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Development of the computational software tools to automate the computational analyses of fusion relevant benchmarks

by S. Simakov, U. Fischer, A. Konobeyev

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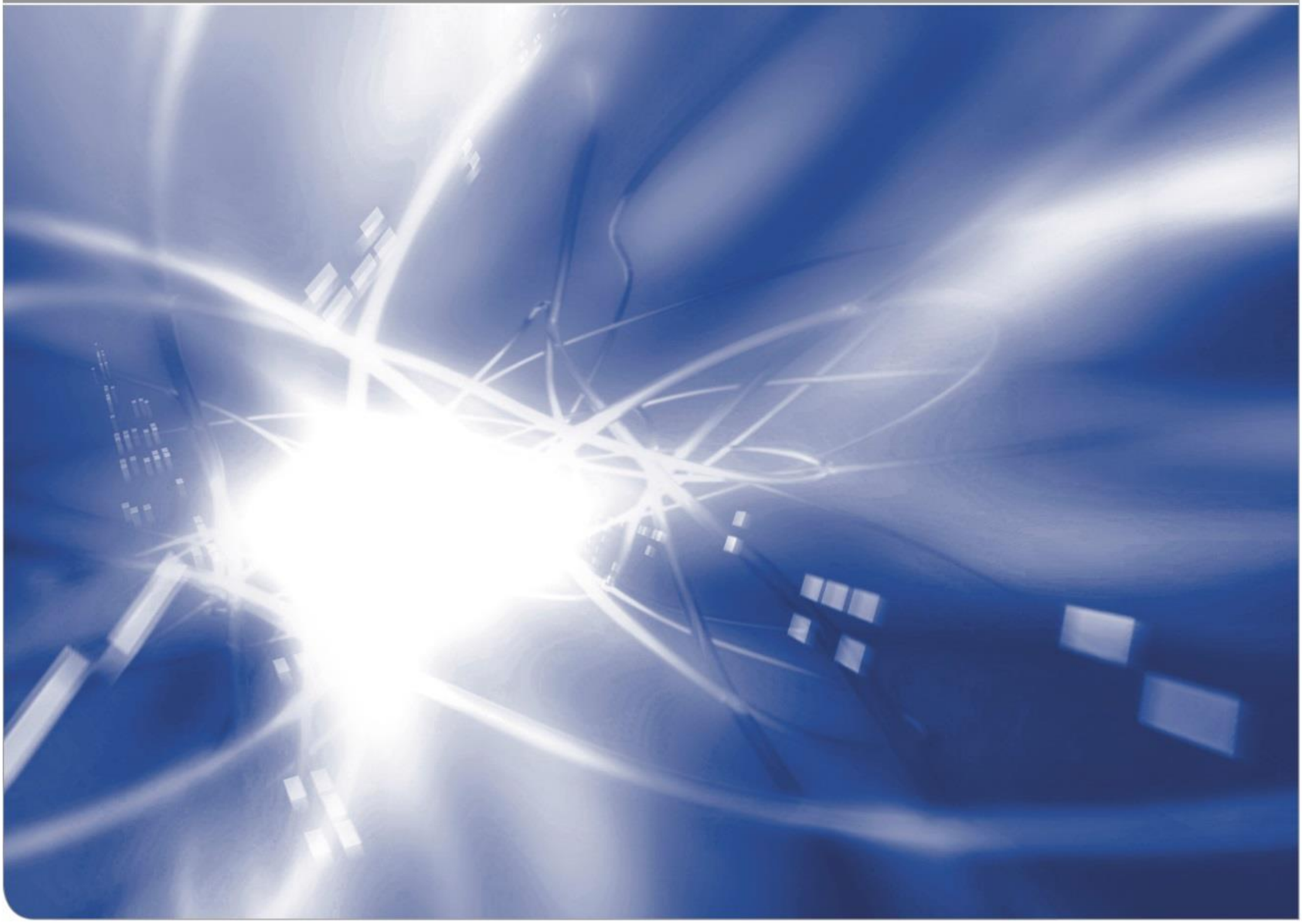

Institut für Neutronenphysik und Reaktortechnik (INR)

Institut für Neutronenphysik und Reaktortechnik
Hermann-von-Helmholtz-Platz 1
76344 Eggenstein-Leopoldshafen
www.inr.kit.edu

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S. Simakov, U. Fischer, A. Konobeyev

Karlsruhe Institute of Technology

Institute for Neutron Physics and Reactor Technology

Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Abstract

The software tool was developed to automate the validation of the evaluated neutron cross sections files against the benchmarks which provide the differential responses. Specifically it was implemented for the energy and time distributions of neutrons and γ-ray spectra measured with the D-T and ^{252}Cf(s.f.) neutron sources and simulated by Monte Carlo code MCNP. The master script modifies the MCNP input deck by selecting the desired evaluation, runs MCNP and compares the calculated spectra with measured ones in user defined intervals. The criteria *chi*-squared, either for intervals or for the whole measured range, was selected to judge about the performance of the evaluated cross section data library. The application of the developed tools for the validation of the ENDF/B-VIII.0, FENDL-3.1d, JEFF.3.3 and JENDL-4.0u libraries against the iron spherical benchmarks with ^{252}Cf and D-T sources has shown that JEFF-3.3 should be considered as superable over all others libraries for the task of the neutron transport. However all tested libraries underestimate the neutron induced γ-rays leakage from bulk iron by factor of two. The reliability of the validation conclusions was strengthened by inter-comparison of the similar benchmarks but carried out in different labs.

November 2020

Content

Introduction

Validation of the evaluated cross sections data files against experimental benchmarks is the substantial and inevitable part of the reliable nuclear data evaluation process. Benchmarks usually have much more complicated geometry and material composition than the cross section measurement experiments and thus require essentially more efforts to simulate them and get a feedback on quality of the tested evaluation. To ease this validation process some kind of automatization was often thought and attempted to implement.

For such important application as the criticality of the simplified assemblies made of fissile material a Database for the International Criticality Safety Benchmark Evaluation Project (DICE) at NEA Data Bank [1] was developed in 2001 and was regular updated since then. The validation of neutron transport data is performed against a single parameter – criticality coefficient K_{eff}. This coefficient and its sensitivities to the neutron cross sections were pre-calculated in DICE for the set of evaluated libraries and could be compared with measured ones. The later were imported for many hundreds relevant experiments from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [2]. The validation of a new evaluation versus the critical benchmarks supposes additional "manual" task: selection of the relevant input information from the DICE database, running benchmark simulation and comparison with measured K_{eff}.

For the benchmarks which provide the spectral responses, i.e. the energy or time-of-flight (TOF) spectra of radiation, the validation is considered so far as an individual "manual" job. It includes searching of measured data and experiment set-up models in the existing databases such as ICSBEP, Shielding Integral Benchmark Archive and Database (SINBAD) [3] or in original publications, computing and comparison in terms of Calculation over Experiment ratio *C/E*. In this case *C/E* is not a single value but an array for the set of secondary particle energies.

The present situation for the neutron data benchmarking against the spectral responses is following. A few collections (suits) of experimental set-up models and measured results united by application or type of measurements do exist, even supplemented in several cases by the "private" scripts to run simulations. As an example we refer to the dozens Livermore 14 MeV pulsed spheres experiments [4 - 7] and collections of the relevant input decks assembled by LANL [8, 10] or NRG [11] for the Monte Carlo code MCNP [12]. These authors compared the calculated neutron time-of-flight or energy spectra with measured ones usually graphically or as C/E ratios for preselected secondary neutron energy domains.

The present report comprises the development of computational software tools to automate the computational analyses of fusion or fission relevant benchmark analyses. The sequence of "on-fly" steps includes: pick-up of desired evaluated data library, running the coupled neutron-photon transport simulation by MCNP, processing of its output and comparison with the experimental data, reporting the results of validation as *C/E* and χ^2 for the user selected energy or time domains or as χ^2 for the full range of experimental data.

