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MCNP modelling of the LMT–006 integral criticality benchmark experiment

Final report

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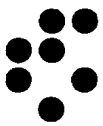

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NASLOV POROČILA: **IJS-DP-12231**
MCNP modeliranje integralnega kritičnega referenčnega eksperimenta LMT-006 **Izdaja:** 0
Bor Kos, mag. jed. teh.; Dr. Peter Schillebeeckx; Dr. Gašper Žerovnik; Dr. Ivo Kodeli

KLJUČNE BESEDE: ICSBEP, referenčni eksperiment, MCNP modeliranje, CAD modeliranje, validacija modela, LMT-006

POVZETEK:

Na podlagi informacij dostopnih v zbirki ICSBEP (International Handbook of Evaluated Criticality Safety Benchmark Experiments) so bili ustvarjeni CAD (Computer Assisted Design) modeli vseh 30 različnih konfiguracij kritičnega referenčnega eksperimenta LMT-006. CAD modeli so bili nato pretvorjeni s pomočjo orodja GRASP v format, primeren za simulacije s programom MCNP (Monte Carlo N-Particle transport code). Novi MCNP modeli so bili validirani s pomočjo rezultatov simulacij drugih kod. Modeli so bili nato uporabljeni za validacijo novejših knjižnic jedrskih podatkov kot na primer JEFF-3.2 in ENDF/B-VII.1.

Zaradi mednarodnega sodelovanja je poročilo pisano v angleščini.

REPORT TITLE: **IJS-DP-12231**
MCNP modelling of the LMT – 006 integral criticality benchmark experiment **Revision:** 0
Bor Kos, MSNE; Peter Shillebeeckx, PhD; Gašper Žerovnik, PhD; Ivo Kodeli, PhD

KEYWORDS: ICSBEP, benchmark experiment, MCNP, modelling, CAD modelling, model validation, LMT-006

ABSTRACT:

Based on the data available from ICSBEP (International Handbook of Evaluated Criticality Safety Benchmark Experiments) handbook CAD (Computer Assisted Design) models of all thirty different configurations of the LMT-006 benchmark experiment were created. Based on these models MCNP (Monte Carlo N-Particle transport code) compatible input files were produced using the GRASP tool. The new MCNP models were validated against the results from existing models. The models were used to validate never nuclear data libraries such as JEFF-3.2 and ENDF/B-VII.1.

DEFINITION OF SYMBOLS, TERMS AND ABBREVIATIONS

IJS	Institut Jožef Stefan (eng. Jožef Stefan Institute – JSI)
JRC	Joint Research Centre
MCNP	Monte Carlo N-Particle Transport Code
Rhino	A commercial 3D computer graphics application software
Grasshopper	A visual scripting language add-on (GH)
CAD	Computer assisted design
MATSSF	A computer code for calculating element and isotope number densities
ICSBEP	International Handbook of Evaluated Criticality Safety Benchmark Experiments
LMT-006	Low enriched uranium fissile material, metal physical form, thermal spectrum benchmark experiment no. 6
GRASP	**G**rasshopper-**R**hino **A**nalyzing **S**urfaces for MCN**P**

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1 INTRODUCTION

1.1 Background and description of the project

The production of input files for the LMT-006 (**L**ow Enriched Uranium fissile material, **M**etal physical form, **T**hermal spectrum) benchmark experiment that are suitable for the MCNP neutron transport code [1] is described. The LMT-006 experiment is included in the ICSBEP handbook [2]. However, only input files for the Apollo2 – MORET4 and Keno neutron transport codes are available at the moment. Since this experiment is very sensitive to the ^{235}U and ^{238}U cross sections in the thermal energy region [3], it provides useful data to validate new evaluated data for ^{235}U and ^{238}U in the resonance region from the CIELO [4] project..

The sensitivity to the total cross section for ^{235}U is presented in Figure 1 and for ^{238}U in Figure 2. This sensitivity plots are taken directly from the DICE [5] software that is distributed with the ICSBEP handbook.

