0.000024	9
11-Na-23	1125	MLBW	+		0.53	9
12-Mg-nat	1200				0.063	8
13-Al-27	1325				0.213	8
15-P-31	1525	MLBW	+		0.17	9
16-S-32	1625	MLBW	+		0.53	9
16-S-32	1628	MLBW	+		0.35	9
16-S34	1631	MLBW	+		0.22	9
16-S-36	1637				0.15	8
17-Cl-nat	1700				33	8
19-K-nat	1900				2.1	8
20-Ca-nat	2000				0.43	8
22-Ti-nat	2200				6.11	8
23-V-nat	2300				5.06	8
27-Co-58	2722	MLBW			1880	2
27-Co-59	2725	MLBW	+			3
30-Zn-64	3025	MLBW			0.76	2[1]
31-Ga-nat	3100				3	2
32-Ge-72	3231	MLBW			1	2
32-Ge-73	3234	MLBW			15	2
32-Ge-74	3237	MLBW			0.4	2
32-Ge-76	3243	MLBW			0.14	2
33-As-75	3325	MLBW			4.3	2
34-Se-74	3125	MLBW				2
34-Se-76	3431	MLBW			85	2
34-Se-77	3434	MLBW			42	2
34-Se-78	3437	MLBW			0.4	2
34-Se-80	3443	MLBW			0.6	2
34-Se-82	3449	MLBW			0.05	2
35-Br-79	3525	MLBW			11	2
35-Br-81	3531	MLBW			2.8	2
36-Kr-78	3625	MLBW			4.7	2
36-Kr-80	3631	MLBW			12	2
36-Kr-82	3637	MLBW			30.2	2
36-Kr-84	3643	MLBW			83	2
36-Kr-85	3646				1.7	2
36-Kr-86	3649	MLBW				2
37-Rb-85	3725	MLBW			0.5	2
37-Rb-86	3728				5	2
37-Rb-87	3731	MLBW				2
38-Sr-84	3825	MLBW				2
38-Sr-86	3831	MLBW			3	2
38-Sr-87	3834	MLBW			16	2
38-Sr-88	3837	MLBW				2
38-Sr-89	3840	MLBW			0.4	2
38-Sr-90	3843				3.67	2
39-Y-89	3925	MLBW			1.3	2
39-Y-90	3928	MLBW			3.5	2
39-Y-91	3931				1.4	2
41-Nb-93	4125	MLBW		+	1.15	2
41-Nb-94	4128	MLBW			13.6	2
42-Mo-nat	4200	MLBW				2
42-Mo-92	4225	MLBW			0.019	2
42-Mo-94	4231	MLBW			0.013	2
42-Mo-96	4237	MLBW			506	2
42-Mo-97	4240	MLBW	+		2.14	3
42-Mo-98	4243	MLBW		+	129	2
42-Mo-99	4246				1.7	2
42-Mo-100	4249	MLBW		+	198.5	2
44-Ru-96	4425				0.25	2
44-Ru-98	4431				8	2
44-Ru-99	4434	MLBW			7	2
44-Ru-100	4437	MLBW			6	2
44-Ru-102	4443	SLBW	+		1.30	3
44-Ru-104	4449	MLBW			0.3	2
44-Ru-105	4452				0.2	2
44-Ru-106	4455				0.15	2
46-Pd-102	4625	MLBW			3.4	2
46-Pd-104	4631	MLBW		+	315	2[1]
46-Pd-106	4637	MLBW		+	300	2[1]
46-Pd-110	4649	MLBW		+	0.2	2[1]
48-Cd-nat	4800				2461	2
48-Cd-106	4825	MLBW	+			3
48-Cd-110	4837	MLBW	+		11	3
48-Cd-111	4840	MLBW	+	+	24	5
48-Cd-112	4843	MLBW	+		2.2	3
48-Cd-113	4846	MLBW	+	+	20615	5
48-CD-114	4849	MLBW	+		0.34	3
48-Cd-115m	4852				31	2
48-Cd-116	4855	MLBW	+		0.1	3
49-In-113	4925	MLBW	+		12	3
49-In-115	4931	MLBW	+		202	3
50-Sn-112	5025	MLBW		+	0.73	2[1]
50-Sn-114	5031	MLBW				2
50-Sn-115	5034	MLBW			50	2
50-Sn-116	5037	MLBW				2
50-Sn-117	5040	MLBW			2.6	2
50-Sn-118	5046	MLBW			2.3	2
50-Sn-119	5046	MLBW			2.3	2
50-Sn-120	5049	MLBW			0.14	2
50-Sn-122	5055	MLBW			0.2	2
50-Sn-123	5058					2
50-Sn-124	5061	MLBW			0.13	2
50-Sn-125	5064				0.6	2
50-Sn-126	5067	MLBW				2
51-Sb-124	5134				6.5	2
51-Sb125	5137	MLBW			1	2
51-Sb-126	5140				5.8	2
52-Te-120	5225				2.3	2
52-Te-122	5231	MLBW			3	2
52-Te-123	5234	MLBW			410	2
52-Te-124	5237	MLBW			7	2
52-Te-125	5240	MLBW			1.6	2
52-Te-126	5243	MLBW			1	2
52-Te-127m	5246				9.4	2
52-Te-128	5249	MLBW			8.4	2
52-Te129m	5252				1.1	2
52-Te-130	5255	MLBW			0.3	2
52-Te-132	5261				0.002	2
53-I-130	5334				18	2
53-I-131	5337	MLBW			0.7	2
54-Xe-124	5425	MLBW			165	2
54-Xe-126	5431	MLBW			2.2	2
54-Xe-128	5437	MLBW			5.36	2
54-Xe-129	5440	MLBW			18	2
54-Xe-130	5443	MLBW			6.2	2
54-Xe132	5449	MLBW			0.5	2
54-Xe-133	5452				190	2
54-Xe-134	5455	MLBW			0.25	2
54-Xe-136	5461				0.16	2
55-Cs-136	5534	MLBW			1.30	2
55-Cs-137	5537	MLBW		+	0.14	2
56-Ba-134	5637	MLBW			2.2	2
56-Ba-135	5640	MLBW			6	2
56-Ba-136	5643	MLBW			0.4	2
56-Ba-137	5646	MLBW			5.1	2
56-Ba-138	5649	MLBW			0.4	2
56-Ba-140	5655	MLBW		+	1.6	2
57-La-140	5731	MLBW			2.7	2
58-Ce-140	5837	MLBW			0.6	2

