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Update of the Evaluated Neutron Cross Section Libraries for the Geant4 Code

(see also INDC(NDS)-0612)

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June 2018

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ABSTRACT

The list of evaluated neutron data libraries in Geant4 format distributed by the IAEA nuclear data service has been updated with six new releases: JEFF-3.3, JEFF-3.2, ENDF/B-VIII.0, ENDF/B-VII.1, BROND-3.1 and JENDL-4.0u (version 2016/1/6). In this report we provide some information concerning the transformation of these six new releases from the ENDF-6 data format into the Geant4 format. In addition, we present a comparison between results obtained with Geant4 and MCNP6 when using these libraries.

June 2018

Contents

1 INTRODUCTION

The so-called High Precision neutron physics model implemented in the Geant4 [1] simulation package allows simulating the transport of neutrons with energies up to 20 MeV. It relies on the G4NDL cross section libraries, prepared by the Geant4 collaboration from evaluated cross section files, originally written in ENDF-6 format [2], and distributed freely together with the code. In order to have more flexibility when performing Monte Carlo simulations we developed a tool for transforming any ENDF-6 format evaluated neutron cross section library into the G4NDL format [3]. In 2012, eight different releases of the ENDF, JEFF, JENDL, CENDL and BROND libraries were translated into the G4NDL format and distributed by the IAEA Nuclear Data Services [4]. Since then, new releases of these libraries have appeared. For this reason, we have updated the list of G4NDL distributed libraries with six new releases, which are: JEFF-3.3 [5], JEFF-3.2 [6], ENDF/B-VIII.0 [7], ENDF/B-VII.1 [8], BROND-3.1 [9] and JENDL-4.0u [10] (version 2016/1/6 [11]).

In this report we provide some information concerning the conversion process of these six new releases into the G4NDL format. In addition, we present a comparison between results obtained with Geant4 and MCNP6 when using these libraries.

2 PRODUCTION OF THE LIBRARIES

The new libraries were produced in a similar way as the older releases, but using PREPRO-2017 [12] instead of PREPRO-2010.

The cross sections used in Geant4 files have to appear in a linear interpolable form. For this reason, it was necessary to pre-process the ENDF-6 format libraries, since the cross section data are given in files MF=2 (resonance parameters) and MF=3 (data points). It was necessary to transform the MF=3 file (which can be expressed also in log-log or linear-log interpolation laws) into a linear-linear interpolable form, and then add the contribution of file MF=2 to file MF=3.

The procedure was performed with the PREPRO software package, a collection of public and standard computing codes distributed by the IAEA which allow converting the ENDF-6 libraries into a form required by many applications. The production scheme used is as follows:

1. First the LINEAR program was applied, in order to change the cross-section data points in file MF=3 into linear-linear interpolation form. The allowable error was set to 0.1%.
2. Then the RECENT program was applied, in order to convert the resonance contribution into cross section data points. The allowable error was set to 0.1%.
3. Then the LINEAR program was applied again, in order to reduce the number of cross section points in file MF=3. The allowable error was set to 1%, since an error smaller than 1% leads to an excessively large number of points (>500.000) for some cross sections.

4. Then the FIXUP program was applied. It reads the ENDF-6 file and performs some format corrections, if needed.
5. Finally the DICTIN program was applied, in order to update the section index in MF=1, MT=451.

Once the ENDF-6 data file is processed with PREPRO, the result (still in ENDF-6 format) is translated with a specific program developed by the authors into the G4NDL data format.

Some specific issues which appeared when creating the libraries are the following:

a) JEFF-3.3:
   - ^{9}Be: secondary neutrons of reaction (n,2n) are described with reaction types MT=875 to MT=891 instead of MT=16. Geant4 is not able to read such data in this format, therefore reaction (n,2n) has been replaced with the (n,2n) appearing in JEFF-3.0, which uses MT=16.
   - ^{232}Th, ^{231,233}Pa: MF=6 data (product energy-angle distributions) for MT=18 (fission) has been converted to MF=4,5,12,14,15 with the PREPRO SIXPAK program before the translation into the G4NDL format, since Geant4 is not able to read such data in MF=6 format.

b) JEFF-3.2:
   - ^{9}Be: secondary neutrons of reaction (n,2n) are described with reaction types MT=875 to MT=891 instead of MT=16. Geant4 is not able to read such data in this format, therefore reaction (n,2n) has been replaced with the (n,2n) appearing in JEFF-3.0, which uses MT=16.
   - ^{46,47,48,49,50}Ti: there is a bug in the ENDF-6 format library in the gamma ray emission after neutron capture. The bug has been corrected by editing the file "by hand".
   - ^{232}Th, ^{231,233}Pa: MF=6 data (product energy-angle distributions) for MT=18 (fission) has been converted to MF=4,5,12,14,15 with the PREPRO SIXPAK program before the translation into the G4NDL format, since Geant4 is not able to read such data in MF=6 format.

c) ENDF/B-VIII.0:
   - ^{232}Th, ^{231,233}Pa: MF=6 data (product energy-angle distributions) for MT=18 (fission) has been converted to MF=4,5,12,14,15 with the PREPRO SIXPAK program before the translation into the G4NDL format, since Geant4 is not able to read such data in MF=6 format.

d) ENDF/B-VII.1:
   - ^{232}Th, ^{231,233}Pa: MF=6 data (product energy-angle distributions) for MT=18 (fission) has been converted to MF=4,5,12,14,15 with the PREPRO SIXPAK program before the translation into the G4NDL format, since Geant4 is not able to read such data in MF=6 format.
   - ^{241,243}Am: MF=5, MT=18 (energy distribution of fission neutrons) are described with LF=12 (energy dependent Madland-Nix spectrum). Geant4 has some problems with this LF=12 energy distribution law so the data were converted to LF=1

(arbitrary tabulated function) with the PREPRO SPECTRA program before the translation into the G4NDL format.

e) BROND-3.1:
- ^{240}Pu: MF=6 data (product energy-angle distributions) for MT=18 (fission) has been converted to MF=4,5,12,14,15 with the PREPRO SIXPAK program before the translation into the G4NDL format, since Geant4 is not able to read such data in MF=6 format.
- ^{241,243}Am, ^{243,244}Cm: MF=5, MT=18 (energy distribution of fission neutrons) are described with LF=12 (energy dependent Madland-Nix spectrum). Geant4 have some problems with this LF=12 energy distribution law so the data was converted to LF=1 (arbitrary tabulated function) with the PREPRO SPECTRA program before the translation into the G4NDL format.

f) JENDL-4.0u:
- No issue to be mentioned.

3 COMPARISON WITH MCNP6

We have verified the integrity of the new G4NDL libraries by performing identical simulations with Geant4 and MCNP6. These simulations are the ones described in [3] (Section III.B.1). The geometry of the simulations consists in a 2 m long cylinder with a radius of 1 µm made of an isotopically pure material with density 1 g/cm^3. The source consists of neutrons isolethargically distributed with energies ranging from 10^{-10} to 19 MeV impinging on the center of the cylinder along its symmetry axis. The small cylinder radius allows to simulate one neutron interaction per event and the secondary particles to leave the cylinder without suffering almost any interaction. The energies and angles of the secondary neutrons, gamma-rays, protons, deuterons, tritons, ^{3}He and alphas are stored in 2-dimensional histograms, one per secondary particle type. The results obtained with these simulations depend on all the partial cross sections and probability distributions present in the libraries.

Two simulations were performed for each isotope present in each of the six converted libraries: one using Geant4 (version geant4.10.04.p01), with 10^7 source neutrons, and the other using MCNP6, with 10^8 source neutrons. In Geant4 the environmental variable "G4NEUTRONHP_DO_NOT_ADJUST_FINAL_STATE" was defined, and in MCNP6 the unresolved resonance range probability table treatment was turned off. These two physics options make the results obtained more comparable with both codes.

An example of the obtained results is presented in Fig. 1, where we present the projection in energies of the 2-dimensional histogram of the secondary neutrons for ^{16}O as the cylinder material (ZA=1000·Z+A=8016). In both Geant4 and MCNP6 simulations the JEFF-3.3 library was used. In this case both results are in good agreement above 1 eV. Discrepancies below 1 eV are due to differences in the thermal treatment of the codes. A similar discrepancy below 1 eV is obtained for all nuclei without large absorption cross sections at low neutron energies, with the exception of ^{1}H where the results obtained with both codes are in agreement.

