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FENDL/C-2.0

Charged-Particle Reaction Data Library for Fusion Applications
Version 1 of March 1997

Data extracted from ENDF/B-6 evaluations
by R.M. White and D.A. Resler, LLNL
and G. M. Hale, LANL

Summary documentation by

A.B. Pashchenko and H. Wienke

Abstract: This document describes the FENDL/C-2.0 charged-particle reaction data library which is a sublibrary of FENDL-2, the evaluated nuclear data library for fusion applications. This file contains evaluated data in ENDF-6 format for the D(d,n), D(d,p), T(d,n), T(t,2n), He-3(d,p) reactions. The processed information, i.e. Maxwellian-averaged reaction rates, and related quantities, calculated from reaction cross-sections, are also included. The data are available from the Nuclear Data Section online via INTERNET by FTP command, or on magnetic tape upon request.

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usernames: ANONYMOUS for FTP file transfer;
FENDL2 for FTP file transfer of FENDL-2.0;
RIPL for FTP file transfer of RIPL
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FENDL/C-2.0

Charged-Particle Reaction Data Library for Fusion Applications
Version 1.0 of March 1997

Data extracted from ENDF/B-6 evaluations
by R.M. White and D.A. Resler, LLNL
and G.M. Hale, LANL

The library FENDL/C-2.0, which is a sublibrary of the improved nuclear data library for fusion applications FENDL-2, contains integrated charged-particle cross-section evaluations and processed data for the following energy-producing fusion gas reactions:

1-H-2(d,n)2-He-3
1-H-2(d,p)1-H-3
2-He-3(d,p)2-He-4
1-H-3(t,2n)2-He-4
1-H-3(d,n)2-He-4

according to the recommendation of the IAEA Advisory Group Meeting on "FENDL-2 and Associated Benchmark Calculations", held in Vienna from 18 to 22 November 1991 [Ref. 1].

Integrated Cross-Section evaluations

The ENDF/B-6 data for the first four deuteron and triton reactions, which were evaluated and compiled by R.M. White and D.A. Resler at the Lawrence Livermore National Laboratory, USA, have been taken over unmodified from the previous version FENDL/C-1.0 [Ref. 2]. The data for the last mentioned 1-H-3(d,n)2-He-4 reaction, compiled and evaluated by G.M. Hale, Los Alamos National Laboratory, USA, and M. Drosg, Vienna University, have been recommended for acception at the IAEA Advisory Group Meeting on "Completion of Fendl-1 and Start of Fendl-2", Del Mar, USA, 5-9 December 1995 [Ref. 3]. These data have been provided to IAEA/NDS by G.M. Hale, February 1997. The commentary sections of the data files (MF=1) include compilations of experimental data by various authors. The data are in ENDF-6 format [Ref. 4].

The FENDL2 subdirectory: [.FUSION.FENDLC]

Contains the following data files and reactions:

a. CPND21.dat, 303 blocks or about 155 kB (1 block = 512 bytes):

1-H-2(d,n)2-He-3	(MF=3, **MT**=50 or MT=4)
1-H-2(d,p)1-H-3	(MF=3, **MT**=103)
2-He-3(d,p)2-He-4	(MF=3, **MT**=103)

Note: In the numerical section MT=4 has been used for the (d,n) reaction, although explanatory section gives MT=50.

CPND22.dat, 74 blocks or. 37.9 kB:

1-H-3(t,2n)2-He-4 (MF=3, MT=16)

b. DTXS.dat, 159 blocks or 81.4 kB

1-H-3(d,n)2-He-4 (MF=3, MT=50 or MT=4)

Processed cross sections

Following the recommendation of the above mentioned IAEA Advisory Group Meeting on "FENDL-2 and Associated Benchmark Calculations", the library FENDL/C-2.0 also contains the data for above mentioned reactions in the processed form, i.e. Maxwellian-averaged reaction rates and related quantities, calculated from the FENDL/C-2.0 pointwise cross sections in ENDF/6 format. The processed information is available in the subdirectory: [.FUSION.PROCESSED].

The data file TDF.new (128 blocks or 65.5 kB) contains the processed data for the first four reactions, which have been generated by the authors of the evaluations, and are taken over from the Livermore Thermonuclear Data File, TDF.dat.

The cross sections for the H-3(d,n)He-4 reaction have been processed by G.M. Hale and are presented in a separate file DT.dat (63 blocks or 32.3 kB).