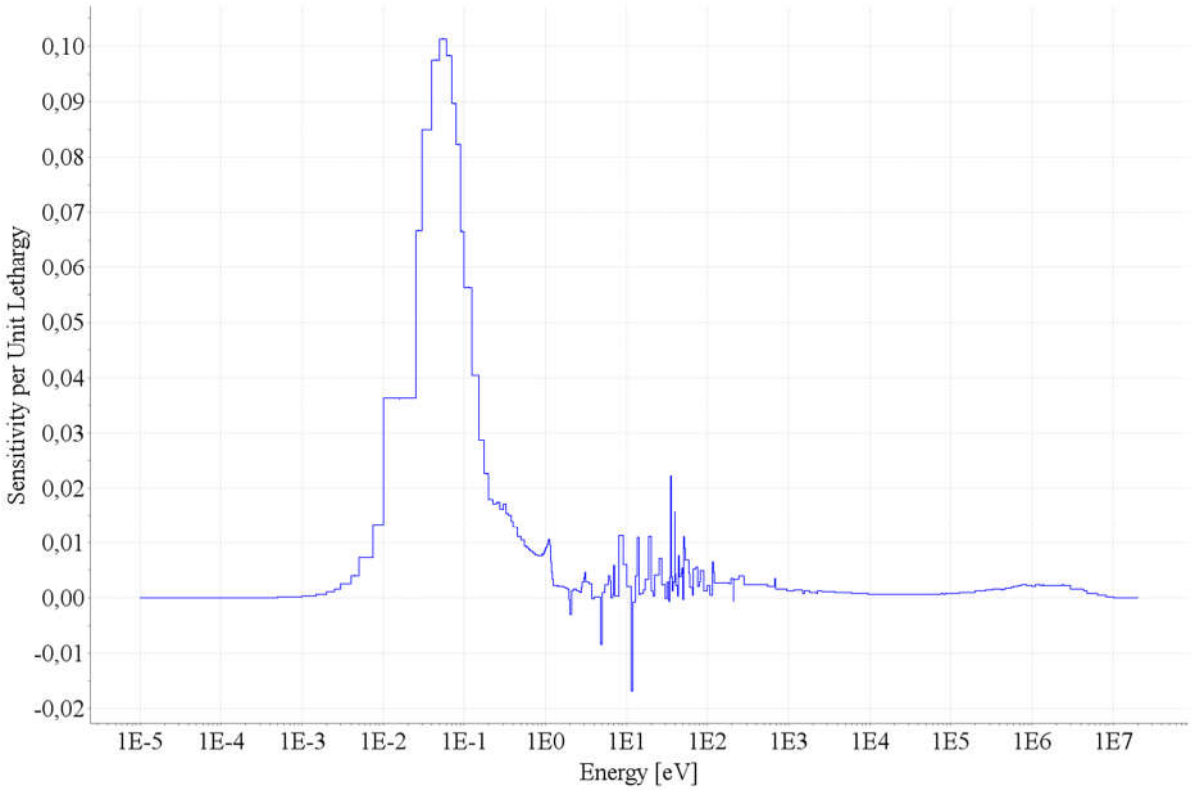

Figure 1: Sensitivity to the total cross section of ^{235}U for case number one of the LMT-006 benchmark.

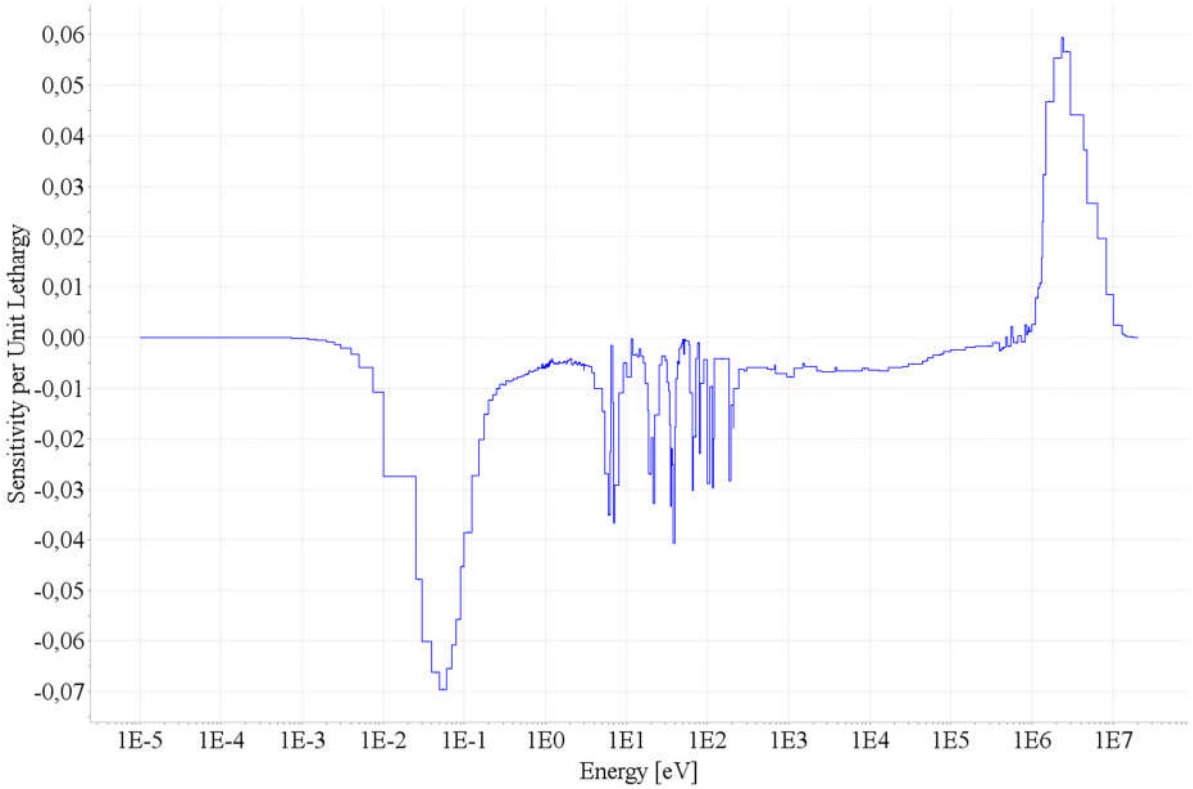

Figure 2: Sensitivity to the total cross section of ^{238}U for case number one of the LMT-006 benchmark.