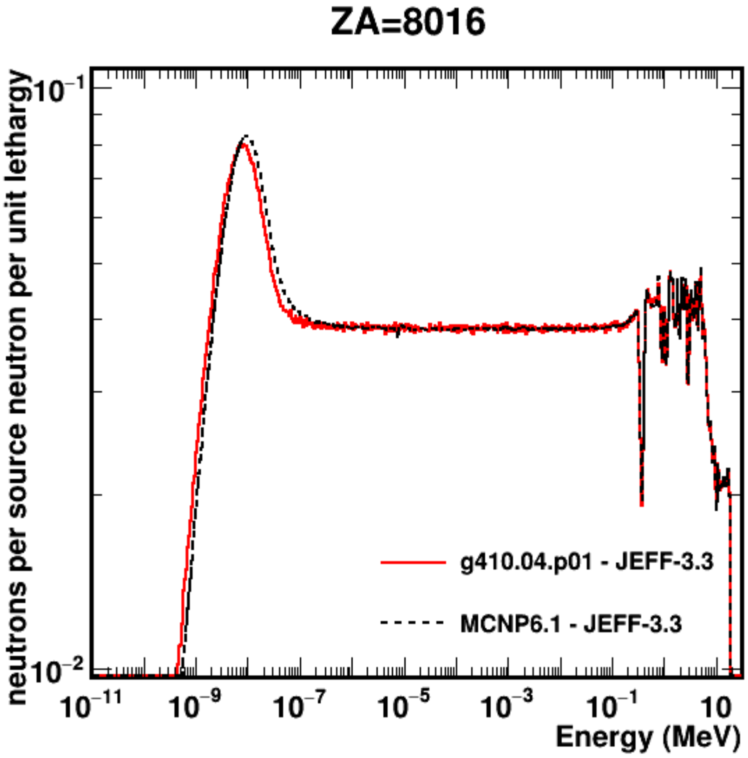

FIG. 1. Energy distributions integrated over all angles of the secondary neutrons obtained with Geant4 and with MCNP6 for ^{16}O (see the text for more details).

The systematic comparison between the results obtained with both codes allow to check the integrity of the G4NDL converted data libraries (the specific issues reported in Section 2 were found after performing these comparisons). It also allows to detect bugs in the Geant4 code. This can be done (and has been done in the past [3]) by identifying in which nuclei there are discrepancies. Then, the format defining the relevant probability distributions for those nuclei is identified. This allows to locate the parts of the code which should be corrected, which are the parts which manage these probability distributions.

In order to quantify the differences in the neutron transport obtained with both codes we have systematically compared the energy distributions integrated over all angles of the secondary neutrons obtained with Geant4 and with MCNP6, i.e. the projection in energies of the 2-dimensional histogram of the secondary neutrons (Fig. 1). This comparison has been performed by computing three different variables for each nuclei of each library, d_1, d_2 and χ^2_{υ}, defined as:

$$d_1 = \frac{1}{N} \sum_{E_i > 1\ eV} \frac{\left|x_i^G - x_i^M\right|}{\frac{1}{2}\left(x_i^G + x_i^M\right)}$$

$$d_2 = \frac{1}{N} \sum_{E_i > 1\ eV, \sigma_i < 1\%} \frac{\left|x_i^G - x_i^M\right|}{\frac{1}{2}\left(x_i^G + x_i^M\right)}$$

$$\chi_{v}^{2}=\frac{1}{N}\sum_{E_i>1\ eV}\left(\frac{x_i^G-x_i^M}{\sigma_i}\right)^2$$

where x_i^G and x_i^M are, respectively, the contents of the i bin of the Geant4 and MCNP6 histograms; σ_i are the uncertainty of the i bin due to counting statistics, computed as the square root of the quadratic sum of the uncertainties in x_i^G and x_i^M; and N is the number of bins considered in the sum. All three variables have been computed for energies above 1 eV, due to the different thermal treatment of the codes mentioned above. d_1 is the average difference between the bin contents. Part of this difference is due to counting statistics, so we defined d_2 same as d_1 but only bins with uncertainties below 1% are considered. χ_v^2 is the reduced chi-squared between both results, and measures the difference between the results in terms of their uncertainties. Note then that a large value of χ_v^2 does not mean a large difference in the obtained results, but a large difference compared with the achieved uncertainties due to counting statistics, which can be reduced by simulating more source neutrons. Indeed, the χ_v^2 is expected to diverge to infinity as the number of source neutrons used in the simulation increases, since the results obtained with both codes are not expected to be exactly the same.

The histogrammed values of d_1, d_2 and χ_v^2 are presented in Figs 5-10 for all the isotopes (but the isomers) present in each of the six transformed libraries. The results are presented in both linear and logarithmic Y axis. Values of d_1 and d_2 greater than 5% have been set to 5%, and χ_v^2 values greater than 5 have been set to 5, for convenience in the representation.

One important note is that in the case of the JENDL library we did not use exactly the same release in MCNP6 (JENDL-4.0, the first release, in 2010) than in Geant4 (JENDL-4.0u version 2016, an updated release). The changes in JENDL-4.0u with respect to JENDL-4.0 are listed in [13].

The results of the simulations performed with both codes deviate less than a few percent in most of the cases. Results with d_1 or d_2 larger than 5% are listed in Table 1. The origin of the discrepancies in ^{135}Cs in JEFF-3.3 has not been identified but the problem seems to be in the MCNP6 result. The results obtained for ^{7}Be in ENDF/B-VII.1 and ^{233}Pa in BROND-3.1 differ significantly, but we did not identify the reason. ^{231}Th in BROND-3.1 appear with a negative elastic cross section at low neutron energies. The differences in the two JENDL isotopes are due to updates in the JENDL library.

TABLE 1. NUCLEI WITH d_1 OR d_2 LARGER THAN 5%, TOGETHER WITH d_1, d_2 AND χ_v^2.

ZA - LIB	d_1	d_2	χ_v^2
55135 – JEFF-3.3	4.04	6.98	122
4007 – ENDF/B-VII.1	5.99	-	33.2
90231 – BROND-3.1	14.4	2.63	20.8
91233 – BROND-3.1	6.96	14.0	134
5010 – JENDL-4.0u	8.69	-	4.58
63156 – JENDL-4.0u	24.1	0.71	626

Other nuclei with smaller but significant discrepancies (isotopes with $\chi_v^2 > 2$ and $d_2 > 1.5\%$) are listed in Table 3 to Table 8. These two conditions in χ_v^2 and d_2 are arbitrary, but we have adopted them to list the discrepant nuclei after testing various types of conditions. The amount and the fraction of isotopes which fulfill these conditions are given in Table 2.

TABLE 2. NUMBER OF ISOTOPES OF EACH OF THE SIX CONVERTED LIBRARIES, TOGETHER WITH THE AMOUNT OF ISOTOPES WITH $\chi_v^2 > 2$ AND $d_2 > 1.5\%$. THE NUMBER OF ISOTOPES TESTED IS NOT THE SAME AS THE TOTAL NUMBER OF ISOTOPES IN EACH LIBRARY SINCE WE DIDN'T TEST THE ISOMERS.

Library	Total number of isotopes	Number of isotopes tested	Number of isotopes with $\chi_v^2 > 2$ and $d_2 > 1.5\%$	Fraction of isotopes with $\chi_v^2 > 2$ and $d_2 > 1.5\%$	Number of isotopes with $\chi_v^2 > 2$	Fraction of isotopes with $\chi_v^2 > 2$
JEFF-3.3	562	546	34	6%	51	9%
JEFF-3.2	472	460	52	11%	78	17%
ENDF/B-VIII.0	556	533	84	16%	114	21%
ENDF/B-VII.1	423	411	90	22%	120	29%
BROND-3.1	372	361	64	18%	78	22%
JENDL-4.0u	406	398	58	15%	87	22%

An example of a good agreement between both simulated results has been presented in 0Fig. 1. In that case $d_1 = 0.9\%$, $d_2 = 0.8\%$ and $\chi_v^2 = 1.4$. Two examples with $\chi_v^2 > 2$ and $d_2 > 1.5\%$ are shown in Fig. 2 (^{138}Ba) and Fig. 3 (^{245}Cm). The discrepancies found for the actinides listed in Table 3 to Table 8 are similar to the one presented in Fig. 3 for ^{245}Cm. This suggests that there could be some bug in Geant4 affecting the energy of the fission neutrons. These discrepancies are not found in all the fission nuclei. As an example, the results obtained for ^{235}U with JEFF-3.3 are provided in Fig. 4.

