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Validation of thermal Pu JEF-2.2 data

The PNL and VALDUC benchmarks

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Abstract

Three PNL and three VALDUC plutonium nitrate critical benchmarks were modelled in MCNP4A. Calculations were performed with the Monte Carlo code MCNP4A, using cross-section data from the EJ2-MCNPlib library. The work was done in the framework of validation of this library (which is based upon the JEF-2.2 evaluation) for criticality applications in thermal Pu systems.

The values of k_{eff} and relevant leakage and reaction rate data were calculated.

The values of k_{eff} are overpredicted by approx. 700 pcm.

Keywords

Criticality calculations
Benchmark calculations
MCNP4A
EJ2-MCNPlib
JEF-2.2 cross-section data
Thermal Pu data

CONTENTS

1. INTRODUCTION

Core neutronics calculations require the benchmarking of nuclear data and neutron transport codes used in the analyses. Data for the important U isotopes have been extensively benchmarked in the previous years, also in the framework of the JEF-project (see *e.g.* [1,2]). However, recent benchmark calculations for thermal Pu data are scarce. These data play an important role if the neutronics behaviour of MOX fuel in overmoderated assemblies is studied. Therefore, a benchmark exercise was initiated by Nouri [3].

In this report the results are presented of several benchmarks in which thermal Pu data play an important role. Calculations were performed with the Monte Carlo neutron transport code MCNP4A, using data from the EJ2-MCNPlib [4] library, which is based on the JEF-2.2 evaluation.

In chapter 2 some details are given on the nuclear data used in the analyses. A short description of the benchmarks is given in chapter 3. The model which is used in the calculations is illustrated in chapter 4. The results of the calculations are given in chapter 5. Finally, in chapter 7 conclusions from this work are drawn.

2. NUCLEAR DATA

Nuclear data used in the calculations performed for this report were taken from the EJ2-MCNPlib library [4]. This library contains high-quality data based on the JEF-2.2 evaluation for calculations with the Monte Carlo code MCNP4A [5].

Recently trouble was stirred up by Dr. Bernat [6], who remarked to several people that data for MCNP4A processed by NJOY would suffer from severe drawbacks. A large drawback would be, that the energy distributions for fission neutrons would be represented in an incorrect way on the MCNP-library. This would have a large effect on calculations in thermal Pu systems (an effect of 1000 pcm was mentioned).

Although this problem may be present in libraries produced at IKE, the EJ2-MCNPlib library does not suffer from this problem. A marked advantage of the EJ2-MCNPlib library is the fact, that energy distributions on the library are as close as possible to the original evaluation. This implies that for ^{239}Pu separate energy distributions for fission neutrons from (n, f), (n, nf), $(n, 2nf)$ and $(n, 3nf)$ are given on the library. MCNP4A has the possibility to sample from Maxwell fission spectra and hence uses exactly the same distributions as given on the evaluation.

3. THE PNL AND VALDUC BENCHMARKS

Benchmark calculations for six thermal Pu systems were performed. The benchmarks were selected by Nouri in [3]. They can be subdivided in two groups:

1. PNL benchmarks:
   Plutonium nitrate in spherical geometry. Reflection by light water.
2. VALDUC experiments:
   Plutonium nitrate in cubic tank. Reflection by light water.

Plutonium concentrations range from 13.2 through 119 g/l. The amount of ^{240}Pu in plutonium ranges from 3.1 through 18.9%.

For all benchmarks two calculations were performed:

1. bare sphere geometry:
   Simple spherical model; no reflection. Equivalent bare sphere radii are provided by Nouri in [3].
2. simple geometry:
   Simplified geometrical model, taking into account the most prominent features of the actual geometry.

The PNL benchmarks all have a water reflector. In the VALDUC experiments two different geometries are studied:

1. water reflection at six sides of the fuel tank
2. water reflection at five sides of the fuel tank

Figures of the geometrical models are given in figs. 4.1 through 4.4.

4. CALCULATIONS

4.1 Geometrical model

Outlines of the PNL and VALDUC geometries are given in figs. 4.1 through 4.4. Data were taken from [7].

4.2 Calculational procedure

Neutron transport calculations for this benchmark were performed using the Monte Carlo code MCNP4A [5]. Continuous-energy cross section data were used, which allow for a very detailed simulation of the neutron transport.