1.2 Purpose and goals of the project

The aim of this project was to produce and validate models of all 30 cases of the LMT-006 criticality benchmark experiment in MCNP format.

2 DESCRIPTION OF THE MODEL AND COMPUTATIONAL STEPS

The first step in the project was the assessment of the available data on the benchmark experiments in the ICSBEP handbook. Models for simulations of the experiment were already available for the Apollo2 – MORET4 and Keno neutron transport codes. The results from the Apollo2 – MORET4 code are used for the validation of the newly developed models in MCNP format.
The geometrical description of the problem was found to be precise and thorough. In addition, the pictures and sketches provide useful information.
The material description was lacking an isotopic composition but an elemental composition was provided. Isotopic definition was available for the crucial elements to the experiment, namely for uranium.
Based on the geometrical data in the ICSBEP handbook for the detailed benchmark model 30 different 3D CAD models were produced using Rhinoceros [6], a commercial 3D computer graphics application software. CAD models are extremely useful in modern computational challenges. They can be used for visualization, structural analysis and in recent years neutron transport codes have been designed to work with CAD models [7]. Scripts such as the GRASP [8] tool have been written to assist in the conversion of CAD models into models suitable for MCNP neutron transport calculations.
In the next step, the 30 CAD detailed models were converted into a MCNP suitable format using the newly developed scripts in the GRASP tool kit. Materials were defined and updated to an isotopic definition for the use with modern nuclear data libraries.
In the last step the models were validated against the results of the Apollo code models.

2.1 CAD models

The CAD models were developed using the Rhinoceros 3D computer graphics application software version 5. The models are based on data for the detailed model described in chapter 3.2 of the official documentation [9] of the benchmark experiment from the ICSBEP handbook.
The case one and thirty CAD models are presented in Figure 3 and Figure 4, respectively. On the left side the 3D model is presented. On the right side a top (XY) view of the models is shown. The green colour represents the critical water level, dark green are the fuel cylinders, red are the bottom supporting structures, yellow is the homogenised water, and the steel support plate and the upper beams are shown in grey colour. Light blue is used to designate the model outside world (water or air) border.
The CAD models will not be distributed for general use but can be requested directly from the author.

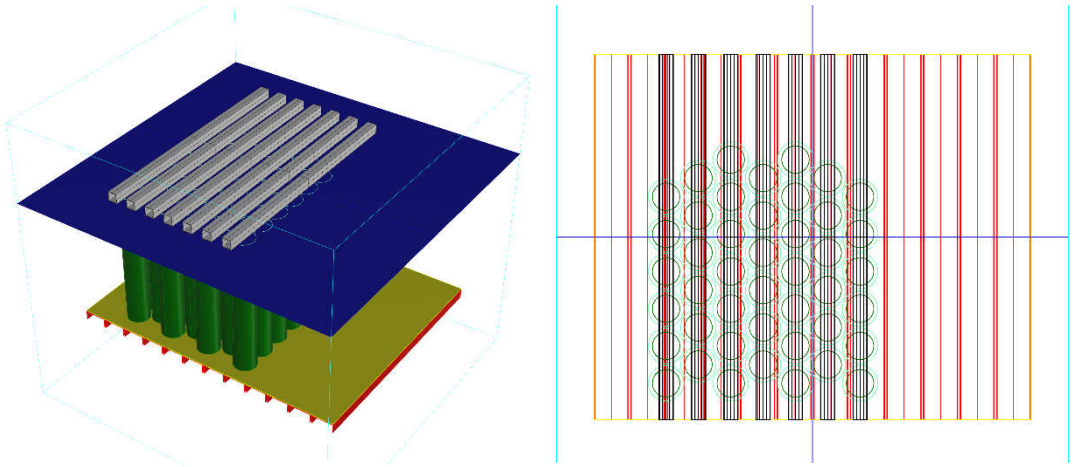

Figure 3: CAD model of case one. On the left side a 3D representation of the experiment and on the right side the top view.

