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FENDL-2.1
Update of an evaluated nuclear data library for fusion applications

Summary documentation prepared by

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December 2004

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Abstract
A description of the work undertaken towards the development of a new version of the FENDL-2 library is given, detailing the selection of the evaluated nuclear data files, the processing performed and the resultant processed files. These include an updated version of the FENDL-2 library (termed FENDL-2.1), the corresponding ACE library for MCNP family of Monte Carlo codes, the MATXS library for deterministic transport codes and the ACEDOP package for Doppler broadening of the resolved resonance cross sections in the ACE files.

December 2004

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Introduction

An IAEA Consultants' Meeting entitled "Maintain FENDL Library for Fusion Application" [1] was held in Vienna on 10-12 November 2003. The main objective of this meeting was to review the status and future developments needed to update FENDL-2. The consultants recommended that a new version of the FENDL-2 library should be released by the end of 2004, to be known as FENDL-2.1.

In order to fulfill the above mentioned recommendations, the IAEA Nuclear Data Section supported the generation of FENDL-2.1 by a Special Service Agreement to Daniel López Aldama. An updated version of FENDL-2 has been made available, and these data are freely available from the IAEA-NDS upon request. They can also be downloaded from the URL: http://www-nds.iaea.org/fendl21/.

A new feature of the FENDL-2.1 package is the availability of the ACEDOP package [2], which allows Döppler broadening of the cross sections in the ACE files, except for the energy region described by unresolved resonance representation in the original ENDF-formatted files.

All of the work carried out to formulate and produce FENDL-2.1 is described in this report. The evaluated nuclear data files were selected according to the recommendations given in Ref. [1]. Processing was performed using NJOY-99.90 [3] at IAEA-NDS, and the resulting processed files are available in ACE format for MCNP and in MATXS format for multi-group transport calculations.

1. FENDL-2.1 Evaluated Nuclear Data Files (FENDL/E-2.1)

Recommendations for replacing evaluations are given in Ref. [1]. The recommendations were implemented, except for the following:

H-2	JENDL-3.3 has no photon production data, therefore ENDF/B-VI Rel.8 was adopted.
He-3	ENDF/B-VI Rel.8 has no photon production data, so JENDL-3.3 was selected.
Be-9	evaluation from JEFF-3.1 was still in progress when the data were processed; therefore, ENDF/B-VI rev. 8 data were adopted instead.
C-12	JENDL-3.3 evaluation uses unit base interpolation law (INT = 22) in File 5 (MF = 5) for MT = 51, which is not allowed according to ENDF-6 formats and procedures [6]. This feature is not yet coded in the NJOY-99.90. After comparing JENDL-FF with JENDL-3.3 data, the decision was taken to use JENDL-FF data.
Cl	Isotopic evaluations in ENDF/B-VI Rel.8 supersede the older elemental evaluation, therefore the more recent isotopic files were adopted.
W	the ENDF/B-VI rev. 8 isotopic evaluations were selected, based on further benchmark testing and the recommendations of Fischer et al [7].

Furthermore, concerning materials from the ENDF/B or JENDL libraries, updated files from the same library were adopted, if available (20 cases).The sources of evaluated data for FENDL-2.1 (FENDL/E-2.1) are presented in Table 1. All the sections with MT numbers in the ranges 152-207 and 219-450 were removed before processing. The deletion process was performed by running sequentially the codes MERGER and DICTIN from the PREPRO2002 Code System [4]. The file was then re-sequenced by the STANEF code from the ENDFUTIL package [5].

Table 1: FENDL-2.1 material selection.

No.	Material	FENDL-2.0	FENDL-2.1	Notes
1	1-H-1	ENDF/B-VI mod 1	JENDL-3.3	
2	1-H-2	BROND-2.1	ENDF/B-VI.8 mod 4	
3	1-H-3	ENDF/B-VI mod 0	ENDF/B-VI.8 mod 0	No photon production
4	2-He-3	ENDF/B-VI mod 1	JENDL-3.3	Photon production added
5	2-He-4	ENDF/B-VI mod 0	ENDF/B-VI.8 mod 1	Minor revisions
6	3-Li-6	ENDF/B-VI mod 0	ENDF/B-VI.8 mod 0	
7	3-Li-7	ENDF/B-VI mod 0	ENDF/B-VI.8 mod 0	
8	4-Be-9	JENDL-FF	ENDF/B-VI.8 mod 8	
9	5-B-10	ENDF/B-VI mod 1	ENDF/B-VI.8 mod 1	
10	5-B-11	ENDF/B-VI mod 0	ENDF/B-VI.8 mod 2	Minor revisions
11	6-C-12	JENDL-FF	JENDL-FF	MF = 14 corrected
12	7-N-14	JENDL-FF	JENDL-FF	
13	7-N-15	BROND-2.1	BROND-2.1	
14	8-O-16	JENDL-FF	ENDF/B-VI.8 mod 3	
15	9-F-19	ENDF/B-VI mod 0	ENDF/B-VI.8 mod 1	Gamma spectra modified
16	11-Na-23	JENDL-3.1	JENDL-3.3	Covariance data
17	12-Mg-nat	JENDL-3.1	JENDL-3.2	
18	13-Al-27	EFF-3.0	JEFF-3.0 (EFF-3.0)	
19	14-Si-28	ENDF/B-VI mod 1	ENDF/B-VI.8 mod 2	MF = 14 corrected
20	14-Si-29	ENDF/B-VI mod 1	ENDF/B-VI.8 mod 3	
21	14-Si-30	ENDF/B-VI mod 1	ENDF/B-VI.8 mod 2	MF = 14 corrected
22	15-P-31	ENDF/B-VI mod 0	ENDF/B-VI.8 mod 0	
23	16-S-nat	ENDF/B-VI mod 0	ENDF/B-VI.8 mod 1	Gamma spectra modified
24	17-Cl-35	ENDF/B-VI mod 0 17-Cl-nat	ENDF/B-VI.8 mod 1	MF = 14 corrected
25	17-Cl-37		ENDF/B-VI.8 mod 1	Minor correction
26	19-K-nat	ENDF/B-VI mod 0	ENDF/B-VI.8 mod 1	Gamma spectra modified
27	20-Ca-nat	JENDL-3.1	JENDL-3.2	MF = 14 corrected
28	22-Ti-46	JENDL-3.1 22-Ti-nat	JENDL-3.3	
29	22-Ti-47		JENDL-3.3	
30	22-Ti-48		JENDL-3.3	
31	22-Ti-49		JENDL-3.3	
32	22-Ti-50		JENDL-3.3	
33	23-V-nat	JENDL-FF	JENDL-3.3	FENDL-2.0: 23-V-51
34	24-Cr-50	ENDF/B-VI mod 1	ENDF/B-VI.8 mod 5	Gamma spectra modified
35	24-Cr-52	ENDF/B-VI mod 1	ENDF/B-VI.8 mod 4	Gamma spectra modified
36	24-Cr-53	ENDF/B-VI mod 1	ENDF/B-VI.8 mod 4	Gamma spectra modified
37	24-Cr-54	ENDF/B-VI mod 1	ENDF/B-VI.8 mod 5	Gamma spectra modified
38	25-Mn-55	ENDF/B-VI mod 1	JENDL-3.3	
39	26-Fe-54	ENDF/B-VI mod 1	ENDF/B-VI.8 mod 5	Gamma spectra modified
40	26-Fe-56	EFF-3.0	JEFF-3.0 (EFF-3.1)	

Table 1: FENDL-2.1 material selection (cont).