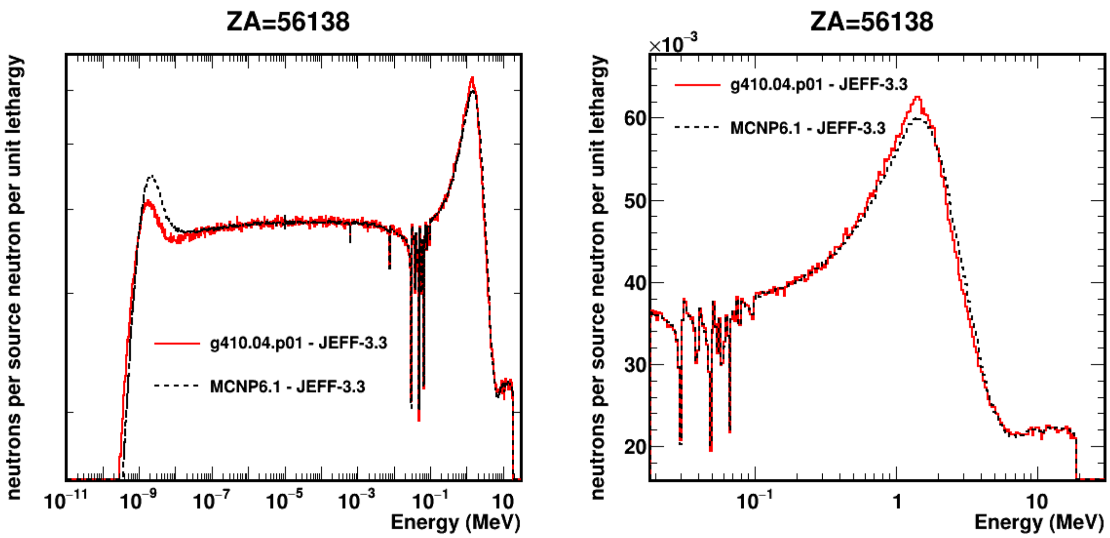

FIG. 2. *Energy distributions integrated over all angles of the secondary neutrons obtained with Geant4 and with MCNP6 using JEFF-3.3 for* ^{138}*Ba (see the text for more details). The right panel is a zoom of the left panel. In this case* $d_1 = 1.13\%$, $d_2 = 1.64\%$ *and* $\chi_v^2 = 2.9$.

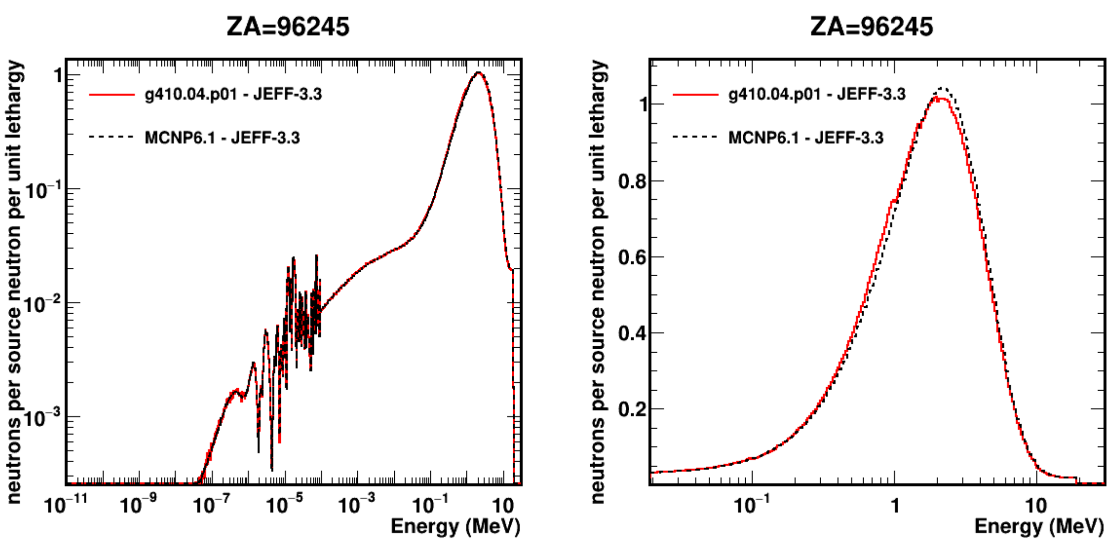

FIG. 3. *Energy distributions integrated over all angles of the secondary neutrons obtained with Geant4 and with MCNP6 using JEFF-3.3 for* ^{245}*Cm (see the text for more details). The right panel is a zoom of the left panel. In this case* $d_1 = 2.81\%$, $d_2 = 3.74\%$ *and* $\chi_v^2 = 72$.

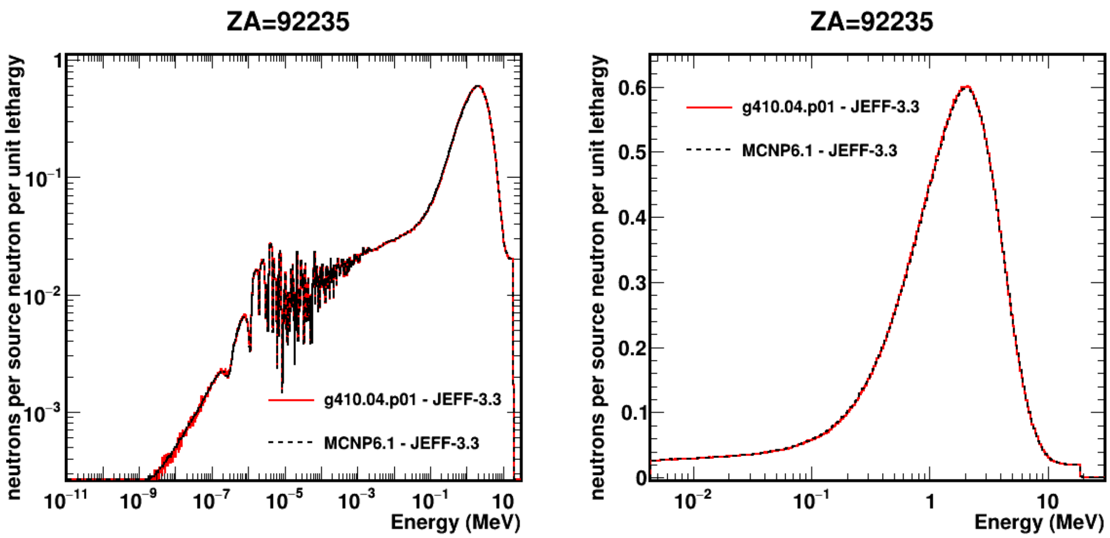

FIG. 4. Energy distributions integrated over all angles of the secondary neutrons obtained with Geant4 and with MCNP6 using JEFF-3.3 for ^{235}U (see the text for more details). The right panel is a zoom of the left panel. In this case $d_1 = 1.80\%$, $d_2 = 1.13\%$ and $\chi_v^2 = 3.2$.

The full set of plots of the energy distributions integrated over all angles of the secondary neutrons obtained with both codes (i.e. similar to the ones presented in Figs 1-4) are available in the IAEA Nuclear Data Services [4] together with the libraries. In addition, similar plots, but with the energy distributions of secondary protons, deuterons, tritons, ^{3}He, alphas and γ-rays, are also provided. There is one plot for each of the mentioned secondary particles, for each nucleus (but the isomers) present in the six distributed libraries.

In the case of secondary particles different from neutrons, we didn't make a systematic comparison between Geant4 and MCNP6 with d_1, d_2 and χ_v^2 similar to the one performed with neutrons and described in this report. This is because in this case the comparison is not so straightforward. In the ENDF-6 format libraries the energy and angles of the secondary neutrons are always provided, but for the rest of the secondary particles these distributions are sometimes omitted. Where they are omitted, Geant4 will use a model to generate them whereas MCNP6 will not produce them.