This procedure was demonstrated for the energy and TOF spectra of neutrons and γ-rays leaking from the iron spherical shells with ^{252}Cf(s.f.) and pulsed D-T sources, measured at IPPE (Obninsk) and LLL (Livermore). The evaluated cross section data from libraries ENDF/B-VIII.0 [13], JEFFF-3.3 [14], JENDL-4.0u [15] or FENDL-3.1 [16] were validated. The *ace* types data required for the MCNP calculations were obtained by processing of the original ENDF6 formatted evaluated files with the help of code NJOY21 [17] or were used as provided (a case of FENDL-3.1).

The present Report gave a special attention to the intercomparison of benchmarks measured at different labs to prove their consistency and representativeness for cross section validation.

The preliminary results were presented at the meeting of Subgroup 45 (SG45) "Validation of Nuclear Data Libraries (VaNDaL) Project" [18] of the Working Party on International Nuclear Data Evaluation Co-operation (WPEC).

1. Description of the nuclear data validation task against the benchmark spectral responses

For developing and demonstration of the automation software, we considered in this report a task of validation of the coupled neutron-photon transport data in the so called clean benchmarks, which have rather simple geometry and consists of practically single material. Concretely, we focused on the Energy and Time of Flight (TOF) spectra of neutrons and γ-rays leaking from the outer surface of iron spheres with the ^{252}Cf(s.f.) or D-T sources in the centre. Obviously the developed automate procedure will work for more complicated benchmarks which also deliver the spectral responses.

1.1. Iron sphere benchmarks with ^{252}Cf source: neutron and γ-ray leakage energy spectra

One of the most well described and documented experiment was carried at IPPE (Obninsk, Russian Federation) where the neutron and γ-ray leakage spectra from six iron spheres with diameter 15, 20, 25, 30, 35 and 40 cm were measured by proportional hydrogen counter and stilbene crystal scintillator [19 - 23]. Fig. 1.1 shows the lay-out of this experiment: the iron sphere configuration with the ^{252}Cf source located in its center, detectors positioned at distance at least equal to three outer radius of sphere and the shadow bar to measure the room returned background. Further details of the IPPE experiment, the numerical experimental data and MCNP model input files are given in the ICSBEP handbook [2] under Entry "ALARM-CF-FE-SCHIELD-001" [23].

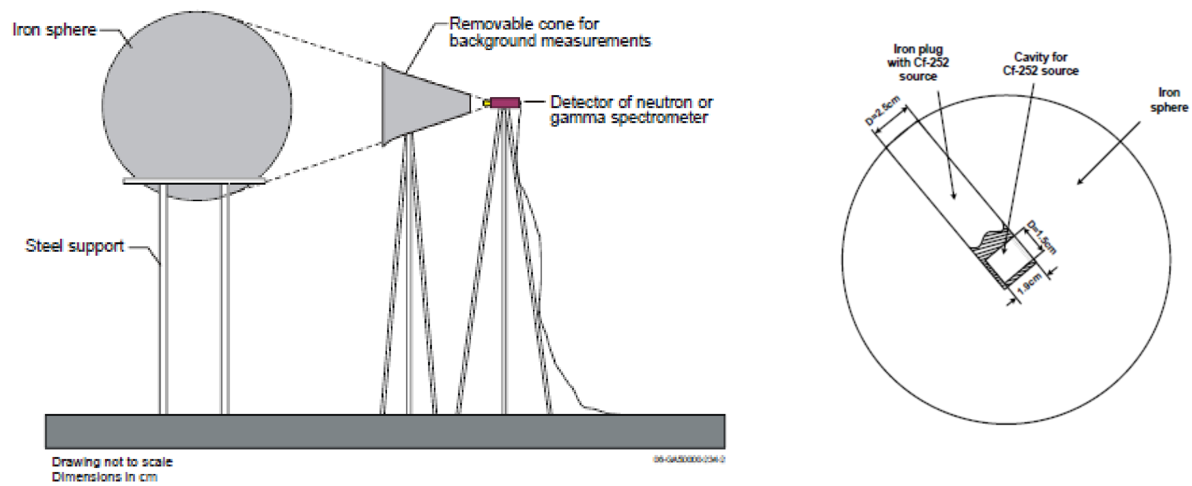

Fig. 1.1. The lay-out of the IPPE experiment (left) and arrangement of the iron sphere with cavity for ^{252}Cf source closed by the iron plug (right) [19 - 23].

As an illustration Fig. 1.2 depicts the IPPE experimental data for the case of two iron spheres (Ø40 cm and Ø 50 cm) and the results of the Monte Carlo calculations performed with ENDF/B-VIII.0 library.

The other known similar benchmarks were carried out at KFK (Karlsruhe, Germany) for three spheres [24 - 26] and at NIST (Gaithersburg, USA) but only for one sphere [27]. Their results are also plotted in Fig. 1.2 and demonstrate in general an agreement between three independent experiments for the spheres of the same diameter. The authors of NIST experiment however wrote "*Agreement in the region below 0.1 MeV is poor and is most likely due to instrumental inaccuracies stemming from calibration problems with the low-energy detector*" [27]. Regarding all this it becomes obvious that the IPPE experiment presents the data for more iron sphere thicknesses and for the larger range of secondary neutron energies. Thus it presents, among others with ^{252}Cf source, the larger interest for nuclear data validation and hence it was used in the present exercise.

Additionally to the neutron spectra the IPPE laboratory has measured and reported the γ-ray spectra. They were measured by stilbene scintillation detector in the energy range 0.4 to 11 MeV. Long time it was a single experiment available for the users who want to benchmark the neutron induced γ-ray production cross sections. From the literature it was known that similar experiment was carried out in 1977 at KFK (Karlsruhe Germany) [25] but its data were not included in the SINBAD database. Such deficiency of SINBAD was reported at several WPEC meetings [28, **Fehler! Verweisquelle konnte nicht gefunden werden.**]. Since then the author (S.S.) of present report has established contact with Prof. S.-H. Jiang, who made the KFK data on γ-ray leakage spectra available for inclusion in SINBAD.

