Use of TRIPOLI-4.3 Lattice Tally to Investigate Assembly Power and Pin Power Maps of PWR Critical Lattices Experiments

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Abstract

Power distribution calculation is a very important task for fuel assembly design and whole core safety analysis. In Monte Carlo power map calculation, both lattice geometry and lattice tally functions are essential. The lattice geometry features of TRIPOLI-4 Monte Carlo code have been reported in previous studies. Lattice tally functions of TRIPOLI-4.3 can be used to tally on some or all cells in a fuel pin lattice and to tally on a fuel assembly lattice with pin-by-pin modeling. In order to study the power maps in pin-by-pin level and in assembly-by-assembly level, this paper using lattice tally of TRIPOLI-4.3 code interprets three PWR critical lattice experiments from LEU-COMP-THERM-008 benchmark. The calculated K_{eff} and relative assembly power maps in a 3 x 3 symmetry configuration have been investigated. The measured relative pin power distributions of 1/8 central assembly with different effects of lattice heterogeneity have been benchmarked against calculated ones.

KEYWORDS: Monte Carlo code, TRIPOLI-4.3, Lattice Tally, Power Map, Criticality, LEU-COMP-THERM-008

1. Introduction

Both pin power distribution calculation in a fuel assembly modeling and fuel assembly power distribution calculation in a whole core modeling are very important for PWR fuel design, radial core reflector evaluation and reactor initial core safety analysis. To reply these power map requirements in a reference Monte Carlo criticality calculation, lattice geometry and lattice tally have been implemented in TRIPOLI-4 Monte Carlo code. [1]

The lattice geometry of TRIPOLI-4 code has been firstly established for PWR lattices and storage arrays. [2, 3] The 3D single lattice, mixed lattice and double-loop-lattice features of TRIPOLI-4.3 have been recently demonstrated with critical configurations. [4]

The 3D lattice tally of TRIPOLI-4.3 can be used to tally on some or all cells in a fuel pin lattice and to tally 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.

To demonstrate and to validate these lattice tally functions of TRIPOLI-4.3, this study interprets three PWR critical lattice experiments with different effects of lattice heterogeneity from LEU-COMP-THERM-008 benchmark. [5] Three loadings with different central configurations have been studied. The calculated K_{eff} and relative assembly power maps in a 3 x 3 symmetry configuration have been validated. The measured relative pin power distributions of 1/8 central assembly are benchmarked against TRIPOLI-4 calculated ones.

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2. Lattice Geometry and Lattice Tally functions of TRIPOLI-4 code

TRIPOLI-4 Monte Carlo transport code has been developed at CEA/Saclay since 1994. It has been extensively applied in reactor physics, criticality safety, radiation shielding and nuclear instrumentation calculations.

The important features of TRIPOLI-4.3 code on reactor physics calculations include: flexible geometry package including 3D lattices geometry and lattice tally, optionally mixed continuous-energy and multi-group libraries, probability tables for unresolved resonance range, perturbations calculations on isotope concentration, material density and cross-section, and multi-processors parallel calculations.

2.1 Lattice Geometry of TRIPOLI-4 code

The geometry of TRIPOLI-4 is designed to cover functionalities of the geometry packages of both TRIPOLI-3 and MORET criticality code so that volumes can be defined with pre-defined shapes and/or with equations of surfaces delimiting them.

Lattice operator 'RESC' was first introduced to deal with the repetition of a parallelepiped fuel cell. Lattice operator 'RESH' was also developed in order to deal with hexagonal cells for fast reactor and high temperature reactor.

In TRIPOLI-4.1, double-loop-lattice concept was introduced and validated in order to deal with storage arrays and fuel assemblies. At that time, water holes and absorbers pins of a PWR fuel assembly had to be set one-by-one by using operator 'ECRASE' (smash) on specific locations of a fuel pin lattice. [2]

To avoid the frequent usage of 'ECRA' operator on lattice configurations and to reduce the computer running time, lattice operators 'EXCEPT', 'REMP' (replace), 'GARDE' (keep), 'RESE' (lattice no.), 'MAILLE' (cell no.) and 'V_ORI' (volume-origin no.) were implemented within TRIPOLI-4.2. These operators simplify the modeling and the verification of mixed lattices geometry.