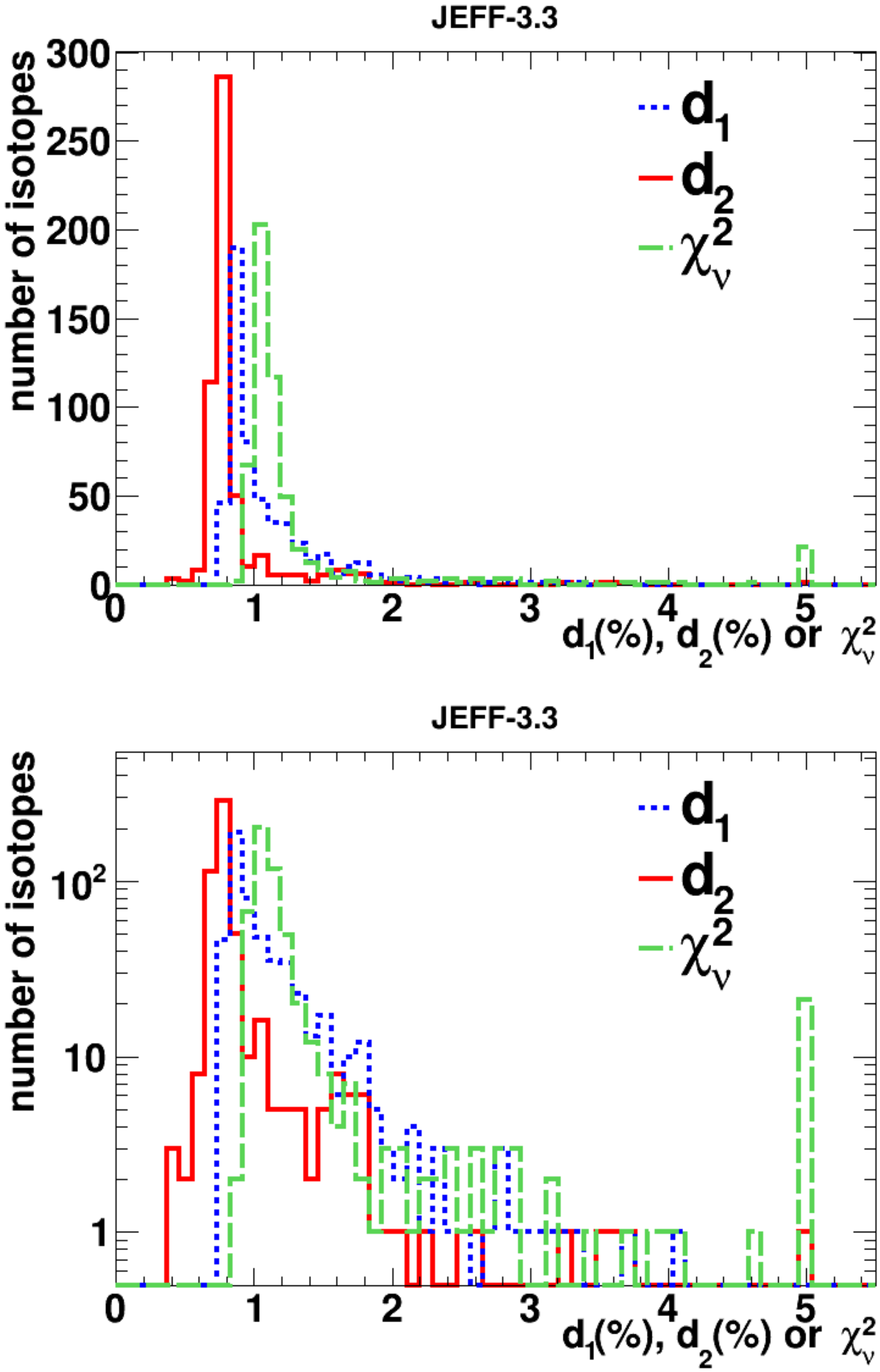

FIG. 5. Number of isotopes with different values of d_1, d_2 and χ_v^2 obtained with JEFF-3.3.

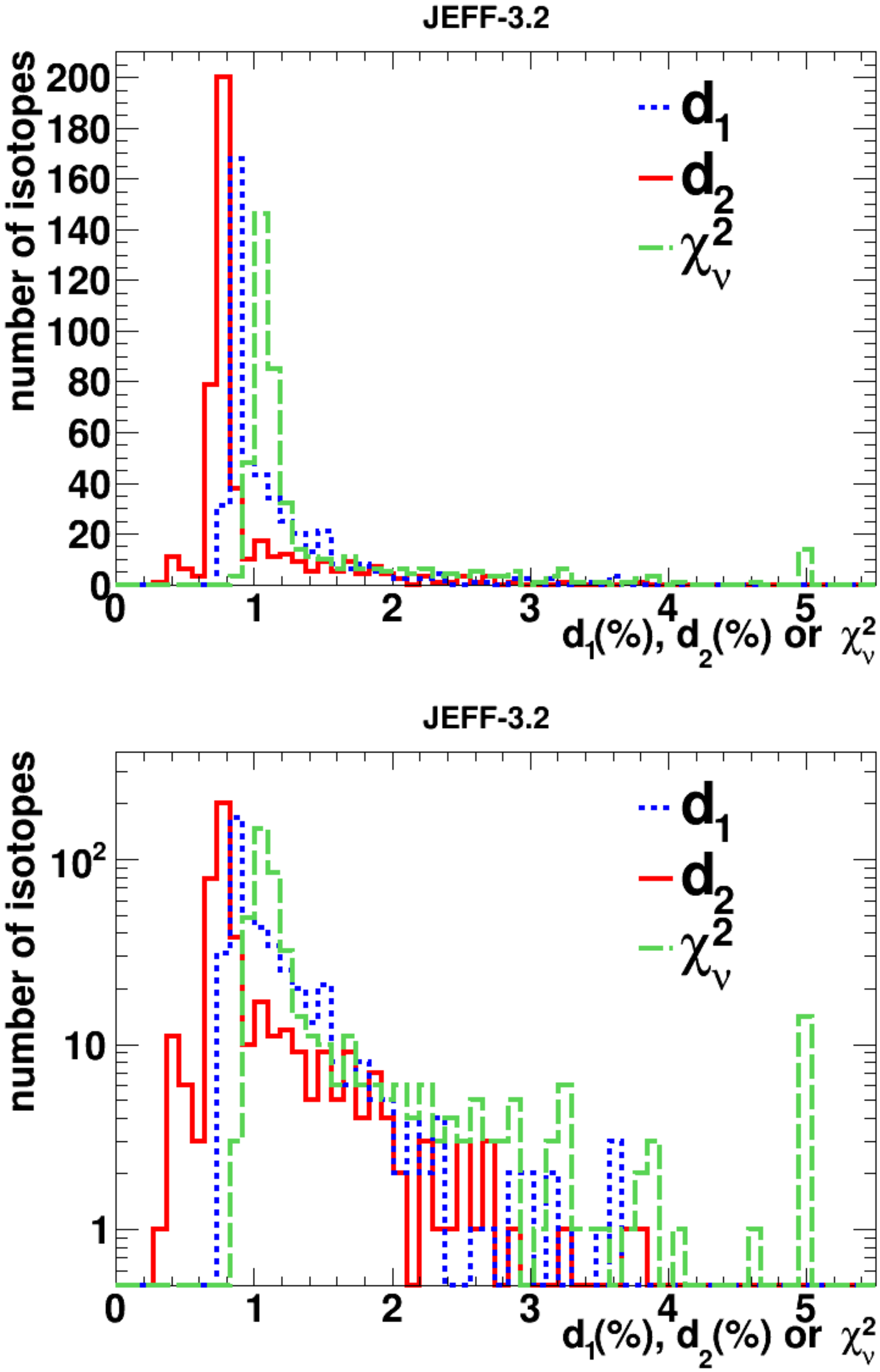

FIG. 6. Number of isotopes with different values of d_1, d_2 and χ_υ^2 obtained with JEFF-3.2.

