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The JEZEBEL benchmark

Results of MCNP4A calculations

A. Hogenbirk

Abstract

In this report the results are presented of JEZEBEL benchmark calculations. The calculations were performed with MCNP4A. JEF-2.2 based cross section data were taken from the EJ2-MCNP library.

Tabulated groupwise reaction rates, leakage data, central fission ratios and central activation ratios are given.

An indication is found for a too high value of $\sigma_{(n,f)}$ for ^{235}U.

Keywords

reactivity calculations
Monte Carlo calculations
MCNP4A
JEF-2.2
JEZEBEL
Plutonium

CONTENTS

1. INTRODUCTION

In this report the results are presented of the JEZEBEL benchmark calculation, as defined in the CSEWG Benchmark Book [1]. The JEZEBEL benchmark consists of a homogeneous, bare (critical) sphere of plutonium metal. The benchmark results can be used to validate Pu cross-section data in the fission source energy range.

The calculations were performed with the Monte Carlo code MCNP4A. JEF-2.2 based cross section data were taken from the EJ2-MCNP library [2], as processed at ECN Petten.

In chapter 2 a short description is given of the method used in the calculations.

Tabulated groupwise reaction rates and spectral indices are given in chapter 3.

A concise discussion of the results is given in chapter 4.

Finally, in chapter 5 the conclusions resulting from this work are given.

2. METHOD

2.1 Geometry

The JEZEBEL benchmark consists of a homogeneous, bare (critical) sphere of plutonium metal. The critical radius amounts to 6.385 cm. The fast spectrum prevailing in the sphere can be used to validate plutonium data in the fission source energy range.

The simple geometrical model for this benchmark calculation was taken from [1]. The composition used in the calculations is given in table 2.1.

2.2 Cross sections

JEF-2.2 based cross section data for all isotopes were taken from the EJ2-MCNP library [2], processed at ECN Petten. For the determination of measured activation ratios data for ^{63}Cu are required, which are not present on the JEF-2.2 evaluation. Therefore, these data were taken from the EFF-2.4 evaluation.

Table 2.1 *JEZEBEL benchmark. Composition of the homogeneous fuel sphere as used in the calculations.*

isotope	density ($*10^{24}$ at cm^{-3})
^{239}Pu	0.03705
^{240}Pu	0.001751
^{241}Pu	0.000117
^{nat}Ga	0.001375

3. RESULTS

Required response parameters are given in [3]. They include k_{eff}, reaction rates, leakage, spectral indices and activation ratios. Reaction rates and cross sections were calculated in the 4-group structure as given in [3] (see table 3.1).

In this chapter tables with calculated results are presented. Values are given with relative percentage errors. Reaction rates (normalised per absorbed neutron) are given in table 3.2. The leakage spectrum (normalised per fission neutron) is given in table 3.3. Experimental and calculated values of central fission ratios are given in table 3.4. In table 3.5 the experimental and calculated values of central activation ratios are given. The experimental data were taken from [1]. It is noted, that data for ^{51}V are not available on either the JEF-2.2 or the EFF-2.4 evaluation. Data for ^{nat}V were used instead in order to determine the activation ratio. Although the abundance of ^{51}V is 99.750%, differences in the activation ratio may occur due to this approximation.

Due to the small size of the fuel sphere, the central region in which the magnitude of the neutron flux is constant, is only small. In this study central fission rates and central activation ratios were determined in a sphere with a radius of 0.2 cm. This value was determined in previous studies [4].