With the mixture of fuel lattice and guide tube lattice for a PWR assembly, the mixed lattices geometry with uniform axial composition have been demonstrated and validated with CRISTO-II storage arrays benchmark. [3] With 3D mixed lattices to define the module configuration of UO_2 powder boxes and double-loop-lattice option to model the array of modules, the case 18 of MARACAS 3D storage array benchmark was modeled and validated with TRIPOLI-4.3. [4]

2.2 Lattice tally options in TRIPOLI-4 code

Following the development of the diverse lattice options in geometry package, lattice tally functions were then available within TRIPOLI-4.3 code in order to tally massively on any cell in big lattice, mixed lattice and multi-loop-lattice. These lattice tally options also offer a convenient way to investigate the power map in a fuel assembly and in a testing reactor core.

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 TRIPOLI-4.3 lattice tally option is not only very economical on computing time but also very easy to use compared with the previous method, using 'ECRASE' operator to define tally volumes. The power maps can be simply obtained by a post-processing program according to calculated fission rate results in associated fuel volumes, lattice identification numbers and normalization factors.

2.3 Examples of lattice tally in TRIPOLI-4.3

The following lines show how the lattice tally in TRIPOLI-4.3 works with the LEU-COMP-THERM-008 benchmark described in section 3. Key word 'GEOMETRIE' and associated lattices and volumes define the 9 central fuel assemblies with pin-by-pin modeling (see Figs. 1 and 10). Key word 'REPONSE' defines the reaction rate calculation. Reaction type '33' corresponds to fission reaction. 'NUCLEI' sums the 3 fission rates from U^{234}, U^{235} and ^{U238}. 'COMPO' asks the macroscopic reaction rates in volumes with composition 'FUEL'.

Key word 'SCORE' defines 2 tallies with the response function **1** defined above and the collision estimator 'COLL'. 'MAILLE' and 'LIST' introduce the lattice tally with 'DEPTH' 1 in the assembly level and 'DEPTH' 2 in the fuel pin level. All tallies associate with the fuel volume **3** defined in fuel pin lattice 4 (15 x 15 x 1) and in fuel assembly lattice 5 (3 x 3 x 1) are taken into account. The fission rates of the 3 x 3 fuel assemblies are fully described and those of the 32 fuel pin (1/8 assembly) are only shown 3 pins in the central fuel assembly location (2, 2, 1).

```
GEOMETRIE
 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 MAILLE LIST  9
       3 DEPTH 1   1 3 1   3 DEPTH 1   2 3 1   3 DEPTH 1   3 3 1
       3 DEPTH 1   1 2 1   3 DEPTH 1   2 2 1   3 DEPTH 1   3 2 1
       3 DEPTH 1   1 1 1   3 DEPTH 1   2 1 1   3 DEPTH 1   3 1 1
1 COLL  DECOUPAGE DEC_INTEGRAL MAILLE LIST  32
       3 DEPTH 2   2 2 1   15 1 1
       3 DEPTH 2   2 2 1   15 2 1   3 DEPTH 2   2 2 1   14 2 1
        ..............                                  FIN_SCORE
```

2.4 TRIPOLI-4.3 running conditions

In this study the continuous-energy cross-section libraries JEF2.2 were prepared by NJOY99-90 processing system with a convergence criteria of 0.1%. As the LEU-COMP-THERM-008 experiments (see section 3) were performed at room temperature, the standard 300K cross–section data were used. Fuel and structure material atomic densities were taken from the ICSBEP Handbook. [5] All TRIPOLI-4.3 models for the critical experiments were explicit and an axially uniform model were 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 distributions according to fitted equations from measurements. [5] With 6 CPUs of 3 GHz, each case took about 12 hour cpu running time to obtain the converged results (standard deviation : K_{eff} < 7 pcm, fuel assembly fission rate < 0.07% and fuel pin fission rate < 0.45 %).

3. PWR critical lattice experiments LEU-COMP-THERM-008 [5, 6]

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. 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 K_{eff} value of 1.0007 (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 core, three loadings, 1, 2 and 8 were selected for this study. These configurations (see Figs. 1-4 and 10-12) 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/cm^3) and soluble boron is evaluated and presented in the benchmark specifications.

In addition to measurements of the critical boron concentrations, the axial flux shapes and the pin power maps were measured. 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 distributions of 1/8 central assembly are available (Fig. 9). Other details of the experiments are described in reference 5.

