

# Jezebel Benchmark Calculations performed with MCNP4A

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## SUMMARY

In this report the results are given of the Jezebel criticality benchmark obtained by using the Monte Carlo code MCNP4A [1]. Results are given for both ENDF/B-V and JEF2.2 data. When JEF2.2 data are used, the resulting value of  $k_{eff}$  appears to be approximately 1 % lower than the result obtained by using ENDF/B-V data. This difference is due to a lower fission rate and a higher capture rate in  $^{239}\text{Pu}$  from JEF2.2 for  $67 \text{ keV} < E_n < 10.0 \text{ MeV}$ .

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# 1. INTRODUCTION

The Jezebel criticality benchmark [2, 3] consists of a sphere of radius 6.385 cm containing metallic plutonium fuel of the following composition:  $^{239}\text{Pu}$ : 0.03705,  $^{240}\text{Pu}$ : 0.001751 and  $^{241}\text{Pu}$ : 0.000117 atoms/barn-cm. The Jezebel Criticality benchmark [4] is a fast benchmark, which can be used for testing Pu cross sections in the high energy range. In this report results are given from MCNP calculations using cross section data from the JEF2.2 and ENDF/B-V library. Extra care was given to a correct procedure to obtain  $k_{eff}$  values from an MCNP criticality calculation. A comparison is given between results from MCNP4A and the previous version MCNP4.2. A comparison with results obtained by GE [4] is given as well.

## 2. USING MCNP FOR CRITICALITY CALCULATIONS

It is known [5] that Monte Carlo criticality calculations in principle suffer from a bias in the calculated value of  $k_{eff}$ . However, by using a stringent procedure, this bias can be made very small. It is essential to use a fission source distribution which is well converged.

Therefore, the following standard procedure was used (MCNP manual [1] page 2-153):

1. Starting from a point source, a fission source distribution was obtained by performing a calculation with a small batch size and a large number of cycles.
2. The fission source produced in step 1 was used in a subsequent calculation with a larger batch size and a smaller number of cycles.
3. Finally, the fission source obtained in step 2 was assumed to be converged and used in a final calculation with an even larger batch size.

Calculations were performed with the following parameters:

1. Batch size: 1000, initial guess of  $k_{eff}$ : 1, number of total cycles: 210, number of active cycles: 200, the first cycle starting from a point source in the center of the model
2. Batch size: 4000, initial guess of  $k_{eff}$ : 1, number of total cycles: 40, number of active cycles: 30, the first cycle uses a fission source produced in the last cycle of the previous MCNP run.
3. As the previous step, except for the batch size, now being 40000.

Proceeding this way, we finally obtain:

$$k_{eff} = 1.00240, \quad \sigma = 0.00017$$

In these calculations ENDF/B-V data were used.

In order to compare the result of this procedure with a calculation of the average value of  $k_{eff}$  obtained from several MCNP runs, the following calculations were done as well:

First  $k_{eff}$  was calculated by MCNP using a point source in the center of the Jezebel model, the batch size being 1000 neutrons. Starting with an initial guess of  $k_{eff} = 1$ , a number of 210 cycles then were used, the first ten being settle cycles so that the last 200 active cycles were used for the calculation of  $k_{eff}$ . Then the final fission source produced by this calculation was used by a next run of MCNP using identical parameters and giving a second estimate for  $k_{eff}$ . Using the fission source of each run in a subsequent run, this procedure was repeated 21 times until a sequence of 23 values of  $k_{eff}$  finally was obtained. These values and their corresponding standard deviations are plotted in fig. 2.1.

From this sequence, mean and standard deviation are:

$$k_{eff} = 1.00242, \quad \sigma = 0.00169$$

As  $k_{eff} = 1.00240 \pm 0.00017$  is well within  $k_{eff} = 1.00242 \pm 0.00169$ , it may be concluded that the proposed standard procedure gives a reliable result for  $k_{eff}$ .

