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USE OF TRIPOLI-4.5 MESH TALLY TO INVESTIGATE POWER MAPS OF THE LEU-COMP-THERM-008 PWR CRITICAL LATTICES

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ABSTRACT

Power distribution calculations are essential for fuel assembly design and whole core safety analysis. In Monte Carlo core power map calculations, both lattice geometry and well-adapted tally functions are necessary. The lattice geometry and lattice tally features of TRIPOLI-4.3 Monte Carlo code for local power map calculation were reported in previous studies. To tally the power distribution on all cells of a whole core in pin-by-pin level, mesh tally can be more efficient on CPU time and more user-friendly on tally input preparation. This paper using the new introduced mesh tally function of TRIPOLI-4.5 interprets the whole core power maps of three PWR critical lattice experiments from LEU-COMP-THERM-008 benchmark. The multiplication factors Keff were calculated by using recent nuclear data libraries, ENDF/B-VII.0 and JEFF3.1, and compared with previous ones using ENDF/B-VI.4 and JEF2.2. The measured pin power distributions of 1/8 central assembly were benchmarked against calculated ones. The whole core power maps including about 5000 fuel pins with different effects of lattice heterogeneity were studied with the parallel computation. Finally, the simulated pin power uncertainty maps were also investigated.

Key Words: Monte Carlo code, TRIPOLI-4, Mesh Tally, Power Map, Criticality, LEU-COMP-THERM-008, ENDF/B-VII.0 and JEFF3.1

1. INTRODUCTION

Several improvements on reactor physics criticality calculation have been recently introduced in continuous energy TRIPOLI-4.5 Monte Carlo code [1] in order to help users study their calculation results. These improvements include: source convergence diagnostics using Boltzmann entropy criterion [2], XML-export file, inter-cycles correlation analysis on multiplication factor Keff and fission rates [3], mesh tally function for whole core power map calculation, and symmetry examination of the calculated power map [3, 4].

Both power map calculation in a fuel assembly modeling and fuel assembly power map calculation in a whole core modeling are essential for LWR fuel design, radial core-reflector evaluation, and reactor initial core safety analysis. In Monte Carlo core power map calculations, both lattice geometry and well-adapted tally functions are necessary. The lattice geometry and lattice tally features of TRIPOLI-4 Monte Carlo code for local power map applications were

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reported in previous studies [4-6]. This paper presents the new mesh tally option of TRIPOLI-4 code used on power map investigation.

The 3D mesh tally of TRIPOLI-4 can be used like the lattice tally to score on some or all cells in a fuel pin lattice and to score on a fuel assembly lattice with pin-by-pin modeling, and thus to obtain the power maps in pin-by-pin level and in assembly-by-assembly level for a PWR core.

Three PWR critical lattice experiments with different effects of lattice heterogeneity from LEU-COMP-THERM-008 benchmark are used in this study [7]. The Keff were calculated by using recent nuclear data libraries, ENDF/B-VII.0 and JEFF3.1, and compared with previous ones using ENDF/B-VI.4 and JEF2.2. Relative assembly power maps in a 3 x 3 symmetry configuration were first investigated. The measured relative pin power distributions of 1/8 central assembly were then benchmarked against calculated ones. Finally the mesh tally function was used to study the three whole core power maps each including about 5000 fuel pins.

2. PWR CRITICAL LATTICE EXPERIMENTS LEU-COMP-THERM-008

The benchmark problems are based upon experiments performed by B&W from 1970 to 1971. To measure the effect of PWR lattice heterogeneity, several experiments were performed inside a large aluminum tank containing borated water, UO2 fuel pins and Pyrex pins. Twelve benchmark experiments have been documented as LEU-COMP-THERM-008 (lct008) in ICSBEP handbook. Three of the most representative experiments, loading 1, 2, and 8, were also taken as ANS reactor physics benchmark [5, 7].

In lct008 experiments, the fuel pins contained low enriched uranium and were clad in aluminum. The active length of fuel pin was 153.4 cm, the water height was fixed at 145 cm, and the boron concentration in the water was adjusted until each experimental configuration was slightly supercritical, with a Keff value of 1.0007 $\pm$ 0.0012 (see Figs. 1 and 2).

The central region of the core resembled a 3 x 3 array of PWR fuel assemblies with fuel pins arranged in a 15 x15 lattice (square pitch of 1.63576 cm). The nine assemblies were surrounded by a driver region of fuel pins identical to those in the central region. The zone between the driver boundary and inner wall of the tank (radius 76.2 cm) contained only borated water. The axial buckling was 0.00037 cm^{-2} which corresponds to an axially uniform model with a height of 163.324 cm.

Among different assembly loadings considered in the lct008 core, three loadings, 1, 2, and 8 were selected for this study. These symmetric configurations (see Figs. 1-4) are named as cases:
A - central 3 x 3 assemblies with fuel pins only,
B - central 3 x 3 assemblies with fuel pins and 3 x 3 x 17 water holes, and
C - central 3 x 3 assemblies with fuel pins, 3 x 3 x 1 water holes, and 3 x 3 x 16 Pyrex pins.