Table 9. (continued)

Isotop	ID JEF2.2	RRP JEF2.2	RRP EJ2	BON	$\sigma_{n,\gamma}^{th}$ (b)	Class
58-Ce-141	5840	MLBW		+	32.7	2
58-Ce-142	5843	MLBW		+	1	2
58-Ve-143	5846	MLBW			6	2
58-Ce-144	5849	MLBW		+	1.13	2
59-Pr-142	5928	MLBW			20	2
59-Pr-143	5931				89	2
60-Nd-142	6025	MLBW			17	2
60-Nd-147	6040	MLBW			440	2
60-Nd-148	6043	MLBW		+	2.5	2[1]
60-Nd-150	6049	MLBW			1.2	2
61-Pm-151	6161				700	2
62-Sm-144	6225				0.7	2
62-Sm-148	6237				5.2	2
62-Sm-153	6252				330	2
62-Sm-154	6255	MLBW			8.4	2
63-Eu-151	6325	MLBW	+	+		5
63-Eu-152	6328	MLBW	+	+		5
63-Eu-156	6340				482	2
63-Eu-157	6343				190	2
64-Gd-160	6449	MLBW	+		0.72	3
65-Tb-159	6525	MLBW		+	23	2
65-Tb-160	6528				525	2
68-Er-166	6837	MLBW			35	2
68-Er-167	6840	MLBW			670	2
71-Lu-175	7125	MLBW		+	25.88	2
71-Lu-176	7128	MLBW		+	1952	2
73-Ta-182	7331	MLBW		+		2
74-W-182	7431	MLBW		+	20.5	2
74-W-183	7434	MLBW		+	10	2
74-W-184	7437	MLBW		+	1.8	2
74-W-186	7443	MLBW		+	37.5	2
75-Re-185	7525	MLBW		+		2
75-Re-187	7531	MLBW		+		2
82-Pb-nat	8200				0.18	2
90-Th-230	9034	MLBW	+			3
90-Th-232	9040	MLBW	+	+	7.4	7
91-Pa-231	9131	MLBW	+	+		7
91-Pa-233	9137	MLBW	+	+	41.5	7
92-U-232	9219	MLBW	+	+	72.7	7
92-U-237	9234	MLBW	+	+		7
94-Pu-236	9428	MLBW	+	+		7
94-Pu-237	9431	MLBW			540	2
94-Pu-243	9449	MLBW	+	+	88.1	7
94-Pu-244	9452	MLBW	+	+		7
95-Am-242	9546	MLBW			5500	2
96-Cm-241	9628	MLBW			251.8	2
96-Cm-246	9643	MLBW	+	+	1.3	7
96-Cm-248	9649	MLBW	+	+		7
98-Cf-251	9858	MLBW	+	+	2862	7

3.2.2 VITAMIN-B6 library

Another new library available for SCALE users is the **VITAMIN-B6 199-group ENDF/B-VI** library [12], which contains data for approximately 120 nuclides. The group structure for this library has been enhanced from the VITAMIN-E 174-group ENDF/B-V library [13] to better cover the thermal range.

