Quantitative and Quality Test of Cross Section Library ENDF/B-b2

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Abstract: This article includes a test or in other words data verification of neutron ENDF/B-VIIb2 sub library. The first part consists from the process of preparation ACE files by NJOY 99.90. The starting point of data verification describes needed patches in NJOY 99.90, which are necessary to do for correctly production of ACE files. After the obtaining ACE files follow the test of all ACE files through GODIVA – input file for MCNP. GODIVA is high enrichment sphere of U-235, where tested material is added as impurity. The aim of GODIVA test is to obtain the certainty if produced ACE files are able to run through MCNP.

The second part of this article begins with choose of benchmarks from "International Handbook of Evaluated Criticality Safety Benchmark Experiments, 2005". From this source of criticality experiments were separated some benchmarks for quality verification of ACE files by MCNP.

Introduction

Data verification in this article is concentrated to neutron ENDF/B-VIIb2 sub library. In the first step of the test is included the using of NJOY 99.90 for ACE files production. In next part of the papers is showed the troubles which the user has to go through for successes run of NJOY. Next MCNP test shows if produced ACE files run or no run successfully through MCNP. In the last section of the test is possible to see results of chosen benchmarks. Benchmarks were calculated by different MCNP codes and also with different ENDF libraries.

1. ENDF format

The ENDF formats were originally developed for use in the US national nuclear data files called ENDF/B (the Evaluated Nuclear Data Files) [1]. These files went through various versions with names like ENDF/B-III, ENDF/B-IV and ENDF/B-VI, each version adding both improved data and new capabilities for representing nuclear data. The current ENDF-7 and ENDF-6 format can represent cross sections for neutrons, photons and charged particles, including particle yields and distributions in angle and energy, for energies up to several hundred MeV, the radioactive decay properties of reaction products and estimated errors and covariances of the various nuclear parameters. The ENDF format is now widely used around the world, including the JEF files in Europe, the JENDL files in Japan and the BROND in Russia. Thus, even though NJOY was originally designed to work with the US ENDF/B libraries all over the world [1]. The ENDF/B-VIIb2 includes 393 neutron evaluations.

2. NJOY 99.90

The NJOY Nuclear Data processing System is a modular computer code designed to transform the data in various ways and output the results as libraries designed to be used in various applications [2]. Each module performs a well defined processing task. The modules are essentially independent programs and they communicate with each other using input and output files, plus a very few common variables.

The NJOY is to convert evaluated nuclear data in ENDF format into forms useful for applications. It is best used by people with some knowledge of things like nuclear reaction theory, resonance theory or scattering theory on one side, and some knowledge of thinks like particle transport codes, reactor core calculations or radiation medicine on the other [2].

Verification process of ENDF/B-VIIb2 and ACE files production includes followed NJOY 99.90 modules:

- **RECONR** reconstructs pointwise (energy-dependent) cross sections from ENDF resonance parameters and interpolation schemes.

- **BROADR** Doppler broadens and thins pointwise cross sections.

- **UNRESR** computes effective self-shielded pointwise cross sections in the unresolved energy range.

- **HEATR** generates pointwise heat production cross sections and radiation-damage cross sections.

- **MODER** converts ENDF "tapes" back and forth between ASCII format and the special NJOY blocked-binary format.

- **ACER** prepares libraries in ACE format for the Los Alamos continuous-energy Monte Carlo code MCNP.

- **VIEWR** takes the output of PLOTR, or special graphics from HEATR, COVR, DTFR, or ACER, and converts the plots into Postscript format for printing or screen display.

- **PURR** generates unresolved-resonance probability tables for use in representing resonance self-shielding effects in the MCNP Monte Carlo code.

- **GASPR** generates gas-production cross sections in pointwise format from basic reaction data in an ENDF evaluation. These results can be converted to multigroup form using GROUPR, passed to ACER, or displayed using PLOTR.

2.1 NJOY 99.90 patches

For successful ACE files calculation from ENDF/B-VIIb2 format is necessary to make two patches in source code of NJOY 99.90. The first one is connect with *Legendre polynomials* in module HEATR, exactly in subroutine H6DDX:

```
File UP90:
             *ident up15
                   *d heatr.3284
                    dimension cnow(*),p(65)
             *ident up30
                   *d up15.11
                    *i heatr.3298
                      data nlmax/65/
```

In this subroutine H6DDX is needed to increase dimension of parameter *p* to around 65 and parameter *nlmax* also to 65. Around thirty fission products need this patch in module HEATR.