Utility routines to read the processed data are present in the file TDFLIB.

Description of contents and format [Ref. 5]

The files TDF.DAT and DT.DAT begin by listing, in sections (2)-(4), the physical constants used, and properties (nuclear masses, Q-value, etc.) for the particles participating in the reaction. Then follows a tabulation, in section (5), of $\langle\sigma v\rangle$ values (in bcm/s) vs. temperature (kT, in MeV). The last column in that tabulation (labeled "EXTR") is the average total incoming energy (in MeV) at each temperature, given by $\langle E_{tot}\sigma v\rangle/\langle\sigma v\rangle$. The next part of the file gives tabulations of the Maxwellian-averaged spectrum in the laboratory system for each of the outgoing particles, as a function of temperature. The temperatures in this part of the file apparently do not have to be same as those given in the $\langle\sigma v\rangle$ tabulation. Section (6) lists values at which the spectrum is "cut" (given as the fractions of the maximum value) in order to determine the energies at which the spectrum is tabulated. Since each cut projects on two energies, in addition to the maximum, there are 2*N+1 energies tabulated for N cuts (labeled "SPECTRUM LEVELS"). Line (7) gives for each temperature the outgoing-particle number and the number of laboratory energies at which the spectrum is tabulated. "AREA" is the numerical integral of the spectrum over energy (which should be unity), scaled by the value of $\langle\sigma v\rangle$ at that temperature, "SIGVB". The spectrum follows in section (8). At each outgoing-particle laboratory energy (in MeV) the "SPECTRUM" (in 1/MeV) is tabulated. This is given by the expression:

$$\langle dN / dE \rangle = \frac{\sqrt{2}}{p} \frac{M'^{3/2}}{\sqrt{m_1 m_2 m_3 m_4}} \int_0^\infty \frac{de}{(kT)^2} \frac{e\, s(e)}{\sqrt{e+Q}} \left[\exp(-J^-) - \exp(-J^+) \right]$$

with

$$J^\pm = \frac{e}{(kT)} + \frac{M'}{(Mm_3 kT)} \left[\sqrt{M'E} \pm \sqrt{m_4 (e+Q)} \right]^2$$

and M = m_1+m_2 = total mass, incident

MN = m3+m4 = total mass, exit

$e = \frac{1}{2} \frac{m_1 m_2}{m_1 + m_2} v^2$ = relative incoming energy,

E = outgoing lab energy, Q=reaction Q-value

This expression was first derived by Talley and Hale in their contribution to the 1988 Mito Nuclear Data Conference [Ref. 2]. The final column in this tabulation, labeled "INTEGRAL" gives the partial integral of the spectrum from E=0 to the tabulated energy for energies up to the maximum of the spectrum. For energies above the maximum, the definition switches to the partial integral from E=4 to the tabulated value, so that those contributions are negative. These partial integrals correspond to unit normalization of the spectrum over all energies, as was mentioned above. Sections (7) and (8) are repeated for all outgoing particles at each temperature in the spectrum grid.

The following comments apply only to the LANL contribution in the data file for the d+t reaction: A temperature grid has been chosen for the <σv> tabulation that is constant in log(kT), giving (the same) 10 points per decade in the tabulated range 10^{-4} MeV to 1 MeV. The spectra are tabulated at every second one of these temperatures, making their grid a subset of the <σv> grid.

The "SPECTRUM LEVELS" (cuts) in the tabulation are only approximate, since this prescription has not be used to establish the outgoing-particle energy grid. The grid is chosen to be constant in $\sqrt{E}$, with 5 points on either side of the energy of the spectral maximum. The quantities "AREA" and "INTEGRAL" were computed analytically between the tabulated energies, using the functional form

$$\langle dN / dE \rangle = A\sqrt{E} \exp\left[-\frac{\left(\sqrt{E-B}\right)^2}{C} \right]$$

to give 3-point interpolation in each interval, and also to extrapolate above and below the range of the tables. The accuracy obtained for these integrals indicates that this functional form is suitable for interpolating and extrapolating the table entries for the spectra.

References

[1] IAEA Advisory Group Meeting on "FENDL-2 and Associated benchmark Calculations", Vienna, Austria, November 1991. Summary report prepared by A.B. Pashchenko and D.W. Muir, and published as report INDC(NDS)-260, 1992.