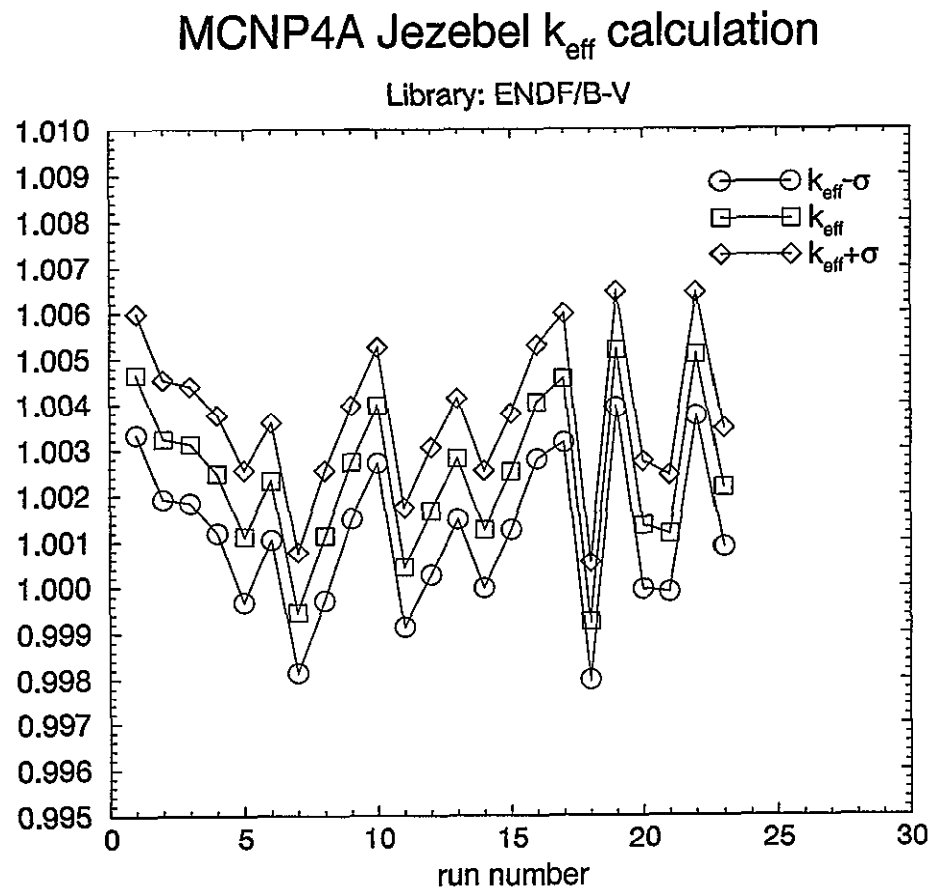


Figure 2.1  $k_{eff}$  and corresponding error boundaries  $k_{eff} \pm \sigma$  for 23 subsequent MCNP runs,  $\sigma$  denoting the standard deviation calculated by MCNP

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### 3. CALCULATIONS

#### 3.1 Comparison MCNP4A - MCNP4.2

In the past several criticality benchmarks have been performed using MCNP4.2. A consistency check was performed in order to be able to relate these results obtained by MCNP4.2 with those obtained by MCNP4A.

#### 3.2 Comparison ECN - GE results

In [4] the results are given of the Jezebel Benchmark as obtained by GE using MCNP4.2 and ENDF/B-V cross section data. Using the procedure mentioned in section 2, calculations were performed by us also using MCNP4.2 and ENDF/B-V data.

#### 3.3 Comparison of JEF2.2 and ENDF/B-V data

Calculations were performed with JEF2.2 and ENDF/B-V cross section data in order to study the dependence on the cross section data used in the calculations. Calculations were again performed using the procedure mentioned in section 2.

## 4. RESULTS

### 4.1 Comparison MCNP4A - MCNP4.2

Using the procedure of section 2, the following results (Table 4.1) were obtained:

Table 4.1  $k_{eff}$  calculated by MCNP4A and MCNP4.2

	$k_{eff}$
MCNP4A	$1.00240 \pm 0.00017$
MCNP4.2	$1.00248 \pm 0.00020$

It can be concluded that there are no statistically significant differences between MCNP4.2 and MCNP4A results.

### 4.2 Comparison ECN - GE results

Table 4.2 shows the results of the comparison between ECN and GE:

Table 4.2  $k_{eff}$  calculation performed by GE and ECN

	$k_{eff}$
GE	$1.00073 \pm 0.00110$
ECN	$1.00248 \pm 0.00020$

These results do not agree within the  $1\sigma$  error bar, but there is no strong disagreement. Moreover, it is not clear which procedure was used by GE to arrive at the results.

### 4.3 Comparison of JEF2.2 and ENDF/B-V data

It appears that there is a substantial difference between the results obtained with JEF2.2 data and those obtained with ENDF/B-V data (table 4.3). The JEF2.2 data result is 0.8 % low, whereas the ENDF/B-V result is only 0.1 % high. The Monte Carlo results obtained with JEF2-2 data are in good agreement with those obtained with deterministic calculations [6]. In the latter calculations, a value of 0.991279 is obtained for  $k_{eff}$ .

Table 4.3  $k_{eff}$  calculated by MCNP4A using JEF2.2 and ENDF/B-V data

	$k_{eff}$
JEF2.2	$0.99232 \pm 0.00039$
ENDF/B-V	$1.00126 \pm 0.00029$

A more detailed analysis can be made by comparing reaction rates in several energy groups. The group structure for representation of the results is given in Table 4.4.