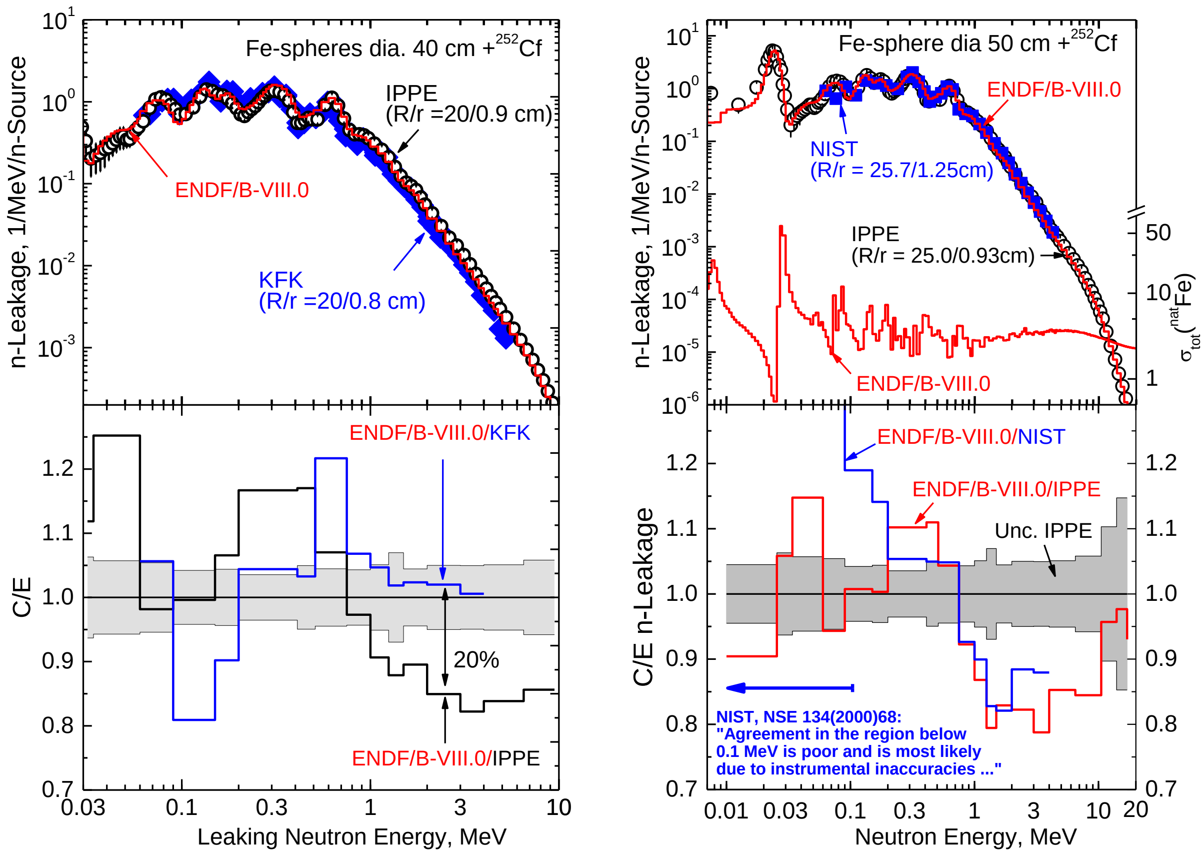

Fig. 1.2. Comparison of the spectra of neutrons leaking from Fe sphere fed by ^{252}Cf(s.f.) source: IPPE and KFK measurements for sphere Ø40 cm (left) and IPPE vs. NIST for sphere Ø50 cm (right). Symbols – measurements; curves – MCNP transport calculations with ENDF/B-VIII.0. The plotted total neutron cross section for ^{nat}Fe allows to observe the anti-correlations with oscillations in leakage spectra. Bottom parts show corresponding C/E ratios integrated in selected energy intervals which capture peaks observed in the energy leakage spectra.

The γ-ray spectra from the IPPE and KFK experiment for the iron shells of the same diameter 30 cm are compared in Fig. 1.3 (left). It is clear seen, that in interval 0.5 - 2 MeV the both experiment data agree within declared uncertainties 10 – 20%. Fig. 1.3 (right) depicts the KFK data for three spheres and results of the MCNP simulation with ENDF/B-VIII.0.

The validation of the evaluated transport data is usually performed in terms of C/E ratio. The bottom parts of Figs. 1.2 and 1.3 plot the C/E ratios after integration of the experimental and calculated neutron leakage spectra in rather broad energy intervals, which cover peaks in spectra. As an intermediate summary we conclude that modern evaluated data libraries ENDF/B-VIII.0 and JEFF-3.3 predict neutron leakage within 20% whereas the γ-ray are underestimated by ≈ 50%. It worthwhile to notice that authors of IPPE experiment has already highlighted such underestimation of γ-ray yield

[22]. We also tried to investigate the reasons and reported intermediate results at series of Nuclear Data experts meetings [36 - 38].

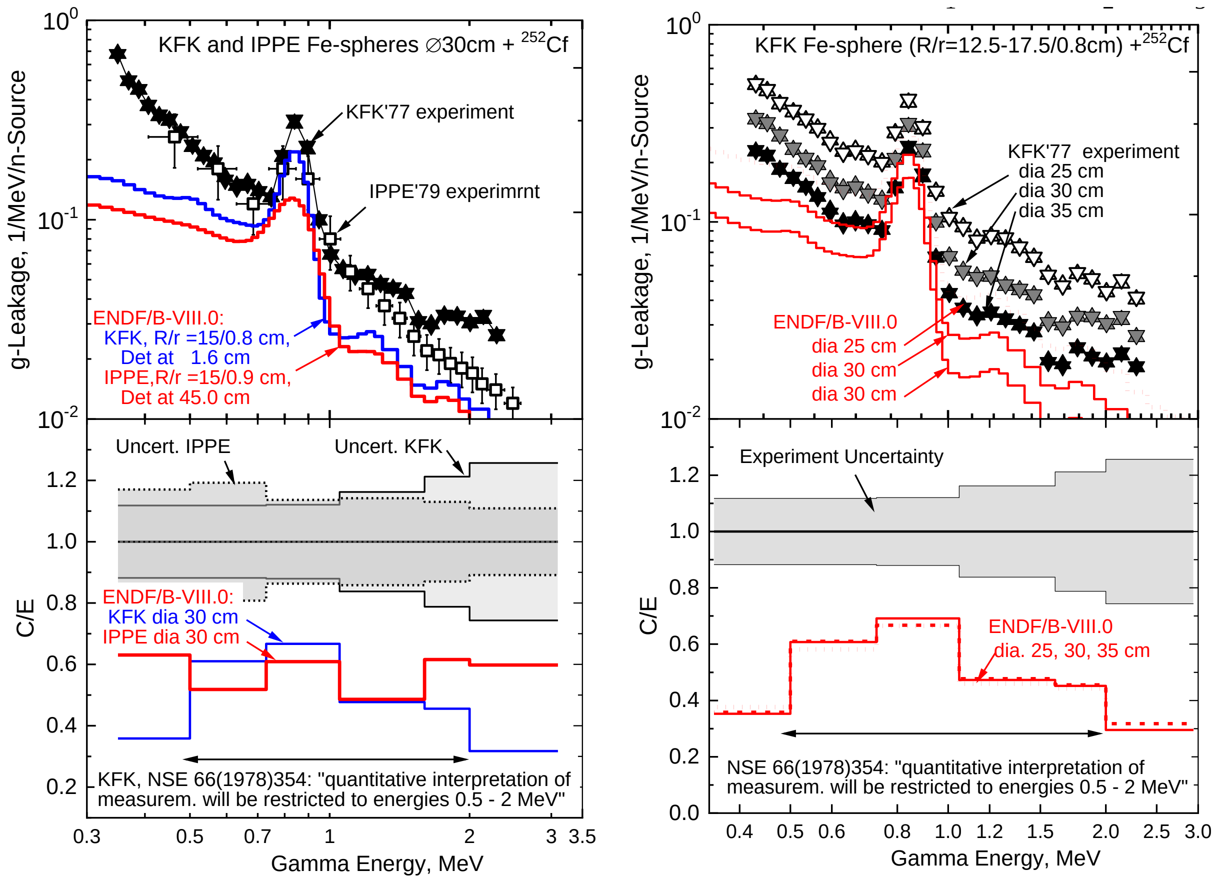

Fig. 1.3. Comparison of the spectra of γ-rays leaking from Fe sphere fed by the ^{252}Cf source: KFK vs. the IPPE measurements for sphere Ø30 cm (left) and all KFK spheres of Ø25 - 35 cm (right). Symbols – measurements; curves – MCNP transport calculations with ENDF/B-VIII.0. Bottom parts plot corresponding C/E ratios integrated in the energy intervals selected to capture the γ-ray spectra features.

1.2. Iron sphere benchmark with D-T source: neutron TOF and energy spectra

The spectra of neutrons emitted from three iron solid spheres of radii 4.46, 13.41 and 22.30 cm for a 14 MeV neutron source have been measured between 10 keV and 14 MeV at Lawrence Livermore Laboratory (LLL) in 1972 [4 - 7]. These radii correspond to the mean free paths of 14 MeV neutrons 0.9, 2.9 and 4.8 mfp which were used by authors of measurements to denote the sphere size. The experimental set-up, Fig. 1.4, shows that the source neutrons were produce by the pulsed d-beam stuck a solid tritium-titanium target. Measurements of the emitted neutron spectra were carried by the time-of-flight technique (TOF) for two different neutron energy regions: between 2 and 15 MeV (high energy spectra) by the NE213 scintillator, and from a few keV to 1 MeV (low energy spectra) by the ^{6}Li glass detector. The high energy spectra were measured using the collimated flight paths at 30 and 120 degrees, while the low energy spectra were measured at 26^{o} in the center of a large enclosure.