The principal physical description of the fuel pin (radius 0.514858 cm), cladding (outer radius 0.602996 cm), Pyrex pin (radius 0.585 cm), water (density 0.99823 g/cm3) and soluble boron is evaluated and presented in the benchmark specifications. In addition to measurements of the critical boron concentrations, the pin power maps were obtained from the measurements of the fission rates derived from collimated counting of gamma ray of fission products in activated fuel pin. For cases B and C, 32 pin power measurements of 1/8 central assembly are available and their positions are shown in Fig. 5. Other details of the experiments are described in reference 7.

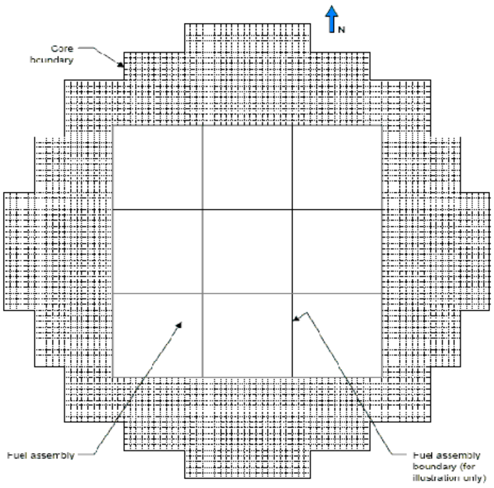

Fig. 1 Core diagram – lct008 [7]

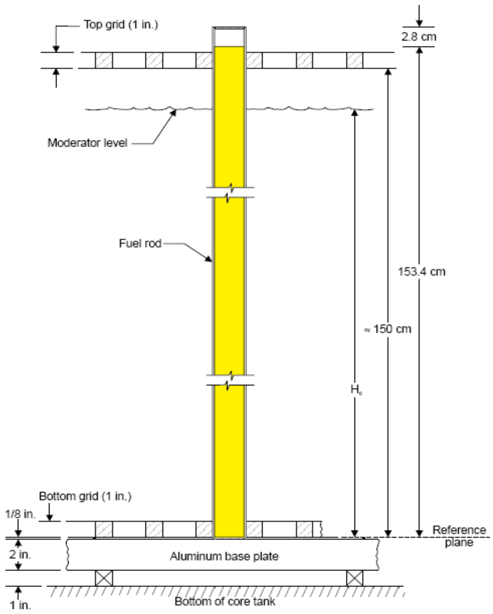

Fig. 2 Vertical diagram of fuel pin [7]

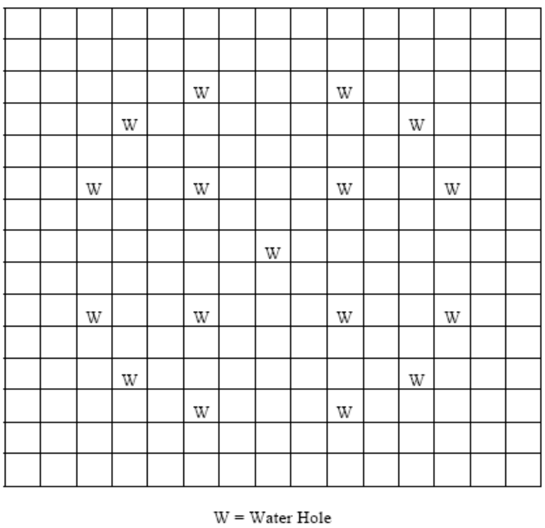

Fig. 3 Assembly loading 2 (Case B, W - water holes)

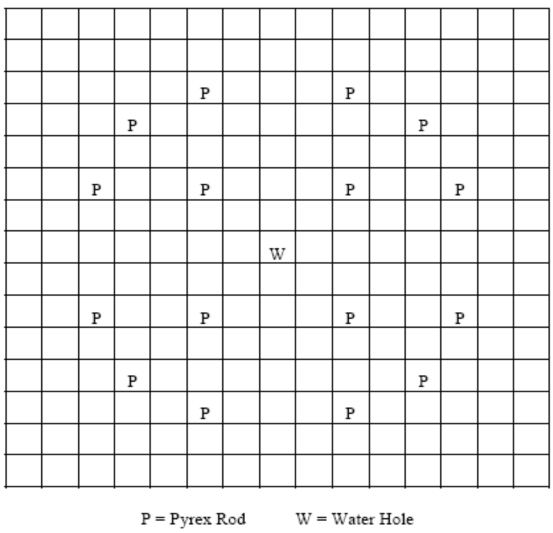

Fig. 4 Assembly loading 8 (Case C, P – Pyrex rods)

3. MESH TALLY OF TRIPOLI-4 CODE

Continuous-energy TRIPOLI-4 Monte Carlo transport code has been widely used on the radiation shielding, criticality safety, and fission reactor physics fields to support French nuclear energy research and industrial applications [1].

Based on international benchmarks and CEA internal measurements, extensive validation studies of TRIPOLI-4 code have been performed on the criticality safety of the fuel cycle, the reactor dosimetry of the PWR, the nuclear heating of research reactors, the radiation damage of reactor grade steels, and the neutron activation for decommissioning activities.