Reaction rates are given in tables 4.5 to 4.7.

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From these results it can be deduced that the main difference in  $k_{eff}$  is due to a significant difference in the fission rate and capture rate of  $^{239}\text{Pu}$  in group 4. This difference is due to differences in  $^{239}\text{Pu}$  cross sections in ENDF/B-V and JEF2.2. In [7], it was already concluded that the  $^{239}\text{Pu}$  cross sections should be modified in the range  $25 \text{ Kev} < E_n < 20 \text{ MeV}$ . The results presented here are not in disagreement with these conclusions. A comparison of the total fission cross section of  $^{239}\text{Pu}$  between JEF2.2 and ENDF/B-V in the relevant energy range is given in fig. 4.1.

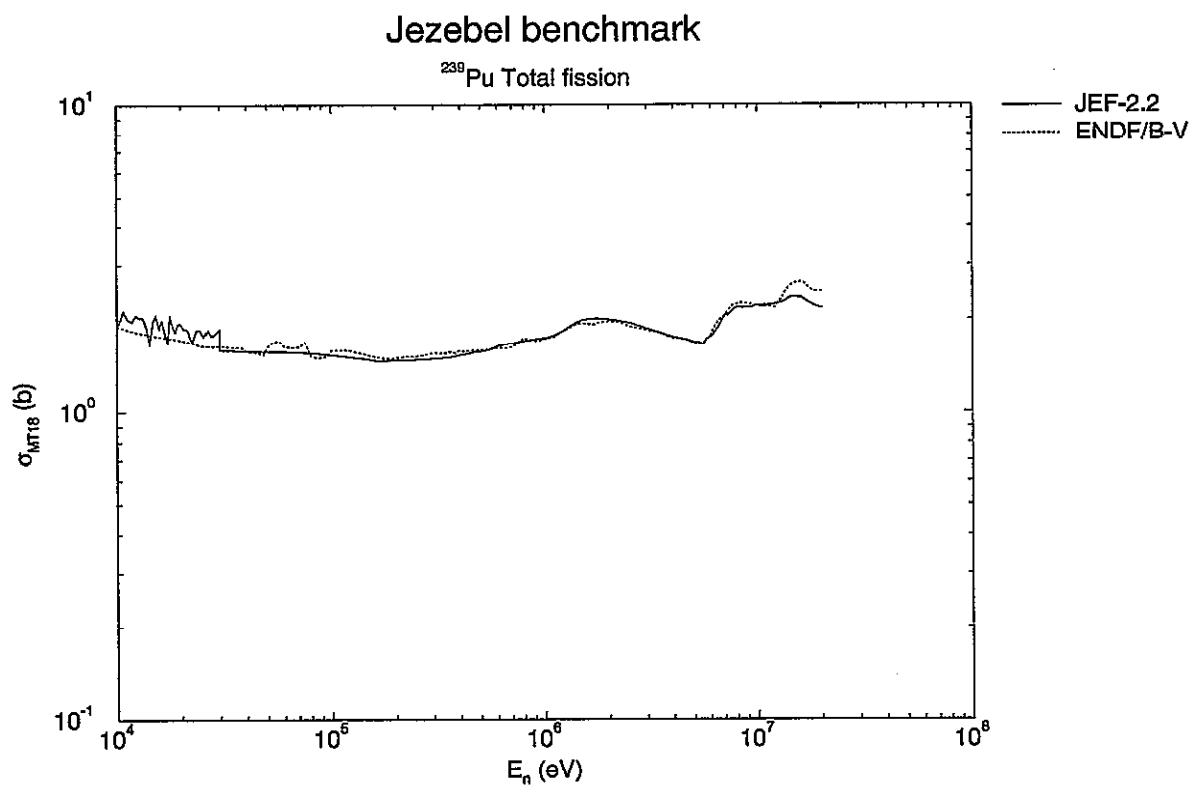


Figure 4.1  $^{239}\text{Pu}$  total fission cross section for JEF2.2 and ENDF/B-V

Table 4.4 Group structure for calculating the reaction rates

group	$E_{low}$ (eV)	$E_{high}$ (eV)
1	$10^{-5}$	0.625
2	0.625	3355
3	3355	$67.38 \cdot 10^3$
4	$67.38 \cdot 10^3$	$10.0 \cdot 10^6$
5	$10.0 \cdot 10^6$	$20.0 \cdot 10^6$