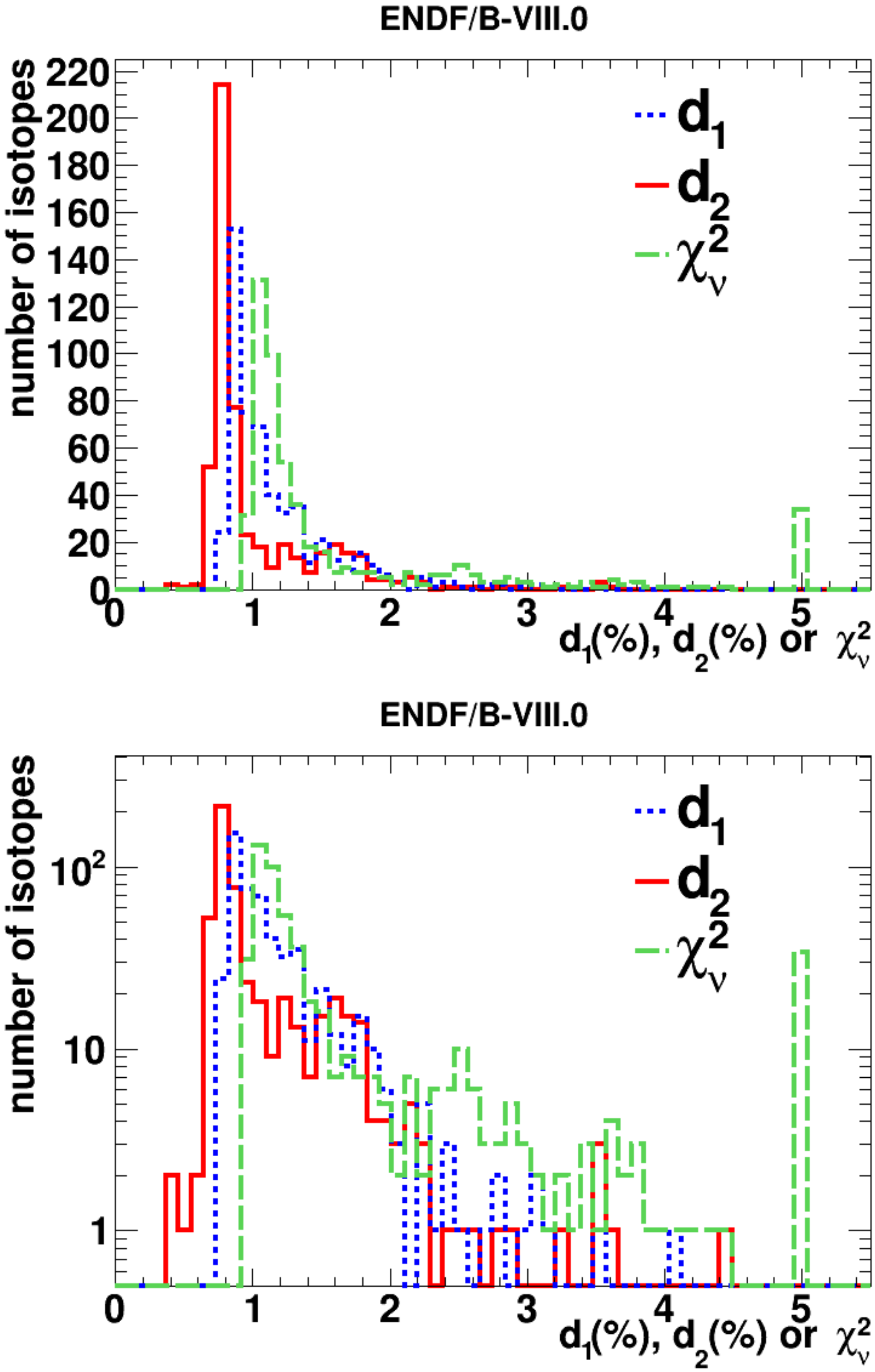

FIG. 7. Number of isotopes with different values of d_1, d_2 and χ^2_υ obtained with ENDF/B-VIII.0.

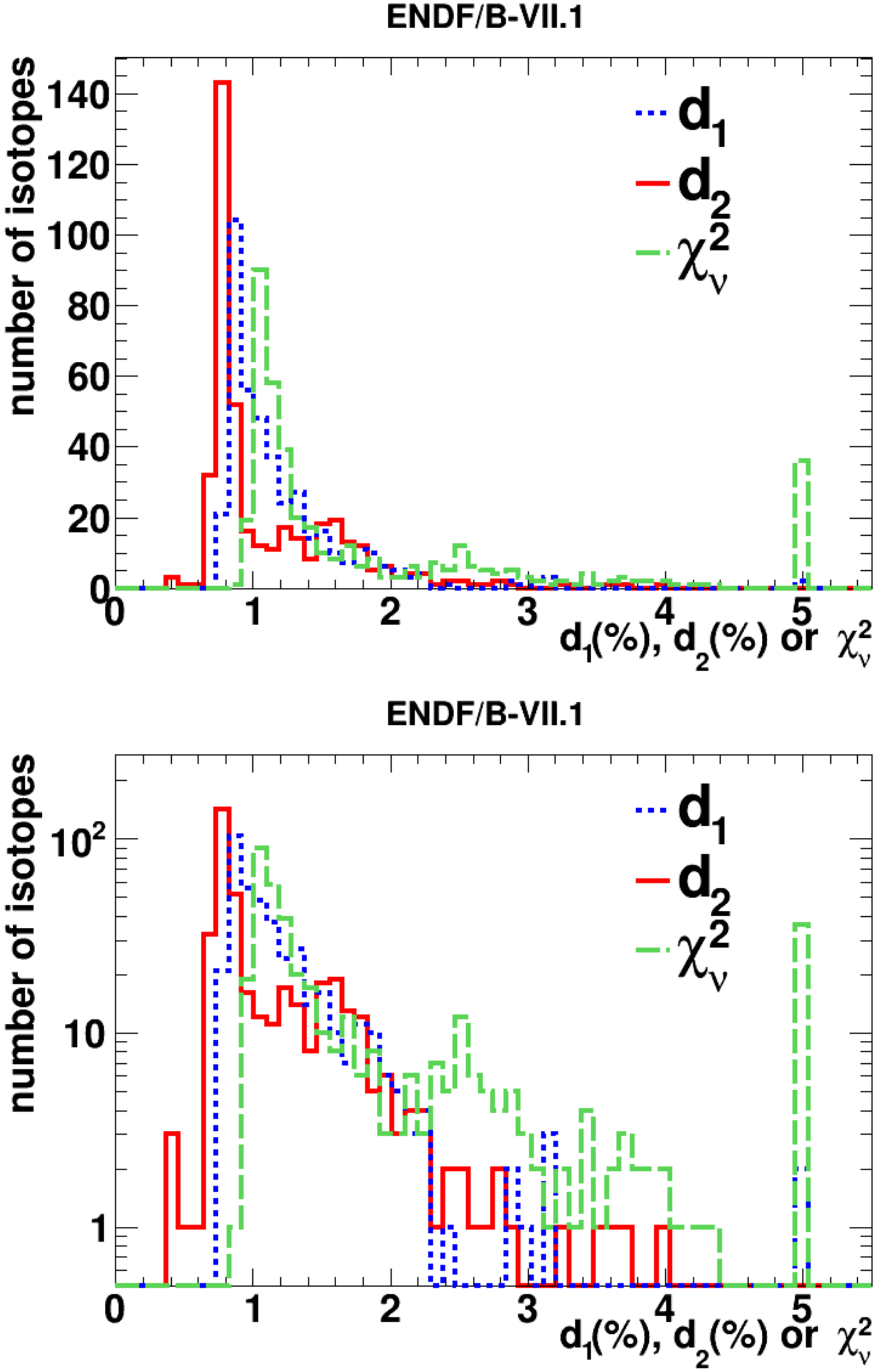

FIG.8. Number of isotopes with different values of d_1, d_2 and χ^2_ν obtained with ENDF/B-VII.1.