No.	Material	FENDL-2.0	FENDL-2.1	Notes
41	26-Fe-57	ENDF/B-VI mod 1	ENDF/B-VI.8 mod 4	Gamma spectra modified
42	26-Fe-58	ENDF/B-VI mod 1	ENDF/B-VI.8 mod 4	Gamma spectra modified
43	27-Co-59	ENDF/B-VI mod 1	ENDF/B-VI.8 mod 1	
44	28-Ni-58	ENDF/B-VI mod 1	JEFF-3.0(EFF-3.0)	
45	28-Ni-60	ENDF/B-VI mod 1	JEFF-3.0(EFF-3.0)	MF = 12 corrected MT51-91
46	28-Ni-61	ENDF/B-VI mod 1	ENDF/B-VI.8 mod 5	Gamma spectra modified
47	28-Ni-62	ENDF/B-VI mod 1	ENDF/B-VI.8 mod 5	Gamma spectra modified
48	28-Ni-64	ENDF/B-VI mod 1	ENDF/B-VI.8 mod 4	Gamma spectra modified
49	29-Cu-63	ENDF/B-VI mod 2	ENDF/B-VI.8 mod 5	Gamma spectra modified
50	29-Cu-65	ENDF/B-VI mod 2	ENDF/B-VI.8 mod 5	Gamma spectra modified
51	31-Ga-nat	JENDL-3.2	JENDL-3.2	No photon production data
52	40-Zr-nat	JENDL-FF	JENDL-FF	
53	41-Nb-93	JENDL-FF	JENDL-FF	MF = 12 corrected MT51-91
54	42-Mo-92	JENDL-FF 42-Mo-nat	JENDL-3.3	
55	42-Mo-94		JENDL-3.3	
56	42-Mo-95		JENDL-3.3	
57	42-Mo-96		JENDL-3.3	
58	42-Mo-97		JENDL-3.3	
59	42-Mo-98		JENDL-3.3	
60	42-Mo-100		JENDL-3.3	
61	50-Sn-nat	BROND-2.1	BROND-2.1	
62	73-Ta-181	JENDL-3.1	JENDL-3.3	
63	74-W-182	JENDL-FF 74-W-nat	ENDF/B-VI.8 mod 2	
64	74-W-183		ENDF/B-VI.8 mod 2	
65	74-W-184		ENDF/B-VI.8 mod 2	
66	74-W-186		ENDF/B-VI.8 mod 2	
67	79-Au-197	ENDF/B-VI mod 1	ENDF/B-VI mod 1	
68	82-Pb-206	ENDF/B-VI mod 0	ENDF/B-VI.8 mod 1	
69	82-Pb-207	ENDF/B-VI mod 1	ENDF/B-VI mod 1	
70	82-Pb-208	ENDF/B-VI mod 0	ENDF/B-VI.8 mod 1	
71	83-Bi-209	JENDL-3.1	ENDF/B-VI.8 mod 2	

As shown in Table 1, the use of isotopic evaluations for Cl, Ti, Mo and W increases the number of materials from 57 in FENDL-2.0 to 71 in FENDL-2.1. The distribution of these materials in terms of the original source of the evaluation is given in Table 2, where NMAT in column 3 represents the number of materials selected from the corresponding library.

As part of the quality assurance procedures, the CHECKR code from the ENDFUTIL package was used to check that the evaluated nuclear data conform to ENDF-6 format. On analysis of the assembled FENDL-2.1 file it was found that in File 14 (MF = 14) for LI = 1 (isotropic distribution), the parameter NK was not consistent with the NK values given in Files 12 (MF = 12) or 13 (MF = 13) for the following materials: C-12, Ca-nat, Cl-35, Si-28 and Si-30.

Table 2: Distribution of materials by original source of evaluation.

No.	Library	NMAT	Materials
1	ENDF/B-VI.8 (E6)	40	^{2}H, ^{3}H, ^{4}He, ^{6}Li, ^{7}Li, ^{9}Be, ^{10}B, ^{11}B, ^{16}O, ^{19}F, $^{28-30}$Si, ^{31}P, S, ^{35,37}Cl, K, $^{50,52-54}$Cr, ^{54,57,58}Fe, ^{59}Co, ^{61,62,64}Ni, ^{63,65}Cu, ^{197}Au, $^{206-208}$Pb, ^{209}Bi, $^{182-184,186}$W
2	JENDL-3.3 (J33)	18	^{1}H, ^{3}He, ^{23}Na, $^{46-50}$Ti, , ^{55}Mn, $^{92,94-98,100}$Mo, ^{181}Ta,V
3	JENDL-3.2 (J32)	3	Mg, Ca, Ga
4	JENDL-FF (JFF)	4	^{12}C, ^{14}N, Zr, ^{93}Nb
5	JEFF-3 (EFF) JEFF3	4	^{27}Al, ^{56}Fe, ^{58}Ni, ^{60}Ni
6	BROND-2.1 (BR2)	2	^{15}N, Sn

Processing Ni-60 caused NJOY-99 failure due to the level energies of the transition probability arrays given in File 12 (MF = 12) for MT = 51-91 not being consistent to within four significant figures with the corresponding values given in File 3 (MF = 3). Furthermore, for Nb-93 the transition probability data were omitted for MT = 51 in File 12. Additionally for Cl-37, the lower energy limit of 0.0 eV in File 5 was changed to 0.00001 eV in order to avoid problems with the initialization algorithm of some NJOY-99 routines.

All these problems were manually fixed in the original evaluated nuclear data file.

Photo-atomic data were taken from the ENDF/B-VI library for all materials as in FENDL-2.0. The evaluated photo-atomic data filename is FENDLEP.DAT.

Table 3 presents a summary of the FENDL/E-2.1 library.

Table 3: FENDL/E-2.1 library-summary.

Neutron data (online *.DAT)				**Photo-atomic data (online FENDLEP.DAT)**	
Material	**MAT No.**	**Source**	**Filename online**	**Element**	**MAT No.**
1-H-1	125	JENDL-3.3	H001J33.DAT	H	100
1-H-2	128	ENDF/B-VI.8 mod 4	H002E6.DAT		
1-H-3	131	ENDF/B-VI.8 mod 0	H003E6.DAT		
2-He-3	225	JENDL-3.3	HE003J33.DAT	He	200
2-He-4	228	ENDF/B-VI.8 mod 1	HE004E6.DAT		
3-Li-6	325	ENDF/B-VI.8 mod 0	LI006E6.DAT	Li	300
3-Li-7	328	ENDF/B-VI.8 mod 0	LI007E6.DAT		
4-Be-9	425	ENDF/B-VI.8 mod 8	BE009E6.DAT	Be	400
5-B-10	525	ENDF/B-VI.8 mod 1	B010E6.DAT	B	500
5-B-11	528	ENDF/B-VI.8 mod 2	B011E6.DAT		
6-C-12	625	JENDL-FF	C012JFFrev.DAT	C	600
7-N-14	725	JENDL-FF	N014JFF.DAT	N	700
7-N-15	720	BROND-2.1	N015BR2.DAT		
8-O-16	825	ENDF/B-VI.8 mod 3	O016E6.DAT	O	800
9-F-19	925	ENDF/B-VI.8 mod 1	F019E6.DAT	F	900
11-Na-23	1125	JENDL-3.3	NA023J33.DAT	Na	1100
12-Mg-nat	1200	JENDL-3.2	MG000J32.DAT	Mg	1200
13-Al-27	1325	JEFF-3.0 (EFF-3.0)	AL027EFF3.DAT	Al	1300
14-Si-28	1425	ENDF/B-VI.8 mod 2	SI028E6rev.DAT	Si	1400
14-Si-29	1428	ENDF/B-VI.8 mod 3	SI029E6.DAT		
14-Si-30	1431	ENDF/B-VI.8 mod 2	SI030E6rev.DAT		
15-P-31	1525	ENDF/B-VI.8 mod 0	P031E6.DAT	P	1500
16-S-nat	1600	ENDF/B-VI.8 mod 1	S000E6.DAT	S	1600
17-Cl-35	1725	ENDF/B-VI.8 mod 1	CL035E6rev.DAT	Cl	1700
17-Cl-37	1731	ENDF/B-VI.8 mod 1	CL037E6rev.DAT		
19-K-nat	1900	ENDF/B-VI.8 mod 1	K000E6.DAT	K	1900
20-Ca-nat	2000	JENDL-3.2	CA000J32rev.DAT	Ca	2000
22-Ti-46	2225	JENDL-3.3	TI046J33.DAT	Ti	2200
22-Ti-47	2228	JENDL-3.3	TI047J33.DAT		
22-Ti-48	2231	JENDL-3.3	TI048J33.DAT		
22-Ti-49	2234	JENDL-3.3	TI049J33.DAT		
22-Ti-50	2237	JENDL-3.3	TI050J33.DAT		
23-V-nat	2300	JENDL-3.3	V000J33.DAT	V	2300
24-Cr-50	2425	ENDF/B-VI.8 mod 5	CR050E6.DAT	Cr	2400
24-Cr-52	2431	ENDF/B-VI.8 mod 4	CR052E6.DAT		
24-Cr-53	2434	ENDF/B-VI.8 mod 4	CR053E6.DAT		
24-Cr-54	2437	ENDF/B-VI.8 mod 5	CR054E6.DAT		

Table 3: FENDL/E-2.1 library-summary (cont).