It has to be noted that authors have derived transmitted spectra from the ratio of measured spectra with sphere and without sphere [4]. It eliminates the necessity to know both the absolute neutron production yield and absolute detector efficiency. The TOF neutron leakage spectra as a number of neutrons per nanoseconds and per source neutron versus the time bins of 2 shakes (20 ns) are presented in tabulated form in Report UCRL-51144 and its Addendum [4, 5] (regrettably these data are not included in SINBAD yet). The iron spheres neutron leakage TOF spectra from this experiment are plotted in Fig. 1.5.

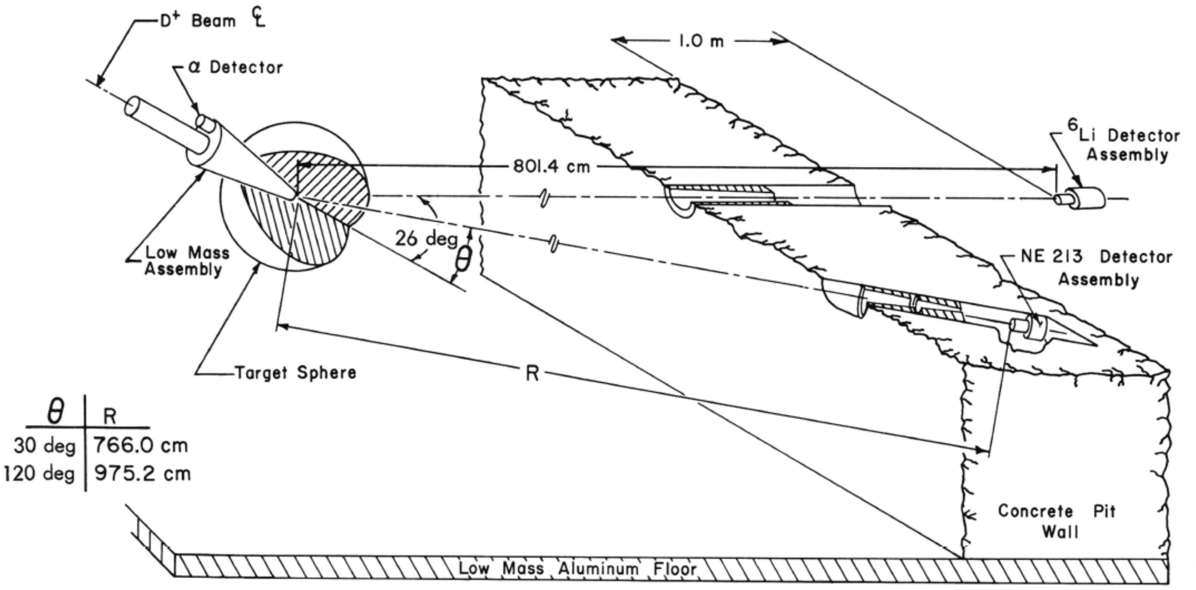

Fig. 1.4. The lay-out of the LLL experiment for with iron spheres and pulsed D-T neutron source [4].

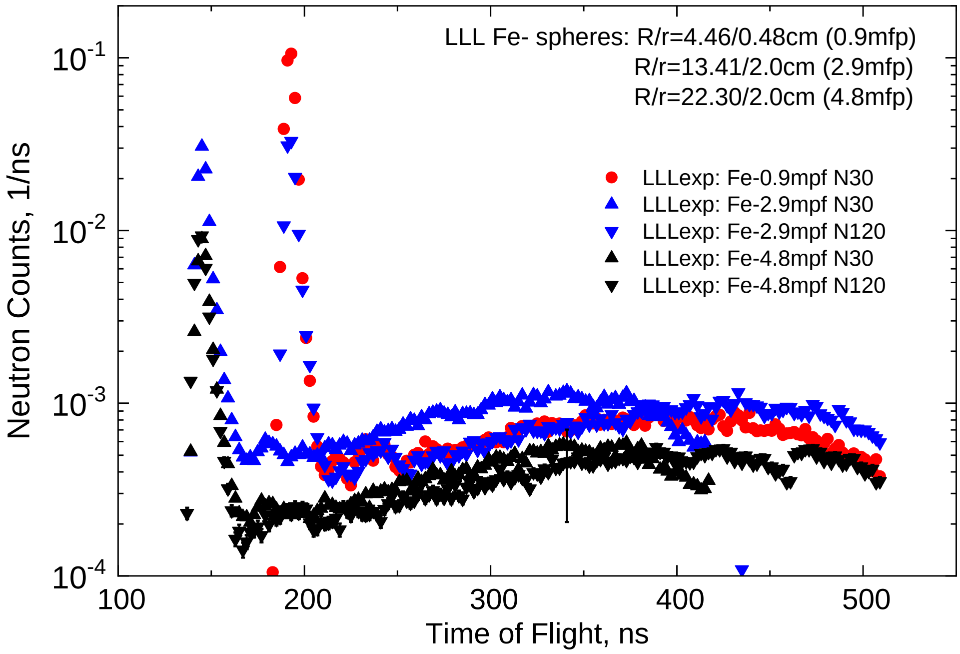

Fig.1.5. The time of flight spectra of neutrons leaking from LLL spheres of different radii fed by a pulsed D-T neutron source and registered by the NE213 scintillation detector positioned at indicated angles.

It is worth to quote the following statement of the LLL experiment made in year 1975 [4] "... *approximate energy spectra were generated from the time-of-arrival spectrum by assuming that all* *interactions occur at the center of the spheres, i.e., by assuming a flight path equal to the detector-to-tritium target distance. This is not a bad assumption, especially for the smaller spheres. However, for the larger spheres and for regions of pronounced structure, comparisons must always be carried out using the time-of-arrival spectrum.*"

Later this point was investigated and confirmed in the IPPE pulsed experiments, where spheres with different sizes and materials were measured by TOF as well as various methodological aspects of this method for massive samples were detailed studied by the Monte Carlo simulation [30 - 35]. Due to the extremely low threshold of the fast scintillator detector, the neutron leakage spectra were measured down to 100 keV, that allowed to observe the resonance structure below ≈ 1 MeV and explain its shift to lower energies when TOF spectra are transformed in energy ones.

We additionally transformed the LLL TOF spectra in the neutron energy distribution. As an example Fig. 1.6 shows the LLL neutron leakage energy spectrum for the thickest sphere (radius 22.3 cm), where it is compared with the similar IPPE pulsed Fe sphere of radius 30.0 cm measured by TOF technique down to 0.1 MeV [35]. Since the IPPE sphere is thicker its spectrum is visibly lower. However the C/E ratios derived from both experiments are similar and both point to underestimation of neutron yield by ENDF/B-VIII.0 in secondary neutron energy interval 1 to 7 MeV. In other words, comparison in terms of C/E demonstrates the agreement between two independent experiments in the overlapping energy interval 1.8 – 14 MeV. Additionally the IPPE experimental and simulation results [31 - 35] demonstrate the shift of resonance structure below 1 MeV to lower energy, when measured TOF spectra are converted in energy representation.