The calculation of k_{eff} and the reaction rates was divided into three subsequent steps:

1. As an initial source S_0 an isotropic point source in the centre of the fuel pin was taken. Using a batch size of 100 neutrons, in 100 cycles a geometrically converged source S_1 was produced, which was used in the second step of the calculation.
2. Starting with S_1 a second calculation was performed, using a batch size of 1000 neutrons. In 100 cycles the initial source S_2 for the final step was produced.
3. In the final run the batch size was extended from 1000 to 10000 neutrons. The values of k_{eff} and the reaction rates were calculated in 100 cycles.

4.3 Cross sections

JEF-2.2 based cross-section data for all isotopes were taken from the EJ2-MCNPlib library [4], processed at ECN Petten.

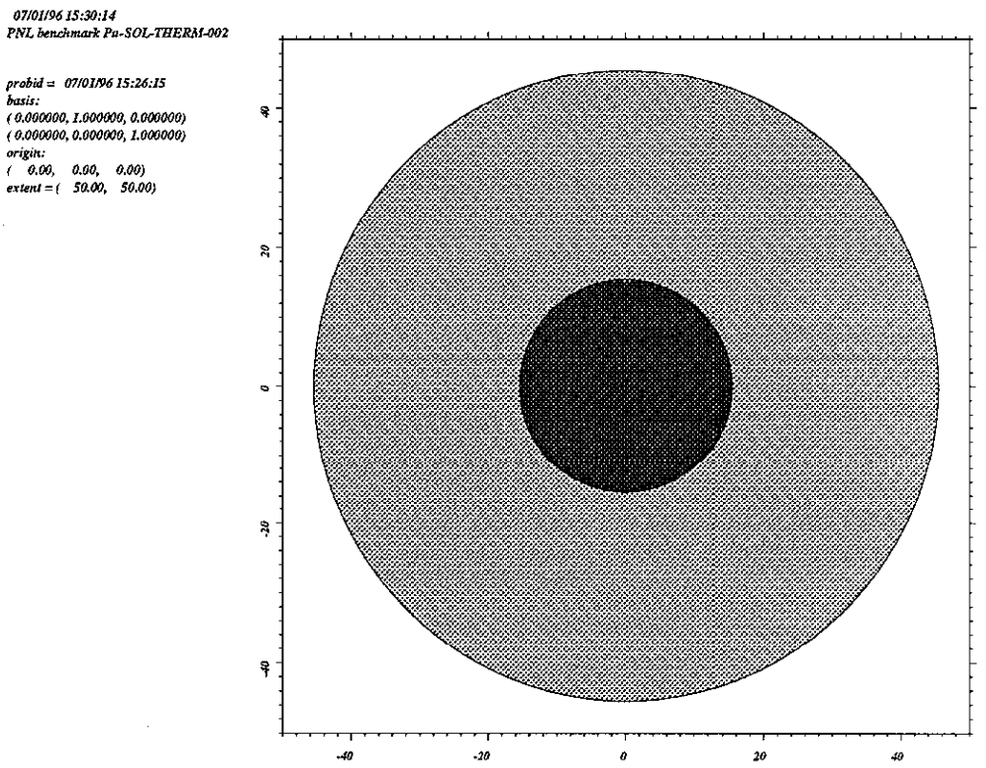

Figure 4.1 *Vertical cross section through the simple MCNP4A model of the PNL geometry (Pu-SOL-THERM-002 case 2). The fuel region is surrounded by a thin shell made of stainless steel and a reflecting water shell.*