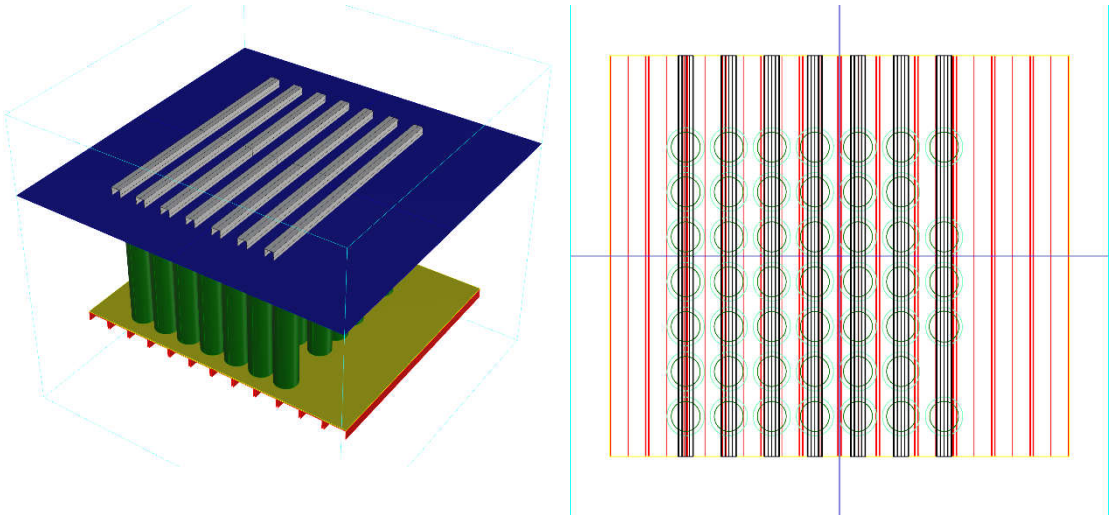

Figure 4: CAD model of case thirty. On the left side a 3D representation of the experiment and on the right side the top view.

2.2 MCNP models

The MCNP models were defined on the basis of the CAD models. The GRASP tool was used for some direct conversion of the CAD surfaces into MCNP surface input card format. All of the surface and cell cards are commented for easier readability of the input file. The MCNP inputs are written for MCNP version 6. Some problems were found when simulating a large number of neutron histories with MCNP version 5.16. The initial source distribution for the eigenvalue calculation is not optimised, thus a larger number of initial cycles is omitted from the final result.

Case one and case thirty MCNP models are presented in the Figure 5 and Figure 6, respectively. On the left side a XZ cross section of the model is presented and on the right side a XY cross section. The models are visualized using VISED [10]. Cyan represents the water, dark blue air, red are the fuel cylinders. Bottom and upper support structures can also be seen shown in orange and yellow.

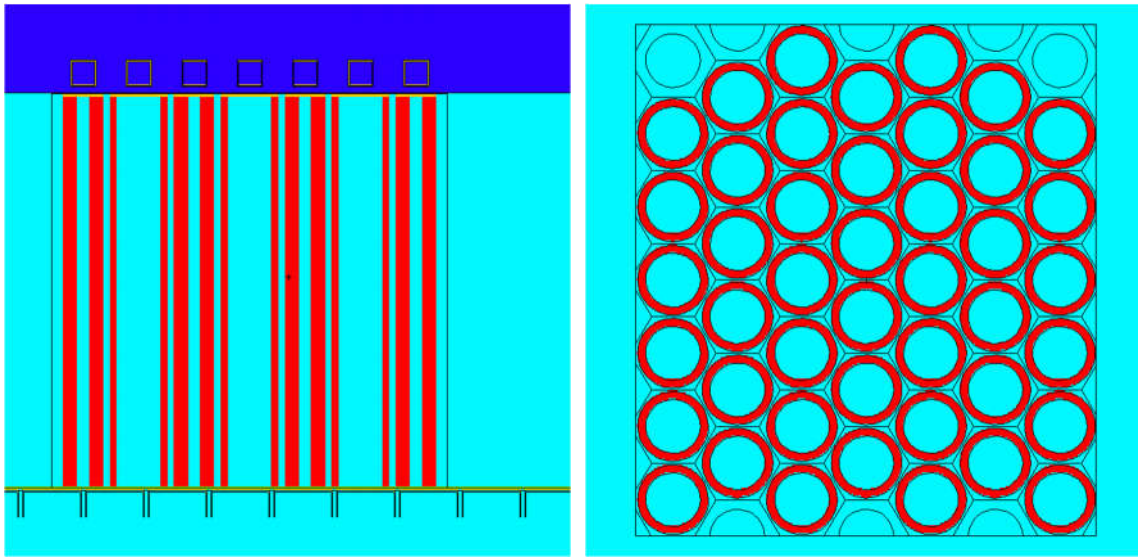

Figure 5: MCNP model of case one. On the left side the XZ cross section of the detailed benchmark experiment model and on the right side the XY cross section.