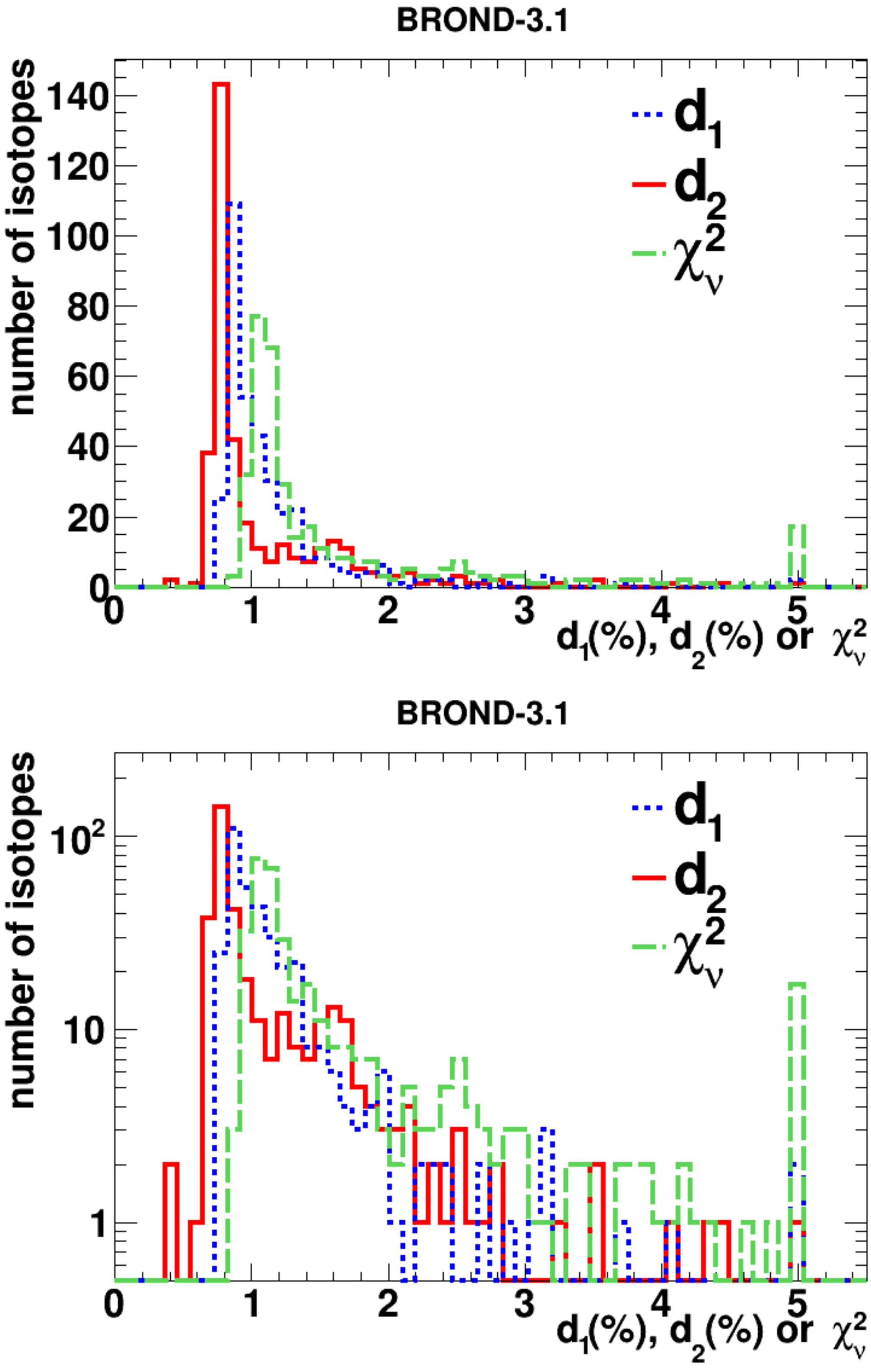

FIG. 9. Number of isotopes with different values of d_1, d_2 and χ^2_ν obtained with BROND-3.1.

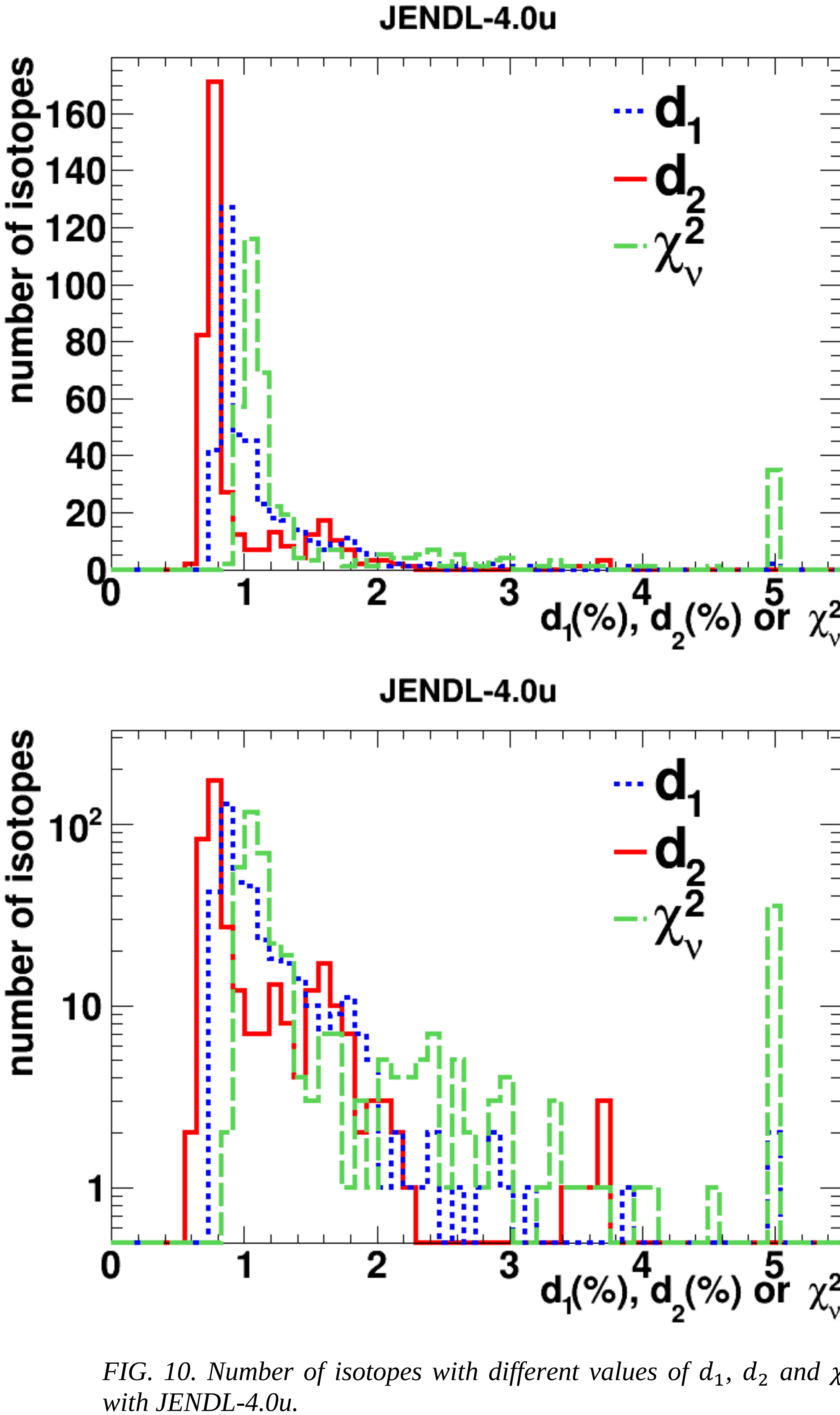

FIG. 10. Number of isotopes with different values of d_1, d_2 and χ_υ^2 obtained with JENDL-4.0u.

TABLE 3. NUCLEI FROM JEFF-3.3 WITH $\chi_v^2 > 2$ AND $d_2 > 1.5$, TOGETHER WITH d_1, d_2 AND χ_v^2.

ZA	d_1(%)	d_2(%)	χ_v^2
46107	1.22	1.64	2.41
53131	1.30	1.81	2.80
55135	4.04	6.98	122
56130	1.16	1.80	2.05
56132	1.18	1.89	2.39
56134	1.14	1.70	2.23
56135	1.24	1.95	2.62
56136	1.14	1.69	2.60
56137	1.10	1.75	2.34
56138	1.13	1.64	2.88
59143	1.26	1.61	3.13
61147	1.55	2.48	3.94
61148	2.36	3.22	6.18
63151	2.18	2.63	3.68
63154	1.97	1.58	2.19
91231	2.00	2.26	4.11
91232	1.76	1.56	5.94
92232	1.49	1.51	5.28
92233	2.77	3.56	51.7
93236	1.95	1.56	7.32
94236	1.90	1.76	9.18
94241	1.73	1.55	7.29
95242	2.18	1.79	18.3
95244	1.73	1.58	6.72
96241	1.83	1.73	10.3
96242	1.62	2.07	7.55
96243	3.29	3.67	64.5
96245	2.81	3.74	72.4
96247	1.87	1.62	8.85
96249	1.72	1.68	8.92
98249	1.74	1.67	9.87
98253	1.87	1.59	9.27
99254	2.29	1.73	12.1
100255	2.17	1.76	12.8

TABLE 4. NUCLEI FROM JEFF-3.2 WITH $\chi_v^2 > 2$ AND $d_2 > 1.5$, TOGETHER WITH d_1, d_2 AND χ_v^2.

ZA	d_1(%)	d_2(%)	χ_v^2
41094	1.30	1.74	2.85
42099	1.28	1.73	2.59
45105	1.36	1.50	3.28
46107	1.28	1.82	2.63
49113	1.45	1.81	2.56
49115	1.49	1.85	2.68
50117	1.36	2.40	3.86
50119	1.08	1.63	2.29
53131	1.31	1.88	2.77
54128	1.12	1.52	2.27
54129	1.25	1.74	2.31
54133	1.29	1.53	2.14
55135	1.27	1.97	3.20
55137	1.22	1.73	3.22
56130	1.22	1.85	2.33
56132	1.18	1.89	2.42
56134	1.10	1.62	2.20
56135	1.20	1.92	2.59
56136	1.13	1.70	2.40
56137	1.11	1.72	2.42
56138	1.25	2.00	3.38
58144	1.17	1.97	2.89
59143	1.20	1.61	2.84
60148	1.58	1.68	3.08
61147	1.55	2.48	3.94
61148	2.36	3.22	6.18
61149	1.96	2.27	3.57
62149	1.90	2.34	3.28
63151	2.17	2.63	3.68
63152	3.60	2.71	17.7
63153	1.83	1.65	2.00
63156	1.52	1.98	3.13
65159	1.58	2.54	3.80
72174	1.52	2.26	2.86
72176	1.32	1.89	2.67
72177	1.79	2.75	3.80
72178	1.66	2.05	3.18
72179	1.50	2.69	3.87
73182	1.46	1.62	2.63
80198	1.25	1.78	3.26
80199	1.60	2.88	5.86
80201	1.45	2.56	5.03
91231	1.69	2.24	4.10
91232	1.76	1.55	5.85
95242	2.25	1.86	18.2
96241	1.81	1.72	10.2
96242	1.43	2.05	7.59
96243	3.40	3.74	65.0
96245	2.94	3.79	72.7
96247	1.86	1.63	8.92
96249	1.73	1.68	8.90
98253	1.87	1.56	9.15

TABLE 5. NUCLEI FROM ENDF/B-VIII.0 WITH $\chi_v^2 > 2$ AND $d_2 > 1.5$, TOGETHER WITH d_1, d_2 AND χ_v^2.