Table 3.1 *Energy group structure used for the representation of the calculated results.*

group	$E_{g,low}$ (eV)	$E_{g,high}$ (eV)
0	1.0000E+7	2.0000E+7
1	2.2313E+6	1.0000E+7
2	497.87E+3	2.2313E+6
3	1.0000E−5	497.87E+3

Table 3.2 *JEZEBEL benchmark. Group reaction rates in fuel sphere. The data are normalised per absorbed neutron.*

$k_{eff} = 0.9952 \pm 0.01\%$					
group	nu*fission	fission	absorption	(n,2n)	capture
^{239}Pu					
total	2.89564E+00 ± 0.01	9.22761E−01 ± 0.01	9.66417E−01 ± 0.01	2.06403E−03 ± 0.19	4.36562E−02 ± 0.03
0	1.16561E−02 ± 0.51	2.54589E−03 ± 0.51	2.54589E−03 ± 0.51	4.80222E−04 ± 0.51	7.51288E−11 ± 0.70
1	9.55966E−01 ± 0.04	2.79634E−01 ± 0.04	2.81260E−01 ± 0.04	1.58381E−03 ± 0.19	1.62652E−03 ± 0.05
2	1.39954E+00 ± 0.03	4.59231E−01 ± 0.03	4.76121E−01 ± 0.03		1.68922E−02 ± 0.03
3	5.28470E−01 ± 0.05	1.81352E−01 ± 0.05	2.06490E−01 ± 0.05		2.51374E−02 ± 0.06
^{240}Pu					
total	9.26750E−02 ± 0.02	2.95248E−02 ± 0.02	3.23878E−02 ± 0.02	1.21389E−04 ± 0.21	2.86307E−03 ± 0.03
0	5.16153E−04 ± 0.51	1.14643E−04 ± 0.51	1.14706E−04 ± 0.51	2.91853E−05 ± 0.52	6.32332E−08 ± 0.52
1	4.05189E−02 ± 0.04	1.20514E−02 ± 0.04	1.22261E−02 ± 0.04	9.22032E−05 ± 0.22	1.74663E−04 ± 0.05
2	4.91869E−02 ± 0.03	1.64932E−02 ± 0.03	1.77387E−02 ± 0.03		1.24540E−03 ± 0.03
3	2.45322E−03 ± 0.06	8.65399E−04 ± 0.06	2.30833E−03 ± 0.05		1.44294E−03 ± 0.06
^{241}Pu					
total	8.66321E−03 ± 0.01	2.72547E−03 ± 0.01	3.13932E−03 ± 0.01	3.87363E−05 ± 0.12	4.13847E−04 ± 0.02
0	3.36006E−05 ± 0.51	7.33863E−06 ± 0.51	7.33863E−06 ± 0.51	1.71233E−06 ± 0.53	1.27506E−13 ± 0.72
1	2.55782E−03 ± 0.04	7.34175E−04 ± 0.04	7.71899E−04 ± 0.04	3.70240E−05 ± 0.12	3.77266E−05 ± 0.05
2	4.02588E−03 ± 0.03	1.29476E−03 ± 0.03	1.52292E−03 ± 0.03		2.28153E−04 ± 0.03
3	2.04590E−03 ± 0.05	6.89195E−04 ± 0.05	8.37164E−04 ± 0.05		1.47968E−04 ± 0.05
^{nat}Ga					
total			6.13751E−04 ± 0.03	1.64659E−05 ± 0.62	5.78240E−04 ± 0.03
0			1.78001E−06 ± 0.51	1.57842E−05 ± 0.65	3.73260E−08 ± 0.51
1			6.98944E−05 ± 0.04	6.81669E−07 ± 0.89	3.63026E−05 ± 0.04
2			2.36271E−04 ± 0.03		2.36093E−04 ± 0.03
3			3.05807E−04 ± 0.05		3.05807E−04 ± 0.05

Table 3.3 *JEZEBEL benchmark. Leakage spectrum at fuel sphere boundary. The data are normalised per fission neutron.*

$k_{eff} = 0.9952 \pm 0.01\%$	
group	leakage
total	6.67902E−01 ± 0.01
0	1.61235E−03 ± 0.52
1	2.06901E−01 ± 0.04
2	3.26896E−01 ± 0.03
3	1.32493E−01 ± 0.05