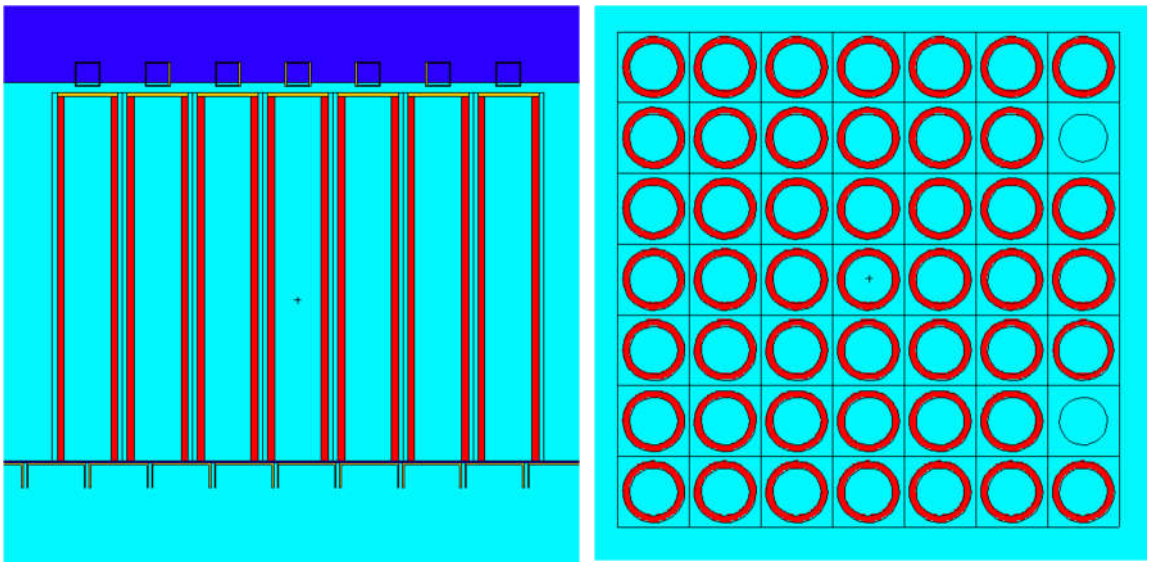

Figure 6: MCNP model of case thirty. On the left side the XZ cross section of the detailed benchmark experiment model and on the right side the XY cross section.

2.3 Material definition

Based on the material elemental information provided in Table 11 in chapter 3.3 of the official documentation of the benchmark experiment from the ICSBEP handbook a nuclide composition was calculated using the MATSSF [11] program code. The composition was derived from the elemental composition combined with the isotopic abundances of natural elements and the isotopic composition for uranium specified in the experiment description.

In Table 1 – Table 5 the atomic volume density of the main nuclides are given. The density is given in atoms/barn/cm which is one of the default units in MCNP. The volume densities for the fuel (ρ = 18.465 g/cm^3), water (ρ = 0.99754 g/cm^3) and water/stainless steel homogenized material (ρ = 6.4697 g/cm^3) were also taken from Table 11. The density for air (ρ = 0.0012 g/cm^3) and steel were found elsewhere in the official documentation (ρ = 7.9017 g/cm^3).

Table 1: Nuclide composition of the fuel with density ρ = 18.465 g/cm^3.

Nuclide	**Atomic density [atoms/(barn cm)]**
C (natural)	$9.2396\ 10^{-4}$
^{27}Al	$2.8722\ 10^{-4}$
^{54}Fe	$3.4846\ 10^{-6}$
^{56}Fe	$5.4700\ 10^{-5}$
^{57}Fe	$1.2633\ 10^{-6}$
^{58}Fe	$1.6812\ 10^{-7}$
^{234}U	$7.0181\ 10^{-6}$
^{235}U	$7.5547\ 10^{-4}$
^{238}U	$4.5866\ 10^{-2}$

Table 2: Nuclide composition of the water with density ρ = 0.99754 g/cm^3.

Nuclide	**Atomic density [atoms/(barn cm)]**
^{1}H	$6.6682\ 10^{-2}$
^{2}H	$7.6693\ 10^{-6}$
^{16}O	$3.3265\ 10^{-2}$
^{17}O	$1.2671\ 10^{-5}$

Table 3: Nuclide composition of the steel with density ρ = 7.9017 g/cm^3.

Nuclide	**Atomic density [atoms/(barn cm)]**
C (natural)	$5.5547\ 10^{-4}$
^{54}Fe	$4.9735\ 10^{-3}$
^{56}Fe	$7.8073\ 10^{-2}$
^{57}Fe	$1.8031\ 10^{-3}$
^{58}Fe	$2.3995\ 10^{-4}$

Table 4: Nuclide composition of a homogenized mixture of stainless steel and water with density $\rho = 6.4697$ g/cm^3.

Nuclide	**Atomic density [atoms/(barn cm)]**
^{1}H	$1.0338\ 10^{-2}$
^{2}H	$1.1890\ 10^{-6}$
C (natural)	$1.0438\ 10^{-4}$
^{16}O	$5.1569\ 10^{-3}$
^{17}O	$1.9644\ 10^{-6}$
^{28}Si	$1.3723\ 10^{-3}$
^{29}Si	$6.9714\ 10^{-5}$
^{30}Si	$4.6010\ 10^{-5}$
^{31}P	$5.3972\ 10^{-5}$
^{32}S	$3.7137\ 10^{-5}$
^{33}S	$2.9322\ 10^{-7}$
^{34}S	$1.6616\ 10^{-6}$
^{36}S	$3.9096\ 10^{-9}$
^{50}Cr	$6.2863\ 10^{-4}$
^{52}Cr	$1.2123\ 10^{-2}$
^{53}Cr	$1.3746\ 10^{-3}$
^{54}Cr	$3.4217\ 10^{-4}$
^{55}Mn	$1.5213\ 10^{-3}$
^{54}Fe	$3.0137\ 10^{-3}$
^{56}Fe	$4.7309\ 10^{-2}$
^{57}Fe	$1.0926\ 10^{-3}$
^{58}Fe	$1.4540\ 10^{-4}$
^{58}Ni	$4.8473\ 10^{-4}$
^{60}Ni	$1.8672\ 10^{-4}$
^{61}Ni	$8.1165\ 10^{-6}$
^{62}Ni	$2.5879\ 10^{-5}$
^{64}Ni	$6.5906\ 10^{-6}$

Table 5: Nuclide composition of the air with density $\rho = 0.0012$ g/cm^3.