Besides the group structure, the ENDF/B version of the data, and the number of nuclides, this library differs from LAW one in other significant ways. The 238-group library was developed for criticality safety applications and was processed from ENDF/B-V using AMPX-77. For most nuclides this library has resonance data for the resolved resonance range and Bondarenko factors for the unresolved range. The processing capabilities of AMPX, coupled with NITAWL-II and BONAMI, have been effective in criticality safety applications. Conversely, VITAMIN-B6 was produced and tested for light-water- reactor (LWR) shielding and reactor pressure vessel dosimetry applications. VITAMIN-B6 was processed using NJOY [3] / SMILER [2], which uses the shielding-factor method and has Bondarenko factors for the entire energy range (all 199 groups) for all nuclides except H, He, Li, ^{9}Be, ^{10}B, and C. Unfortunately AMPX and NITAWL-II cannot process several of the resonance parameter formalisms in ENDF/B-VI.

Predecessors to the VITAMIN-B6 library contained almost no data in the thermal-energy range and were designed primarily for shielding applications. With the addition of thermal-energy data, **VITAMIN-B6 is the first ENDF/B-VI multigroup library available that may be used for criticality safety analysis applications**. **The VITAMIN-B6 library, like the 238-group library, is a general-purpose library with adequate group structure for most fast and thermal criticality safety applications.** Initial testing of the library with Cross-Section Evaluation Working Group (CSEWG) criticals [13] indicated good agreement with the critical condition. One of the limitations of the VITAMIN-B6 library, though, is that it contains data for only 120 nuclides.

3.3 Validation of SCALE libraries

The SCALE 238- and 44-group ENDF/B-V libraries were validated very intensively on a large number of critical experiments for both thermal and fast systems (see e.g. [1, 4, 5, 10,11 and 15]). All these validations proved that both libraries describe the systems with sufficient accuracy. As an example, results of validation tests are presented in Table 10 [1].

Unfortunately, we have not any validation results for the EIJ-XMAS library.

One of the most recent sets of validation results is listed in Tables 11 and 12 [4]. In this work, three libraries were tested, namely the 238- and 44-group SCALE libraries and 199-group VITAMIN-B6 library.

Since earlier validation results with the ENDF/B-V libraries, some enhancements have been made. Resolved resonance data for p-wave and d-wave resonances were added to the ENDF/B-V libraries because it was found that they could have a significant effect on results for unmoderated, intermediate-energy problems. Another discovery that has been made is that there are several ENDF “nonresonance” materials that have important resonance structures that need to be taken into account. Resonance structures in some light-to-intermediate-mass nuclides, such as ^{7}Li, ^{28}Si, ^{19}F, and ^{27}Al, are now accounted for using Bondarenko shielding factors. These improvements can have significant effects on certain types of systems, in particular where the intermediate-energy range is important.

There are some conclusions derived from the validation:

The majority of the experiments that were analyzed are low-enriched UO_2 LWR-type fuel rod lattices. Also included are several mixed-oxide (MOX) LWR-type and fast-reactor fuel rod lattices, four homogenous UF_4 green blocks, two highly enriched UO_2 F_2 solutions, and two highly enriched UO_2 $(NO_3)_2$ solutions.

As can be seen from Table 11, a generally good agreement exists between all three libraries. The **mean calculated k_{eff} value for each library is within 0.2% of unity**, as shown in Table 12. There are three cases, *baw1645*s, *baw1645*t, and *pnl19*4, where the 44-group and the 199-group libraries produce k_{eff} values that are more than 1% greater than the 238-group results. Note that the average energy-causing fission (AEF) is greater than 1 eV for these cases, whereas the AEF for almost all other cases is less than 1 eV and generally an order of magnitude less than those for the three cases mentioned. These fuel pin lattice experiments are less thermalized due to the very low moderator-to-fuel-volume ratios (approximately 0.5 or less). All other fuel pin lattice experiments have moderator-to-fuel-volume ratios greater than 1.

The last four cases in Table 11, beginning with the prefix *ydr*, are the homogenous UF_4 green blocks. The 199-group results for these cases are 2% higher than the 238-group and the 44-group results. These are low-enriched thermal homogeneous systems with low H/U ratios (8 or less). This same phenomenon has been noted in calculations performed for other critical experiments with the same general characteristics. A statistical summary of the results in Table 11 is given in Table 12, both with and without the YDR green block benchmarks.

Table 10. Comparison of 44- and 238-group results [15]