Neutron data (online *.DAT)				**Photo-atomic data (online FENDLEP.DAT)**	
Material	**MAT No.**	**Source**	**Filename online**	**Element**	**MAT No.**
25-Mn-55	2525	JENDL-3.3	MN055J33.DAT	Mn	2500
26-Fe-54	2625	ENDF/B-VI.8 mod 5	FE054E6.DAT	Fe	2600
26-Fe-56	2631	JEFF-3.0 (EFF-3.1)	FE056JEFF3.DAT		
26-Fe-57	2634	ENDF/B-VI.8 mod 4	FE057E6.DAT		
26-Fe-58	2637	ENDF/B-VI.8 mod 4	FE058E6.DAT		
27-Co-59	2725	ENDF/B-VI.8 mod 1	CO059E6.DAT	Co	2700
28-Ni-58	2825	JEFF-3.0(EFF-3.0)	NI058JEFF3.DAT	Ni	2800
28-Ni-60	2831	JEFF-3.0(EFF-3.0)	NI060JEFF3rev.DAT		
28-Ni-61	2834	ENDF/B-VI.8 mod 5	NI061E6.DAT		
28-Ni-62	2837	ENDF/B-VI.8 mod 5	NI062E6.DAT		
28-Ni-64	2843	ENDF/B-VI.8 mod 4	NI064E6.DAT		
29-Cu-63	2925	ENDF/B-VI.8 mod 5	CU063E6.DAT	Cu	2900
29-Cu-65	2931	ENDF/B-VI.8 mod 5	CU065E6.DAT		
31-Ga-nat	3100	JENDL-3.2	GA000J32.DAT	Ga	3100
40-Zr-nat	4000	JENDL-FF	ZR000JFF.DAT	Zr	4000
41-Nb-93	4125	JENDL-FF	NB093JFFrev.DAT	Nb	4100
42-Mo-92	4225	JENDL-3.3	MO092J33.DAT	Mo	4200
42-Mo-94	4231	JENDL-3.3	MO094J33.DAT		
42-Mo-95	4234	JENDL-3.3	MO095J33.DAT		
42-Mo-96	4237	JENDL-3.3	MO096J33.DAT		
42-Mo-97	4240	JENDL-3.3	MO097J33.DAT		
42-Mo-98	4243	JENDL-3.3	MO098J33.DAT		
42-Mo-100	4249	JENDL-3.3	MO100J33.DAT		
50-Sn-nat	5000	BROND-2.1	SN000BR2.DAT	Sn	5000
73-Ta-181	7328	JENDL-3.3	TA181J33.DAT	Ta	7300
74-W-182	7431	ENDF/B-VI.8 mod 2	W182E6.DAT	W	7400
74-W-183	7434	ENDF/B-VI.8 mod 2	W183E6.DAT		
74-W-184	7437	ENDF/B-VI.8 mod 2	W184E6.DAT		
74-W-186	7443	ENDF/B-VI.8 mod 2	W186E6.DAT		
79-Au-197	7925	ENDF/B-VI mod 1	AU197E6.DAT	Au	7900
82-Pb-206	8231	ENDF/B-VI.8 mod 1	PB206E6.DAT	Pb	8200
82-Pb-207	8234	ENDF/B-VI mod 1	PB207E6.DAT		
82-Pb-208	8237	ENDF/B-VI.8 mod 1	PB208E6.DAT		
83-Bi-209	8325	ENDF/B-VI.8 mod 2	BI209E6.DAT	Bi	8300

2. Processing FENDL/E-2.1 data to ACE and MATXS formats

The evaluated nuclear data files selected for FENDL/E-2.1 were processed using the NJOY-99.90 modular code system with local updates at IAEA-NDS (Appendix 1). The processing sequence for generating the FENDL/MC-2.1 and FENDL/MG-2.1 libraries is shown in Figure 1. FENDL/MC-2.1 is an ACE-formatted library suitable for use by the MCNP family of Monte-Carlo codes [8]. FENDL/MG-2.1 is a multi-group-formatted library, intended for use in deterministic transport codes like DORT and TORT [9].

The FENDL-2.1 transport sub-libraries were processed following the specifications given in Refs. [1, 10]. A summary of the main processing options is presented below for completeness:

- Reconstruction tolerance in RECONR: 0.1%.
- Resonance-integral-check tolerance in RECONR: 0.3%.
- Maximum resonance integral error in RECONR: 5.0E-08 (default for 0.1%).
- Temperature: 300K = 2.5852E-08 MeV.
- Thinning tolerance in BROADR: 0.1%.
- Integral criterion tolerance in BROADR: 0.3%.
- Integral thinning tolerance in BROADR: 5.0E-0.8 (default for 0.1%).
- Maximum energy in BROADR: 2 MeV.
- Number of probability bins in PURR: 20.
- Number of resonance ladders: 100.
- Bondarenko σ_0 values: 10^{10}, 10^5, 10^4, 10^3, 300, 100, 30, 10, 3, 1, 0.3, 0.1, 0.001 barns, not more than 10 out of this list (Table 4).
- No thermal data.
- No thinning in ACER.
- ACE-type 1 file.
- Suffix for zaid in ACER: .21.
- New cumulative angle distributions in ACER.
- Detailed photon calculation in ACER.
- Neutron groups: 175 in Vitamin-J structure.
- Gamma groups: 42 in Vitamin-J structure.
- Neutron weight function: VITAMIN-E (IWT=11 in NJOY).
- Gamma weight function: 1/E with roll-offs (IWT=3 in NJOY).
- Legendre order: P-6 for transport correction to P-5.
- Reactions included: all reactions contained in the evaluated FENDL/E-2.1 file, energy balance heating (MT = 301), kinematic heating (MT = 443), damage (MT = 444) and gas production. For MATXS-formatted files, MT = 251 (μ), MT = 252 (χ), MT = 253 (γ) and MT = 259 (1/v) are also included.

Some examples of NJOY input options are given in Appendix 2. Complete set of inputs is available on the web or through CD-ROM distribution.