The second patch is connected with *negative probabilities* in module ACER, subroutine PTLEG2:

```
Module ACER:
               */ subroutine ptleg2
               *d acer.6951
                   dimension aco(3600), cprob(3600), cumm(3600)
               *d acer.7031
                   if (ii.gt.3600) call error('ptleg2','too many angles',' ')
```

After these changes is the NJOY 99.90 able to successfully produce ACE files for MCNP.

3. GODIVA test

A unreflected sphere of highly enriched uranium called GODIVA was used as input deck for MCNP 4C2. The nuclides in this model are U-235, U-238 and tested material was added as impurity.

The composition of the sphere:

U-235: **94.889 %**
U-238: **5.111 %**
Tested material as impurity: **0.001 %**

3.1 MCNP patch

During the running of GODIVA for all materials in ENDF/B-VIIb2 was recorded for **Rh-103** dimension overflow in subroutine EXPUNG for parameter *m3*. Parameter *m3* is necessary to increase to value 1500.

```
Subroutine: EXPUNG
             (Line 15)
        integer, parameter : : m3 = 1500
        integer, parameter : : m4 = 200
        integer : :   jx(27), m2(m3), jf(m4), nx(8)
```

In ENDF/B-VII**b1** format – **Gd-155** and **Rh-103**

4. Quality test - benchmarking

The source of benchmarks is International Handbook of Evaluated Criticality Safety Benchmark Experiments, 2005 [4]. In this papers are situated four calculated benchmarks:

1. HEU-MET-FAST-001 (1 case, 'Godiva') [4]
- A bare sphere of highly enriched uranium (LANL, 1950s).
- The uranium enrichment was 94% U-235.
- The isotopes in this benchmark model are U-234, U- 235, U-238.

2. HEU-SOL-THERM-004 (6 cases) [4]
- Reflected uranyl-fluoride solutions in heavy water (LANL, 1950s). The D/235U ratio varied from 34 to 431.
- The uranium enrichment was 94% U-235.
- The isotopes in these benchmark models are H-1, H-2, O-16, F-19, Si-28, Si-30, Cr-50, Cr-52, Cr-54, Mn-55, Fe-54, Fe-56, Fe-58, Ni-58, Ni-60, Ni-62, Ni-64, U-234, U-235 and U-238.
  Thermal scattering data for D in D2O is used.

3. HEU-SOL-THERM-013 (4 cases, 'ORNL-1', : : :, 'ORNL-4') [4]
- Uranyl nitrate solutions poisoned with boric acid in an unreflected sphere (at ORNL, 1950s).
- The uranium enrichment was 93% 235U.
- The isotopes in these benchmark models are H-1, N-14, O-16, Al-27, Si-28, Si-30, Mn-55, Cu-63, Cu-65, U-234, U-235, U-236 and U-238.
  Thermal scattering data for H in H2O is used.
  For cases 1 _ 3 B-10, B-11 is also present.

4. HEU-SOL-THERM-042 (8 cases) [4]
- Unreflected cylinders (5 ft and 9 ft diameter) of highly enriched uranyl nitrate solution. The uranium concentration was varied.
- The uranium enrichment was 93% 235U.
- The isotopes in these benchmark models are H-1, C-nat, N-14, O-16, Cr-50, Cr-52, Cr-54, Fe-54, Fe-56, Fe-58, Ni-58, Ni-60, Ni-62, Ni-64, Mo-92, Mo-94, Mo-98, Mo-100, U-234, U-235, U-236, U-238.
  Thermal scattering data for H in H2O is used.

1. **HEU-MET-FAST-001** (1 case, 'Godiva')

GODIVA	MCNP	MCNP 5	MCNP 5	MCNP 4C3	MCNP 4C3	MCNP 5	MCNP 5	MCNP 4C3	MCNP 4C2
	ENDF-V	ENDF-V	ENDF-VI (6.6)	ENDF-VI (6.8)	ENDF/B-VIIb1	ENDF/B-VIIb1	ENDF/B-VIIb1	ENDF/B-VIIb2	ENDF/B-VIIb2
	LANL	NNDC BNL	NNDC BNL	NRG Petten	NRG Petten	NNDC BNL	LANL	NRG Petten	VUJE / FEI SUT
CASE (k_{eff})	0.9968 (90)	0.99751 (60)	0.99827 (61)	0.99644 (40)	0.99980 (19)	1.00004 (33)	0.9994 (30)	0.99988 (20)	1.00001 (22)

2. **HEU-SOL-THERM-004** (6 cases)