Nuclide	**Atomic density [atoms/(barn cm)]**
^{14}N	$3.9349\ 10^{-5}$
^{15}N	$1.4375\ 10^{-7}$
^{16}O	$1.0568\ 10^{-5}$
^{17}O	$4.0258\ 10^{-9}$

2.4 Computer codes

In the following sections the computer codes used are briefly described. For a more detailed description of each of the codes the reader should address the provided reference literature.

2.4.1 Monte Carlo simulations

The main program for Monte Carlo neutron transport simulation is the Monte Carlo N-Particle (**MCNP**) program code [1]. This code is widely used for the simulation of benchmark experiments.
For visualization of the geometry of the MCNP input file the Visual Editor (**VISED**) [10] was used.

2.4.2 CAD drawing manipulation

For drawing the CAD models a commercial 3D computer graphics application software called **Rhinoceros 3D** [6] was used. It is combined with a freeware add-on called **Grasshopper** [12]. The **GRASP** [8] tool is based on a combination of Rhinoceros 3D and Grasshopper. It provides the user with an easy to use set of analysis tools designed to produce MCNP compatible surface card entries.

2.4.3 Material definition

For material definition **MATSSF** [11] was used. The program helps the user to calculate the element and isotope number densities, given the chemical composition of the components, their weight fraction in the mixture, the mass and the dimensions of the sample or the density.

3 VALIDATION OF THE MCNP MODELS

The models were validated against the results for eigenvalues from the Apollo2-Moret4 results from the official documentation for the detailed benchmark model. The Apollo2-Moret4 simulations used nuclear data cross sections from the JEF-2.2 library in a 172 group structure.

The MCNP6 version 1.0 simulated 115 cycles with 10^5 neutrons per cycle and skipping the first 15 cycles when calculating the final eigenvalue. The MCNP simulations were done on 56 computer cores. Each simulation took approximately 15 min[1]. Thermal scattering libraries were used for water and the materials consisting of a stainless steel/water mixture. The nuclear data library (JEF-2.2) in continuous energy form was used in the MCNP calculations.

The eigenvalue results of the two codes with statistical uncertainties of the simulations are given in Table 6. The results are also visualised in Figure 7. A good agreement between the models for the two codes is seen. For some cases a larger difference between the two codes is observed which cannot be explained at this time.