Case No.	Case designation	44-Group k_{eff}	238-Group k_{eff}	Δk_{eff} (%)	Case No.	Case designation	44-Group k_{eff}	238-Group k_{eff}	Δk_{eff} (%)
1	ANS33AL1	1.0027	1.0036	-0.09	48	EPRU65	0.9977	0.9900	0.77
2	ANS33AL2	1.0129	1.0092	0.37	49	EPRU65B	0.9985	0.9965	0.20
3	ANS33AL3	1.0035	0.9991	0.44	50	EPRU75	0.9974	0.9941	0.33
4	ANS33EB1	0.9979	0.9906	0.73	51	EPRU75B	1.0023	1.0004	0.19
5	ANS33EB2	1.0096	1.0073	0.23	52	EPRU87	0.9986	0.9974	0.12
6	ANS33EP1	0.9964	0.9941	0.23	53	EPRU87B	0.9985	0.9968	0.17
7	ANS33EP2	1.0020	0.9984	0.36	54	NSE71H1	0.9982	0.9939	0.43
8	ANS33SLG	0.9964	0.9960	0.04	55	NSE71H2	1.0009	0.9973	0.36
9	ANS33STY	0.9909	0.9876	0.33	56	NSE71H3	1.0036	0.9979	0.57
10	B1645SO1	0.9976	0.9947	0.29	57	NSE71SQ	1.0014	0.9959	0.55
11	B1645SO2	1.0007	0.9983	0.24	58	NSE71W1	0.9993	0.9919	0.74
12	BW1231B1	0.9969	0.9936	0.33	59	NSE71W2	0.9976	0.9957	0.19
13	BW1231B2	0.9985	0.9947	0.38	60	P2438AL	0.9951	0.9943	0.08
14	BW1273M	0.9947	0.9943	0.04	61	P2438BA	0.9972	0.9958	0.14
15	BW1484A1	0.9965	0.9948	0.17	62	P2438CU	0.9957	0.9958	-0.01
16	BW1484A2	0.9954	0.9888	0.66	63	P2438SLG	0.9997	0.9954	0.43
17	BW1484B1	0.9973	0.9964	0.09	64	P2438SS	0.9978	0.9987	-0.09
18	BW1484B2	0.9973	0.9940	0.33	65	P2438ZR	0.9956	0.9937	0.19
19	BW1484B3	0.9992	0.9955	0.37	66	P2615AL	1.0004	0.9940	0.64
20	BW1484C1	0.9937	0.9914	0.23	67	P2615BA	0.9970	0.9961	0.09
21	BW1484C2	0.9936	0.9937	-0.01	68	P2615CD1	0.9985	0.9986	-0.01
22	BW1484S1	0.9981	0.9947	0.34	69	P2615CD2	0.9990	0.9930	0.60
23	BW1484S2	0.9989	0.9980	0.09	70	P2615CU	1.0003	0.9968	0.35
24	BW1484SL	0.9966	0.9911	0.55	71	P2615SS	0.9998	0.9969	0.29
25	BW1645S1	1.0010	0.9906	1.04	72	P2615ZR	0.9980	0.9940	0.40
26	BW1645S2	1.0035	0.9940	0.95	73	P2827L1	1.0023	1.0006	0.17
27	BW1645T1	1.0062	0.9951	1.11	74	P2827L2	0.9997	0.9964	0.33
28	BW1645T2	1.0068	0.9965	1.03	75	P2827L3	1.0081	1.0088	-0.07
29	BW1645T3	1.0007	0.9924	0.83	76	P2827L4	1.0073	1.0044	0.29
30	BW1645T4	0.9986	0.9888	0.98	77	P2827SLG	0.9948	0.9939	0.09
31	BW1810A	0.9971	0.9945	0.26	78	P2827U1	1.0004	0.9955	0.49
32	BW1810B	0.9980	0.9969	0.11	79	P2827U2	0.9998	0.9979	0.19
33	BW1810C	1.0005	0.9984	0.21	80	P2827U3	1.0018	0.9999	0.19
34	BW1810D	0.9999	0.9962	0.37	81	P2827U4	1.0042	1.0011	0.31
35	BW1810E	0.9976	0.9940	0.36	82	P3314AL	0.9973	0.9944	0.29
36	BW1810F	1.0032	0.9983	0.49	83	P3314BA	1.0002	1.0075	-0.73
37	BW1810G	0.9971	0.9949	0.22	84	P3314BC	1.0008	1.0072	-0.64
38	BW1810H	0.9973	0.9939	0.34	85	P3314BF1	1.0022	1.0055	-0.33
39	BW1810I	1.0022	0.9953	0.69	86	P3314BF2	0.9981	0.9985	-0.04
40	BW1810J	0.9980	0.9970	0.10	87	P3314BS1	0.9970	0.9965	0.05
41	CR1071AS	1.0207	1.0125	0.82	88	P3314BS2	0.9959	0.9926	0.33
42	CR1653AS	1.0169	1.0097	0.72	89	P3314BS3	0.9972	0.9936	0.36
43	CR2500S	1.0194	1.0129	0.65	90	P3314BS4	1.0005	0.9941	0.64
44	DSN399-1	1.0056	0.9973	0.83	91	P3314CD1	1.0001	0.9939	0.62
45	DSN399-2	1.0010	0.9948	0.62	92	P3314CD2	0.9929	0.9910	0.19
46	DSN399-3	1.0024	0.9977	0.47	93	P3314CU1	0.9941	0.9877	0.64
47	DSN399-4	0.9965	0.9910	0.55	94	P3314CU2	1.0005	0.9953	0.52

Table 10. (continued)