	MCNP	MCNP 5	MCNP 4C3	MCNP 5	MCNP 4C3	MCNP 4C2
	ENDF-VI (6.0)	ENDF-VI (6.6)	ENDF/B-VIIb1	ENDF/B-VIIb1	ENDF/B-VIIb2	ENDF/B-VIIb2
	LANL	NNDC BNL	NRG Petten	NNDC BNL	NRG Petten	VUJE / FEI SUT
CASE 1 (k_{eff})	1.0089 (80)	0.98512 (50)	0.98500 (84)	0.98375 (56)	0.98487(91)	0.98426 (53)
CASE 2 (k_{eff})	1.0043 (100)	0.97981 (58)	0.97938 (93)	0.98054 (59)	0.98306(102)	0.97945 (54)
CASE 3 (k_{eff})	1.0082 (110)	0.98457 (102)	0.98580 (106)	0.98626 (111)	0.98655(95)	0.98585 (53)
CASE 4 (k_{eff})	1.0079 (110)	0.98294 (52)	0.98808 (102)	0.99052 (55)	0.99088(94)	0.99002 (60)
CASE 5 (k_{eff})	1.0035 (110)	0.97392 (58)	0.98857 (93)	0.98833 (57)	0.98722(104)	0.98911 (59)
CASE 6 (k_{eff})	0.9998 (120)	0.95376 (115)	0.98473 (123)	0.98411 (59)	0.98597(103)	0.98661 (60)

3. HEU-SOL-THERM-013 (4 cases, 'ORNL-1', : : :, 'ORNL-4')

	MCNP 4a ENDF-V GIT/WSR	MCNP 5 ENDF-VI (6.6) NNDC BNL	MCNP 4C3 ENDF-VI (6.8) NRG Petten	MCNP 4C3 ENDF/B-VIIb1 NRG Petten	MCNP 5 ENDF/B-VIIb1 NNDC BNL	MCNP 4C3 ENDF/B-VIIb2 NRG Petten	MCNP 4C2 ENDF/B-VIIb2 VUJE / FEI SUT
CASE 1 (k_{eff})	1.0001 (40)	0.99934 (39)	0.99899(60)	0.99789 (58)	0.99876 (38)	0.99777(57)	0.99868 (37)
CASE 2 (k_{eff})	0.9991 (40)	0.99799 (41)	0.99824(70)	0.99731 (56)	0.99765 (40)	0.99741(74)	0.99761 (42)
CASE 3 (k_{eff})	0.9960 (40)	0.99613 (47)	0.99573(80)	0.99330 (71)	0.99310 (45)	0.99421(69)	0.99372 (43)
CASE 4 (k_{eff})	0.9971 (40)	0.99682 (51)	0.99708(60)	0.99638 (71)	0.99469 (45)	0.99726(54)	0.99632 (47)

4. HEU-SOL-THERM-042 (8 cases)

	MCNP 4b ENDF-V WSMS LLC	MCNP 5 ENDF-VI (6.6) NNDC BNL	MCNP 4C3 ENDF-VI (6.8) NRG Petten	MCNP 4C3 ENDF/B-VIIb1 NRG Petten	MCNP 5 ENDF/B-VIIb1 NNDC BNL	MCNP 4C3 ENDF/B-VIIb2 NRG Petten	MCNP 4C2 ENDF/B-VIIb2 VUJE / FEI SUT
CASE 1 (k_{eff})	0.9976 (30)	0.99649 (56)	0.99641(53)	0.99573 (50)	0.99664 (38)	0.99577(48)	0.99750 (27)
CASE 2 (k_{eff})	0.9979 (30)	0.99811 (53)	0.99798(41)	0.99580 (47)	0.99674 (26)	0.99623(56)	0.99636 (28)
CASE 3 (k_{eff})	1.0017 (20)	1.00073 (41)	0.99947(39)	0.99862 (37)	1.00021 (23)	1.00101(43)	1.00185 (22)
CASE 4 (k_{eff})	1.0023 (20)	1.00102 (38)	1.00088(38)	1.00076 (35)	1.00128 (28)	1.00176(40)	1.00343 (20)
CASE 5 (k_{eff})	0.9995 (20)	0.99767 (33)	1.00081(29)	0.99964 (29)	0.99881 (22)	0.99944(36)	1.00082 (17)
CASE 6 (k_{eff})	1.0002 (20)	1.00027 (36)	1.00076(29)	0.99937 (30)	0.99995 (18)	1.00031(36)	1.00089 (18)
CASE 7 (k_{eff})	1.0017 (20)	1.00097 (32)	0.99972(23)	1.00012 (31)	1.00087 (22)	0.99933(29)	1.00105 (17)
CASE 8 (k_{eff})	1.0016 (10)	1.00073 (27)	1.00127(27)	1.00081 (26)	1.00152 (17)	1.00055(30)	1.00146 (14)