Figure 1: Core diagram

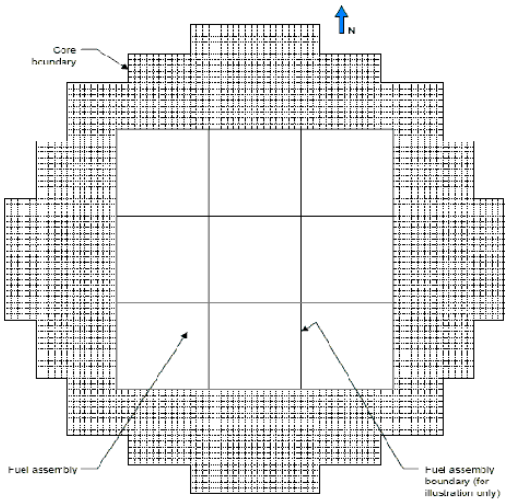


Figure 2: Vertical diagram of fuel pin

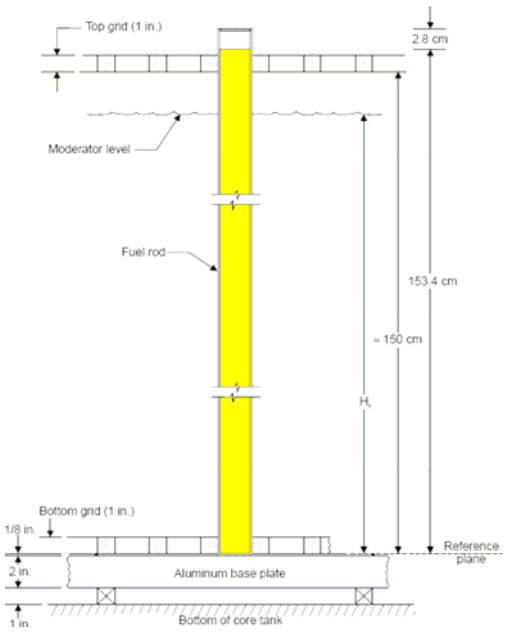


Figure 3: Assembly loading 2 for core (Case B)

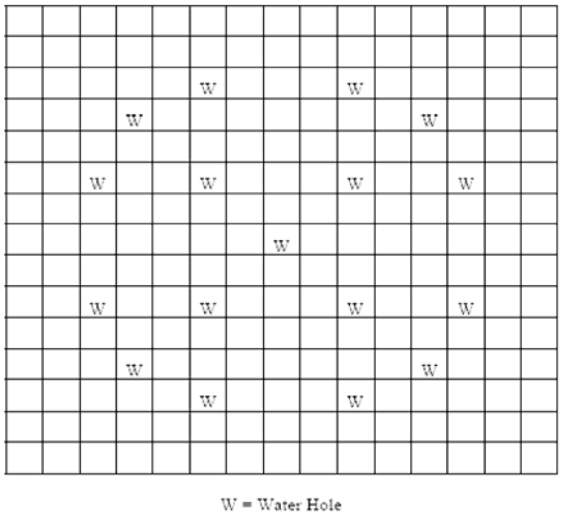
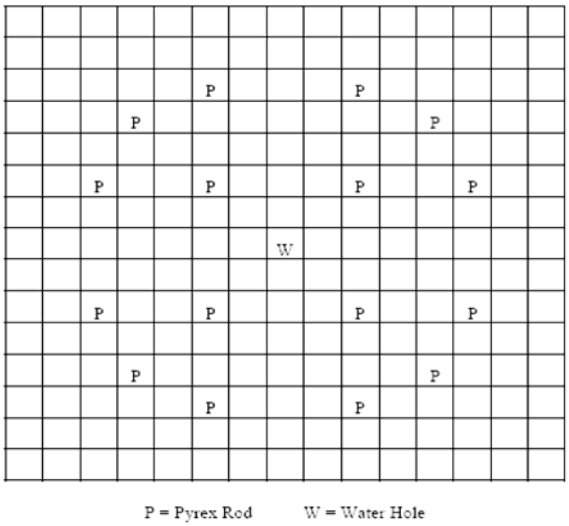


Figure 4: Assembly loading 8 for core (Case C)



4. Results and Discussion

Using JEF2.2 data library, the calculated K_{eff} of A, B and C cases are shown in following Table. First column gives the results taken from previous study using TRIPOLI-4.1 and second column presents the results of present study. Clearly the K_{eff} obtained with TRIPOLI-4.3 in this study are in 2-4 standard deviations of those obtained with TRIPOLI-4.1.

