

Validation of the Monte Carlo code COSMC by 3-D Venus-2 MOX Core Benchmark

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1. Introduction

Due to its advantages of dealing with continuous energy cross sections and arbitrary geometry, the Monte Carlo (MC) method is becoming widely used in the field of transport calculations in reactor physics. A new 3D Monte Carlo transport code which named COSMC, specifically intended for reactor physics analysis, has been developed jointly by the Department of Engineering Physics in Tsinghua University and State Nuclear Power Software Development Center. Now, the COSMC is an internal test version [1,2]. The COSMC code uses the method known as the delta-tracking method to simulate neutron transport, the advantages of which include fast simulation in complex geometries and relatively simple handling of complicated geometrical objects. Some other techniques such as computational-expense oriented method and hash-table method [3] have been developed and implemented in COSMC to decrease the computational time consuming. To meet the requirements of reactor analysis, the COSMC code has the capability of criticality calculation and burnup calculation.

In this study, the criticality calculation capability of COSMC is tested on the basis of VENUS-2 3D MOX core benchmark. There are three types of fuels, i.e., 3/0 UO₂(with 3.0wt% enrichment UO₂ fuel), 4/0 UO₂(with 4.0wt% enrichment UO₂ fuel), 2/2.7 MOX(with 2.0 wt% enrichment UO₂ fuel and PuO₂ fuel weight 2.7 wt%), in the VENUS-2 core. The infinite multiplication factors and the absorption and fission reaction rates for each actinide were calculated and the comparisons were made between the benchmark results and those of COSMC code and MCNP. Large discrepancy between the code results and the measurements were found due to the nuclear data library. The pin-by-pin power distributions and the axial fission rate distributions tallies of the benchmark were performed, as well as the comparisons between calculation results and benchmark results. The comparison in the calculation efficiency was made between COSMC and MCNP in the cell calculation and assembly calculation. The time consuming of COSMC is less than that of MCNP, especially for large tally cases.

2. Benchmark description

The benchmark based on the VENUS-2 MOX core measurement data has been initiated in order to understand better the behavior of the fuel and to identify possible improvements in nuclear data and physics modeling methods. The VENUS (Vulcain Experimental

NUclear Study) facility[4,5] is a zero power critical reactor located at SCK.CEN in Belgium. The central part of the core consists of UO₂ fuel pins 3.3 wt% enriched in ²³⁵U (3.3/0) and Pyrex pins. There are UO₂ fuel pins 4.0 wt% enriched in ²³⁵U (4.0/0) on the periphery of the core and MOX fuel pins enriched 2.0 wt.% in ²³⁵U and 2.7 wt.% in high grade plutonium (2.0/2.7) on the most external part of the core. Three dimensional models have been made in COSMC as shown in Fig.1 and Fig.2.

In addition, to verify the calculation efficiency and accuracy of neutron flux of COSMC, a typical PWR UO₂ and MOX assemblies are adopted. The PWR UO₂ fuel assembly is the same geometrical configuration as a 17×17 type fuel design. The average ²³⁵U enrichment is 6.2% and the assembly is composed of UO₂ and UO₂-Gd₂O₃ (Gd) fuel rods. As shown in Fig.3. The PWR MOX fuel assembly is also the same geometrical configuration as a 17×17 type PWR fuel design as shown in Fig.3. The average Pu fissile content is 11wt.% and the assembly is composed of low, middle and high Pu content fuel rods. The atomic number densities and fuel rod specifications of the UO₂ and MOX fuel are shown in Table I and Table II, respectively. Other parameters related to the assembly can be found in reference [6].

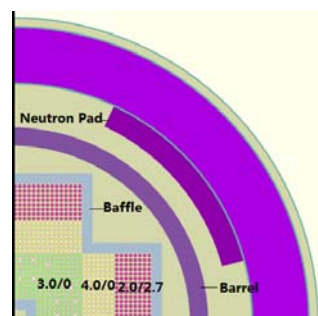


Fig. 1 Quarter VENUS-2 core loading configuration

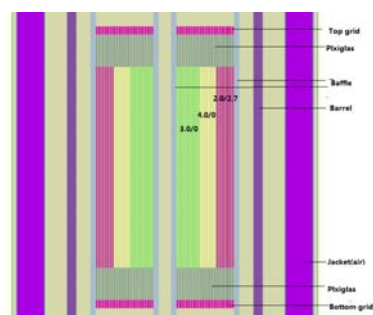


Fig. 2 Core description (vertical cross-section)

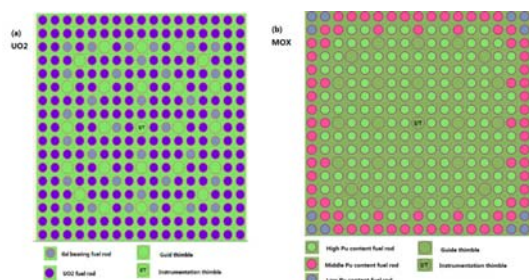


Fig. 3 Configuration of PWR UO₂ and MOX assembly

Table I Atomic number density and fuel rod specification of UO₂

UO ₂ fuel rod	
²³⁵ U enrichment	6.50%
UO ₂ density	10.3 g/cc
Atomic number density(#/barn/cm)	
²³⁵ U	1.5122E-03
²³⁸ U	2.1477E-02
¹⁶ O	4.5945E-02