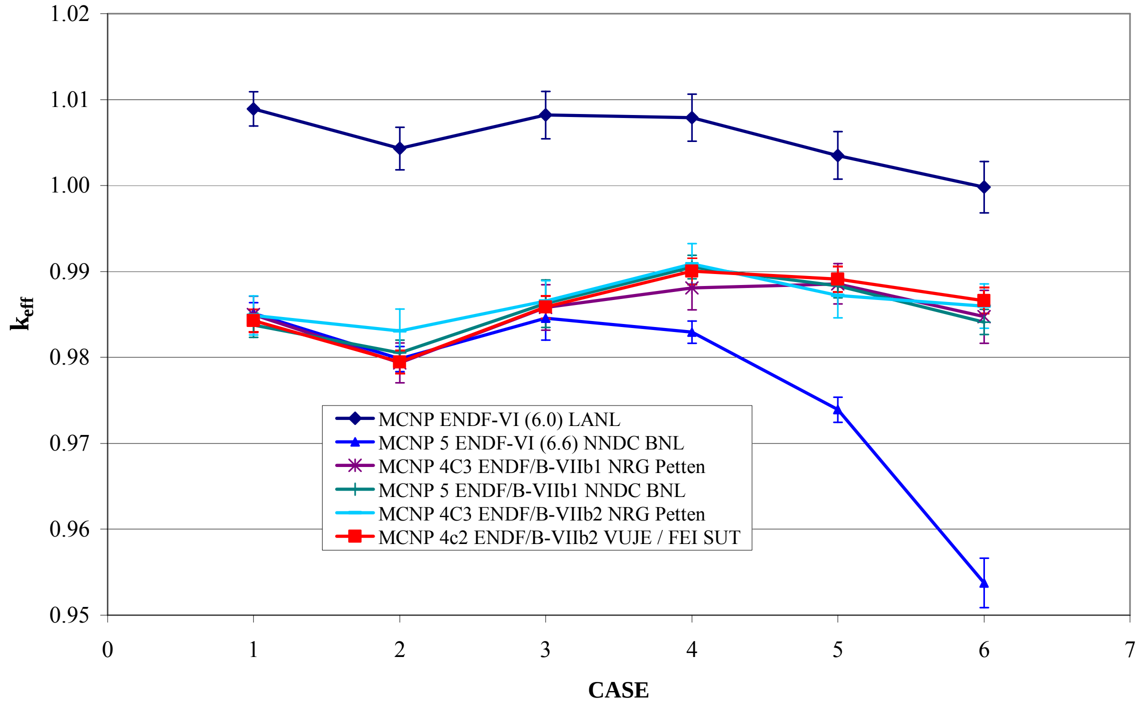

Fig. 1: HEU-SOL-THERM-004 *- reflected uranyl-fluoride solutions in heavy water.*