For reactor physics and criticality calculation with TRIPOLI-4, the fission neutron sources distribution is an important issue and many useful options of the code are available. These options include: flexible geometry package including 3D lattices geometry, lattice tally, and mesh tally functions. Automatic discards initial cycles for K_{eff} and for reaction rate tally are also basic. Advanced options include: source convergence diagnostics, inter-cycles correlation analysis on fission rates, and symmetry examination of the calculated power map [2-4]. All these advanced options need the well-adapted 3D tally functions.

Using the 3D lattices geometry, figures 5-8 show the TRIPOLI-4 modeling of the cases A, B, and C of lct008 cores. The modeling and the validation of mixed lattices geometry including the guide tube lattice and the absorber pins for a PWR fuel assembly were presented in previous CRISTO-II studies. The 3D lattice of lattice modeling and validation for the storage arrays MARACAS and for the PWR critical lattices were also demonstrated with TRIPOLI-4 [4, 6].

Lattice tally functions were then available within TRIPOLI-4 code in order to tally massively on any cell in big lattice, mixed lattice, and multi-loop-lattice. As the lattice identification numbers are different for fuel pin lattice and fuel assembly lattice, and as the lattice cell locations must be specified according to the pre-defined lattice geometry, the lattice tally for the whole core power map calculation needs to generate an important input and a case-dependent post-processing program according to the calculated fission rate results in the associated fuel volumes.

Mesh tally was designed to have an independent score geometry for tally purpose. The development and the application of mesh tally of TRIPOLI-4.5 were presented in reference 3. Generally this tally option is helpful for fission source convergence study, power distribution map calculation, neutron flux distribution, and dose map applications.

Both collision and track-length estimators are considered with mesh tally of TRIPOLI-4. These estimators are useful to tally on different material zones when using mesh tally. 3D Cartesian mesh tally have been implemented and validated. Cylindrical and prismatic mesh tally options have also been developed and they can be used on various fuel and geometry conditions.

Mesh tally is easy to use in input data preparation and the post-processing of simulation results to construct the power map is also user-friendly. In this study, the post-processing was programmed with the open source graphic software from OpenDX [8].

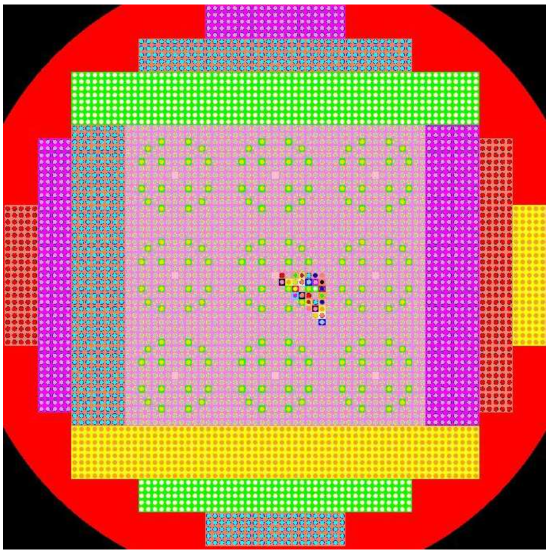

Fig. 5 Previous modeling (1997 – case C) (With pin power measurement volumes stamped on 1/8 central assembly)

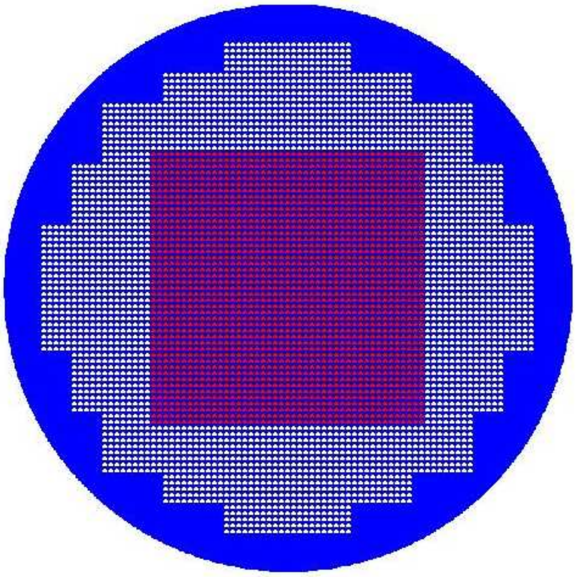

Fig. 6 TRIPOLI-4.5 modeling - case A (Central assemblies with fuel pins only)

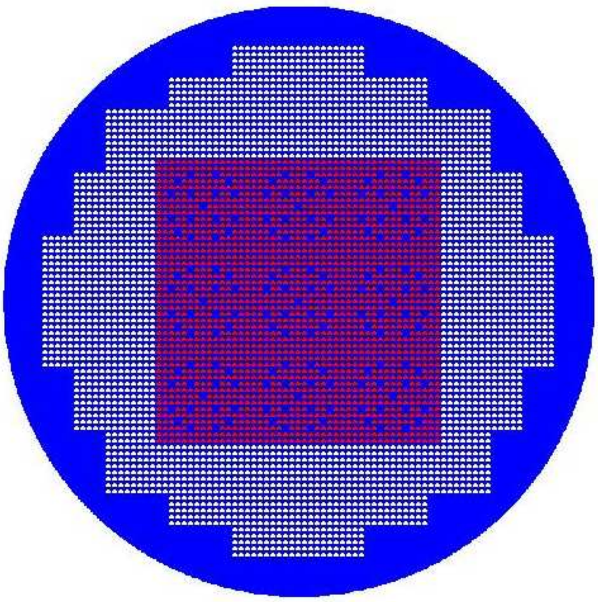

Fig. 7 TRIPOLI-4.5 modeling - case B (Central 9 assemblies with water holes)