Case No.	Case designation	44-Group k_{eff}	238-Group k_{eff}	Δk_{eff} (%)	Case No.	Case designation	44-Group k_{eff}	238-Group k_{eff}	Δk_{eff} (%)
95	P3314CU3	0.9972	0.9989	-0.17	141	P3926SL1	0.9942	0.9926	0.16
96	P3314CU4	0.9992	0.9950	0.42	142	P3926SL2	0.9990	0.9928	0.62
97	P3314CU5	0.9938	0.9926	0.12	143	P3926U1	0.9979	0.9939	0.40
98	P3314CU6	0.9958	0.9910	0.48	144	P3926U2	0.9980	0.9931	0.49
99	P3314SLG	0.9982	0.9942	0.40	145	P3926U3	1.0001	0.9959	0.42
100	P3314SS1	0.9969	0.9946	0.23	146	P3926U4	1.0026	0.9974	0.52
101	P3314SS2	1.0011	0.9960	0.51	147	P3926U5	0.9999	0.9998	0.01
102	P3314SS3	0.9990	0.9926	0.64	148	P3926U6	1.0024	0.9970	0.54
103	P3314SS4	0.9957	0.9957	0.00	149	P4267B1	0.9969	0.9981	-0.12
104	P3314SS5	0.9944	0.9875	0.69	150	P4267B2	1.0035	1.0010	0.25
105	P3314SS6	1.0003	0.9935	0.68	151	P4267B3	1.0025	1.0053	-0.28
106	P3314W1	1.0015	0.9992	0.23	152	P4267B4	0.9993	0.9977	0.16
107	P3314W2	0.9958	0.9927	0.31	153	P4267B5	1.0031	1.0007	0.24
108	P3314ZR	0.9978	0.9957	0.21	154	P4267SL1	0.9974	0.9940	0.34
109	P3602BB	0.9988	0.9947	0.41	155	P4267SL2	0.9993	0.9958	0.35
110	P3602BS1	1.0000	0.9928	0.72	156	P49-194	1.0081	0.9981	1.00
111	P3602BS2	1.0001	0.9977	0.24	157	P62FT231	1.0005	0.9958	0.47
112	P3602CD1	0.9988	0.9943	0.45	158	P71F14F3	1.0029	0.9944	0.85
113	P3602CD2	1.0002	0.9931	0.71	159	P71F14V3	0.9973	0.9929	0.44
114	P3602CU1	0.9964	0.9945	0.19	160	P71F14V5	0.9977	0.9959	0.18
115	P3602CU2	0.9980	0.9926	0.54	161	P71F214R	1.0010	0.9949	0.61
116	P3602CU3	1.0039	0.9938	1.010	162	PAT80L1	1.0031	0.9987	0.44
117	P3602CU4	1.0040	0.9944	0.96	163	PAT80L2	0.9920	0.9954	-0.34
118	P3602N11	1.0003	0.9918	0.85	164	PAT80SS1	1.0004	1.0003	0.01
119	P3602N12	0.9963	0.9943	0.20	165	PAT80SS2	0.9926	0.9946	-0.20
120	P3602N13	0.9957	0.9939	0.18	166	W3269A	0.9934	0.9920	0.14
121	P3602N14	0.9984	0.9951	0.33	167	W3269B1	0.9963	0.9900	0.63
122	P3602N21	0.9995	0.9972	0.23	168	W3269B2	0.9964	0.9898	0.66
123	P3602N22	0.9967	0.9972	-0.05	169	W3269B3	0.9948	0.9878	0.70
124	P3602N31	1.0010	0.9966	0.44	170	W3269C	0.9986	0.9946	0.40
125	P3602N32	1.0015	0.9967	0.48	171	W3269SL1	0.9952	0.9919	0.33
126	P3602N33	1.0045	0.9976	0.69	172	W3269SL2	1.0040	0.9947	0.93
127	P3602N34	1.0027	0.9961	0.66	173	W3269W1	0.9957	0.9938	0.19
128	P3602N35	1.0036	0.9960	0.76	174	W3269W2	1.0009	0.9995	0.14
129	P3602N36	1.0009	0.9964	0.45	175	W3385SL1	0.9964	0.9918	0.46
130	P3602N41	1.0002	0.9948	0.54	176	W3385SL2	1.0005	0.9995	0.10
131	P3602N42	1.0019	0.9995	0.24	177	YDR14PL2	1.0011	1.0011	0.00
132	P3602N43	0.9994	0.9967	0.27	178	YDR14PL3	1.0115	1.0089	0.26
133	P3602SS1	0.9978	0.9904	0.74	179	YDR14UN2	1.0047	1.0024	0.23
134	P3602SS2	1.0012	0.9962	0.50	180	YDR14UN3	1.0163	1.0128	0.35
135	P3926L1	0.9996	0.9966	0.30		**MEAN**	**0.9999**	**0.9964**	
136	P3926L2	1.0028	0.9994	0.34		**MEDIAN**	**0.9993**	**0.9957**	
137	P3926L3	1.0017	0.9959	0.58		**STD. DEV.**	**0.0045**	**0.0064**	
138	P3926L4	1.0055	1.0114	-0.59		**MIN.**	**0.9909**	**0.9875**	
139	P3926L5	1.0070	1.0032	0.38		**MAX.**	**1.0207**	**1.0129**	
140	P3926L6	1.0026	0.9994	0.32					