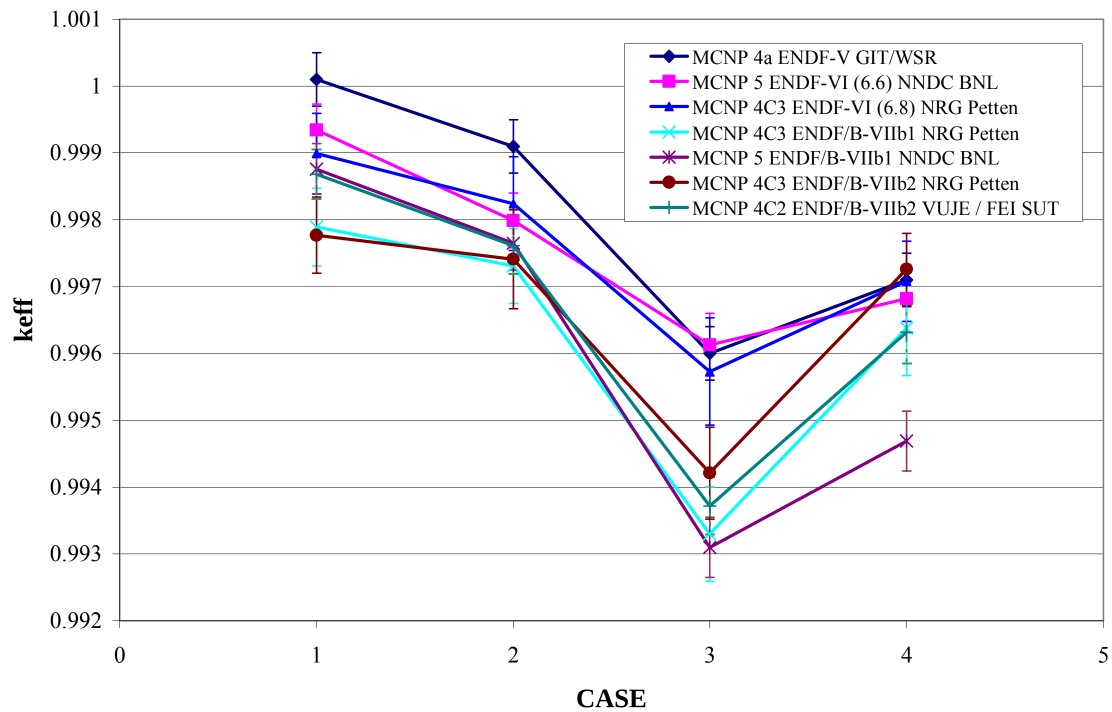

Fig. 2: HEU-SOL-THERM-013 *- uranyl nitrate solutions poisoned with boric acid in an unreflected sphere.*

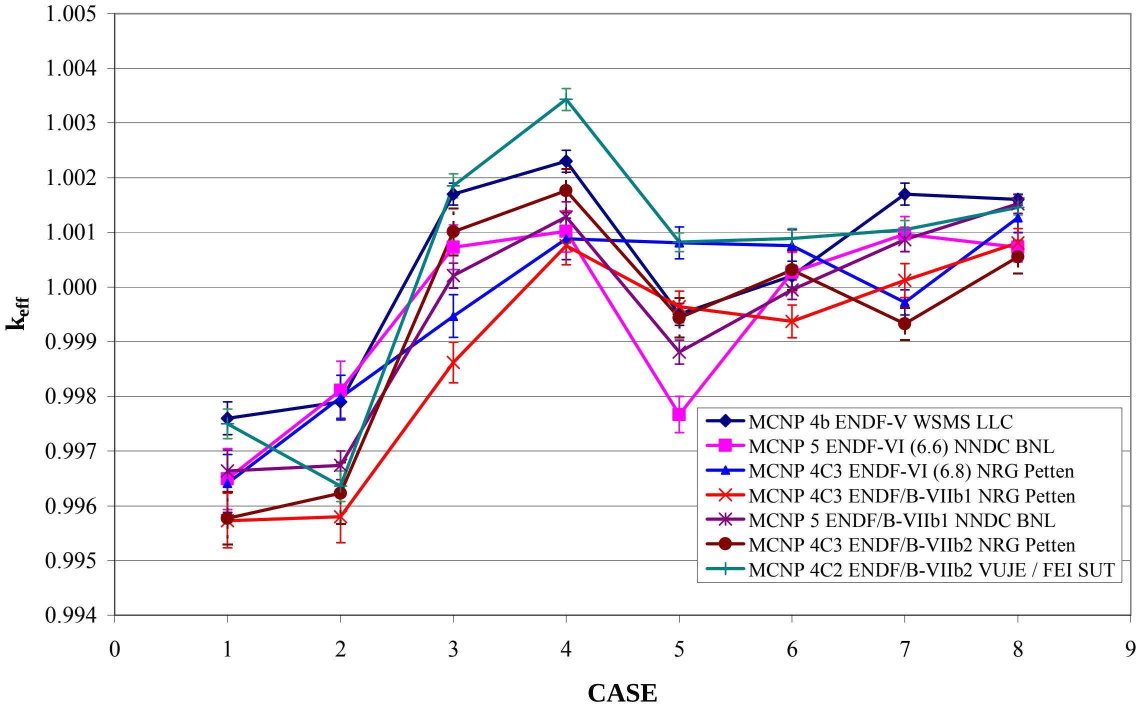

Fig. 3: HEU-SOL-THERM-042 *- unreflected cylinders (5 ft and 9 ft diameter) of highly enriched uranyl nitrate solution.*

5. Results and Conclusions

The application of NJOY 99.90 on ENDF/B-VIIb2 plus two small patches results 391 ACE files from 393 ENDF evaluations. ACE files for Th-232 and Pa-231 were not produced because for these materials are needed special NJOY patch. All 391 ACE files run through GODIVA test successfully, only for Rh-103 is needed one MCNP patch.

The second part of this study shows that majority lines in figures have very similar development for all of cases. Some curves mainly in fig. 1 are out of the trend. These lines are still object of the study and interest.

Acknowledgement

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