Case	Previous study - 1997 [2]		Present study - 2006	
	K_{eff}	Std.	K_{eff}	Std.
A	0.9992	± 0.00027	1.00033	± 0.00007
B	0.9995	± 0.00032	1.00015	± 0.00007
C	0.9983	± 0.00035	0.99963	± 0.00007

The calculated power maps in 3 x 3 symmetrical assemblies are shown in the Figs 5 and 6 for cases A, B and C. Fig. 5 shows the relative power distributions of the assemblies in each case. Fig. 6 shows the normalized power maps. Normalization in Fig. 6 has been done to the central assembly power for each case. Calculated standard deviations in assembly level are very small, lower than 0.05% for cases A and B and 0.07% for case C.

Figure 5: Lattice tally calculated 3 x 3 assembly power distributions (arbitrary unit)

Case A			Case B			Case C		
2.3242	2.8549	2.3179	2.4331	2.9207	2.4480	1.8655	1.9162	1.8811
2.8576	3.4362	2.8563	2.9202	3.3935	2.9355	1.9112	1.7086	1.9303
2.3197	2.8614	2.3239	2.4457	2.9333	2.4549	1.8687	1.9190	1.8825

From these calculated assembly power maps, satisfactory symmetry results have been obtained using lattice tally in assembly level. 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 lower 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 in the Monte Carlo simulations. This means that not only the convergence levels in K_{eff} and in local fission rates but also the convergence level of symmetry power map should be considered in the simulation.

Other test calculations for asymmetry factors of assembly power map have been run. The asymmetry factors depend on the rejected initial cycles of neutron histories and the number of used cycles in simulation. The initial 3D neutron source distribution is also helpful to reduce the asymmetry in power map calculation. Comparing to arbitrary setting of fission source like a point source or an uniform distributed source, the experimental determined neutron flux shapes in radial and axial directions are really useful.

Figure 6: Normalized 3 x 3 assembly power distributions

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

In Fig. 6, the central assembly power and the corner one of case A present about 32.5% difference. This is the biggest one among the three cases and it is due to the accumulation of thermal neutron in the central zone without water holes and Pyrex pins.

For case B, the central assembly power and the corner one present about 28.0% difference. Comparing to case A, this difference is smaller thanks to introduced 3 x 3 x 17 water holes.

For case C, the central assembly power and the nearby one present about 9-12% difference and the peak power assembly is not in the central one thanks to introduced Pyrex absorber pins. From Fig. 5, it is clear that the case C has the smallest fission rate because of the Pyrex pins. Pyrex pins also play a more important role to reduce power in the central assembly than in the corner one due to a radial cosine power distribution in fundamental mode.

4.1 Pin power maps

The measurement results of relative pin power distributions of the central 1/8 assembly (32 fuel pins) and the differences in percentage between calculation and measurement are shown in Figs 7 and 8 for cases B and C. (see also Figs. 3, 4, 9, 11 and 12). In Fig. 7, the pin power map has been normalized to 1.0338, the average pin power of measurements for case B. In Fig. 8, it has been normalized to 1.0416, the average pin power of measurements for case C.

Generally the pin power distributions produced by TRIPOLI-4.1 using volume tally at 1997 and by TRIPOLI-4.3 using lattice tally at 2006 are similar. Both can calculate correctly the fission rates near water holes and Pyrex absorber pins which introduce larger gradient of thermal flux and clear fluctuation of neutron spectrum.

In this study, the uncertainty of calculated fission rate in fuel pin level has been reduced to lower than 0.3% in case B and 0.45% in case C. The global differences between calculation and measurement are represented by the RMS errors of 32 fuel pins. For case C this RMS error has been reduced from 1.9% at 1997 to 1.2% at 2006 but for case B, it keeps 1.7%. This

can be explained by our previous observation that, due to the experimental quality of one fuel pin located on the right hand side of Fig. 7, the over-estimation by calculations of +6.0% at 1997 using volume tally has been reproduced with +5.3% at 2006 using lattice tally.