Table 11. Validation Results [4]

Case designation	238g k_{eff}	238g std. Dev.	238g AEF (eV)	44g k_{eff}	199g k_{eff}	Δk (238g-44g)	Δk (238g-199g)
ans33bb2	1.0059	0.0011	0.21007	1.0084	1.0066	-0.0025	-0.0007
ans33bh2	1.0103	0.0011	0.19792	1.014	1.0095	-0.0037	0.0008
ans33bp2	0.996	0.0011	0.22838	1.0001	0.9971	-0.0041	-0.0011
ans33h2	0.9952	0.0012	0.19796	0.9976	0.9948	-0.0024	0.0004
baw1231a	0.9925	0.001	0.7384	0.9942	0.9981	-0.0017	-0.0056
baw1231b	0.9942	0.001	1.20499	0.997	1.0017	-0.0028	-0.0075
baw1273m	0.9908	0.0011	0.53765	0.9957	1.0004	-0.0049	-0.0096
baw1484a	0.9913	0.001	0.19302	0.9932	0.9927	-0.0019	-0.0014
baw1484b	0.9918	0.0013	0.14075	0.9974	0.9896	-0.0056	0.0022
baw1484c	0.9941	0.0014	0.19646	0.9949	0.9965	-0.0008	-0.0024
baw1484d	0.9886	0.0014	0.15571	0.9932	0.9887	-0.0046	-0.0001
baw1645s	0.9946	0.0012	1.44406	1.0046	1.0069	-0.01	-0.0123
baw1645t	0.997	0.001	2.30048	1.0057	1.0107	-0.0087	-0.0137
bnw1810a	0.9965	0.0011	0.35955	0.9984	0.9986	-0.0019	-0.0021
bw1645so	0.9986	0.0012	0.41653	0.9989	1.0024	-0.0003	-0.0038
epru615b	0.9954	0.0014	0.3239	0.9988	1.0022	-0.0034	-0.0068
epri70b	0.9985	0.0015	0.769	1.0002	0.9975	-0.0017	0.001
epri70un	0.9965	0.0015	0.579	0.9981	0.9948	-0.0016	0.0017
epri87b	1.0041	0.0013	0.282	1.0088	1.0015	-0.0047	0.0026
epri87un	1.0015	0.0011	0.193	1.0034	0.9938	-0.0019	0.0077
epri99b	1.006	0.001	0.182	1.0081	1.0009	-0.0021	0.0051
epri99un	1.0024	0.0016	0.136	1.0078	1.0004	-0.0054	0.002
epru75	0.9973	0.001	0.11538	0.9973	0.9964	0	0.0009
epru75b	0.9977	0.001	0.14369	1.0014	0.9961	-0.0037	0.0016
epru87b	0.9969	0.0012	0.0938	1.0014	0.996	-0.0045	0.0009
ft214r	0.9931	0.0016	0.37036	0.9977	0.999	-0.0046	-0.0059
ft214v3	0.9936	0.0011	0.37366	0.9971	0.9962	-0.0035	-0.0026
or260901	1.0061	0.0014	0.0334	1.0073	1.0041	-0.0012	0.002
or260906	1.0009	0.0012	0.0322	1.0039	1.0009	-0.003	0
or2968al	1.007	0.001	0.0499	1.0085	1.0107	-0.0015	-0.0037
or2968s1	0.9915	0.0016	0.054	0.993	0.9915	-0.0015	0
or2968s2	1	0.001	0.0393	0.9998	1.0027	0.0002	-0.0027
p2438x05	0.9928	0.0014	0.0967	0.9956	0.9925	-0.0028	0.0003
p2438x17	0.9944	0.001	0.0997	0.9964	0.9949	-0.002	-0.0005
p2438x28	0.9953	0.0014	0.0979	0.996	0.9939	-0.0007	0.0014
p2615x14	0.9956	0.0015	0.11467	0.9982	0.9926	-0.0026	0.003
p2615x23	0.9987	0.0016	0.11559	0.9992	0.9966	-0.0005	0.0021
p2615x31	0.9957	0.0015	0.11615	0.9986	0.9918	-0.0029	0.0039
p2827non	0.9926	0.0013	0.0967	0.9942	0.9919	-0.0016	0.0007
p2827u2a	0.9958	0.0013	0.17423	1.0024	0.9951	-0.0066	0.0007
p2827u2b	0.9976	0.0015	0.2787	1.0049	0.9961	-0.0073	0.0015
p3314a	0.9974	0.0015	0.31604	1.003	1.0051	-0.0056	-0.0077
p3314b	0.9974	0.0011	0.32215	1.0028	0.9989	-0.0054	-0.0015
p3602b4	0.9921	0.0016	0.30714	0.9955	0.9968	-0.0034	-0.0047
p3602c4	0.9958	0.0011	0.30888	0.9997	0.9971	-0.0039	-0.0013
p3602a2	0.9952	0.0014	0.0993	0.9991	0.9964	-0.0039	-0.0012
p3602non	1	0.0016	0.29088	1.0027	0.9972	-0.0027	0.0028
p3602s4	0.9968	0.0017	0.30277	1.0015	0.9956	-0.0047	0.0012
p3926a2	0.9936	0.0014	0.16301	0.9924	0.9927	0.0012	0.0009
p3926nob	0.9978	0.0016	0.27956	1.0007	0.9938	-0.0029	0.004
p3926u2a	0.9923	0.0014	0.34961	0.9965	0.9944	-0.0042	-0.0021
p3926u4a	0.9983	0.0016	0.51584	1.0012	0.9981	-0.0029	0.0002