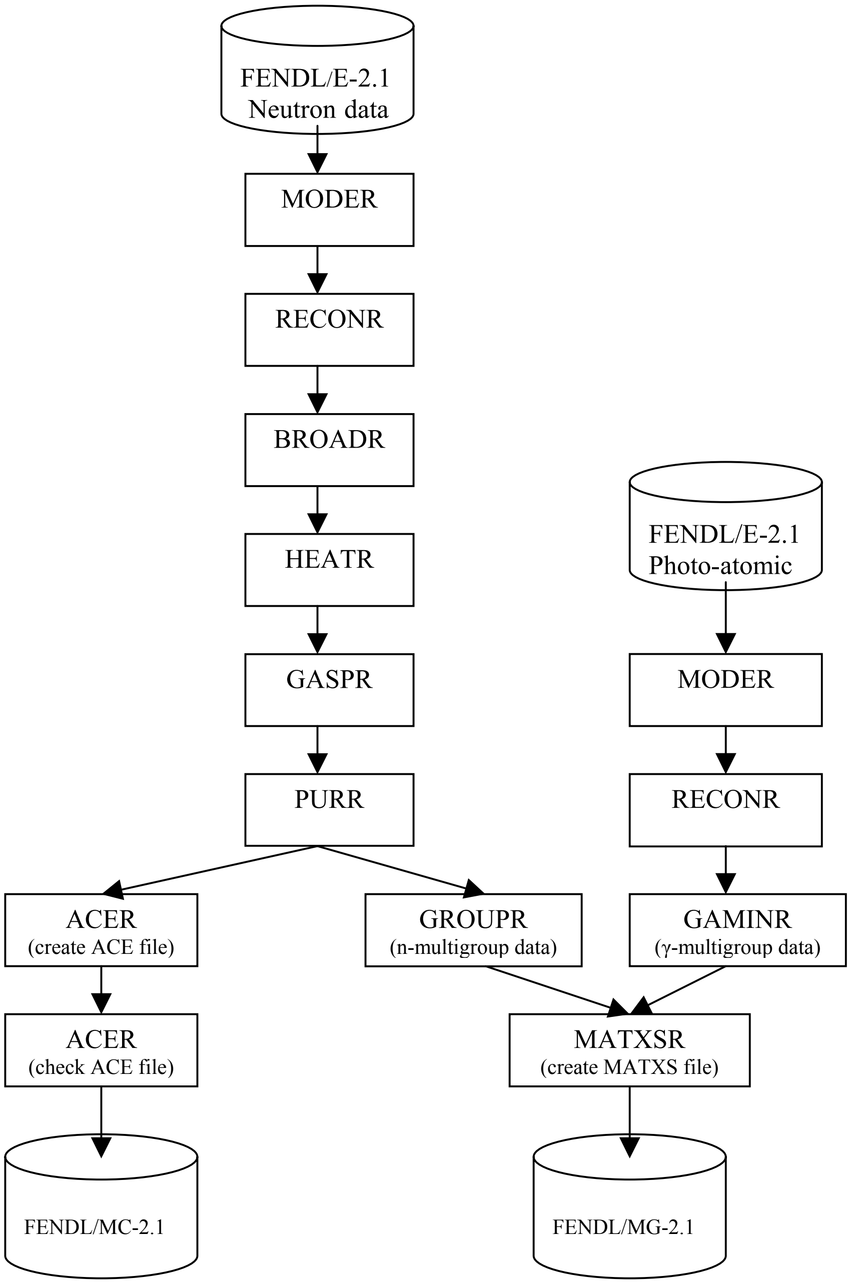

Figure 1: NJOY processing sequence for FENDL/MC-2.1 and FENDL/MG-2.1.

Table 4: Bondarenko σ_0 values for the multi-group data files.

Material	**10^{10}**	**10^5**	**10^4**	**10^3**	**300.**	**100.**	**30.**	**10.**	**3.**	**1.**	**0.3**	**0.1**	**.001**
H-1	X												
H-2	X		X	X		X		X		X			
H-3	X												
He-3	X												
He-4	X												
Li-6	X												
Li-7	X												
Be-9	X		X	X	X	X	X	X		X		X	X
B-10	X												
B-11	X												
C-12	X		X	X	X	X	X	X		X		X	X
N-14	X		X	X	X	X	X	X		X		X	X
N-15	X												
O-16	X		X	X	X	X	X	X		X		X	X
F-19	X												
Na-23	X												
Mg-nat	X												
Al-27	X												
Si-28	X					X		X		X			
Si-29	X					X		X		X			
Si-30	X					X		X		X			
P-31	X												
S-nat	X			X	X	X	X	X					
Cl-35	X			X	X	X	X	X					
Cl-37	X			X	X	X	X	X					
K-nat	X			X	X	X	X	X					
Ca-nat	X			X	X	X	X	X	X	X			
Ti-46	X		X	X	X	X	X	X	X	X			
Ti-47	X		X	X	X	X	X	X	X	X			
Ti-48	X		X	X	X	X	X	X	X	X			
Ti-49	X		X	X	X	X	X	X	X	X			
Ti-50	X		X	X	X	X	X	X	X	X			
V-nat	X		X	X	X	X	X	X		X		X	X
Cr-50	X			X	X	X	X	X	X	X			
Cr-52	X			X	X	X	X	X	X	X			
Cr-53	X			X	X	X	X	X	X	X			
Cr-54	X			X	X	X	X	X	X	X			
Mn-55	X	X		X		X		X		X			
Fe-54	X	X	X	X		X		X					
Fe-56	X	X	X	X		X		X	X	X	X	X	
Fe-57	X	X	X	X		X		X					
Fe-58	X	X	X	X		X		X					

Table 4: Bondarenko σ_0 values for the multi-group data files (cont).

Material	10^{10}	10^5	10^4	10^3	300.	100.	30.	10.	3.	1.	0.3	0.1	.001
Co-59	X	X	X	X		X		X					
Ni-58	X			X	X	X	X	X	X	X			
Ni-60	X			X	X	X	X	X	X	X			
Ni-61	X			X	X	X	X	X	X	X			
Ni-62	X			X	X	X	X	X	X	X			
Ni-64	X			X	X	X	X	X	X	X			
Cu-63	X		X		X	X	X	X		X		X	
Cu-65	X		X		X	X	X	X		X		X	
Ga-nat	X		X	X	X	X	X	X		X		X	X
Zr-nat	X		X	X	X	X	X	X		X		X	X
Nb-93	X		X	X	X	X	X	X		X		X	X
Mo-92	X		X	X	X	X	X	X		X		X	X
Mo-94	X		X	X	X	X	X	X		X		X	X
Mo-95	X		X	X	X	X	X	X		X		X	X
Mo-96	X		X	X	X	X	X	X		X		X	X
Mo-97	X		X	X	X	X	X	X		X		X	X
Mo-98	X		X	X	X	X	X	X		X		X	X
Mo-100	X		X	X	X	X	X	X		X		X	X
Sn-nat	X		X	X		X		X		X			
Ta-181	X		X	X		X		X					
W-182	X		X	X	X	X	X	X		X		X	X
W-183	X		X	X	X	X	X	X		X		X	X
W-184	X		X	X	X	X	X	X		X		X	X
W-186	X		X	X	X	X	X	X		X		X	X
Au-197	X		X	X	X	X	X	X		X			
Pb-206	X			X		X		X		X			
Pb-207	X			X		X		X		X			
Pb-208	X			X		X		X		X			
Bi-209	X		X	X		X		X					

3. Continuous-energy data library FENDL/MC-2.1 for MCNP

FENDL/MC-2.1 contains pointwise cross section data files for use in the Monte Carlo code MCNP. Two files are given for each material: one with extension "`.ace`" for the cross section data file in the ACE type 1 (ASCII) format, and the second one with extension "`.dir`" with the information required by the XSDIR file of the MCNP code system. Both files are prepared by the ACER module of NJOY-99. The `.dir` files were rewritten by the UpdXSDIR code to give the correct ACE filename and to update the route to 0. Table 5 summarizes the information on the FENDL/MC-2.1 library. All the files were created at 300K, and probability tables (PT) were generated for those materials with unresolved resonance data.

Table 5: FENDL/MC-2.1 library-summary.