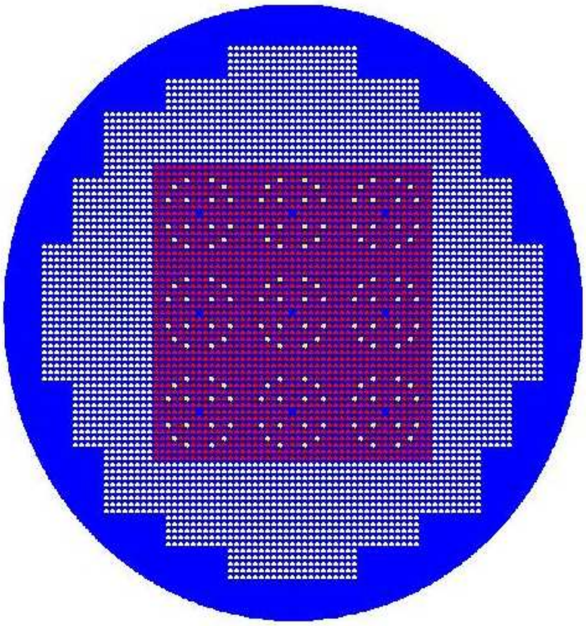

Fig. 8 TRIPOLI-4.5 modeling - case C (Central 9 assemblies with Pyrex pins)

3.1 Example of mesh tally in TRIPOLI-4.5

The following lines show how the mesh tally in TRIPOLI-4.5 works with the lct008 benchmark. Under module ‘GEOMETRIE’, the 9 central fuel assemblies of case A with pin-by-pin modeling were defined with lattice of lattice conception (see Figs. 1 and 8). Fuel pin lattice (VOLU 4) was first introduced by using operator ‘RESC’ to deal with the 15 x 15 array of fuel cell. Fuel assembly lattice (VOLU 5) was then created by using operator ‘RESC’ to deal with the 3 x 3 array of the central assemblies. The driven fuel pins around the 9 central fuel assemblies are not defined here. Keyword ‘ECRA’ (smash) was used to define the relationship between two VOLU cells. The fuel arrays (VOLU 4 and VOLU 5) were also smashed into the boron water reflector.

Under module ‘REPONSE’, the reaction rate calculation data were defined. Reaction type ‘33’ corresponds to fission reaction. ‘NUCLEI’ sums the 3 fission rates from U234, U235 and U238. ‘COMPO’ asks the macroscopic reaction rates in volumes with composition ‘FUEL’.

Under module ‘SCORE’, 2 tallies with the response function **1** defined above were prepared. The collision estimator ‘COLL’ and the mesh tally ‘MAILLAGE’ were then introduced with a geometry reference ‘REPERE’ placed in the center of the corner fuel pin. The fission rates of the 81 x 81 mesh array were used for lct008 whole core pin-by-pin tally and those of the 8 x 8 for local mesh tally of the central 1/4 assembly.

```
GEOMETRIE   (case A - central 3 x 3 fuel assemblies)

 TYPE 1 BOITE 1.63576        1.63576   163.324    // Lattice cell - Water
 TYPE 2 CYLZ   0.602996     81.662                // cladding
 TYPE 3 CYLZ   0.514858     81.662                // FUEL
 TYPE 4 CYLZ  76.2          81.662                // Borated water

 VOLU 1000 COMBI 4   0. 0. 0.  FINV               // reflector
 VOLU 1 COMBI 1 -35.98672 -35.98672   0 ECRA  1 1000 FINV
 VOLU 2 COMBI 2 -35.98672 -35.98672   0 ECRA  1    1  FINV
 VOLU 3 COMBI 3 -35.98672 -35.98672   0 ECRA  1    2  FINV
 VOLU 4 RESC VOLU   1   15  15  1    ECRA  1 1000  FINV
 VOLU 5 RESC VOLU   4    3   3  1    ECRA  1 1000  FINV // 3X3 central part
 .......

 REPONSE     1  REACTION NEUTRON
          NUCLEI 3    U234 COMPO  FUEL   INTERACTION 1 33
                      U235 COMPO  FUEL   INTERACTION 1 33
                      U238 COMPO  FUEL   INTERACTION 1 33   FIN_REPONSE

 SCORE       2

     1 COLL   DECOUPAGE DEC_INTEGRAL MAILLAGE
       81 81 1    1.63576    1.63576  163.324
       REPERE   -65.4304    -65.4304    0.
     1 COLL   DECOUPAGE DEC_INTEGRAL MAILLAGE
       8 8 1    1.63576    1.63576  163.324
       REPERE      0.    -11.45032    0.        FIN_SCORE
```

3.2 TRIPOLI-4.5 running conditions

In this study the continuous-energy cross-section libraries JEFF3.1 and ENDF/B-VII.0 were prepared by NJOY99-259 processing system with the convergence criteria of 0.1 %. The lct008 experiments were performed at room temperature so the standard 300 K cross–section data were used. Fuel and structure material atomic densities were taken from the ICSBEP Handbook [7].