Figure 7: Relative pin power distributions of central 1/8 assembly for case B
(Measurements and differences between calculations and measurements)

M : Measurement pin power [5]
Diff 1 = (C_{1997} – M) x 100 / M, C_{1997} : previous calculated pin power with volume tally [2]
Diff 2 = (C_{2006} – M) x 100 / M, C_{2006} : TRIPOLI-4.3 calculated pin power with lattice tally

	1.107	1.026	1.000	1.025	1.026	0.980	0.983
W	+1.5	+3.2	+1.1	-0.8	-0.4	-0.4	-0.3
	+0.6	+2.4	+2.2	-1.2	-1.1	+1.1	-0.9
	1.068	1.075	1.036	1.047	1.098	1.026	1.003
	+1.4	+2.7	+1.6	+0.1	-1.3	+0.2	-2.3
	+1.0	+3.1	+1.1	- 0.7	-1.6	- 1.3	-3.2
			1.116	1.118		1.070	0.967
		W	+0.8	+0.2	W	+0.7	+2.4
			+0.4	+0.3		+0.5	+1.8
			1.091	***1.145***	1.133	1.032	0.924
			+0.2	-2.1	-0.7	-1.7	**+6.0**
			+0.4	-0.1	-0.5	-0.9	+5.3
					1.109	1.007	0.974
				W	-1.9	-1.9	-1.3
					-1.4	-1.2	-0.9
					1.015	0.973	0.971
					-0.3	-0.2	-1.9
					+0.4	+0.4	-1.7
						0.970	0.950
						-0.5	-1.4
						-2.3	-1.0
							0.920
							-0.4
							+1.6

Max. standard deviation of calculation in fuel pin : 1.2 % (C_{1997}) and 0.3% (C_{2006}).
RMS errors of 32 fuel pins : 1.29 % (Measurement), 1.7 % (C_{1997}) and 1.7% (C_{2006}).

Calculated power maps are normalized to 1.0338, the average pin power of the measurements. [6] W is the water hole.

Figure 8: Relative pin power distributions of central 1/8 assembly for case C
(Measurements and differences between calculations and measurements)

M : Measurement pin power [5]
Diff 1 = (C_{1997} – M) x 100 / M, C_{1997} : previous calculated pin power with volume tally [2]
Diff 2 = (C_{2006} – M) x 100 / M, C_{2006} : TRIPOLI-4.3 calculated pin power with lattice tally

	1.148	1.027	1.045	1.057	1.047	1.088	1.124
W	-3.2	**+5.0**	+1.0	-3.3	+0.2	-1.8	+1.1
	+0.2	+0.5	- 1.6	-2.6	- 1.2	-0.4	- 0.4
	1.036	0.945	1.001	0.982	0.962	1.070	1.105
	+0.8	+1.2	-1.9	- 0.5	-0.6	-1.8	+0.6
	+1.7	+1.0	-1.1	+1.5	+0.2	-1.6	+0.2
			0.901	0.900		1.001	1.087
		P	+0.3	+0.4	P	- 2.1	+0.4
			- 0.1	- 0.4		- 1.4	+0.7
			0.914	***0.854***	0.933	1.049	1.088
			+1.0	**+5.9**	-0.6	+0.4	+2.3
			+0.9	+2.4	-1.2	+0.1	+3.2
					0.970	1.097	1.138
				P	+0.2	+0.8	+0.4
					+0.5	- 0.4	+0.5
					1.071	1.140	1.195
					+0.2	- 0.3	-1.3
					- 0.6	+0.3	-2.0
						1.164	1.199
						+0.1	-2.4
						+1.2	-0.7
							1.206
							- 0.3
							+0.1

Max. standard deviation of calculation in fuel pin : 1.7 % (C_{1997}) and 0.45% (C_{2006}).
RMS errors of 32 fuel pins : 1.10 % (Measurement), 1.9 % (C_{1997}) and 1.2% (C_{2006}).

Calculated power maps are normalized to 1.0416, the average pin power of the measurements. [6] W is the water hole and P the Pyrex absorber pin.

5. Perspective and Conclusion

Another way to calculate the power map with TRIPOLI-4 code is to use the new introduced mesh tally option. This new mesh tally option is still under development and validation. Implemented into TRIPOLI-4.4, new mesh tally option has been first used to study the fission source convergence test in criticality calculations. [7]

Both lattice tally and mesh tally are important tools for power map calculations. Using lattice tally on a big core needs to generate an important input file to specify each pin and each assembly locations in the related lattice geometry but post-processing of simulation results to construct the power map is relative easy.

Mesh tally is easy to use in input data preparation but post-processing of simulation results to construct the power map needs to combine several sets of mesh tally results in real case. This is due to real fuel assemblies including different types of fuel pins (UO_2/MOX, enrichments for new fuel and different burn-ups for irradiated fuel).