No.	Material	ZAID	PT tables	ACE filename	XSDIR filename
1	1-H-1	1001.21c	-	H001.ACE	H001.DIR
2	1-H-2	1002.21c	-	H002.ACE	H002. DIR
3	1-H-3	1003.21c	-	H003.ACE	H003. DIR
4	2-He-3	2003.21c	-	HE003.ACE	HE003. DIR
5	2-He-4	2004.21c	-	HE004.ACE	HE004. DIR
6	3-Li-6	3006.21c	-	LI006.ACE	LI006.DIR
7	3-Li-7	3007.21c	-	LI007.ACE	LI007.DIR
8	4-Be-9	4009.21c	-	BE009.ACE	BE009.DIR
9	5-B-10	5010.21c	-	B010.ACE	B010.DIR
10	5-B-11	5011.21c	-	B011.ACE	B011.DIR
11	6-C-12	6012.21c	-	C012.ACE	C012.DIR
12	7-N-14	7014.21c	-	N014.ACE	N014.DIR
13	7-N-15	7015.21c	-	N015.ACE	N015.DIR
14	8-O-16	8016.21c	-	O016.ACE	O016.DIR
15	9-F-19	9019.21c	-	F019.ACE	F019.DIR
16	11-Na-23	11023.21c	-	NA023.ACE	NA023.DIR
17	12-Mg-nat	12000.21c	-	MG000.ACE	MG000.DIR
18	13-Al-27	13027.21c	-	AL027.ACE	AL027.DIR
19	14-Si-28	14028.21c	-	SI028.ACE	SI028.DIR
20	14-Si-29	14029.21c	-	SI029.ACE	SI029.DIR
21	14-Si-30	14030.21c	-	SI030.ACE	SI030.DIR
22	15-P-31	15031.21c	-	P015.ACE	P015.DIR
23	16-S-nat	16000.21c	-	S000.ACE	S000.DIR
24	17-Cl-35	17035.21c	-	CL035.ACE	CL035.DIR
25	17-Cl-37	17037.21c	-	CL037.ACE	CL037.DIR
26	19-K-nat	19000.21c	-	K000.ACE	K000.DIR
27	20-Ca-nat	20000.21c	-	CA000.ACE	CA000.DIR
28	22-Ti-46	22046.21c	-	TI046.ACE	TI046.DIR
29	22-Ti-47	22047.21c	-	TI047.ACE	TI047.DIR
30	22-Ti-48	22048.21c	-	TI048.ACE	TI048.DIR
31	22-Ti-49	22049.21c	-	TI049.ACE	TI049.DIR
32	22-Ti-50	22050.21c	-	TI050.ACE	TI050.DIR
33	23-V-nat	23000.21c	-	V000.ACE	V000.DIR
34	24-Cr-50	24050.21c	-	CR050.ACE	CR050.DIR
35	24-Cr-52	24052.21c	-	CR052.ACE	CR052.DIR
36	24-Cr-53	24053.21c	-	CR053.ACE	CR053.DIR
37	24-Cr-54	24054.21c	-	CR054.ACE	CR054.DIR
38	25-Mn-55	25055.21c	-	MN055.ACE	MN055.DIR

Table 5: FENDL/MC-2.1 library-summary (cont).

No.	Material	ZAID	PT tables	ACE filename	XSDIR filename
39	26-Fe-54	26054.21c	-	FE054.ACE	FE054.DIR
40	26-Fe-56	26056.21c	-	FE056.ACE	FE056.DIR
41	26-Fe-57	26057.21c	-	FE057.ACE	FE057.DIR
42	26-Fe-58	26058.21c	-	FE058.ACE	FE058.DIR
43	27-Co-59	27059.21c	-	CO059.ACE	CO059.DIR
44	28-Ni-58	28058.21c	-	NI058.ACE	NI058.DIR
45	28-Ni-60	28060.21c	-	NI060.ACE	NI060.DIR
46	28-Ni-61	28061.21c	-	NI061.ACE	NI061.DIR
47	28-Ni-62	28062.21c	-	NI062.ACE	NI062.DIR
48	28-Ni-64	28064.21c	-	NI064.ACE	NI064.DIR
49	29-Cu-63	29063.21c	-	CU063.ACE	CU063.DIR
50	29-Cu-65	29065.21c	-	CU065.ACE	CU065.DIR
51	31-Ga-nat	31000.21c	-	GA000.ACE	GA000.DIR
52	40-Zr-nat	40000.21c	X	ZR000.ACE	ZR000.DIR
53	41-Nb-93	41093.21c	X	NB093.ACE	NB093.DIR
54	42-Mo-92	42092.21c	X	MO092.ACE	MO092.DIR
55	42-Mo-94	42094.21c	X	MO094.ACE	MO094.DIR
56	42-Mo-95	42095.21c	X	MO095.ACE	MO095.DIR
57	42-Mo-96	42096.21c	X	MO096.ACE	MO096.DIR
58	42-Mo-97	42097.21c	X	MO097.ACE	MO097.DIR
59	42-Mo-98	42098.21c	X	MO098.ACE	MO098.DIR
60	42-Mo-100	42100.21c	X	MO100.ACE	MO100.DIR
61	50-Sn-nat	50000.21c	X	SN000.ACE	SN000.DIR
62	73-Ta-181	73181.21c	X	TA181.ACE	TA181.DIR
63	74-W-182	74182.21c	X	W181.ACE	W181.DIR
64	74-W-183	74183.21c	X	W183.ACE	W183.DIR
65	74-W-184	74184.21c	X	W184.ACE	W184.DIR
66	74-W-186	74186.21c	X	W186.ACE	W186.DIR
67	79-Au-197	79197.21c	-	AU197.ACE	AU197.DIR
68	82-Pb-206	82206.21c	-	PB206.ACE	PB206.DIR
69	82-Pb-207	82207.21c	-	PB207.ACE	PB207.DIR
70	82-Pb-208	82208.21c	-	PB208.ACE	PB208.DIR
71	83-Bi-209	83209.21c	-	BI209.ACE	BI209.DIR

4. Multi-group cross section data library FENDL/MG-2.1

FENDL/MG-2.1 contains neutron-photon coupled multi-group cross section data in MATXS (ASCII) format. These data can be easily processed by the code TRANXS [11] for further use in deterministic transport codes such as DORT and TORT. The vitamin-J energy structure was used for neutrons as well as photons to give 175 energy groups between 0.00001 eV and 19.64 MeV for neutrons, and 42 groups between 1 keV and 50 MeV for photons. Table 6 summarizes the FENDL/MG-2.1 data.

Table 6: FENDL/MG-2.1 library-summary.

No.	Material	MATXS ID	MATXS (*.m)	GROUPR (*.g)	GAMINR (*.gam)
1	1-H-1	h1	H001.M	H001.G	H000.GAM
2	1-H-2	d	H002.M	H002.G	
3	1-H-3	h3	H003.M	H003.G	
4	2-He-3	he3	HE003.M	HE003.G	HE000. GAM
5	2-He-4	he4	HE004.M	HE004.G	
6	3-Li-6	li6	LI006.M	LI006.G	LI000.GAM
7	3-Li-7	li7	LI007.M	LI007.G	
8	4-Be-9	be9	BE009.M	BE009.G	BE000.GAM
9	5-B-10	b10	B010.M	B010.G	B000.GAM
10	5-B-11	b11	B011.M	B011.G	
11	6-C-12	c12	C012.M	C012.G	C000.GAM
12	7-N-14	n14	N014.M	N014.G	N000.GAM
13	7-N-15	n15	N015.M	N015.G	
14	8-O-16	o16	O016.M	O016.G	O000.GAM
15	9-F-19	f19	F019.M	F019.G	F000.GAM
16	11-Na-23	na23	NA023.M	NA023.G	NA000.GAM
17	12-Mg-nat	mgnat	MG000.M	MG000.G	MG000.GAM
18	13-Al-27	al27	AL027.M	AL027.G	AL000.GAM
19	14-Si-28	si28	SI028.M	SI028.G	SI000.GAM
20	14-Si-29	si29	SI029.M	SI029.G	
21	14-Si-30	si30	SI030.M	SI030.G	
22	15-P-31	p31	P015.M	P015.G	P015.GAM
23	16-S-nat	snat	S000.M	S000.G	S000.GAM
24	17-Cl-35	cl35	CL035.M	CL035.G	CL000.GAM
25	17-Cl-37	cl37	CL037.M	CL037.G	
26	19-K-nat	knat	K000.M	K000.G	K000.GAM
27	20-Ca-nat	canat	CA000.M	CA000.G	CA000.GAM
28	22-Ti-46	ti46	TI046.M	TI046.G	TI000.GAM
29	22-Ti-47	ti47	TI047.M	TI047.G	
30	22-Ti-48	ti48	TI048.M	TI048.G	
31	22-Ti-49	ti49	TI049.M	TI049.G	

Table 6: FENDL/MG-2.1 library-summary (cont).