All TRIPOLI-4.5 models for the lct008 experiments were explicit and an axially uniform model was taken. In each run, 20 initial cycles of 50 000 neutron histories per cycle were skipped in order to obtain converged fission source. Initial cosine radial and axial neutron flux shapes were set for neutron source distribution in case A and a point source for cases B and C. With 16 CPUs of 2.8 GHz, each case took about 6 hours CPU run time to obtain the tally results (standard deviation : Keff < 7 pcm, fuel assembly fission rate < 0.07% and fuel pin fission rate < 0.45 %).

4. RESULTS AND DISCUSSION

4.1 Keff benchmarks with JEF and ENDF/B libraries

Using JEF2.2 and JEFF3.1 nuclear data libraries, Table I shows the calculated Keff of cases A, B and C. First two columns of the Table I present the results taken from previous studies using TRIPOLI-4.1 (JEF2.2) [5] and TRIPOLI-4.3 (JEF2.2) [4]. The third column shows those from TRIPOLI-4.5 (JEFF3.1) of present study.

Clearly the Keff calculated with TRIPOLI-4.5 (JEFF3.1) in this study are in 2 to 4 standard deviations of those obtained with TRIPOLI-4.1 (JEF2.2) and TRIPOLI-4.3 (JEF2.2). The libraries effect between JEF2.2 and JEFF3.1 is not obvious and it is swamped by the uncertainties of simulations.

Table I. Keff of LEU-COMP-THERM-008 calculated with TRIPOLI-4 (JEF libraries)

Case	JEF2.2 - 1997 [5] Keff Std.	JEF2.2 - 2006 [4] Keff Std.	JEFF3.1 – 2009 Keff Std.
A	0.99920 ± 0.00027	1.00033 ± 0.00007	0.99999 ± 0.00007
B	0.99950 ± 0.00032	1.00015 ± 0.00007	1.00013 ± 0.00007
C	0.99830 ± 0.00035	0.99963 ± 0.00007	0.99959 ± 0.00007

Using ENDF/B-VI.2, ENDF/B-VI.4, and ENDF/B-VII.0 nuclear data libraries, Table II shows the calculated Keff of cases A, B and C. First column of Table II presents the results taken from previous study using TRIPOLI-4.1 (ENDF/B-VI.2) [5]. Second and third columns present those from TRIPOLI-4.5 (ENDF/B-VI.4) and TRIPOLI-4.5 (ENDF/B-VII.0) of this study.

Unlike the Keff obtained with JEF libraries, the libraries effect of three ENDF/B evaluations is obvious and the improvement of calculated Keff is clear when comparing to the experimental ones: 1.0007 ± 0.0012. Previous Keff comparisons between JEF2.2 and ENDF/B-VI.2 revealed a discrepancy of 380 ± 34 pcm to 440 ± 43 pcm for the three cases [5]. Present comparisons between two new libraries JEFF3.1 and ENDF/B-VII.0 show that their disagreements have been reduced to 86 ± 10 pcm for case C and 138 ± 10 pcm for case A.

Table II. Keff of LEU-COMP-THERM-008 calculated with TRIPOLI-4 (ENDF/B libraries)

Case	ENDF/B-VI.2 - 1997 [5] Keff Std.	ENDF/B-VI.4 - 2009 Keff Std.	ENDF/B-VII.0 - 2009 Keff Std.
A	0.99480 ± 0.00021	0.99810 ± 0.00007	1.00138 ± 0.00007
B	0.99570 ± 0.00028	0.99822 ± 0.00007	1.00143 ± 0.00007
C	0.99430 ± 0.00025	0.99695 ± 0.00007	1.00045 ± 0.00007

In summary, it can be concluded that the improvement of nuclear data on U-238, U-235, Al-27, O-16, and H-1 in the past decade is really helpful for the lct008 PWR critical lattice benchmarks. The software stability of the TRIPOLI-4 code in three versions has also been confirmed.

4.2 Power map benchmarks

Using mesh tally of TRIPOLI-4.5, power maps are calculated in three levels in this study:
- the 3 x 3 fuel assemblies power distributions,
- the fuel pin power distributions of the central 1/8 assembly for cases B and C, and
- the pin-by-pin whole core power maps.

The calculated power maps in fuel assembly level for cases A, B, and C in 3 x 3 symmetrical structures were performed. Satisfactory symmetry results have been obtained. Table III shows the normalized central 3 x 3 fuel assembly power distributions of lct008.

Table III. Normalized 3 x 3 fuel assembly power distributions of LEU-COMP-THERM-008

Case A			Case B			Case C		
0.6764	0.8308	0.6746	0.7170	0.8607	0.7214	1.0918	1.1215	1.1010
0.8316	1.0000	0.8312	0.8605	1.0000	0.8650	1.1186	1.0000	1.1298
0.6751	0.8327	0.6763	0.7207	0.8644	0.7234	1.0937	1.1231	1.1018

Maximum asymmetry factors among the four diagonal corner assemblies are 0.27% for case A, 0.89% for case B, and 0.92% for case C. As the calculated errors in fission rate have been reduced to less than 0.07% in assembly level, small but clear asymmetry factors observed in cases B and C are probably due to the convergence level of fission source and the under estimation of the simulation uncertainty on fission rate in the Monte Carlo simulations [2, 3].