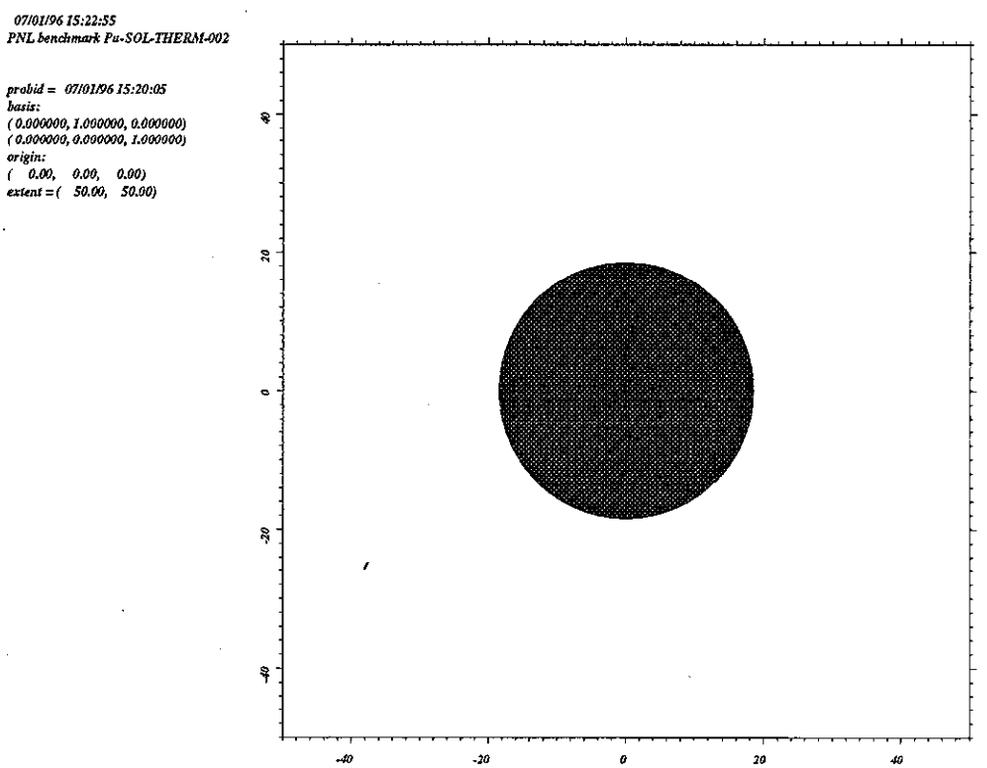

Figure 4.2 *Vertical cross section through the bare sphere MCNP4A model of the PNL geometry (Pu-SOL-THERM-002 case 2). The Pu nitrate solution is contained in a sphere without reflection.*

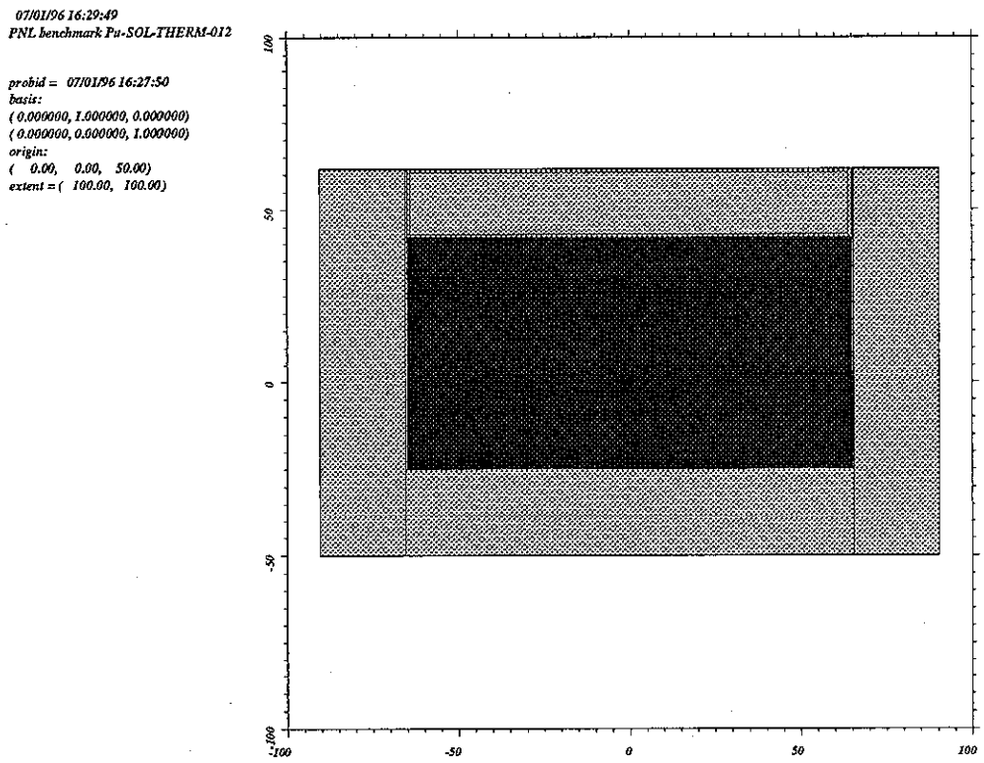

Figure 4.3 *Vertical cross section through the simple MCNP4A model of the VALDUC geometry with reflection on six sides (Pu-SOL-THERM-012 case 5). The fuel region is surrounded by a tank made of stainless steel. On top is a lucoflex box, filled with water. The fuel tank is placed in a pool filled with water.*