No.	Material	MATXS ID	MATXS (*.m)	GROUPR (*.g)	GAMINR(*.gam)
32	22-Ti-50	ti50	TI050.M	TI050.G	TI000.GAM
33	23-V-nat	vnat	V000.M	V000.G	V000.GAM
34	24-Cr-50	cr50	CR050.M	CR050.G	CR000.GAM
35	24-Cr-52	cr52	CR052.M	CR052.G	
36	24-Cr-53	cr53	CR053.M	CR053.G	
37	24-Cr-54	cr54	CR054.M	CR054.G	
38	25-Mn-55	mn55	MN055.M	MN055.G	MN000.GAM
39	26-Fe-54	fe54	FE054.M	FE054.G	FE000.GAM
40	26-Fe-56	fe56	FE056.M	FE056.G	
41	26-Fe-57	fe57	FE057.M	FE057.G	
42	26-Fe-58	fe58	FE058.M	FE058.G	
43	27-Co-59	co59	CO059.M	CO059.G	CO000.GAM
44	28-Ni-58	ni58	NI058.M	NI058.G	NI000.GAM
45	28-Ni-60	ni60	NI060.M	NI060.G	
46	28-Ni-61	ni61	NI061.M	NI061.G	
47	28-Ni-62	ni62	NI062.M	NI062.G	
48	28-Ni-64	ni64	NI064.M	NI064.G	
49	29-Cu-63	cu63	CU063.M	CU063.G	CU000.GAM
50	29-Cu-65	cu65	CU065.M	CU065.G	
51	31-Ga-nat	ganat	GA000.M	GA000.G	GA000.GAM
52	40-Zr-nat	zrnat	ZR000.M	ZR000.G	ZR000.GAM
53	41-Nb-93	nb93	NB093.M	NB093.G	NB000.GAM
54	42-Mo-92	mo92	MO092.M	MO092.G	MO000.GAM
55	42-Mo-94	mo94	MO094.M	MO094.G	
56	42-Mo-95	mo95	MO095.M	MO095.G	
57	42-Mo-96	mo96	MO096.M	MO096.G	
58	42-Mo-97	mo97	MO097.M	MO097.G	
59	42-Mo-98	mo98	MO098.M	MO098.G	
60	42-Mo-100	mo100	MO100.M	MO100.G	
61	50-Sn-nat	snnat	SN000.M	SN000.G	SN000.GAM
62	73-Ta-181	ta181	TA181.M	TA181.G	TA000.GAM
63	74-W-182	w182	W181.M	W181.G	W000.GAM
64	74-W-183	w183	W183.M	W183.G	
65	74-W-184	w184	W184.M	W184.G	
66	74-W-186	w186	W186.M	W186.G	
67	79-Au-197	au197	AU197.M	AU197.G	AU000.GAM
68	82-Pb-206	pb206	PB206.M	PB206.G	PB000.GAM
69	82-Pb-207	pb207	PB207.M	PB207.G	
70	82-Pb-208	pb208	PB208.M	PB208.G	
71	83-Bi-209	bi208	BI209.M	BI209.G	BI000.GAM

Three files are supplied for each material: one with extension "`.m`" containing the MATXS-formatted cross section data, and two additional files with extensions "`.g`" and "`.gam`" containing the GROUPR and GAMINR output respectively in GENDF format (last two files are useful for sensitivity analysis).

5. Verification of FENDL/MC-2.1 and FENDL/MG-2.1

The main verification technique used in this work was to check the NJOY output file for each material. A total of 556 messages were generated by NJOY, of which 29 were produced in the second ACER run and 3 in the MATXSR run. All the "messages" generated were understood, and most of them are related to incomplete evaluations. Some comments about the major issues are given below:

- Evaluations for H-3, He-4 and Ga-nat do not have photon production data.
- For several evaluations, particularly evaluations from JENDL-3.3 and the elemental evaluations, File 6 (MF = 6) is used, although incomplete: the energy distribution is not given for the recoil nucleus. NJOY-99 applied one particle approximation in these cases. Negative values of the total heating cross section (MT = 301) were found (Table 7) in 10 cases.
- The corrective actions performed in the second run of ACER were considered appropriate.
- For evaluations with energy limits greater than 20 MeV, usually the warning messages come from the higher energies.

Table 7: Materials with negative values of MT = 301 (heat).

No.	Material	Energy range where MT=301 is negative [MeV]
1	Ti-47	2.54 - 11.70
2	Mo-92	0.43 - 8.99
3	Mo-94	0.60 - 16.29
4	Mo-95	2.99 - 14.60
5	Mo-96	1.00 – 17.10
6	Mo-97	2.52 – 13.68
7	Mo-98	0.42 -19.90
8	Mo-100	0.42 – 19.90
9	Sn-nat	2.10 – 2.93
10	Ta-181	3.37 – 8.81

A second verification technique was used for all the ACE-formatted files. Processed data were converted back to ENDF-6 format using the code ACELST [12]. The original evaluation was processed using the PREPRO-2002 code system (LINEAR+RECENT+SIGMA1), and the two ENDF-6 formatted files were compared using COMPLOT. No significant deviations in the cross section data were found.

After running these basic verification procedures, the processed data were judged to be acceptable.

6. Special purpose libraries

According to Ref. [1], the following recommendations are given for the FENDL-2.1 special purpose libraries:

- Existing FENDL-2 file for dosimetry is not be updated - use of IRDF-2002 is recommended instead (http://www-nds.iaea.org/irdf2002/html/).
- FENDL-2 activation library is not to be updated - use of EAF-2003 is recommended instead. The cross section library will be available in both EAF and ENDF format (same as used for JEFF-3.0) through IAEA-NDS, including the decay data library.
- No changes are recommended to the FENDL-2 charged-particle library.

7. Accessing FENDL-2.1 data

The FENDL-2.1 data library is freely available from the IAEA-NDS upon request, and is also readily accessible at http://www-nds.iaea.org/fendl21/ web site.

FENDL-2.1 package includes the following information:

- FENDL/E-2.1 data files for neutron and photo-atomic interaction data.
- FENDL/MC-2.1: continuous energy data files for MCNP calculations.
- FENDL/MG-2.1: coupled neutron-photon multi-group data library for transport calculations.
- NJOY inputs for generation of FENDL-2.1.
- Auxiliary programs and MSDOS/WINDOWS batch procedures used in the generation and verification of the FENDL-2.1 transport libraries.
- ACEDOP code package for Döppler broadening of ACE-formatted files.
- Documentation: IAEA report INDC(NDS)-467 (this document).

8. Final remarks and recommendations

An updated version of FENDL-2 (termed FENDL-2.1) has been assembled and made available for fusion applications. All evaluated nuclear data files from FENDL/E-2.1 were processed using the NJOY-99.90 code system. FENDL/MC-2.1 and FENDL/MG-2.1 libraries were also assembled. Materials with unresolved resonance data in FENDL/MC-2.1 include probability tables.

FENDL-2.1 libraries, input files and reports as well as the ACEDOP package are freely available on the web site http://www-nds.iaea.org//fendl21/, or can be requested on CD-ROM from the IAEA-NDS.

An extensive and intensive benchmarking of the updated transport libraries is strongly recommended, analysing the same set of benchmarks that was used to validate FENDL-2.0.

References

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4. Cullen, D. E., "PREPRO 2002: 2002 ENDF/B Pre-processing codes", IAEA-NDS-39, Rev. 11, 5 February 2003.

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7. Fischer, U., Forrest, R.A., Sublet, J.-C., Private communication on tungsten evaluations, December 2004.

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11. MacFarlane, R. E., "TRANSX 2: A Code for Interfacing MATXS Cross Section Libraries to Nuclear Transport Codes", Los Alamos National Laboratory, LA-12312-MS, 1992.