Table 11. (continued)

Case designation	238g k_{eff}	238g std. dev.	238g AEF (eV)	44g k_{eff}	199g k_{eff}	Δk (238g-44g)	Δk (238g-199g)
p4267a	0.9934	0.0011	0.28105	0.9985	0.9944	-0.0051	-0.001
p4267b	1.0017	0.0013	0.61372	1.0047	1.0026	-0.003	-0.0009
p4267c	0.9952	0.0011	0.5294	1.0013	0.9973	-0.0061	-0.0021
p4267d	0.9916	0.0013	1.17106	0.9964	0.9979	-0.0048	-0.0063
p5803x21	1.0008	0.0011	0.8919	1.0051	0.9981	-0.0043	0.0027
p5803x32	1.0071	0.0017	0.11345	1.0087	0.9997	-0.0016	0.0074
p5803x43	1.003	0.0011	0.28961	1.003	0.9993	0	0.0037
p5803x67	0.9947	0.0011	2.90878	1.0004	0.9967	-0.0057	-0.002
p5803x68r	1.0026	0.0016	0.16572	1.0057	0.9953	-0.0031	0.0073
pnl194	0.9984	0.0014	3.52691	1.0093	1.0121	-0.0109	-0.0137
rfp2710r	1.0031	0.0021	0.2241	1.0088	1.01	-0.0057	-0.0069
rfp2710u	1.0066	0.0021	0.08	1.0075	1.005	-0.0009	0.0016
saxtn104	1.0037	0.0016	0.10144	1.0037	0.9962	0	0.0075
saxtn56b	0.995	0.0016	0.64781	1.0019	0.9944	-0.0069	0.0006
saxtn735	1.0016	0.0016	0.19013	1.0001	0.9935	0.0015	0.0081
saxtn792	1.0019	0.0017	0.15514	1.0034	0.9932	-0.0015	0.0087
saxton52	0.9968	0.0011	0.90107	1.0026	0.9929	-0.0058	0.0039
saxton56	0.9953	0.0017	0.55471	0.9995	0.9937	-0.0042	0.0016
saxu56	0.9884	0.0016	0.29855	0.9964	0.9971	-0.008	-0.0087
saxu792	0.9956	0.0011	0.10365	0.9989	0.9923	-0.0033	0.0033
w3269b	0.9968	0.0015	0.43864	1.0031	1.0052	-0.0063	-0.0084
ydr14pl2	1.0003	0.0013	0.0869	1.003	1.0206	-0.0027	-0.0203
ydr14pl3	1.0116	0.0015	0.24078	1.015	1.0384	-0.0034	-0.0268
ydr14un2	1.0024	0.0015	0.13709	1.0023	1.0243	0.0001	-0.0219
ydr14un3	1.0125	0.0015	0.32832	1.0186	1.0447	-0.0061	-0.0322

Table 12. Statistical summary of results from Table 11

44 g results		**238 g results**		**199 g results**	
Mean	1.0014	Mean	0.9979	Mean	0.9998
Standard error	0.0006	Standard error	0.0006	Standard error	0.0011
Median	1.0007	Median	0.9968	Median	0.9971
Count	77	Count	77	Count	77
44 g results, no YDRs		**238 g results, no YDRs**		**199 g results, no YDRs**	
Mean	1.0009	Mean	0.9975	Mean	0.9980
Standard error	0.0006	Standard error	0.0006	Standard error	0.0006
Median	1.0002	Median	0.9968	Median	0.9968
Mode	0.9964	Mode	0.9952	Mode	0.9971
Count	73	Count	73	Count	73

Conclusions

(1) The 238-, 44-, and 199-group libraries demonstrate **good agreement for the vast majority of the benchmark cases analyzed**. However, **the 44- and 199-group results for severely undermoderated LWR-type fuel pin lattices are approximately 1% higher than the 238-group library**. **Results obtained with the 199-group library for homogeneous thermal systems with low H/U ratios are approximately 2% high** and indicate a failure in the narrow resonance approximation used to generate the cross sections in this library. The narrow resonance approximation, which has proven satisfactory for shielding analysis, can produce unreliable results for criticality calculations. Broad resonances, such as those that occur in some nuclides near thermal energies, are not satisfactorily represented using the narrow resonance approximation. Therefore, **the 199-group VITAMIN-B6 library with the shielding-factor method (e.g., NJOY/BONAMI) should not be used for homogeneous thermal systems with low H/U ratios**. The validation results presented here highlight the **importance of validation using benchmark critical experiments that are in the area of applicability for systems that are to be analyzed**.