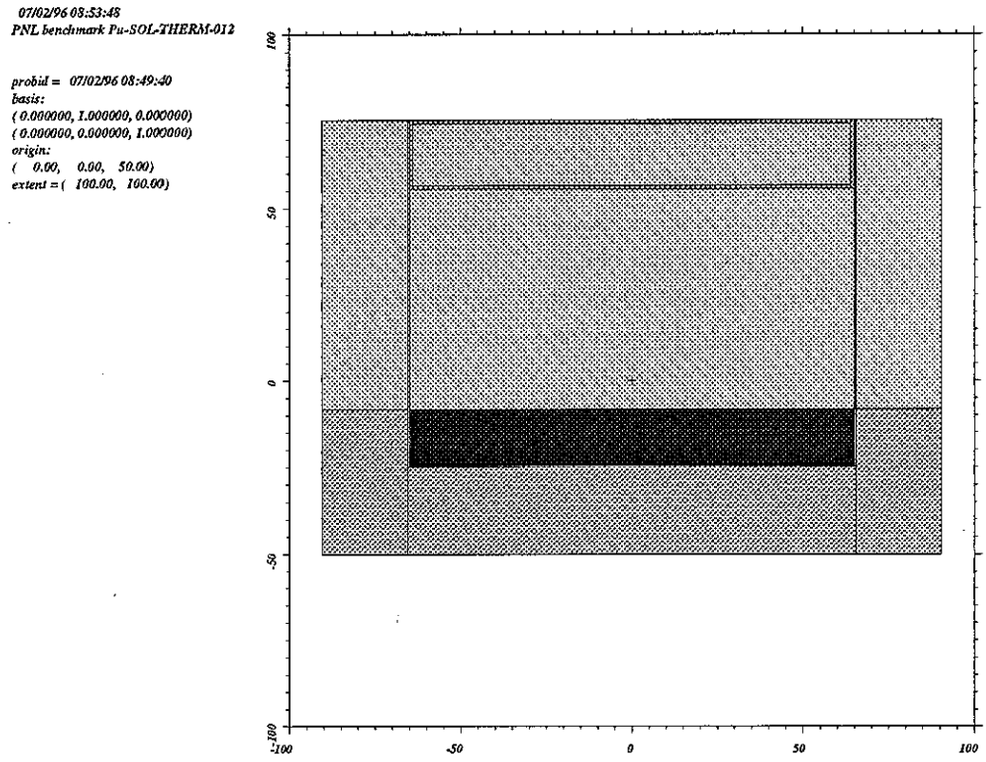

Figure 4.4 *Vertical cross section through the simple MCNP4A model of the VALDUC geometry with reflection on five sides (Pu-SOL-THERM-012 case 6). The fuel region is surrounded by a tank made of stainless steel. On top is a lucoflex box, filled with air. The fuel tank is placed in a pool filled with water.*

5. RESULTS

The neutron flux spectrum calculated in the fuel zone for several benchmarks is given in fig. 5.1. From this fig. it is clear, that in this benchmark exercise a broad range of spectra in thermal Pu systems is probed.