12. Trkov, A., Private communication on ACELST code, December 2002.

APPENDIX 1: NJOY local updates at IAEA-NDS.

```
*ident upiaea1
*/ groupr - A.Trkov, IAEA
*/         Local updates from NJOY97 that were not implemented
*/ Need more space for the flux calculator (Case: U-238)
*d up89.6
      dimension a(400000)
*d up89.8
      iamax=400000
*/
*ident upijs57
*/ groupr  A.Trkov, 9-March-1999
*/ groupr is caught in an infinite loop for Be-9 from ENDF/B-VI
*/ on a PC with Lahey compiler.
*/ It seems the products inside an "if" statements are
*/ computed differently than outside. The program does not
*/ recognise that ep EQUALS "test" when written as a product.
*d groupr.6054
      test=shade*epn
      if (idis.gt.0.and.ep.lt.test) epn=test
*/
*/ Old proposal from C.Dean
*d groupr.2745,2746
               b(iz+3+li)=(sigz(iz)-sam)*wtf*(1-beta)
*/
*ident upijs59
*/ acer   A.Trkov 20-aug-1999
*/ If pointwise representation in CM system, csn should be used
*/ (pointed out by Harry Wienke).
*d acer.3394,3396
                        if (csn.ge.a(ll).and.csn.le.a(ll+2))
     &                    call terp1(a(ll),a(ll+1),a(ll+2),a(ll+3),
     &                    csn,fmu,lang-10)
*/
*ident upijs61
*/ acer   A.Trkov 3-dec-1999
*/        fix6 may run out of space without warning
*d acer.3247
      dimension a(2000)
*d up3.38
      data namax/2000/
*i acer.3262
      if(nw.gt.namax) call error('fix6','storage exceeded.',' ')
*i acer.3272
      if(nw.gt.namax) call error('fix6','storage exceeded.',' ')
*i acer.3278
      if(nw.gt.namax) call error('fix6','storage exceeded.',' ')
*i acer.3280
      if(nw.gt.namax) call error('fix6','storage exceeded.',' ')
*i acer.3282
      if(nw.gt.namax) call error('fix6','storage exceeded.',' ')
*i acer.3284
      if(nw.gt.namax) call error('fix6','storage exceeded.',' ')
*i acer.3290
      if(nw.gt.namax) call error('fix6','storage exceeded.',' ')
*i acer.3296
      if(nw+l.gt.namax) call error('fix6','storage exceeded.',' ')
*i acer.3299
      if(nw+l.gt.namax) call error('fix6','storage exceeded.',' ')
*/
*ident upijs62
*/ groupr  A.Trkov, 29-Apr-2002
*/         - Fix inconsistent usage of output weighting flux unit number
```

```
*/         - Fix logic when searching for the right flux point
*i groupr.80
c     *            note: weighting flux file is always written binary  *
*d groupr.99
c     *    ninwt   tape unit for flux parameters (binary)              *
*d groupr.272
*d groupr.2290
         ninwt=iabs( ninwt)
         call openz(-ninwt,1)
*d groupr.2294
     &     ehi,sigpot,nflmax,-ninwt,jsigz
*d groupr.2307,2308
         call openz(-ninwt,0)
         write(nsyso,'(/'' ninwt......'',i4)') -ninwt
*d groupr.3037
      if (e.gt.el*(1-small).and.e.lt.en*(1+small)) go to 230
*/
*ident upijs63
*/ purr  A.Trkov, May 2002
*/       Increase scratch space to process Pu-239 from JEF-2.2
*d purr.95
      maxscr=12000
*/
*ident upijs64
*/ groupr  A.Trkov, July 2002
*/         There is an error in Cl-37 in ENDF/B-VI Rev.8
*/         MAT 1731 MF 15 MT 102
*/         The first energy for the gamma yields is zero. It
*/         redefines enext in getsed to zero, which is
*/         interpreted as a flag to do initialisation in
*/         getgyl (called from getff). Since 'yl' is
*/         already reserved, groupr crashes.
*d groupr.8697
            if (elo.gt.0 .and. elo.lt.enext) enext=elo
*ident upiaea2
*/ groupr - A.Trkov, IAEA, Feb-2003
*/          Increase array size for Legendre coefficients
*i groupr.4756
c     maximum legendre coefficients
      parameter (mxlg=65)
*d groupr.4764
      dimension term(mxlg),terml(mxlg)
*i groupr.5209
c     maximum legendre coefficients
      parameter (mxlg=65)
*d groupr.5212
      dimension term(mxlg),x(10),y(10,mxlg)
*d groupr.5329,5330
c     maximum legendre coefficients
      parameter (mxlg=65)
      dimension cnow(*),term(*),p(mxlg)
      dimension x(10),y(10,mxlg),yt(mxlg)
*d groupr.5333
      external f6ddx,f6psp,f6dis,legndr,error
*i groupr.5358
      if(nl.gt.mxlg) call error('f6cm','nl>mxlg',' ')
*d groupr.5586
c     maximum legendre coefficients
      parameter (mxlg=65)
      dimension cnow(*),p(mxlg)
*d groupr.5768
c     maximum legendre coefficients
      parameter (mxlg=65)
      dimension cnow(*),p(mxlg)
*i groupr.5630
```

```
         if(nl.gt.mxlg) call error('f6ddx','nl>mxlg',' ')
*i groupr.5992
c     maximum legendre coefficients
      parameter (mxlg=65)
*d groupr.5995
      dimension term(mxlg),p(mxlg),amu(50),fmu(50),qp(8),qw(8)
*i groupr.6130
c     maximum legendre coefficients
      parameter (mxlg=65)
*d groupr.6133,6134
      dimension term1(mxlg),term2(mxlg),p(mxlg)
      dimension qp(8),qw(8)
*i groupr.6733
c     maximum legendre coefficients
      parameter (mxlg=65)
*d groupr.6740
      dimension flo(mxlg),fhi(mxlg)
*i groupr.7314
c     maximum legendre coefficients
      parameter (mxlg=65)
*d groupr.7318
      dimension b(6),alo(mxlg),ahi(mxlg)
*i groupr.7929
c     maximum legendre coefficients
      parameter (mxlg=65)
*d groupr.7942
      dimension fl(mxlg)
*/
*ident upiaea3
*/ acer   - A.Trkov, IAEA, Feb-2003
*/             declare "error" external to avoid conflict with intrinsic
function
*i up69.66
      external error
*/
*ident upfndl1
*/ matxsr - D. L. Aldama, NDS/IAEA Consultant, Nov-2004
*/ Need more space  (Case: 1-H-2 from JENDL-3.3)
*/  subroutine band
*d matxsr.1973
      dimension b(5000)
*d matxsr.1978
      maxb=5000
*/  subroutine shufl
*d matxsr.2078
      dimension b(5000)
*d matxsr.2080
      maxb=5000
*/
*ident upfndl2
*/ gaspr - D. L. Aldama, NDS/IAEA Consultant, Nov-2004
*/ Need more space (case Ni-058 from JEFF-3.0)
*d gaspr.28
      dimension egas(80000),sgas(5,80000)
*d gaspr.41
      maxg=80000
*ident upfndl3
*/ purr - D. L. Aldama, NDS/IAEA Consultant, Nov-2004
*/ to allow PT for multi-isotope materials when
*/ not all the isotopes have unresolved resonance data
*d purr.624
*i purr.651
      if (ier.eq.ner) go to 110
*/
*ident upfndl4
```

```
*/ acer - D. L. Aldama, NDS/IAEA Consultant, Nov-2004
*/ Format extension for negative energies (overlap)
*d acer.4947,4948
            write(nsyso,'(''   energy range: '',1p,e11.4,
     &        '' - '',e11.4,'' ev'')') urlo,urhi
*/
*ident upfndl5
*/ groupr - D. L. Aldama, NDS/IAEA Consultant, Nov-2004
*/ Needed to process Be-9 from JEFF-3.0 evaluation
*/  MT=875-891 for (n,2n) splitted reaction
*i groupr.1147
         else if (mtd.ge.875.and.mtd.le.884) then
            write(reac,'(''2n0'',i1)') mtd-875
         else if (mtd.ge.885.and.mtd.le.890) then
            write(reac,'(''2n'',i2)') mtd-875
         else if (mtd.eq.891) then
            reac='2nc'
*i groupr.3964
         if (iverf.ge.6.and.mtd.ge.875.and.mtd.le.891) mt=mtd
*i groupr.4331
      if (mfd.ge.31.and.mfd.le.36.and.iverf.ge.6.and.
     &   (mtd.ge.875.and.mtd.lt.891)) go to 400
*i groupr.8014
         if (mth.ge.875.and.mth.lt.891) za2=1
*i groupr.8330
      if (iverf.ge.6.and.mth.ge.875.and.mth.le.890) mt0=875
*/
*/ matxsr - D. L. Aldama, NDS/IAEA Consultant, Nov-2004
*/ Needed to process Be-9 from JEFF-3.0 evaluation
*/  MT=875-891 for (n,2n) splitted reaction
*d matxsr.1418
  290 if (mt.gt.891) go to 300
*i matxsr.1433
      if (mt.ge.875.and.mt.lt.885) write(strng,'(''2n0'',i1)') mt-875
      if (mt.ge.885.and.mt.lt.891) write(strng,'(''2n'',i2)') mt-875
      if (mt.eq.891) write(strng,'(''2ncn'')')
*i matxsr.1504
      k016=0
*i matxsr.1652
      if (mt.eq.16) k016=1
      if (k016.eq.1.and.mt.ge.875.and.mt.le.891) go to 310
*/
*ident upfndl6
*/ groupr - D. L. Aldama, NDS/IAEA Consultant, Nov-2004
*/ subroutine namer corrected for mt=659, reac=d09
*/ It's only affect groupr printout
*d groupr.1124
         else if (mtd.ge.650.and.mtd.le.659) then
*/
```