(2) Minimal attention has been given in the past to the preparation of multigroup libraries that have the structure and parameters necessary to be applicable for all types of systems. Reasons include computational limitations and focus on specific types of applications. **Presently, no system is available to process ENDF/B-VI data into multigroup cross sections that are effective for all types of systems requiring criticality safety analyses.** NJOY can process ENDF/B-VI data but uses the narrow resonance approximation. AMPX has not been updated for compatibility with the ENDF/B-VI formats. For these reasons, there are plans to update AMPX and process and test a complete ENDF/B-VI library with at least 300 energy groups.

For more detailed discussion of the problem see [4].

4 Feasibility of preparing new SCALE libraries for VVER applications

4.1 Fine-group libraries

Fine-group SCALE libraries contain so many groups (usually about 200 or more) that they can be generated using standard Maxwellian, 1/E and fission spectra and are, therefore, completely independent on the type of the reactor core lattice geometry. A library suitable for PWR is suitable for VVER as well and there is no need to generate a special fine-group library for VVER. Nevertheless, it is generally desirable to have a library that is generated from the last version of ENDF.

Generally, there is hardly a need to generate a new fine-group library unless at least one of the following conditions is fulfilled:

(1) A new version of the Evaluated Nuclear Data Files (ENDF) appears.

(2) There is a serious upgrade of the data processing system (e.g. NJOY or AMPX) that allows either more precise description of neutron interactions or better utilisation of data from ENDF. (Alternatively, there can be a requirement to do such upgrade in order to utilise new data incorporated in ENDF.)

(3) There is a reason to change the library group structure (more groups and/or group boundary changes) in order to achieve better precision or generality.

In case of the 238-group SCALE ENDF/B-V library, the first of the above conditions is obviously fulfilled because there is a new version ENDF/B-VI. As it was discussed in section 3.3, the ORNL staff have an intention to upgrade the AMPX system and to generate new fine-group library (probably 300 groups) in order to better utilise data from ENDF/B-VI (e.g. Reich-Moore formalism) and make the library more general. A similar upgrade of the NJOY system is probable in near future. It is obvious that the codes improvements and library generation and validation can be performed much easier by the teams of ORNL and LANL than by the institutes from VVER-operating countries. They are much more experienced in this field, have prepared input data for validation tasks and results for comparisons etc. For us the task would be much more difficult and expensive.

Although libraries based on ENDF/B-VI and JEFF2.2 already exist, they are from different reasons not so easily available and they would also require very intensive validation.

So our conclusion is to use the SCALE 238-group library until a new one will appear.

4.2 Broad-group libraries

In the case of broad-group libraries the situation is a little bit different. The only broad-group library available and recommended is the 44-group ENDF/B-V one collapsed from the 238-group library with a typical PWR spectrum. There is a requirement to generate such a library using spectrum typical for VVER in order to have the SCALE system licensed in our and other Central and Eastern Europe countries. This task is fully feasible and we dispose with all necessary means (including a new version of MALOCS module) for generating and validation of a new broad-group library.

Still there is a problem. We can generate the new library only from the 238-group ENDF/B-V one but it is probable that a new fine-group library will be released in near future. The question is if we should generate the new library on base of the old fine-group one or wait until a new fine-group library will be available.

On the other hand one should not await a dramatically improved precision of criticality calculations with the new VVER broad-group library because the spectra in PWRS and VVERs are very similar. It can even appear that differences between the two libraries will be so small that it will not be worth to use two different libraries. But this assumption should be proved.

The new library should be validated not only on benchmarks for VVERs but also on test cases prepared for the original 44-group library validation (see e.g. [4, 10, 11, 15]). It is necessary for the comparison of both libraries and verification that the new library is prepared properly. There is plenty of testing cases for the VVER hexagonal lattices for critical experiments carried out on ZR-6 In Budapest, Hungary, and LR-0 in NRI Řež which are currently used for codes validation.

5 Conclusions

Considering all aspects of using the SCALE code system for the VVER systems we came to the following conclusions:

1. Use the 238-group ENDF/B-V library until a new one based on ENDF/B-VI library is released.
2. Perform calculations of VVER test cases with the original 44-group library.
3. Generate a new VVER 44-group library collapsed from 238 ENDF/B-V one at least for those isotopes that are needed for criticality calculation (both VVER and PWR cases).
4. Generate a full version broad-group library whenever a new ENDF/B-VI fine-group library will be available.
5. Possibility of generating a fine-group library based on the European files JEFF2.2 will be discussed and solved later.

The second task is already in progress with the aim not only validate the library but also the new module KENO VI for hexagonal geometry. Task 3 will start next year.

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