This means that not only the convergence levels in Keff and in local fission rates but also the convergence level of symmetry power map should be considered in the simulation. If we take into account the inter-cycles correlation the calculated errors of the fission rate may increase. The asymmetry factors depend also on the rejected initial cycles of neutron histories and the number of used cycles in simulation. The initial 3D neutron source distribution is also important.

Table III shows that the central assembly power and the corner one of case A present about 32.5% difference. It is due to the accumulation of thermal neutron in the central zone. For case B, this difference is reduced to 28 % thanks to introduced 3 x 3 x 17 water holes. For case C, the peak power assembly is not in the central one due to introduced Pyrex absorber pins.

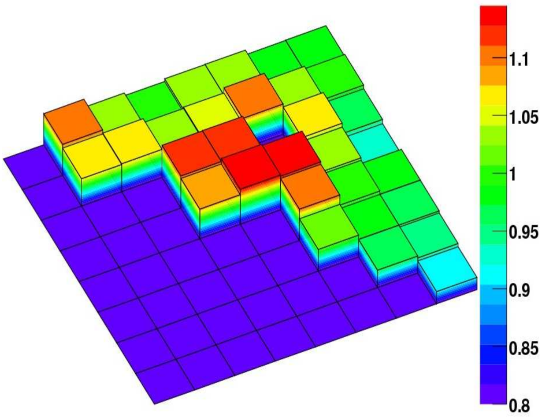

Fig. 9 Pin power map of central 1/8 assembly (Case B with water holes – W)

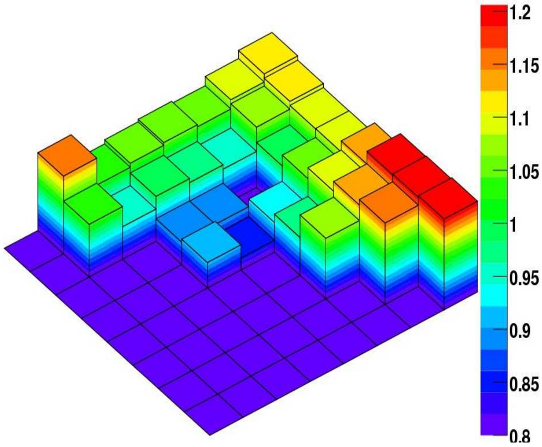

Fig. 10 Pin power map of central 1/8 assembly (Case C with Pyrex rods - P)

Figures 9 and 10 present the relative pin power distributions of central 1/8 assembly for cases B and C (see also Fig. 5). For case B, the peak pin power is near the water holes. For case C, the peak pin power zones are near the central water hole and the assembly corners. Pyrex pins zone presents power sink. Water holes and Pyrex absorber pins introduce larger gradient of thermal flux and important fluctuation of neutron spectrum and TRIPOLI-4.5 calculates them correctly.

The uncertainty of calculated fission rate in fuel pin level is below 0.30 % in case B and 0.45 % in case C. Discrepancies between the calculations and the measurements are represented by the RMS (root mean square) error of 32 fuel pins. For case C this RMS error is 1.2 % but for case B, it is 1.7%. This discrepancy can be explained by our previous observation that, due to the experimental quality of one fuel pin in case B, the RMS error of case B is higher [4, 5].

Figures 11 to 13 show the whole core power maps of cases A, B, and C based on the pin-by-pin mesh tally results. Power maps with symmetric shapes have been obtained for these three cases. The pin power maps of cases A and B present a radial cosine power distribution in fundamental mode and the water holes in case B introduce discrete peak zones in the central fuel assemblies.

Due to Pyrex pins in case C, the radial cosine power distribution was disappeared in Fig. 13 and the minimum power zone appears on the central assembly (cf. Table III.). In fact power reduction in the central assembly is more important than in the corner assembly due to the original radial cosine power distribution. Due to the central power collapse, the peak power zones in Fig. 13 move symmetrically to the driver regions of the core.