[2] R.M. White and D.A. Resler, "FENDL/C-1.0, Charged-particle reaction data library for fusion applications", Summary documentation by A.B. Pashchenko, report IAEA-NDS-166, (International Atomic Energy Agency, Jan. 1995).

[3] IAEA Advisory Group Meeting on "Completion of FENDL-1 and Start of FENDL-2", Del Mar, California, USA, 5-9 December 1995. Summary report prepared by A.B. Pashchenko and published as report INDC(NDS)-352, March 1996.

[4] P.F. Rose (Editor), "ENDF-6 Summary Documentation", 4th Edition of BNL-NCS-17541(=ENDF-201) (October 1991), U.S. National Nuclear Data Center, Brookhaven National Laboratory, Upton, N.Y., USA. The IAEA documentation is presented in "ENDF-6 - The U.S. Evaluated Nuclear data Library for Neutron Reaction Data by the U.S. National Nuclear Data Center including revisions up to June 1993", IAEA-NDS-100, Rev. 6, June 1995.

[5] G.M. Hale, private communication, 29 January 1997.

[6] T.L. Talley, G.M. Hale, Proceedings of the International Conference on Nuclear Data for Science and Technology, Mito, Japan, May/June 1988, pp. 299-302.

Status of evaluations

The status of the important energy-producing charged-particle reactions for fusion applications was discussed at the IAEA Consultants' Meeting hosted in October 1992 by the U.S. Brookhaven National Laboratory, (see INDS(NDS)-268 document) and at the IAEA Specialists' Meeting held in April 1994 at the Smolenice Castle, Slovakia (see INDC(NDS)-306).

It was concluded at the Brookhaven Meeting that the three sets of integrated cross-sections evaluated at Arzamas, Russia, at Los Alamos and Livermore, USA, are, in general, in a good agreement. However, a difference exists in the low-energy cross section for T(d,n)He-4 reaction. This difference is about four percent, which is larger than the uncertainty assigned to this cross-section by the evaluators. Both, the Brookhaven and Smolenice meetings recommended that the ENDF/B-6 charged-particle sublibrary be adopted for the FENDL project and that the current low-energy difference of ~ 4% in the T(d,n)He-4 reaction be investigated by evaluators from Arzamas, Livermore, Los Alamos, and Vienna, so that it can be resolved. The jointly agreed-upon evaluation (Los Alamos-Vienna/Livermore/Arzamas) will be accepted for FENDL-2.0 to replace previous one.

Attachment

DISTRIBUTION OF THE FENDL2 LIBRARY

(As recommended at the IAEA Advisory Group Meeting on FENDL,
held at IAEA Headquarters, Vienna, Austria, March 1997.)

The master copy of the FENDL-2 library resides with the Nuclear Data Section of the International Atomic Energy Agency. To facilitate user access to the library the official copy of FENDL-2 will be distributed in XXX to the major nuclear data centres in Europe (NEA Data Bank, Paris), Japan (JNDC, Tokai-mura), Russia (CJD,Obninsk) and USA (NNDC, Brookhaven and RSIC, Oak Ridge). As agreed between data centers, sharing common FENDL information, the recipients are receiving now the same products from all above centers. The data are available and may be further distributed to the user community according to the customer service options given below. Each FENDL sub-library will be in a single data set, i.e. Activation, Decay, etc. in the 8 mm tape, 6 mm tape, 4 mm tape or standard 9 track magnetic tape (6250 bpi or 1600 bpi) and CD-ROM options. The interested scientists may request FENDL-2 (or parts of it) directly from the IAEA/NDS or from one of these centers.

FENDL CUSTOMER SERVICE OPTIONS

MEDIA	FORMAT	By WHOM
Electronic	FTP	IAEA, NEADB, NNDC
4 mm tape	UNIX TAR	CJD, IAEA, NEADB, NNDC, RSIC
	VAX BACKUP	CJD, IAEA, NEADB, NNDC
	ASCII	NEADB
6 mm tape	UNIX TAR	NEADB
	VAX BACKUP	NEADB
	ASCII	NEADB
8 mm tape	UNIX TAR	NEADB, NNDC, RSIC
	VAX BACKUP	NEADB, NNDC
	ASCII	NEADB
9 track	ASCII	CJD, IAEA
	EBCDIC	CJD, IAEA
CD-ROM	UNIX TAR	RSIC
	ASCII	NEADB

Table notes

1) NNDC will distribute FENDL unprocessed data
2) RSIC will distribute FENDL processed data
3) RSIC offers cost free service to ITER customers