ZA	d_1(%)	d_2(%)	χ_v^2
8018	4.08	4.47	94.7
35081	1.17	1.57	2.55
38087	1.34	1.56	3.44
41094	1.25	1.67	2.67
41095	1.34	2.80	4.00
42099	1.27	1.67	2.53
44099	1.18	1.54	2.10
45105	1.52	1.62	4.40
46107	1.19	1.75	2.42
48111	1.24	1.80	2.61
49113	1.44	1.87	2.50
49115	1.47	1.93	2.90
50115	1.30	2.01	3.43
50116	1.13	1.63	2.38
50117	1.33	2.29	3.78
50118	1.06	1.57	2.16
50119	1.12	1.62	2.48
50123	1.20	1.59	2.60
50126	1.17	1.59	2.74
51124	1.74	2.18	3.61
51125	1.31	1.73	2.38
52123	1.30	1.61	2.04
52124	1.07	1.80	2.29
52125	1.15	1.68	2.27
52128	1.10	1.69	2.37
53129	1.11	1.73	2.46
53131	1.32	1.97	2.87
54128	1.09	1.54	2.15
54129	1.20	1.75	2.31
54135	1.22	1.89	2.99
55134	1.35	2.14	2.89
55135	1.20	1.88	3.15
55136	1.29	2.19	3.89
55137	1.22	1.77	3.40
56130	1.32	2.02	2.40
56132	1.20	2.17	2.58
56135	1.20	1.81	2.54
56136	1.12	1.75	2.53
56137	1.12	1.98	2.49
57138	1.35	2.12	3.09
58140	1.21	1.73	2.70
58144	1.16	2.05	3.01
59143	1.17	1.61	2.79
61147	1.47	2.47	3.72
61148	2.23	3.25	6.13
61149	1.89	2.21	3.56
63152	2.43	3.56	4.32
63154	2.00	1.67	2.14
63156	1.53	1.85	3.08
65159	1.59	2.49	3.81
71175	1.79	1.55	4.27
71176	1.98	1.82	4.18

ZA	$d_1(\%)$	$d_2(\%)$	χ_v^2
73182	1.47	1.65	2.63
80198	1.25	1.77	3.26
80199	1.60	2.89	5.87
80201	1.45	2.57	5.02
91230	1.81	1.60	6.44
91231	1.69	2.23	4.10
91232	1.76	1.55	5.84
92231	1.88	1.65	7.53
92233	2.71	3.55	52.0
93234	1.92	1.68	9.17
93236	2.22	1.76	9.75
93238	2.04	1.64	8.12
94236	1.91	1.75	9.16
94237	1.89	1.63	9.17
94238	1.92	1.61	3.66
95240	1.78	1.65	9.29
95242	2.08	1.83	18.5
96241	1.88	1.64	9.18
96242	1.40	2.06	6.96
96243	3.08	3.57	62.7
96244	1.29	1.65	3.80
96245	2.80	3.66	72.4
96247	1.81	1.56	7.60
96249	1.51	1.52	8.41
97246	2.07	1.66	9.04
97248	1.93	1.69	9.50
98249	1.72	1.65	10.2
98251	1.49	1.53	7.85
98253	1.91	1.53	9.74
99252	2.22	1.78	13.8
99254	2.01	1.70	11.2
100255	2.21	1.82	13.1

TABLE 6. NUCLEI FROM ENDF/B-VII.1 WITH $\chi_v^2 > 2$ AND $d_2 > 1.5$, TOGETHER WITH d_1, d_2 AND χ_v^2.

ZA	d_1(%)	d_2(%)	χ_v^2
4007	5.99	-	33.2
26057	2.28	3.96	23.3
35081	1.17	1.57	2.55
38087	1.34	1.56	3.44
41094	1.25	1.67	2.67
41095	1.34	2.80	4.00
42099	1.26	1.68	2.53
44099	1.18	1.54	2.10
44106	1.07	1.50	2.16
46107	1.19	1.75	2.42
48111	1.24	1.80	2.61
49113	1.44	1.87	2.50
49115	1.47	1.93	2.90
50115	1.30	2.01	3.43
50116	1.13	1.64	2.38
50117	1.33	2.29	3.78
50118	1.06	1.57	2.15
50119	1.12	1.62	2.48
50123	1.20	1.59	2.60
50126	1.17	1.58	2.72
51124	1.76	2.32	3.72
51125	1.31	1.73	2.38
52123	1.30	1.61	2.04
52124	1.07	1.80	2.30
52125	1.15	1.68	2.27
52128	1.10	1.69	2.38
53129	1.11	1.73	2.46
53131	1.32	1.97	2.87
54128	1.09	1.54	2.15
54129	1.20	1.75	2.31
54135	1.22	1.89	2.99
55134	1.35	2.14	2.89
55135	1.19	1.88	3.15
55136	1.29	2.19	3.89
55137	1.22	1.77	3.40
56130	1.32	2.02	2.39
56132	1.20	2.17	2.58
56135	1.20	1.81	2.54
56136	1.12	1.75	2.53
56137	1.12	1.98	2.49
57138	1.35	2.12	3.09
58140	1.21	1.73	2.70
58144	1.16	2.05	3.01
59143	1.17	1.61	2.79
61147	1.47	2.47	3.72
61148	2.23	3.25	6.12
61149	1.89	2.21	3.56
63152	2.43	3.56	4.33
63154	2.02	1.65	2.16
63156	1.53	1.85	3.08
65159	1.59	2.49	3.81
71175	1.79	1.55	4.27

ZA	d_1(%)	d_2(%)	χ_v^2
71176	1.98	1.82	4.18
72174	1.30	2.07	2.66
72176	1.37	1.97	2.70
72177	1.80	2.80	4.01
72178	1.46	1.87	2.90
72179	1.58	2.67	3.87
72180	1.11	1.56	2.48
73182	1.47	1.65	2.63
80198	1.25	1.77	3.26
80199	1.60	2.89	5.86
80201	1.45	2.57	5.02
91230	1.81	1.60	6.44
91231	1.69	2.23	4.10
91232	1.76	1.55	5.85
92231	1.88	1.65	7.53
93234	1.92	1.68	9.17
93236	2.01	1.56	7.35
93238	1.85	1.59	7.12
94236	1.91	1.75	9.16
94237	1.89	1.63	9.17
94238	1.88	1.61	3.65
95240	1.78	1.65	9.29
95241	2.15	2.49	7.48
95243	1.93	2.28	5.64
96241	1.96	1.65	9.79
96242	1.53	2.09	7.59
96243	3.13	3.63	63.4
96244	1.50	1.53	3.33
96245	2.87	3.70	72.8
96247	1.72	1.52	8.01
96249	1.46	1.54	7.35
97246	1.98	1.61	8.49
97248	2.14	1.69	9.57
98249	1.63	1.64	9.64
98251	1.64	1.55	7.98
98253	1.88	1.56	9.16
99252	2.19	1.78	13.6
99254	2.27	1.74	12.0
100255	2.10	1.73	12.6

TABLE 7. NUCLEI FROM BROND-3.1 WITH $\chi_v^2 > 2$ AND $d_2 > 1.5$, TOGETHER WITH d_1, d_2 AND χ_v^2.