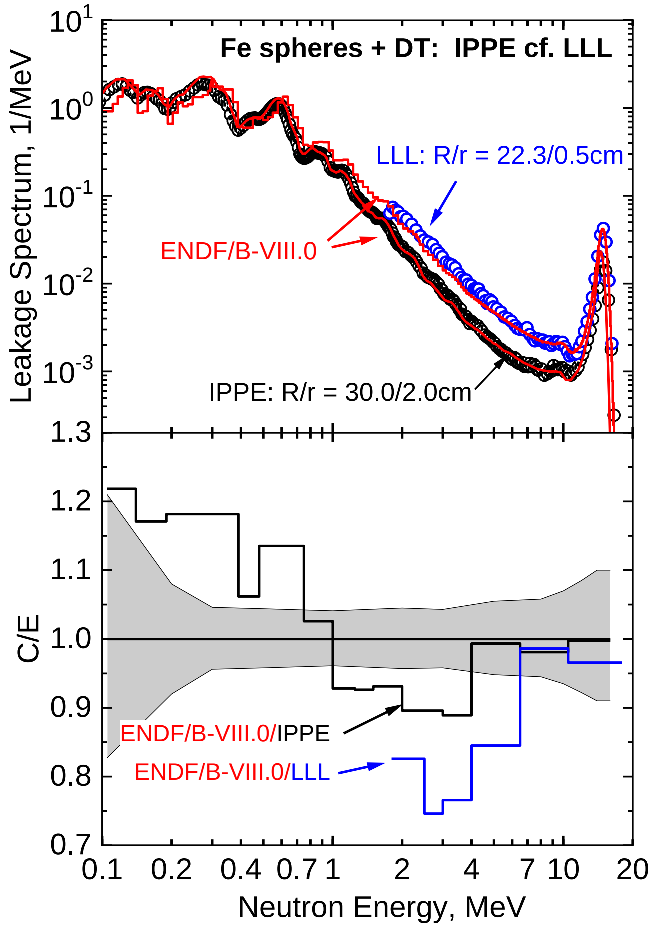

Fig. 1.6. Comparison of the spectra of neutrons leaking from Fe sphere fed by pulsed D-T neutron source: measurements - LLL sphere of outer radius 22.3 cm (4.8 mfp) [4, 5] and IPPE sphere of radius 30 cm [35]; calculations - MCNP with ENDF/B-VIII.0. Bottom part shows the C/E ratios obtained from integration in the selected energy intervals.

Taking into account the abovementioned studies and since the LLL TOF spectra have been measured only above 1.6 MeV were transformed the LLL TOF distributions in energy to demonstrate how automatization procedure works both with TOF and energy spectra. The validation of the 4.8 mfp thick LLL iron sphere experiment (high energy spectra at 30 degree) was selected as example (see next Sections). The MCNP model of the LLL benchmark was taken from Reports [8 - 10].

2. Modifications of the MCNP input decks for IPPE and LLL Iron spheres necessary for automatization

To allow automation of the validation procedure the original MCNP input decks, given for the IPPE experiment in ICSBEP [23] or for LLL in [9], has to be modified. It was done as following (see example in Fig. 2.1).

(1) Default material card for all nuclides in the task was added:

```
m0  nlib=   plib=04c  $  setting default neutron and photon libraries for
                         all materials in problem
```

(2) Elemental carbon was replaced by isotopes ^{12}C and ^{13}C, since major modern evaluated cross section libraries have no data for natural carbon (in the cases of the JEFF-3.3 and JENDL-4.0u evaluations ^{12}C was substituted by ^{00}C):

```
m1   6012   0.000388870 $ 6000 .000393076 was replaced by .000393076*0.9893
     6013   0.000004206 $ 6013            was added       .000393076*0.0107
```

(3) To get the MCNP results in the broader energy range and for more fine groups than those usually specified in the original input decks the new neutron or photon Tallies were added with finer energy bins, Fig. 2.1.

(4) To perform validation of neutron and γ-ray leakage spectra in one run, the photon tallies were included in the IPPE iron input deck (in the ICSBEP database the IPPE decks for neutron and photon leakage are given separately). In the present auto-validation exercise we omitted the γ-rays from decay of ^{252}Cf(s.f.). However it is still a reasonable approximation for the rather thick iron spheres, of diameter 50 cm or more, as was shown in [36, 37]. The reason is that for thick iron layer the Fe(n,x)γ reactions make the dominant contribution to the leaking γ-rays, whereas the direct gammas from ^{252}Cf source will be absorbed.

It is important to stress that further modifications of the original input decks are usually required to perform the nuclear data validation on the up-to-day level of knowledge. In particular, the prompt fission neutron spectrum of ^{252}Cf(s.f.) given in ISCBEP decks for IPPE experiment is represented by the Watt distribution - it should be replaced by standard one [39]. Moreover since the neutron leakage spectrum was measured without time analysis (i.e. the prompt fission events were not separated from all others) the spectrum of delayed neutrons from the ^{252}Cf(s.f.) decay should be added as it was done in [36 - 38].

After all modifications the MCNP input decks renamed as **`IPPE_Fe_Cf`** and **`LLL_Fe_DT_48`** were used in the automation nuclear data validation procedure. As an example Fig. 2.1 lists the fragment of the **`IPPE_Fe_Cf`** input deck (note that the added tallies 202 and 222 will be used for comparison with experimental data).

Fig. 2.1. Fragment of the MCNP input file **IPPE_Fe_Cf** with modifications (highlighted by colour) necessary for the automation of nuclear data validation.

```
message: datapath =
xsdir             =

Fe,d50cm,b8(Cf252 Benchmark Model, p.103 ALARM-CF-FE-SHIELD-001)
1 0             -1  imp:n,p=1
2 1  0.0848605 1 -2  imp:n,p=1  $ Iron
3 0            2 -3  imp:n,p=1  $ vacuum
4 2  0.0843428 3 -4  imp:n,p=1  $ Cu
5 0            4 -5  imp:n,p=1  $ vacuum
6 1  0.0848605 5 -6  imp:n,p=1  $ Iron sphere
7 0            6 -7  imp:n,p=1  $ vacuum
8 0            7 -8  imp:n,p=1
9 0            8     imp:n,p=0

1 so   0.21
2 so   0.53
3 so   0.61
4 so   0.84
5 so   0.93
6 so  25.      $ Iron   Sphere, Outer Radius R = 10,15,20,25,30, 35cm
7 so  75       $ Detector at distance  r = 3*R = 30,45,60,75,90,105cm
8 so 110       $ instead of 100.cm

c
m0  nlib=   plib=04c  $ setting default n and g libraries for all materials
c
m1    6012  0.000388870 $ 6000 0.000393076 was replaced by .000393076*0.9893
      6013  0.000004206 $ 6013             was added       .000393076*0.0107
      25055       0.000343751
      26054       0.005051712
      26056       0.077013534
      26057       0.001815183
      26058       0.000243262
m2    29063       0.058340421  $ Copper
      29065       0.026002379
c
c Source Cards
sdef pos=0 0 0 erg=d2
sp2 -3 1.175 1.04            $ Watt fission spectrum
c sp2 -3 1.025 2.926
c
c Tallies
fc2  Neutron Leakage 0.005 - 0.75 MeV   $ it is original Tallies
f2:n 7
e2    0.005 0.01  0.015 0.02 0.021 0.022 0.023 0.024 0.025 0.026
      0.027 0.028 0.029 0.03 0.032 0.034 0.036 0.038 0.04  0.042
      0.044 0.046 0.048 0.05 0.052 0.054 0.056 0.058 0.06  0.065
      0.07  0.075 0.08  0.085 0.09 0.095 0.1   0.11  0.12  0.13
      0.14  0.15  0.16  0.17  0.18 0.19  0.2   0.21  0.22  0.23
      0.24  0.25  0.26  0.27  0.28 0.29  0.3   0.32  0.34  0.36
      0.38  0.4   0.42  0.44  0.46 0.48  0.5   0.55  0.6   0.65
      0.7   0.75
ft2 geb 0 0.002 10000
sd2 1
fc12  Neutron Leakage 0.085 - 17 MeV   $ it is original Tallies
f12:n 7
e12   0.085 0.09 0.095 0.1  0.11  0.12 0.13 0.14 0.15 0.16
      0.17  0.18 0.19  0.2  0.21  0.22 0.23 0.24 0.25 0.26
      0.27  0.28 0.29  0.3  0.32  0.34 0.36 0.38 0.4  0.42
```

```
      0.44  0.46 0.48  0.5   0.55  0.6   0.65 0.7   0.75 0.8
      0.85  0.9  0.95  1     1.1   1.2   1.3  1.4   1.5  1.6
      1.7   1.8  1.9   2     2.25  2.5   2.75 3     3.25 3.5
      3.75  4    4.25  4.5   4.75  5     5.5  6     6.5  7
      7.5   8    8.5   9     9.5   10    10.5 11    12   13
      14    15   16    17
ft12 geb 0 0.125 0
sd12  1
c
fc122  Gamma Leakage 0.407 - 11.1 MeV   $ it is original Tallies
f122:p 7
e122  0.407  0.52  0.63   0.74   0.846   0.951   1.055   1.16   1.26  1.365
      1.467  1.57  1.67   1.77   1.87    1.98    2.08    2.18   2.38  2.58
      2.78   2.98  3.19   3.39   3.59    3.79    3.99    4.19   4.49  4.79
      5.09   5.39  5.69   5.99   6.29    6.59    6.89    7.2    7.5   7.9
      8.3    8.7   9.1    9.5    9.9    10.3    10.7    11.1
ft122 geb 0 0.15 0
sd122 1
c
 ……

c ----  Tallies for Validation automatization procedure ---
c
fc202  Neutron Leakage 0.001 - 14.0 MeV with fine bins
f202:n 7
e202  0.0010 0.0012 0.0015 0.0020 0.0023 0.0025
      0.003  6i  0.010  $ step = 0.001 MeV
            19i  0.030  $ step = 0.001 MeV
            14i  0.060  $ step = 0.002 MeV
            15i  0.14   $ step = 0.005 MeV
            15i  0.30   $ step = 0.010 MeV
            14i  0.60   $ step = 0.020 MeV
             7i  1.00   $ step = 0.050 MeV
            39i  5.00   $ step = 0.100 MeV
            24i 10.00   $ step = 0.200 MeV
            19i 14.00   $ step = 0.200 MeV
ft202 geb 0 0.002 10000
sd202 1
c
fc222  Gamma Leakage 0.003 - 14.0 MeV with fine bins
f222:p 7
e222  0.003  6i  0.010  $ step = 0.001 MeV
            19i  0.030  $ step = 0.001 MeV
            14i  0.060  $ step = 0.002 MeV
            15i  0.14   $ step = 0.005 MeV
            15i  0.30   $ step = 0.010 MeV
            14i  0.60   $ step = 0.020 MeV
             7i  1.00   $ step = 0.050 MeV
            39i  5.00   $ step = 0.100 MeV
            29i 11.00   $ step = 0.200 MeV
            14i 14.00   $ step = 0.200 MeV
ft222 geb 0 0.15 0
sd222 1
c -------------------------------------------------
mode n p
c
c  Print Tallies   Dump to runtp   Print mctal   MaxDumps runtp   MaxRendez
c prdmp    1.E+9            1.E+9             1                3           0
prdmp       j                  j             1                j       1.E+9
print
c
nps 1.E+8        $ nps = 1.E+9  4x48=192cpu = 5 min
```