Table 4.5 Fission rate of  $^{239}\text{Pu}$  and  $^{240}\text{Pu}$ 

group	Fission rate of $^{239}\text{Pu}$		Fission rate of $^{240}\text{Pu}$	
	JEF2.2	ENDF/B-V	JEF2.2	ENDF/B-V
1	0.000E+00	0.000E+00	0.000	0.000
2	4.943E-08	1.051E-08	1.378E-09	4.128E-13
3	7.386E-06	6.957E-06	1.627E-08	1.568E-08
4	5.179E-04	5.253E-04	1.670E-05	1.715E-05
5	1.348E-06	8.850E-07	6.071E-08	4.176E-08

Table 4.6 Fission rate of  $^{241}\text{Pu}$  and capture rate of  $^{239}\text{Pu}$ 

group	Fission rate of $^{241}\text{Pu}$		Capture rate of $^{239}\text{Pu}$	
	JEF2.2	ENDF/B-V	JEF2.2	ENDF/B-V
1	0.000	0.000	0.000	0.000
2	3.442E-10	1.193E-10	3.538E-08	1.659E-08
3	3.732E-08	3.418E-08	2.282E-06	2.172E-06
4	1.517E-06	1.515E-06	2.294E-05	1.591E-05
5	3.886E-09	2.512E-09	3.971E-14	9.059E-10

Table 4.7 Total flux

group	Total flux	
	JEF2.2	ENDF/B-V
1	0.000	0.000
2	3.627E-07	1.201E-07
3	1.197E-04	1.134E-04
4	7.947E-03	8.064E-03
5	1.629E-05	1.074E-05

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## 5. CONCLUSIONS

- In our report the results are given for the JEZEBEL criticality benchmark, performed with MCNP4A using JEF2.2 and ENDF/B-V cross section data.
- Using ENDF/B-V data, agreement is found between our results and those obtained by GE [4].
- A good agreement is found between results from MCNP4A and those from MCNP4.2
- The results obtained with JEF2.2 data agree with results from deterministic calculations [6].
- The results obtained with JEF2.2 data differ significantly from those obtained with ENDF/B-V data. This difference is due to a lower fission rate and a higher capture rate in  $^{239}\text{Pu}$  from JEF2.2 for  $67 \text{ keV} < E_n < 10.0 \text{ MeV}$ . Modifications of the  $^{239}\text{Pu}$  JEF2.2 cross sections, as already suggested in [7], seem to be necessary.

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## REFERENCES

- [1] Briesmeister, J.G., Ed.: *MCNP - A General Monte Carlo N - Particle Transport Code*, Version 4A, LA-12625-M, Los Alamos National Laboratory, November 16, 1993.
- [2] Hansen, G.E. and Paxton, H.C.: *Reevaluated specifications of some LANL Fast Neutron Systems*, LA-4208, Los Alamos National Laboratory, 1969.
- [3] Cross Section Evaluating Group Benchmark Specifications, BNL-19302 (ENDF-202), November 1974/Revised October 1978.
- [4] Sitaraman, S.: *MCNP: Light Water Reactor Critical Benchmarks*, NEDO-32028 Class I, GE Nuclear Energy, San Jose, March 1992.
- [5] Gelbard, E.M. and Prael, R.: *Computation of standard deviations in eigenvalue calculations*, Progress in Nuclear Energy, Vol. 24, pp. 237-241, 1190.
- [6] Oppe, J. and Janssen A.J.: *Fast Reactor Benchmarking with JEF2 data*, ECN internal report NFA-ENGINE-94-01, Petten, January 1994.
- [7] Fort, E., Mounie, C. and Okajima, S.: *JEF2 Validation, Action Sheet 2: Validation in the high energy range  $100 \text{ KeV} < E < 10 \text{ MeV}$* , JEF/DOC - 439.

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## APPENDIX A. JEZEBEL MCNP BENCHMARK INPUT

message: ixr

jezebel fuel sphere based on endfb5 lib. (300 k)

c

c     infinite dilute 239Pu cross sections used

c

1	1	.038918	-1
2	1	.038918	1 -2
3	1	.038918	2 -3
4	0	3	

1	so	1.0
2	so	3.0
3	so	6.385

imp:n 1 1 1 0

kcode 40000 1.0 10 70

m1 94239.50c 0.03705 94240.50c 0.001751 94241.50c 0.000117

m2 94239.50c 1.0

m3 94240.50c 1.0

m4 94241.50c 1.0

vol 4.18879 108.9085 977.2662 0

ctme 3000

print

e0 .625e-6 3.355e-3 6.7379e-2 10. 20.0

f1:n 3

f4:n 1 2 3 t

fc4 fission reaction rates in the three Pu isotopes

units: fissions/cm3\*source neutron

(n,gamma) in 239Pu

units: captures/cm3\*source neutron

flux

units: neutrons/cm2\*source neutron

fm4 (0.03705 2 -6)

(0.001751 3 -6)

(0.000117 4 -6)

(0.03705 2 102)

(1)

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