ZA	d_1(%)	d_2(%)	χ_v^2
4009	3.21	2.50	31.8
8018	4.08	4.48	94.7
26057	2.46	4.09	23.4
35081	1.17	1.57	2.54
38087	1.34	1.54	3.43
41094	1.25	1.66	2.66
41095	1.35	2.80	4.01
42099	1.27	1.66	2.53
44099	1.18	1.54	2.10
46107	1.18	1.74	2.41
49113	1.44	1.87	2.50
49115	1.48	1.93	2.90
50115	1.29	2.02	3.43
50116	1.13	1.61	2.36
50117	1.34	2.30	3.79
50118	1.06	1.56	2.15
50119	1.12	1.62	2.48
50123	1.20	1.59	2.59
50126	1.16	1.59	2.72
51124	1.76	2.31	3.71
51125	1.31	1.73	2.38
52123	1.30	1.61	2.03
52124	1.07	1.80	2.28
52125	1.15	1.69	2.27
52128	1.10	1.69	2.40
53129	1.11	1.73	2.46
53131	1.32	1.96	2.88
54128	1.09	1.53	2.14
54129	1.20	1.75	2.29
54135	1.22	1.89	3.00
55134	1.35	2.14	2.89
55135	1.20	1.88	3.15
55136	1.29	2.19	3.89
55137	1.22	1.76	3.39
56130	1.33	2.02	2.41
56132	1.20	2.18	2.58
56135	1.20	1.81	2.54
56136	1.11	1.73	2.51
56137	1.13	1.98	2.50
58140	1.21	1.74	2.70
58144	1.16	2.06	3.02
59143	1.18	1.61	2.80
61147	1.47	2.47	3.73
61148	2.23	3.26	6.13
61149	2.28	2.82	4.07
63152	2.43	3.56	4.32
63154	2.01	1.65	2.16
63156	1.53	1.85	3.08
65159	1.59	2.49	3.82
71175	1.78	1.54	4.26
71176	1.98	1.82	4.17
73182	1.48	1.65	2.63
90231	14.40	2.63	20.8

ZA	d_1(%)	d_2(%)	χ_v^2
91233	6.96	14.05	134
93236	3.70	1.57	8.59
93238	1.89	1.64	7.28
94237	1.72	1.69	9.11
94242	1.64	2.21	4.63
95241	1.96	2.49	6.81
95243	1.94	2.19	5.67
96243	2.73	3.54	122
96244	1.55	2.70	11.5
96245	2.91	4.32	37.6
96249	1.62	1.53	5.90

TABLE 8. NUCLEI FROM JENDL-4.0U WITH $\chi_v^2 > 2$ AND $d_2 > 1.5$, TOGETHER WITH d_1, d_2 AND χ_v^2.

ZA	d_1(%)	d_2(%)	χ_v^2
43099	1.36	1.67	2.43
44101	1.25	1.60	2.43
44103	1.27	1.83	2.64
44099	1.15	1.52	2.08
45103	1.64	1.75	2.88
45105	1.94	1.54	7.24
51124	1.73	2.17	3.58
51125	1.28	1.66	2.20
52123	1.35	1.81	2.21
52125	1.13	1.67	2.17
52130	1.11	1.65	2.33
53127	1.30	2.20	2.99
53129	1.18	1.91	2.60
53131	1.33	1.98	2.92
56130	1.20	1.83	2.26
56132	1.20	1.92	2.46
56134	1.08	1.69	2.08
56135	1.20	1.93	2.60
56136	1.14	1.65	2.43
56137	1.05	1.60	2.19
56138	1.20	1.69	3.30
57138	1.38	2.08	3.02
57139	1.12	1.66	2.70
59141	1.40	2.00	4.04
59143	1.25	1.53	3.02
73181	1.32	1.61	2.15
80199	1.36	2.13	3.48
80201	1.24	2.05	3.56
91230	1.82	1.59	6.43
91232	1.76	1.56	5.94
92231	1.85	1.65	7.46
92233	2.65	3.68	56.0
92235	3.91	3.57	57.6
93234	1.94	1.69	9.23
93236	1.95	1.56	7.33
93238	1.82	1.61	7.13
94236	1.91	1.75	9.14
94237	1.91	1.61	9.09

ZA	d_1(%)	d_2(%)	χ_v^2
94239	2.42	3.40	44.2
94241	1.79	1.58	7.52
95240	1.76	1.64	9.30
95242	3.01	3.72	68.7
95244	1.73	1.57	6.69
96241	1.95	1.65	9.80
96242	1.53	2.10	7.59
96243	3.14	3.65	64.1
96244	1.51	1.51	3.26
96245	2.86	3.69	72.7
96247	1.70	1.52	7.96
96249	1.46	1.52	7.36
97246	1.97	1.61	8.51
97248	2.13	1.69	9.54
98249	1.68	1.64	9.61
98251	1.66	1.54	7.91
98253	1.87	1.59	9.25
99252	2.23	1.80	13.7
99254	2.30	1.73	12.1
100255	2.14	1.76	12.8

4 The PHP_AS_HP flag

At compilation time it is possible to define the following flag in Geant4: PHP_AS_HP. If this flag is defined then the sampling procedure to generate secondary particles will be slightly different (see [14]). We have performed the same test described in the previous section with and without defining this flag, using the JEFF-3.3 library. The obtained results are presented in Fig. 11, showing that according to this test the default behavior is closer to MCNP6. Note that this does not mean that the results are closer to MCNP6 for every situation.

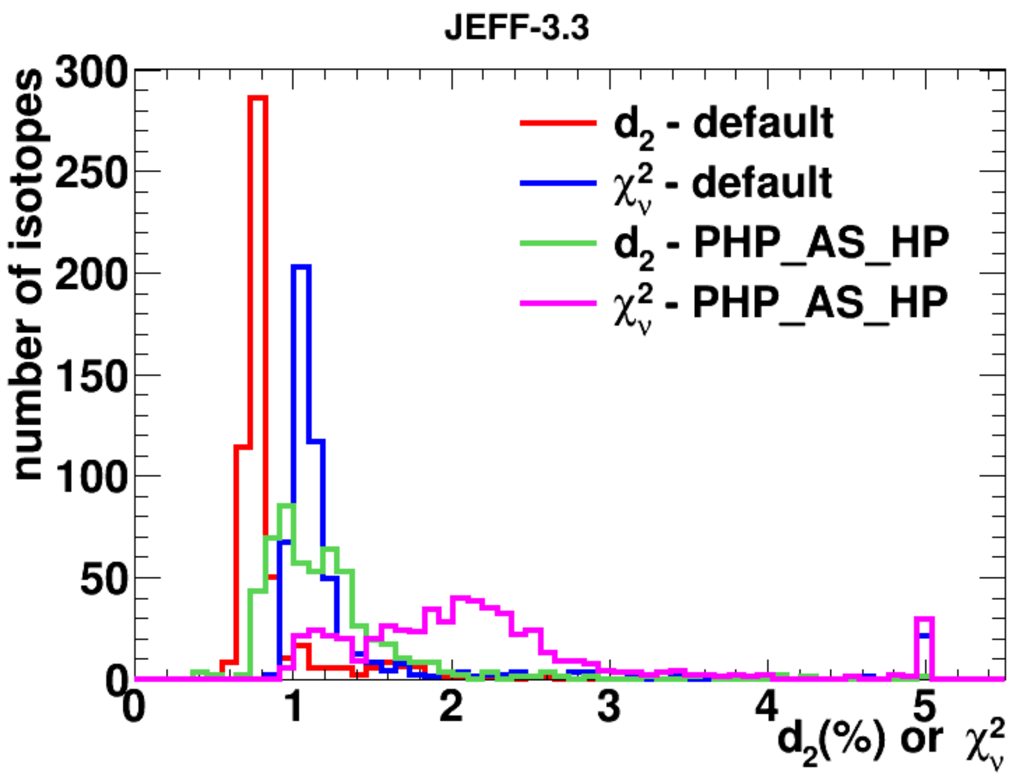

FIG. 11. Values of d_2 and χ^2_υ obtained using JEFF-3.3 with the default Geant4 compilation ("default") and with a compilation performed with the option PHP_AS_HP turned on ("PHP_AS_HP").

5 SUMMARY AND CONCLUSIONS

The list of G4NDL libraries distributed by the IAEA Nuclear Data Services has been updated with six new releases: JEFF-3.3, JEFF-3.2, ENDF/B-VIII.0, ENDF/B-VII.1, BROND-3.1 and JENDL-4.0u (version 2016/1/6).

A comparison between Geant4 and MCNP6 when using these six new releases has been performed concerning the neutron transport. The differences between the obtained results have been quantified, showing a reasonable agreement between both codes and assuring the integrity of the converted libraries. Those isotopes showing larger discrepancies have been listed, together with the parameter values defining these discrepancies.

A large set of plots containing energy distributions obtained from Geant4 and MCNP6 simulations of the secondary neutrons, γ-rays, p, d, t, ^{3}He and α have been generated and are available from the IAEA Nuclear Data Services together with the libraries.

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