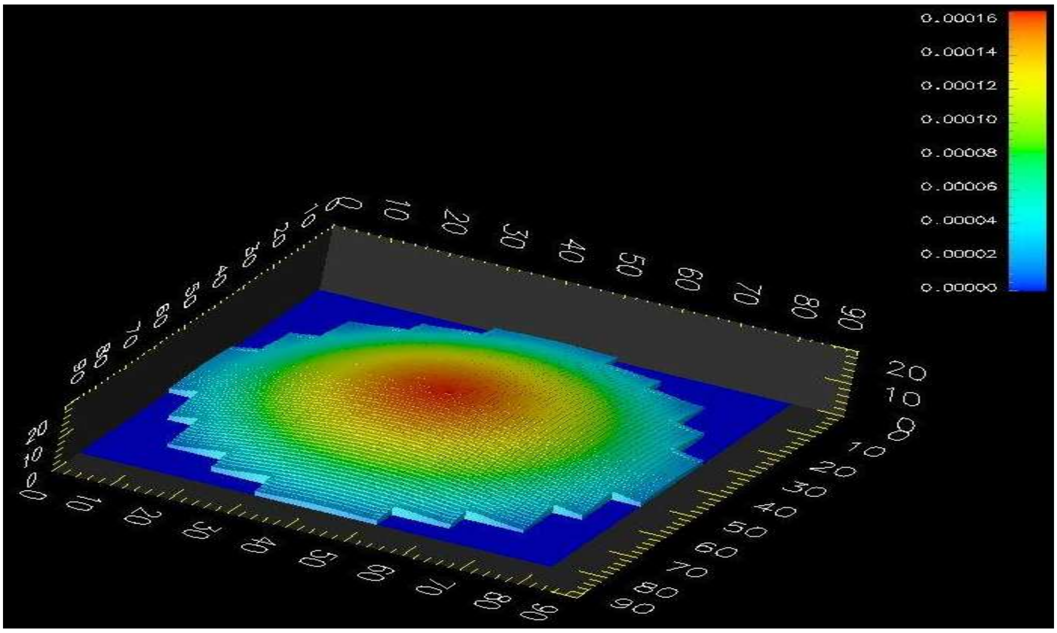

Fig. 11 Pin power map of the LEU-COMP-THERM-008 PWR critical lattice, Case A (Mesh tally results of the TRIPOLI-4.5 simulation)

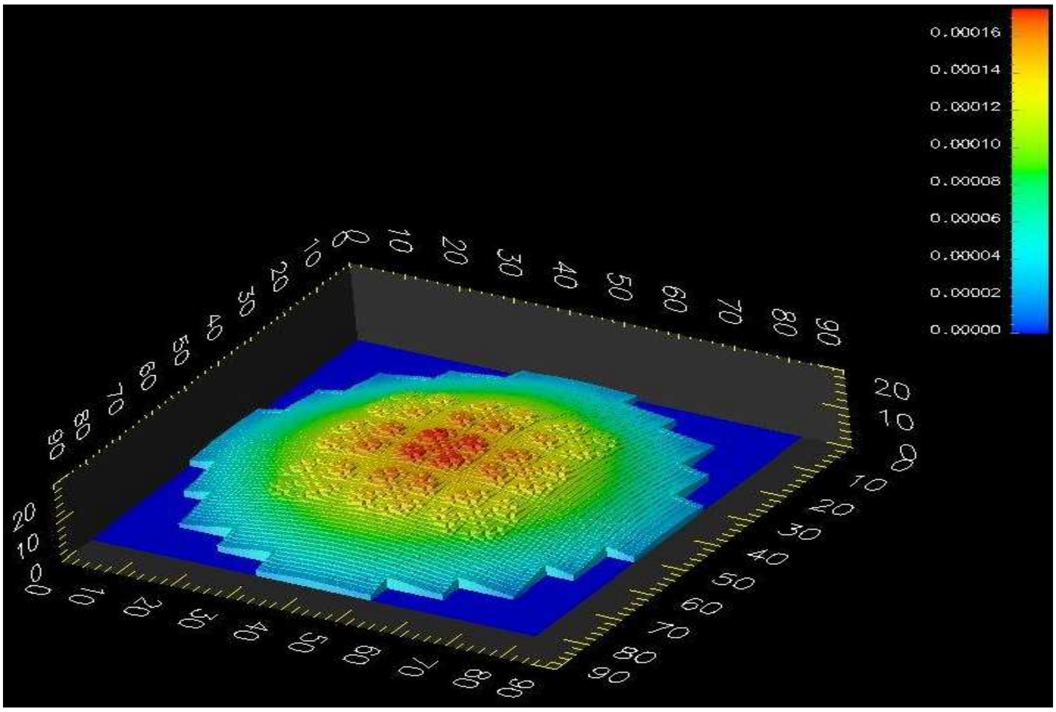

Fig. 12 Pin power map of the LEU-COMP-THERM-008 PWR critical lattice, Case B (4 x 4 x 3 X 3 water holes introduced)