3. Batch script `run_auto` for on-fly modifications of the input deck, running MCNP and post processing

Linux batch script `run_auto` is a master of automation procedure. It performs following sequence of operations on-fly:

1) pick-ups the specific Benchmark and Evaluated transport Data for validation purpose;
2) modifies the basic MCNP deck and creates temporary file `mcnp.inp`;
3) runs MCNP with file `mcnp.inp` as input;
4) invokes the *ValiDat* code which reads and process the MCNP output (`mctal`) and experimental data files, then performs *Vali*dation of nuclear *Dat*a in terms of C/E and criteria χ^2;
5) saves results in the files which will have names relevant to the validation task.

Below are the corresponding fragments of the Linux batch script `run_auto`.

(1) As the first step the user has to select in script `run_auto` the desirable Benchmark and Evaluation by ordering the proper benchmark name and extension of the ACE files. In this example the LLL_Fe_DT_48 and *ace* files with ext = 03 (JEFF-3.3) will be picked-up by MCNP (in this example since they are listed as the last ones):

```
echo " 1: =*= Selection of Benchmark and Evaluated (ace) data library =*="
  benchmark="IPPE_Fe_Cf"                        # selection of IPPE benchmark
  benchmark="LLL_Fe_DT_48"                      # selection of LLL  benchmark
  ext="31"                                      # selection of FENDL-3.1
  ext="04"                                      # selection of JENDL-4.0u
  ext="80"                                      # selection of ENDF/B-VIII.0
  ext="03"                                      # selection of JEFF-3.3
```

(2) At the second step, the Linux stream editor *`sed`* will replace the string “`nlib=`” by the ordered library “`nlib=03c`” and will produce the temporary input file `mcnp.inp` for MCNP:

```
 echo " 2: =*=*=  modification/creation of mcnp.inp with selected library:
           ext= ${ext}  =*=*= "
  sed  "s/nlib=/nlib=${ext}c/g"  ${benchmark}  >  mcnp.inp
```

(3) Then the batch script launches the MCNP code *`mcnp6.mpi`*, which will generate the outputs (important for the further processing is a file `mctal`):

```
echo " 3: =*=*=  run mcnp6.20  =*=*= "
  mpirun   mcnp6.mpi   i = mcnp.inp   o = output   m = mctal   x = xsdir
```

(4) At the fourth step, the Fortran code *ValiDat* will be invoked together with its input file `ValiDat_${benchmark}.inp`. Code *ValiDat* will produce output file `ValiData.res` with results of processing and comparison with experiment:

```
echo " 4: =*= run ValiDat with input ValiDat.inp to perform validation =*="
  ./ValiDat  ValiDat_${benchmark}.inp
```

(5) As the last step the Linux script copies `mctal` and `ValiDat.res` into files which names will contain information about selected `benchmark` and evaluated data library extension `ext` for archiving and checking off-line.

```
echo " 5: =*= save results under names with ${benchmark} and ${ext} =*="
  cp   mctal             mctal_${benchmark}_${ext}
  cp   output            output_${benchmark}_${ext}
  cp   ValiDat.res       ValiDat_${benchmark}_${ext}.res
```

4. Code *ValiDat* to read and process the MCNP output and experimental data

The purpose of code *ValiDat.f95* is to read file `mctal` produced by MCNP and file with experimental data and then compare them in terms of C/E ratio and criteria χ^2. The code was written in the Fortran-95 language and compiled by two Fortran compilers: *GNU gfortran* and *Intel ifort* (to force *ifort* to recognise the Fortran source extension *.f95*, the compilation was performed with flags "-fpp -free -Tf").

The *ValiDat.f95* code reads the MCNP computed quantity array (Tally) from file `mctal,` reads the experimental spectrum and computes the C/E ratio for every Energy or TOF interval given in file `Edges.dat`. It is worthwhile noticing that energy bins of MCNP tally should NOT be identical to the grid used for experimental spectrum and NOT necessary coincide with Edges of intervals, since *ValiDat* first computes integrals and their uncertainties for simulated and experimental spectra in the intervals given in `Edges.dat`, then calculates arrays of C/E and χ^2.

It is supposed that uncertainties, if given at all, are statistical ones. It is always true for the MCNP tally, but not for the experimental data. During integrations of the experimental spectrum the statistical uncertainties are quadratically summed and thus relative statistical uncertainties decreases as interval of integration increases. To avoid this and take into account the non-vanished systematic uncertainty of the experimental data, the latter was considered as an additional input parameter for the *ValiDat* code.

To qualify the level of agreement we employed the standard metric for testing nuclear data libraries - the “reduced” chi-squared parameter:

$$\chi^2(n) = \frac{1}{n}\sum_{i=1}^{n}\frac{({}^{C_i}/_{E_i} - 1)^2}{\sigma_i^2}$$

where the calculated and experimental values *Ci* and *Ei* for interval *i* are compared with unity mediated by the sum of the total MCNP simulation and experimental relative uncertainty σ_i. The degree of freedom, *n*, is considered to be equal to the number of Energy or TOF intervals (given in `Edges.dat`) in which the experimental and calculated neutron leakage spectra will be integrated. We also considered the partially cumulated $\chi^2(n)$ when the number of intervals *n* is lesser than maximal number necessary to cover the full Energy or TOF range of experimental data.