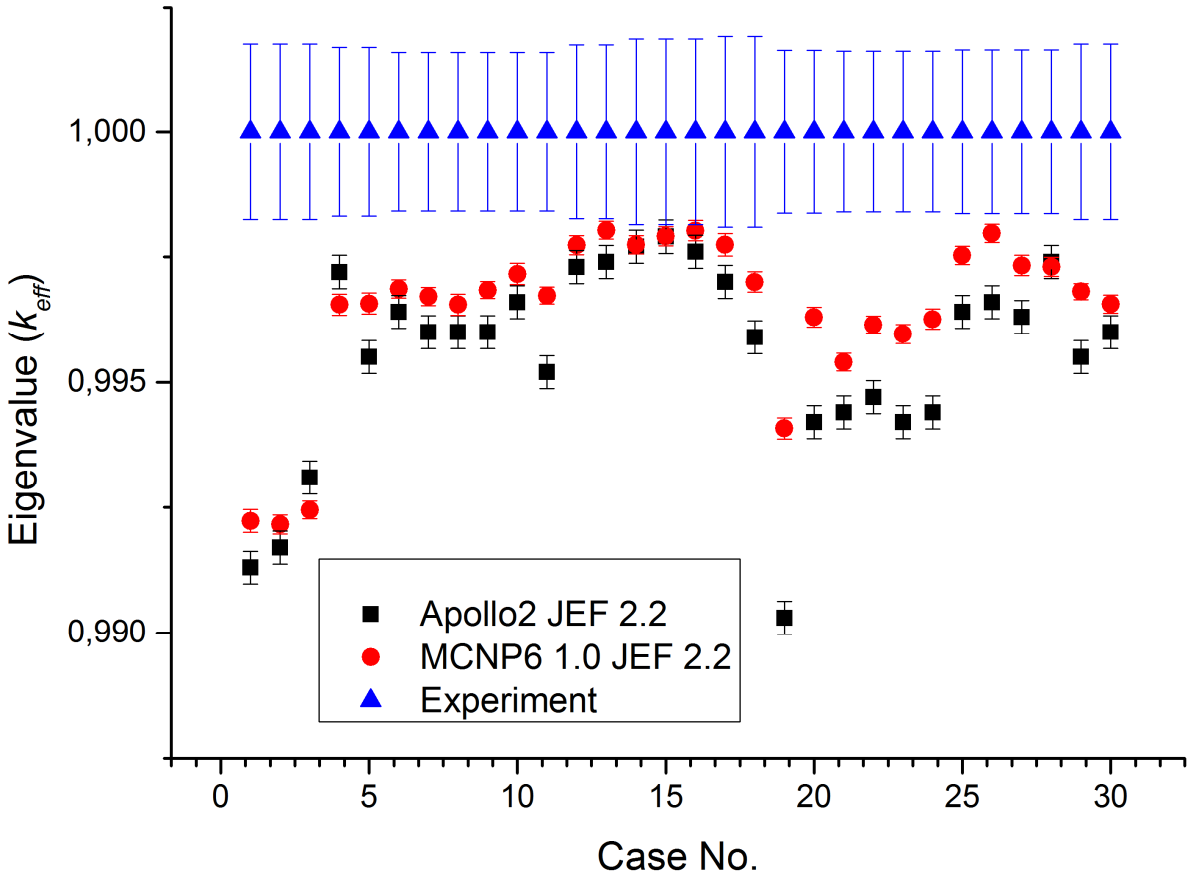

Figure 7: Eigenvalue (k_{eff}) results with statistical uncertainties of the calculations for the Apollo2 model and the new MCNP models together with the experimental results.

[1] Wall clock.

Table 6: Eigenvalue (k_{eff}) results with statistical uncertainties of calculations for the Apollo2 model and the new MCNP models.

Case no.	Apollo2-Moret4	Apollo2 uncertainty	MCNP 6 ver. 1.0	MCNP 6 ver. 1.0 uncertainty
1	0.9913	$3.27129\ 10^{-4}$	0.99223	$2.29368\ 10^{-4}$
2	0.9917	$3.27261\ 10^{-4}$	0.99216	$1.89576\ 10^{-4}$
3	0.9931	$3.27723\ 10^{-4}$	0.99245	$1.7966\ 10^{-4}$
4	0.9972	$3.29076\ 10^{-4}$	0.99655	$2.10454\ 10^{-4}$
5	0.9955	$3.28515\ 10^{-4}$	0.99657	$2.10351\ 10^{-4}$
6	0.9964	$3.28812\ 10^{-4}$	0.99686	$1.80319\ 10^{-4}$
7	0.996	$3.2868\ 10^{-4}$	0.99671	$1.80371\ 10^{-4}$
8	0.996	$3.2868\ 10^{-4}$	0.99655	$2.10428\ 10^{-4}$
9	0.996	$3.2868\ 10^{-4}$	0.99684	$1.7042\ 10^{-4}$
10	0.9966	$3.28878\ 10^{-4}$	0.99716	$2.10582\ 10^{-4}$
11	0.9952	$3.28416\ 10^{-4}$	0.99673	$1.69444\ 10^{-4}$
12	0.9973	$3.29109\ 10^{-4}$	0.99773	$1.90513\ 10^{-4}$
13	0.9974	$3.29142\ 10^{-4}$	0.99803	$1.80607\ 10^{-4}$
14	0.9977	$3.29241\ 10^{-4}$	0.99774	$1.8072\ 10^{-4}$
15	0.9979	$3.29307\ 10^{-4}$	0.99791	$1.9084\ 10^{-4}$
16	0.9976	$3.29208\ 10^{-4}$	0.99802	$2.00838\ 10^{-4}$
17	0.997	$3.2901\ 10^{-4}$	0.99774	$2.20849\ 10^{-4}$
18	0.9959	$3.28647\ 10^{-4}$	0.997	$2.00674\ 10^{-4}$
19	0.9903	$3.26799\ 10^{-4}$	0.99408	$2.09738\ 10^{-4}$
20	0.9942	$3.28086\ 10^{-4}$	0.9963	$2.00372\ 10^{-4}$
21	0.9944	$3.28152\ 10^{-4}$	0.9954	$1.80203\ 10^{-4}$
22	0.9947	$3.28251\ 10^{-4}$	0.99615	$1.70258\ 10^{-4}$
23	0.9942	$3.28086\ 10^{-4}$	0.99596	$1.90266\ 10^{-4}$
24	0.9944	$3.28152\ 10^{-4}$	0.99626	$2.0034\ 10^{-4}$
25	0.9964	$3.28812\ 10^{-4}$	0.99753	$1.80572\ 10^{-4}$
26	0.9966	$3.28878\ 10^{-4}$	0.99797	$1.80603\ 10^{-4}$
27	0.9963	$3.28779\ 10^{-4}$	0.99733	$2.0065\ 10^{-4}$
28	0.9974	$3.29142\ 10^{-4}$	0.9973	$1.90692\ 10^{-4}$
29	0.9955	$3.28515\ 10^{-4}$	0.99681	$1.60499\ 10^{-4}$
30	0.996	$3.2868\ 10^{-4}$	0.99656	$1.80623\ 10^{-4}$

4 RESULTS USING CURRENT NUCLEAR DATA LIBRARIES

A significant difference between the experimental results and the results of the benchmark model can be seen in Figure 7. To test if the current nuclear data libraries perform better on this benchmark experiment, the MCNP simulations were repeated using the ENDF/B-VII.1 and JEFF-3.2 nuclear data libraries.