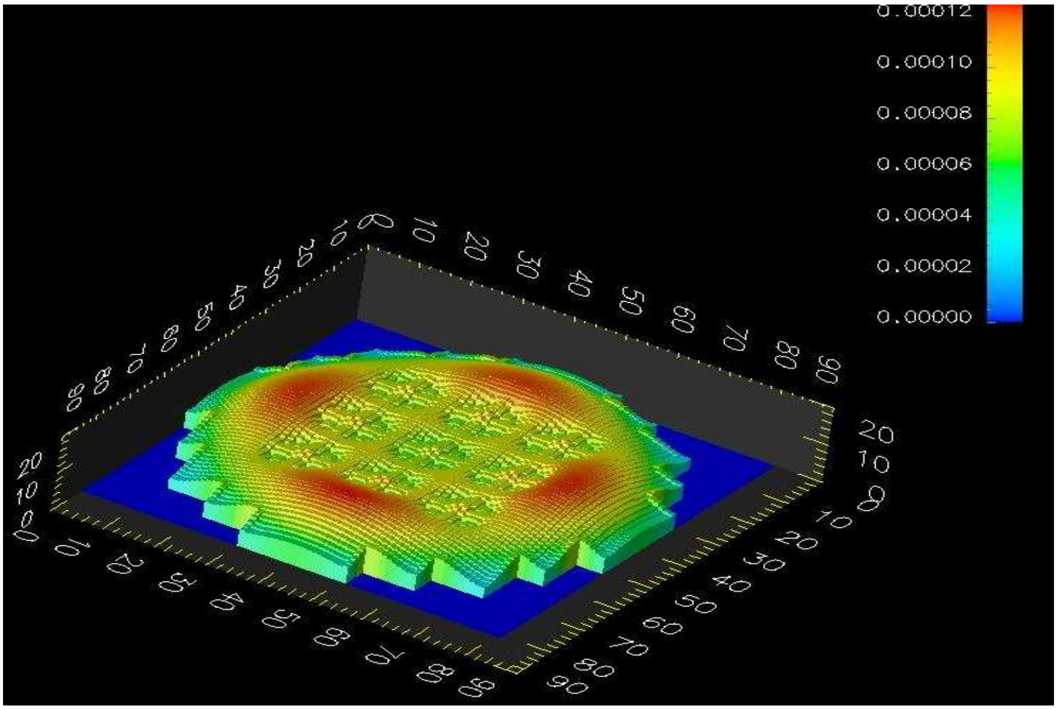

Fig. 13 Power map of the LEU-COMP-THERM-008 PWR critical lattice, Case C (4 x 4 x 3 X 3 Pyrex absorber rods introduced)

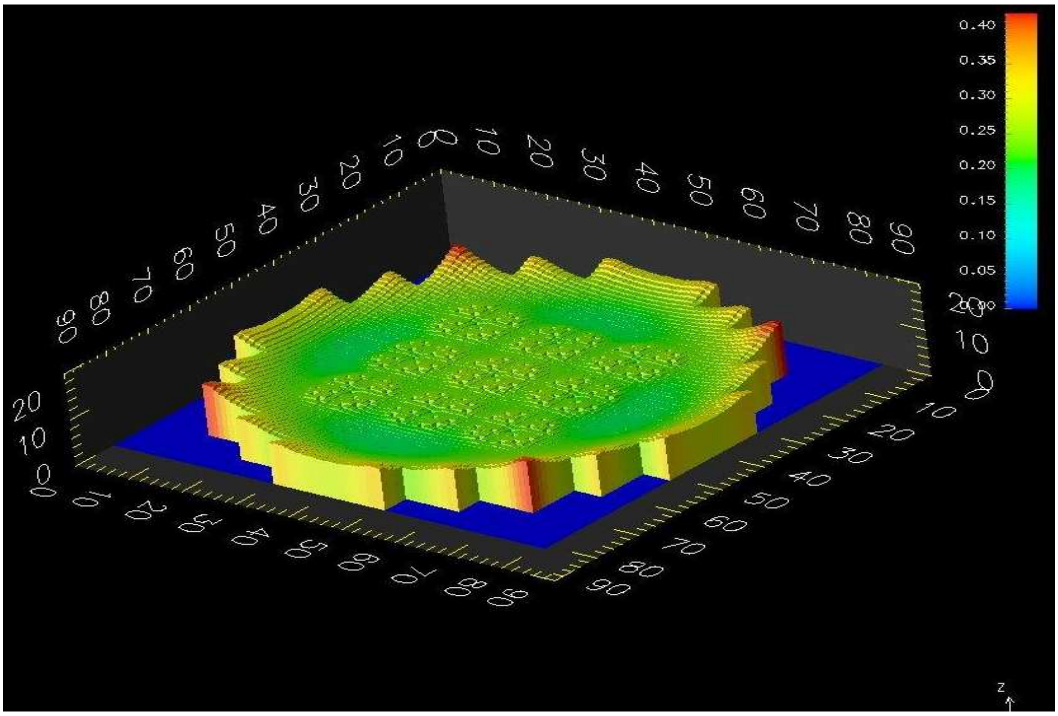

Fig. 14 Pin power uncertainty map of the LEU-COMP-THERM-008 - Case C (Standard deviation map – one sigma up to 0.45 %)

Fig. 14 presents the simulated pin power uncertainty map of case C. Due to the Pyrex pins, the thermal flux gradient and the neutron spectrum fluctuation increase in the central assemblies and the simulation uncertainties increase. So the 3 x 3 fuel assemblies image also floats on the pin power uncertainty map. The boundary fuel power presents a higher uncertainty due to the neutron leakage from the core and the neutron absorption in the surrounding boron water. In addition, symmetric shapes of the pin power uncertainty maps have been obtained for cases A, B, and C.

5. CONCLUSIONS

Mesh tally is a practical tally tool to calculate the whole core power map and to study the fission source convergence in reactor criticality calculations. This paper demonstrates the new introduced mesh tally in TRIPOLI-4.5 code and its application on lct008 PWR lattices. This study also confirms the contribution from the new data libraries, JEFF3.1 and ENDF/B-VII.0 on lct008 benchmark and improved C/E ratios on Keff are available now. For a power reactor whole core calculation, the mesh tally of TRIPOLI-4.5 code becomes basic; however, the inter-cycles correlation is evident and the fission source convergence is difficult to obtain. In the future, more work will be performed on the symmetry problems in whole core power map calculations.

ACKNOWLEDGMENTS

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