As an example, the input file `ValiDat_IPPE_Cf.inp` for *ValiDat.f95* is listed in Fig. 4.1. The meaning of input parameters is explained by comments (NB: the comments should start from column 40 or larger). In the example given, two runs will be performed employing the same file *mctal* (which however contains the results for both neutron and γ-ray leakage spectra) but two different corresponding experimental data sets with own energy boundaries (Edges) for integration and calculation of C/E and χ^2.

It has to be noted that the original experimental data could be presented by authors in the deferent ways: as the Spectrum [1/MeV] or Yield [1/bin] arrays versus of two (low and upper bin boundaries) or one (middle) argument. To distinguish between them the input parameter "`No. of Argument columns in Exp. Data`" is used, whereas its negative sign indicates the spectrum rather than yield.

Fig. 4.1. Input file `ValiDat_IPPE_Fe_Cf.inp` for code *ValiDat.f95*.

```
mctal_IPPE_Fe_Cf          Name of File mctal produced by MCNP
1.                         Scaling Factor for Tally, Fn (default = 1.)
0                          is it Spectrum [1/MeV] or Yield [1/bin] ? (1/0)
0                          Reverse order of argument or not, KeyRev (1/0)
202                        Tally Number to be processed, NumTally
IPPE_Fe_Cf_d50n.dat       Name of File with Experimental Data
-2                         No. of Argument columns in Exp. Data file ? (2/1)
2                          Error type for Exp. Data: Abs/Rel/No ? (2/1/0)
0.03                       Systematic Relative Error, ErSys = ?
Edge_IPPE_Cf_n.dat         File with Edges for Spectrum Integration
1                         Repeat calculations with other Files  ? (1/0)
mctal_IPPE_Fe_Cf          Name of File mctal produced by MCNP
1.                         Scaling Factor, Fn  (default = 1.)
0                          is it Spectrum [1/MeV] or Yield [1/bin] ? (1/0)
0                          Reverse order of argument or not, KeyRev  (1/0)
222                        Tally Number to be processed, NumTally
IPPE_Fe_Cf_d50g.dat       Name of File with Experimental Data
-2                         No. of Energy columns Exp. Data file  ? (2/1)
2                          Error type for Exp. Data: Abs/Rel/No ? (2/1/0)
0.05                       Systematic Relative Error, ErSys  = ?
Edge_IPPE_Fe_Cf_g.dat      File with Edges
0                         Repeat calculations with other Files  ? (1/0)
```

5. Results of validation

The neutron and photon leakage energy spectra simulated by MCNP for the IPPE iron sphere of Ø50 cm fed by ^{252}Cf source and visual comparison with measurements are shown in Fig. 5.1: the energy spectra, C/E ratios and partial criteria χ^2 cumulated from the lowest energies to the maximal ones.

The quality of evaluation could be judged from the consideration of the C/E ratios for energy intervals which boundaries should be selected by user to capture the observed specific future in spectra, such as peaks, change of slope etc. Thus Fig. 5.1 (left) shows that C/E for neutron leakage indicates underestimation of ENDF/B-VIII.0 by 20% above ≈ 1 MeV (pointing to such deficiency was included in paper [40] and proper corrections were undertaken afterwards). The cumulated $\chi^2(n)$ (the *chi*-squared parameter summed until interval number *n*) shows the better behaviour of ENDF/B-VIII.0 in comparison with JEFF-3.3 up to ≈ 1 MeV. However this 20% underestimation by ENDF/B-VIII.0 results to the total χ^2 (computed for the whole energy range) to be ≈ 2 times larger than with JEFF-3.3, see Table 5.1.

Both library ENDF/B-VIII.0 and JEFF-3.3 underestimate the γ-ray spectrum by factor of 2. As a result criteria χ^2 is substantially different from unity, see also Fig. 5.1 (right plot). It worth to notice that JEFF-3.3 stronger than ENDF/B-VIII.0 underestimates the yield of γ-rays above 6 MeV (these gammas originate from the neutron capture reaction on iron) - that is also reflected in the rise of cumulated $\chi^2(n)$ above 6 MeV.

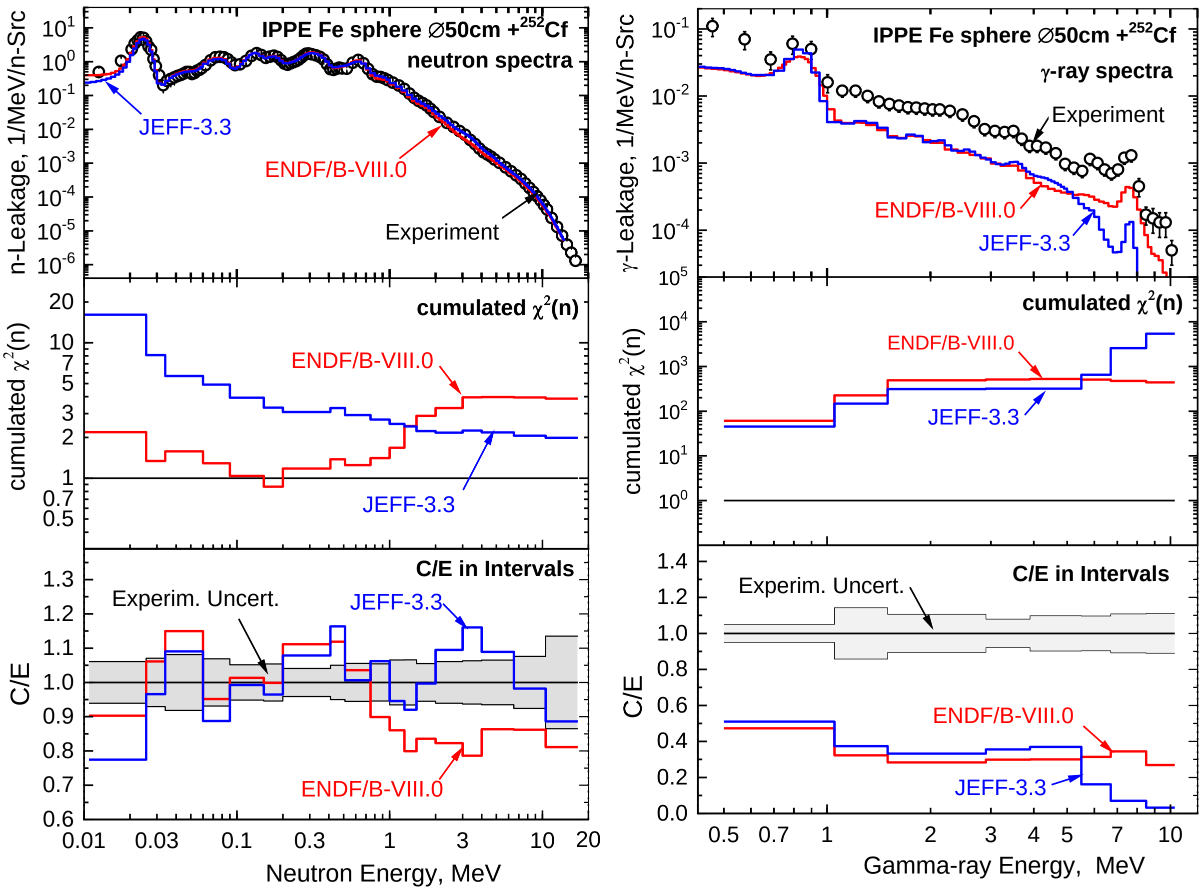

Fig. 5.1. The neutron (left) and γ-ray (right) leakage spectra from the IPPE iron sphere Ø50 cm with ^{252}Cf(s.f.) source: open circle - experiment [21, 23], curves - MCNP simulation with nuclear data from ENDF/B-VIII.0 (red) and JEFF-3.3 (blue). Upper part of figures – energy spectra, middle – χ^2 cumulated over n integration intervals, bottom – C/E for these intervals.

Table 5.1. The total criteria χ^2 for the MCNP simulation of the neutron and photon leakage spectra (in whole energy range) for iron spheres measured at IPPE with ^{252}Cf(s.f.) and at LLL with D-T sources. The green or red colours highlight the best or worse evaluations.