Table 3.4 *JEZEBEL benchmark. Central fission ratios. Experimental data were taken from [1].*

$k_{eff} = 0.9952 \pm 0.01\%$			
index	exp. value	calc. value	C/E
$\sigma_f(^{238}\mathrm{U})/\sigma_f(^{235}\mathrm{U})$	2.137E−01 ± 1.08	2.003E−01 ± 1.23	9.372E−01 ± 1.64
$\sigma_f(^{233}\mathrm{U})/\sigma_f(^{235}\mathrm{U})$	1.578E+00 ± 1.71	1.524E+00 ± 0.96	9.656E−01 ± 1.96
$\sigma_f(^{237}\mathrm{Np})/\sigma_f(^{235}\mathrm{U})$	9.620E−01 ± 1.66	9.154E−01 ± 1.05	9.516E−01 ± 1.97
$\sigma_f(^{239}\mathrm{Pu})/\sigma_f(^{235}\mathrm{U})$	1.448E+00 ± 2.00	1.427E+00 ± 0.97	9.855E−01 ± 2.22

Table 3.5 *JEZEBEL benchmark. Central activation ratios. Experimental data were taken from [1].*

$k_{eff} = 0.9952 \pm 0.01\%$			
index	exp. value	calc. value	C/E
$\sigma_{(n,\gamma)}(^{51}\mathrm{V})/\sigma_f(^{235}\mathrm{U})$	2.300E−03 ± 13.04	1.726E−03 ± 2.52	7.506E−01 ± 13.29
$\sigma_{(n,\gamma)}(^{55}\mathrm{Mn})/\sigma_f(^{235}\mathrm{U})$	2.400E−03 ± 12.50	3.515E−03 ± 1.53	1.464E+00 ± 12.59
$\sigma_{(n,\gamma)}(^{63}\mathrm{Cu})/\sigma_f(^{235}\mathrm{U})$	1.000E−02 ± 6.00	1.063E−02 ± 3.28	1.063E+00 ± 6.84
$\sigma_{(n,\gamma)}(^{93}\mathrm{Nb})/\sigma_f(^{235}\mathrm{U})$	2.300E−02 ± 8.70	2.797E−02 ± 1.32	1.216E+00 ± 8.80
$\sigma_{(n,\gamma)}(^{197}\mathrm{Au})/\sigma_f(^{235}\mathrm{U})$	8.300E−02 ± 2.41	8.084E−02 ± 1.18	9.740E−01 ± 2.69

4. DISCUSSION

The calculated data presented in chapter 3 show that

- the value of k_{eff} is underpredicted by approximately 0.5% in calculations with JEF-2.2 data. This was already observed in several other JEZEBEL benchmark calculations.
- the values of central fission ratios are systematically underpredicted by at least 2%. This could indicate, that the fission cross section for ^{235}U in the JEF-2.2 evaluation is too high.
- some experimental values of central activation ratios are reproduced, but a strong overprediction of $\sigma_{(n,\gamma)}(^{55}\text{Mn})$ is observed. This agrees with other calculations (see e.g. [4]). The underprediction of $\sigma_{(n,\gamma)}(^{51}\text{V})$ may be due to the fact, that in the calculations data for ^{nat}V were used.

The values of central reaction rates depend on the definition of the central region, because of small size of the critical system. More experimental information is needed for a better geometrical modelling of the system.

5. CONCLUSIONS

In this report the results are presented of the JEZEBEL benchmark calculation. Calculations were performed with MCNP4A, using cross section data from the JEF-2.2 evaluation. Group cross section data and group reaction rates were generated in the group structure defined by Rowlands in [3].

It is observed, that the value of k_{eff} is underpredicted by approximately 0.5% in calculations with JEF-2.2 data.

Some indication is found for a too high value of the fission cross section for ^{235}U on the JEF-2.2 evaluation.

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