A compilation of calculated values for k_{eff} is given in table 5.1

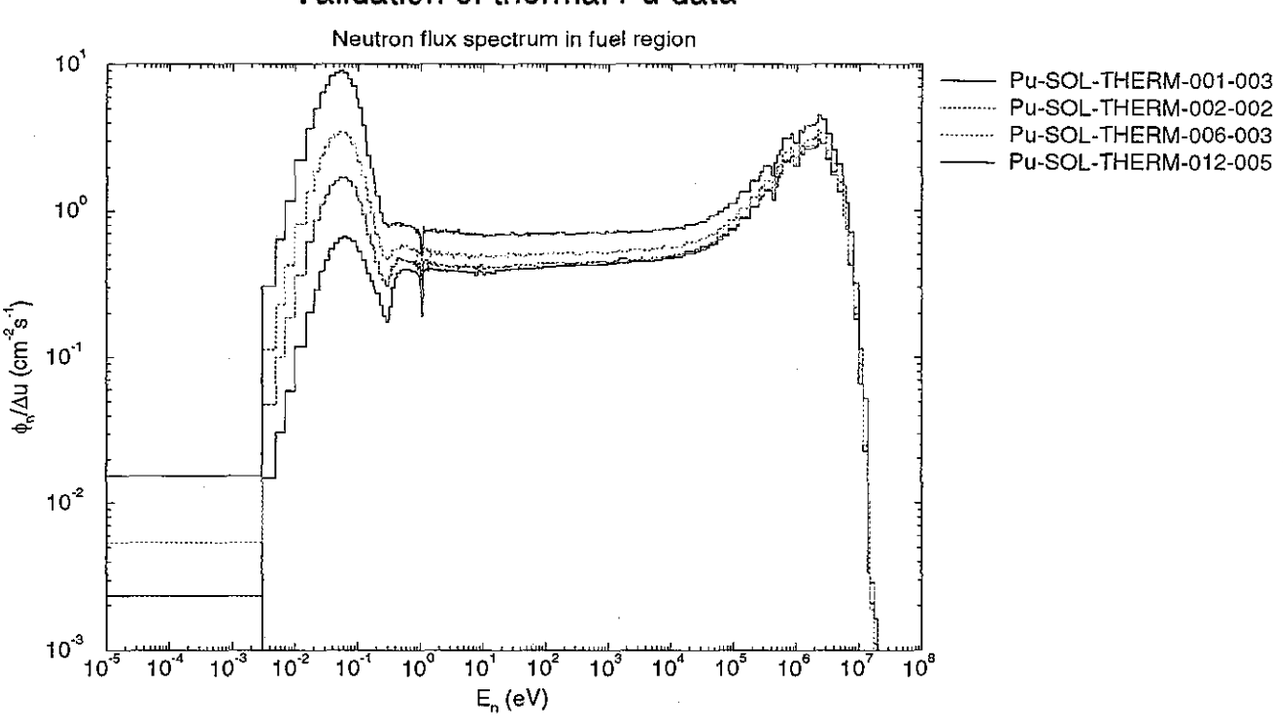

Figure 5.1 *Neutron flux spectrum calculated in the fuel zone in several benchmark geometries.*

Table 5.1 *Results from thermal Pu benchmark calculations. The bare sphere results refer to simplified equivalent bare sphere calculations. Note that for some results the statistical uncertainty is still high; more accurate results will be obtained. Calculations for the missing data are underway.*

identification	case #	C[Pu] (g/l)	geometry	bare sphere radius (cm)	$k_{eff} \pm \sigma$ [%]
Pu-SOL-THERM-001	case 3	119	bare sphere	17.91	1.0077 ± 0.07
Pu-SOL-THERM-001	case 3	119	simple geom.	-	1.0143 ± 0.06
Pu-SOL-THERM-002	case 2	51.42	bare sphere	18.47	1.0032 ± 0.10
Pu-SOL-THERM-002	case 2	51.42	simple geom.	-	1.0029 ± 0.29
Pu-SOL-THERM-006	case 3	26.97	bare sphere	22.09	1.0057 ± 0.27
Pu-SOL-THERM-006	case 3	26.97	simple geom.	-	1.0013 ± 0.24
Pu-SOL-THERM-012	case 5	13.2	bare sphere	53.52	1.0006 ± 0.12
Pu-SOL-THERM-012	case 5	13.2	simple geom.	-	1.0099 ± 0.16
Pu-SOL-THERM-012	case 6	105	bare sphere	21.41	- ± -
Pu-SOL-THERM-012	case 6	105	simple geom.	-	- ± -
Pu-SOL-THERM-012	case 8	52.7	bare sphere	22.25	- ± -
Pu-SOL-THERM-012	case 8	52.7	simple geom.	-	- ± -

6. DISCUSSION

From the results presented in chapter 5 it is clear, that with current data from the JEF-2.2 evaluation the value of k_{eff} in thermal Pu systems is overpredicted in analyses with MCNP4A.

This overpriction is consistent with the results obtained with the group Monte Carlo code MONK (see [3]), although the magnitude is markedly smaller. Analyses with French codes (APOLLO-1 + MORET, APOLLO-2 + TRIMARAN-2, TRIPOLI-4) show a much smaller overprediction, and in some cases even an underprediction.

A (sometimes rather large) discrepancy is observed between the results from analyses in a bare sphere geometry and analyses in a simple realistic geometry. This is probably due to a different calculation of neutron leakage in the analyses with MCNP4A compared to the analyses with deterministic codes with which the equivalent bare sphere radii were determined.

7. CONCLUSIONS

In this report the results are presented of Monte Carlo analyses of thermal Pu systems. Results are given for three PNL systems (Pu nitrate in reflected spherical geometry) and three VALDUC systems (Pu nitrate in reflected cubic geometry). The analyses were performed with MCNP4A using JEF-2.2 based data from the EJ2-MCNPlib library.

In all calculations the value of k_{eff} is overpredicted (by approx. 700 pcm). The overprediction is consistent with results from independent calculations with the group Monte Carlo code MONK, but disagrees with results from calculations with several French code systems.

Further analysis of leakage and relevant reaction rates is needed in order to explain the results.

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