Figure 8 shows the results of the eigenvalue calculations with these libraries in comparison with the experimental data and JEF-2.2 results. The results obtained with JEFF-3.2 are in better agreement, while the ENDF/B-VII.1 library produces a clear overestimation of k_{eff}.

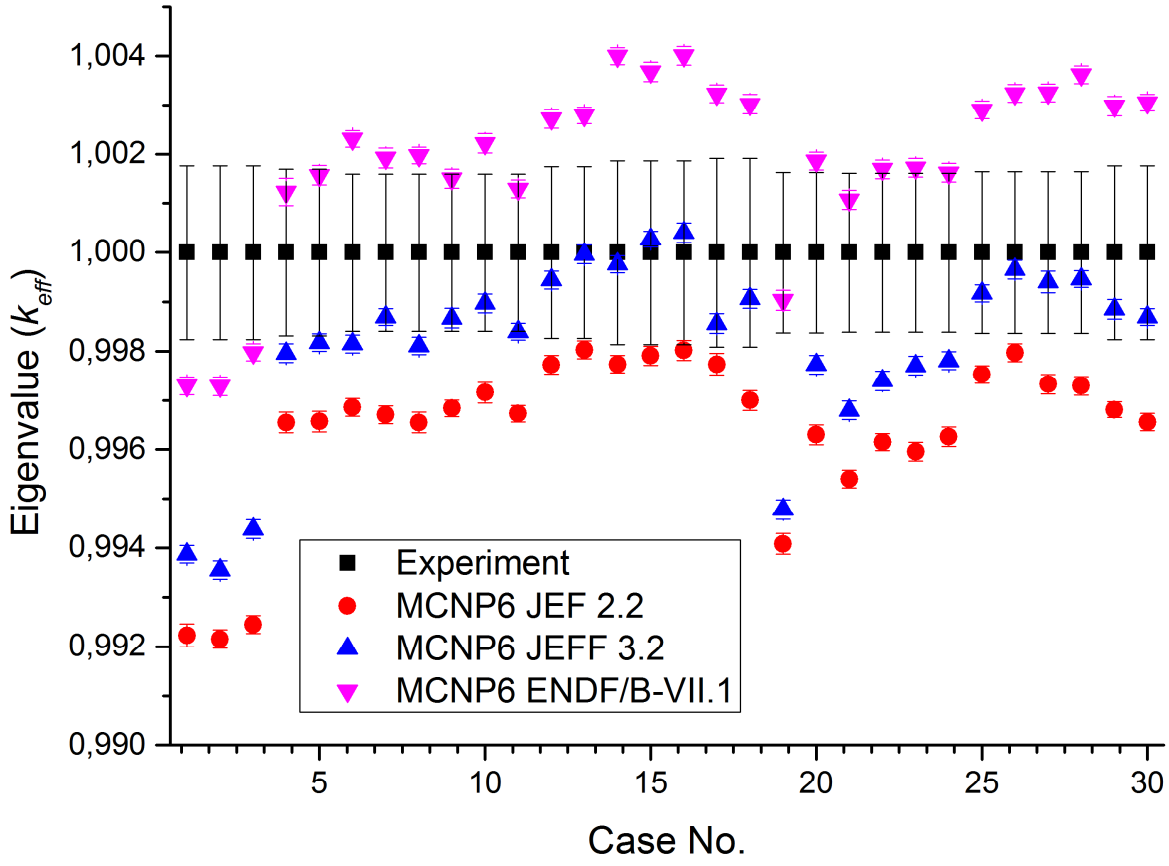

Figure 8: Eigenvalue (k_{eff}) results with statistical uncertainties of the MCNP calculation for never nuclear data libraries, JEFF-3.2 and ENDF/B-VII.1, compared to the experimental result and the JEF-2.2 MCNP simulation.

5 SUMMARY

In this report a detailed description of the conversion process of the LMT-006 benchmark experiment into a format compatible for MCNP neutron transport simulations was presented. In the first step all data from the official documentation in the ICSBEP handbook about the geometry, material definition and results from simulations with other codes were studied.
Based on these data CAD models for all 30 different experimental cases of this benchmark were produced. The CAD models were then converted into a MCNP compatible format.
In the last part of the report a validation of the 30 MCNP models was presented. Good agreement with the results from the Apollo2-Moret4 was observed except for a few cases. Current official neutron data libraries such as JEFF-3.2 and ENDF/B-VII.1 were also tested on the models and a better agreement between the experiment and model can be seen.
The models should be used as part of the numerous benchmark experiments which are currently used to validate new nuclear data. They are especially interesting to test ^{235}U and ^{238}U cross section differences in the thermal energy region.

6 ACKNOWLEDGEMENT

This work has been carried out within the framework of GENTLE program and has received funding from the GENTLE research and training program. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

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