APPENDIX 2: Examples of NJOY-99.90 inputs for FENDL-2.1.

2.1 NJOY-99.90 input options for Fe-56

```
moder / Extract/convert neutron evaluated data
1 -21
'26-Fe-56 from FENDLE-2.1'/
20 2631
0/
moder / Extract/convert photo-atomic data
1 -41
'26-Fe-56 from FENDLE photo-atomic'/
40 2600
0/
reconr / Reconstruct XS for neutrons
-21 -22
'FENDL-2.1 PENDF for 26-Fe-56'/
2631 2/
0.001 0. 0.003/
'FENDL-2.1: 26-Fe-56 from JEFF-3.0'/
'Processed by NJOY-99.90 at NDS/IAEA Nov2004'/
0/
broadr / Doppler broaden XS
-21 -22 -23
2631 1 0 0 0./
0.001 2.0e6 0.003/
300.
0/
heatr / Add heating kerma and damage energy
-21 -23 -24/
2631 2 0 0 0 2/
443 444/
gaspr / Add gas production
-21 -24 -25
purr / Process Unresolved Resonance Range if any
-21 -25 -26
2631 1 10 20 100/
300.
1.E+10 1.E+05 1.E+04 1.E+03 1.E+02 1.E+01 3.E+00 1.E+00 3.E-01 1.E-01
0/
acer / Prepare ACE files
-21 -26 0 27 28
1 0 1 .21/
'26-Fe-56 from FENDL-2.1(JEFF-3.0) NJOY 99.90 NDS/IAEA Nov2004'/
2631 300.
1 1/
/
acer / Check ACE files
0 27 0 29 30
7 1 1 -1/
/
groupr / Prepare multigroup data for neutrons
-21 -26 0 31
2631 17 10 11 6 1 10 1/
'26-Fe-56 from FENDL-2.1(JEFF-3.0) NJOY 99.90 NDS/IAEA Nov2004'/
300.
1.E+10 1.E+05 1.E+04 1.E+03 1.E+02 1.E+01 3.E+00 1.E+00 3.E-01 1.E-01
3/
3  251 'mubar'/
3  252 'xi'/
3  253 'gamma'/
3  259 '1/v'/
6/
16/
```

```
0/
0/
reconr / Reconstruct photo-atomic data
-41 -42
'FENDL-2.1 photo-atomic PENDF TAPE for 26-Fe-56'/
2600 2/
0.001 0. 0.003/
'FENDL-2.1: 26-Fe-56 from ENDF/B-VI'/
'Processed by NJOY-99.90 at NDS/IAEA Nov2004'/
0/
gaminr / Prepare multigroup data for photons
-41 -42 0 43/
2600 10 3 6 1/
'26-Fe-56 from FENDL-2.1(ENDF/B-VI) NJOY-99.90 NDS/IAEA Nov2004'/
-1/
0/
matxsr / Produce MATXS file
31 43 44/
1 'fendl-2.1 fe56'/
2 3 3 1
'FENDL-2.1: 26-Fe-56 from JEFF-3.0'/
'Photo-atomic data from ENDF/B-VI'/
'Processed by NJOY-99.90 at NDS/IAEA Nov2004'/
'n' 'g'/
175 42
'nscat' 'ng' 'gscat'/
1 1 2/
1 2 2/
'fe56' 2631 2600/
stop
```

2.1 NJOY-99.90 input options for W-184.

```
moder / Extract/convert neutron evaluated data
1 -21
'74-W-184 from FENDLE-2.1'/
20 7437
0/
moder / Extract/convert photo-atomic data
1 -41
'74-W-184 from FENDLE photo-atomic'/
40 7400
0/
reconr / Reconstruct XS for neutrons
-21 -22
'FENDL-2.1 PENDF for 74-W-184'/
7437 2/
0.001 0. 0.003/
'FENDL-2.1: 74-W-184 from ENDF/B-VI'/
'Processed by NJOY-99.90 at NDS/IAEA Nov2004'/
0/
broadr / Doppler broaden XS
-21 -22 -23
7437 1 0 0 0./
0.001 2.0e6 0.003/
300.
0/
heatr / Add heating kerma and damage energy
-21 -23 -24/
7437 2 0 0 0 2/
443 444/
gaspr / Add gas production
-21 -24 -25
purr / Process Unresolved Resonance Range if any
-21 -25 -26
7437 1 10 20 100/
300.
1.E+10 1.E+04 1.E+03 3.E+02 1.E+02 3.E+01 1.E+01 1.E+00 1.E-01 1.E-03
0/
acer / Prepare ACE files
-21 -26 0 27 28
1 0 1 .21/
'74-W-184 from FENDL-2.1(ENDF/B-VI) NJOY 99.90 NDS/IAEA Nov2004'/
7437 300.
1 1/
/
acer / Check ACE files
0 27 0 29 30
7 1 1 -1/
/
groupr / Prepare multigroup data for neutrons
-21 -26 0 31
7437 17 10 11 6 1 10 1/
'74-W-184 from FENDL-2.1(ENDF/B-VI) NJOY 99.90 NDS/IAEA Nov2004'/
300.
1.E+10 1.E+04 1.E+03 3.E+02 1.E+02 3.E+01 1.E+01 1.E+00 1.E-01 1.E-03
3/
3  251 'mubar'/
3  252 'xi'/
3  253 'gamma'/
3  259 '1/v'/
6/
16/
0/
0/
reconr / Reconstruct photo-atomic data
```

```
-41 -42
'FENDL-2.1 photo-atomic PENDF TAPE for 74-W-184'/
7400 2/
0.001 0. 0.003/
'FENDL-2.1: 74-W-184 from ENDF/B-VI'/
'Processed by NJOY-99.90 at NDS/IAEA Nov2004'/
0/
gaminr / Prepare multigroup data for photons
-41 -42 0 43/
7400 10 3 6 1/
'74-W-184 from FENDL-2.1(ENDF/B-VI) NJOY-99.90 NDS/IAEA Nov2004'/
-1/
0/
matxsr / Produce MATXS file
31 43 44/
1 'fendl-2.1 w184'/
2 3 3 1
'FENDL-2.1: 74-W-184 from ENDF/B-VI'/
'Photo-atomic data from ENDF/B-VI'/
'Processed by NJOY-99.90 at NDS/IAEA Nov2004'/
'n' 'g'/
175 42
'nscat' 'ng' 'gscat'/
1 1 2/
1 2 2/
'w184' 7437 7400/
stop
```

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