For a real PWR new core power map calculation, 3D Monte Carlo simulation using lattice tally and mesh tally of TRIPOLI-4 code has also been performed recently. As tally in fuel pin level in present Monte Carlo simulation is still very computer time consuming and as the fission source convergence in a power reactor K_{eff} calculation is still a challenge using Monte Carlo calculation, more efforts are needed in order to improve the Monte Carlo tally performance and the fission source convergence.

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Figure 9: Previous modeling (1997 – case C) (With pin power measurement volumes stamped on 1/8 central assembly)

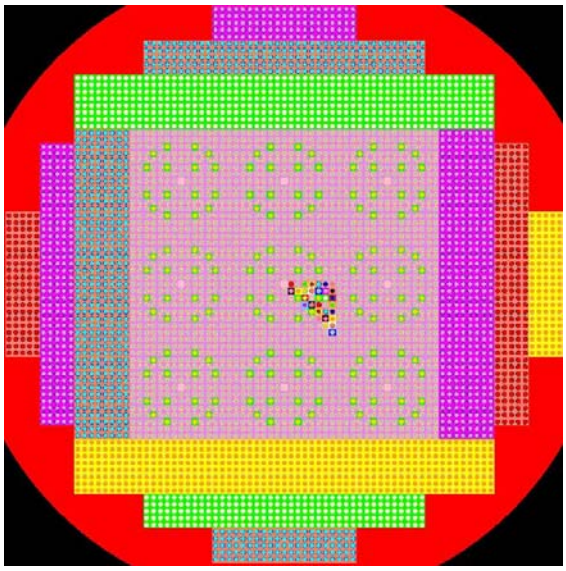

Figure 10: TRIPOLI-4.3 modeling - case A (Central 3x3 assemblies with fuel pins only)

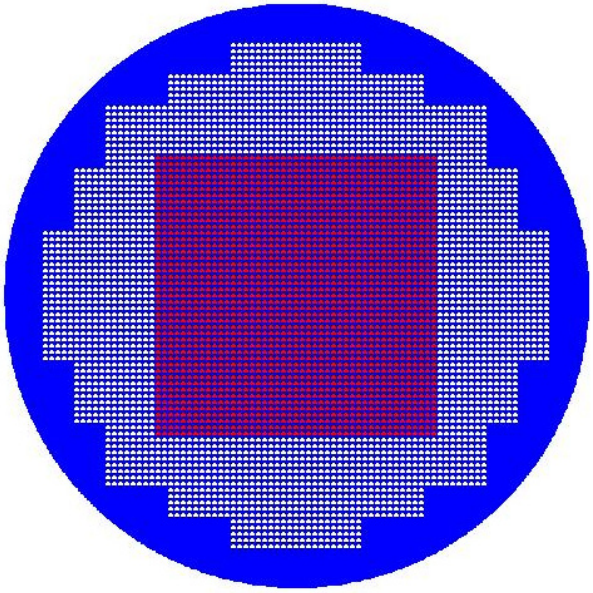

Figure 11: TRIPOLI-4.3 modeling - case B (Central 3x3 assemblies with water holes, pin power map from lattice tally)

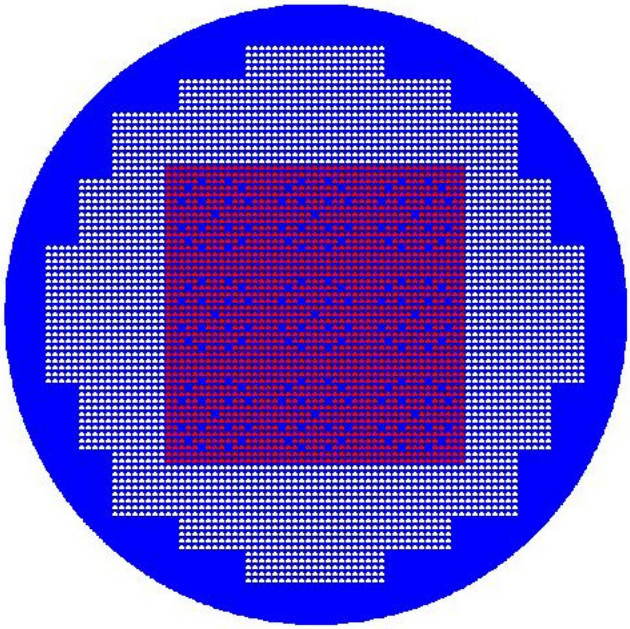

Figure 12: TRIPOLI-4.3 modeling - case C (Central 3x3 assemblies with Pyrex pins and water holes, pin power from lattice tally)