Benchmark	Leaking Radiation	Energy or TOF range	No. of Intervals for C/E	total χ^2 computed for whole measured spectrum			
				ENDF/B -VIII.0	JEFF -3.3	FENDL -3.1d	JENDL -4.0u
IPPE Fe Ø50 cm with ^{252}Cf	neutrons	0.01 – 17.0 MeV	18	3.87	**1.99**	**3.48**	1.64
	γ-rays	0.50 – 10.3 MeV	8	4.41E+2	5.40E+03	6.49E+2	4.15E+2
LLL Fe Ø44.6 cm with D-T	neutrons	12.9 – 40.9 shake	6	12.0	**0.89**	**0.37**	4.48
	neutrons	1.8 – 18.0 MeV	6	8.16	**0.39**	**0.59**	3.26

The validation results for the thickest 4.8 mfp LLL iron pulsed sphere are shown in Fig. 5.2 for the time of flight (left) and energy (right) spectra. The later was calculated from TOF to demonstrate the energy distribution of secondary neutrons, which is more convenient for the interpretation. Then the energy integration intervals were selected and corresponding them the TOF integration limits were computed. Since the lowest values of TOF results to the highest neutron energies, the cumulated $\chi^2(n)$ increases as function of TOF but decreases versus the neutron energy. For the whole TOF or Energy ranges the values of χ^2 should be approximately equal (it depends how TOF uncertainties were transformed into energy ones).

For the analysed LLL Fe benchmark the total criteria χ^2 turns out to be several times lesser for the JEFF-3.3 library than for ENDF/B-VIII.0, see Table 5.1.

At the end we have performed automatic validation of the latest versions of Fusion (FENDL-3.1d) [16] and Japanese (JAENDL-4.0u) [15] evaluated data libraries. In this case it was done fully automated or “blind”, i.e. without any spectra comparison or analysis of C/E and χ^2 for each integration interval. The obtained total χ^2 for neutron leakage are summarised in Table 5.1 for both benchmarks. They point to a better quality of FENDL-3.1d and JENDL-4.0u versus ENDF/B-VIII.0 but comparable or a bit worse performance versus JEFF-3.3. The considered libraries also underestimate the yield of leaking γ-rays substantially larger than uncertainties reported in experiments.

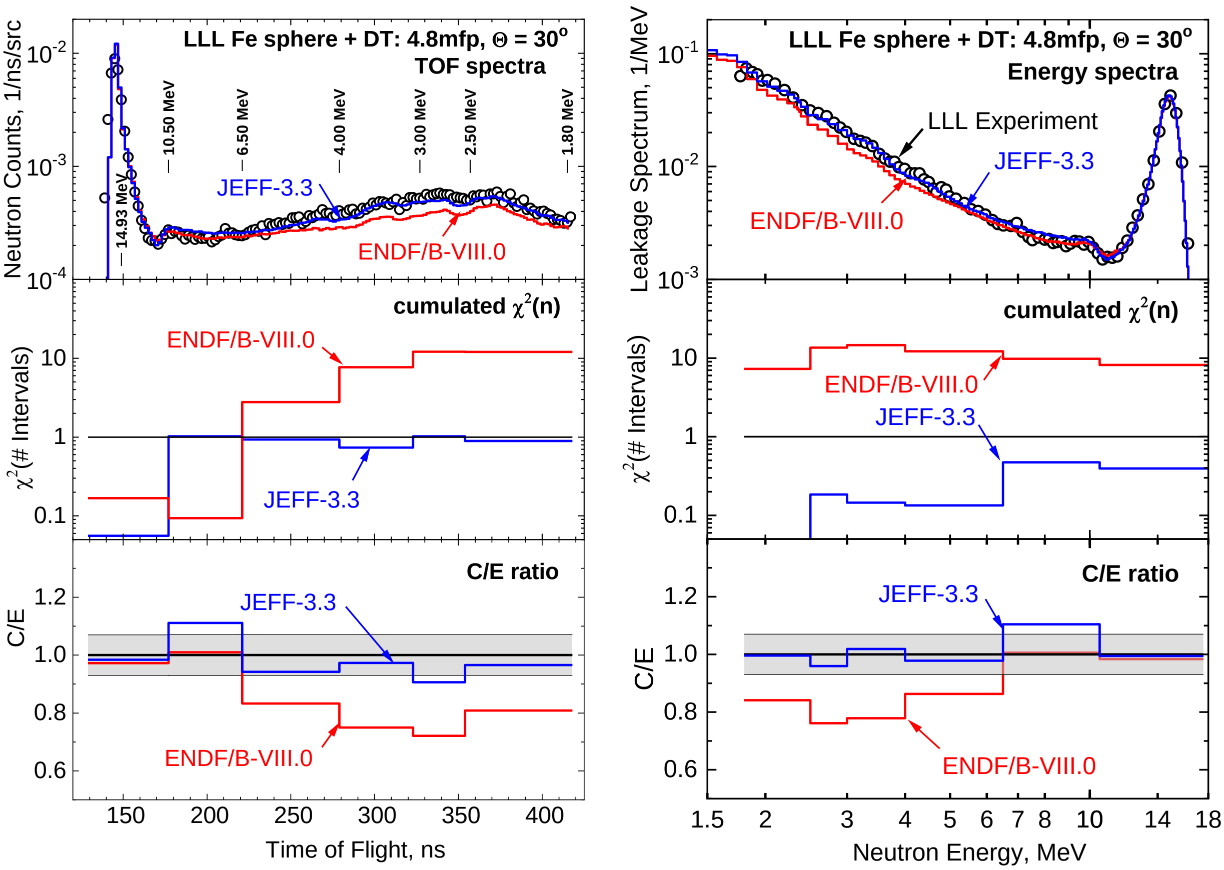

Fig. 5.2. The TOF (left) and energy (right) neutron leakage spectra for the LLL iron sphere with wall thickness 4.8 mfp (Ø44.6 cm) pulsed by the D-T source and measured at angle 30°: open circle - experiment [4], curves - MCNP simulation with nuclear data from ENDF/B-VIII.0 (red) and JEFF-3.3 (blue). Upper part of figures – energy spectra, middle – χ^2 cumulated over n integration intervals, bottom – C/E for these intervals.

Summary

The computational software tools to automate the validation of the evaluated neutron cross section libraries in fusion or fission relevant benchmarks have been developed. The novel element of this approach consists in application to the benchmarking versus the spectral responses (arrays), such as energy or time distributions of the emitted neutrons or γ-rays, and usage of criteria χ^2 for qualification of evaluation. So far existing analogues software tools and databases deal with the validation of evaluated data validation versus a single parameter such as the critically coefficient of fissile system.

The elaborated Linux shell script and Fortran code allow in one automatic sequence to modify the MCNP input deck for the experimental benchmark to pick-up desired evaluated cross section files, run MCNP simulation, process its output and compare with the experimental data. Finally the procedure delivers the C/E and *chi*-squared criteria to judge about the quality of the used neuron-photon transport data library in the preselected energy or time intervals or in the whole measured range.

For automation of validation process itself, several manual modifications of the original input decks are necessary, e.g.: replacing of the element by isotopes, inserting tallies with extended range and more fine group structure, more accurate representation of source, etc. Besides this the more deep investigation of validation task is often inevitable: selection of the reliable benchmarks, understanding of the measuring technique and derived quantities, defining the range of the response validity, analysis of the uncertainty components, etc. – all this was done in the present report for considered cases.

The developed tools were applied for validation of ENDF/B-VIII.0, FENDL-3.1d, JEFF.3.3 and JENDL-4.0u in two benchmarks with iron spherical shells fed by spontaneously fissile ^{252}Cf and pulsed fusion D-T sources. As a result of automated validation based on criteria χ^2, we conclude that JEFF-3.3 should be considered as superable over all others libraries for neutron transport simulation in the thick iron. However the quality of all tested libraries to predict the neutron induced γ-rays generation and propagation in iron is not acceptable and requires further analysis.

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