Table II Atomic number density and fuel rod specification of MOX fuel

	Low Pu content fuel	Middle Pu content fuel	High Pu content fuel
MOX density (g/cc)	10.4	10.4	10.4
²³⁵ U enrichment (wt%)	0.2	0.2	0.2
Pu concentration (wt%)	7.5	14.4	19.1
Pu concentration (wt%)	4.8	9.2	12.2
²³⁵ U	4.3463E-05	4.0212E-05	3.8000E-05
²³⁸ U	2.1408E-02	1.9812E-02	1.8724E-02
²³⁸ Pu	3.6652E-05	7.0521E-05	9.3169E-05
²³⁹ Pu	9.4712E-04	1.8154E-03	2.4075E-03
²⁴⁰ Pu	4.3265E-04	8.2927E-04	1.0997E-03
²⁴¹ Pu	1.6026E-04	3.0720E-04	4.0739E-04
²⁴² Pu	1.0984E-04	2.1052E-04	2.7920E-04
²⁴¹ Am	4.6536E-05	8.9200E-05	1.1828E-04
¹⁶ O	4.6358E-02	4.6338E-02	4.6325E-02

Note: Definition of Puf content is $(^{239}\text{Pu} + ^{241}\text{Pu}) / (^{235}\text{U} + ^{238}\text{U} + ^{238}\text{Pu} + ^{239}\text{Pu} + ^{240}\text{Pu} + ^{241}\text{Pu} + ^{242}\text{Pu} + ^{241}\text{Am})$

3. Methodology

The fission source iteration method is used for critical calculation of Monte Carlo, and the convergence rate of the fission source distribution is determined by the system dominance ratio. The source convergence module of COSMC has a statistical function of Shannon entropy, it can qualitatively reflect convergence trend of fission source distribution and helpfully determine the reasonable neutron quantity in inactive generation [7].

The newly proposed Cell-Mapping method provides a fast scheme to match the tracking cell with the tally

cells, and it is efficient in reducing the time required to treat massive tally cells [8]. Most of the existing MC codes including MCNP and COSMC adopt a universe-based geometry system, which allows any cells to be filled with a different universe and provides flexibility useful in describing lattice geometry. Given a track length that occurs in certain cell, the tally-cell list need be searched to find the matched tally cell and the tallies will be updated accordingly. When using a sequential search method whereby one has judge the equality between two sectors, and thus the overall procedure can become prohibitively expensive when the tally-cell list is large.

In general, the time consuming of COSMC is decreased significantly comparing with that of MCNP for all the cases as shown in Table III. For the assembly calculation, if the K_{inf} was calculated without tally flux, the time consuming ratio of COSMC to MCNP is about 0.65. However, if K_{inf} was calculated with tally flux, the time ratio of COSMC to MCNP is about 0.48. The time consuming increasing of MCNP is more significant than that of COSMC. This shows that the tally efficiency of COSMC is higher than that of MCNP, because the Cell-Mapping method has been utilized in COSMC.

Table III Comparison of computing time between COSMC and MCNP (min)

Cases	Particles	COSMC	MCNP	COSMC/MCNP
UO ₂ (wt 3.3%)	5000×300	2.65	4.87	0.54
UO ₂ (wt 4.0%)	5000×300	2.67	5.34	0.5
MOX(wt 2.0/2.7%)	5000×300	2.82	6.62	0.43
assembly(No tally)	5000×1000	8.6	13.15	0.65
MOX assembly(No tally)	5000×1000	8.9	14.02	0.63
UO ₂ assembly	5000×1000	9.35	19.48	0.48
MOX assembly	5000×1000	9.8	22.4	0.44

4. Results

4.1 Infinite multiplication factors and energy integrated reaction rate

The infinite multiplication factors of cell calculations of benchmark, MCNP and COSMC as well as associated standard deviation are shown in Table IV. Large discrepancies of the multiplication factor between MCNP, COSMC and experiment were found. The infinity multiplication factors discrepancies between MCNP and COSMC are less than 100 pcm for the three cases based the same library ENDF/B-VII.0. The results of COSMC are consistent with that of MCNP. Therefore, that differences results from nuclear data library.

The energy integrated absorption and fission reaction rates per actinides in the fuels is shown in Table V. In this table, the absorption reaction rate is expressed as

sum of fission and capture reaction rates. The energy integrated reaction rates deviation between COSMC and MCNP is shown in Table VI. The energy integrated reaction rates of COSMC agreed well with that of MCNP, and the largest deviation is less than 0.52% with 0.5% uncertainty of MCNP and 0.3% uncertainty of COSMC.

Table IV Benchmark, MCNP, and COSMC eigenvalue results for cell calculation

Type of Fuel	Source	Eigenvalue	Vs.Benchmark (pcm)	Vs.MCNP (pcm)
UO ₂ (wt 3.3%)	Benchmark(Average)	1.40786±0.00277	-	-
	MCNP	1.41568±0.00050	788	-
	COSMC	1.41475±0.00024	688	-93
	Benchmark(Average)	1.33925±0.00395	-	-
UO ₂ (wt 4.0%)	MCNP	1.35641±0.00053	1716	-
	COSMC	1.35644±0.00025	1737	21
	Benchmark(Average)	1.258±0.00429	-	-
MOX(wt 2.0/2.7%)	MCNP	1.28112±0.00059	1716	-
	COSMC	1.28012±0.00029	1737	100

Table V Energy integrated reaction rates in fuel cells (reactions/cm³/sec)

	2/2.7 MOX		3/0 UO ₂		4/0 UO ₂	
	Abs	Fiss	Abs	Fiss	Abs	Fiss
²³⁵ U	3.52E+0 2	9.12E+ 01	1.49E+ 02	7.18E +02	1.26E+ 02	5.63E +02
²³⁸ U	1.49E+0 0	1.05E+ 01	1.09E+ 01	1.20E +00	1.11E+ 01	1.38E +00
²³⁹ Pu	6.23E+0 2	3.17E+ 02	-	-	-	-
²⁴⁰ Pu	8.09E+0 0	8.44E+ 02	-	-	-	-
²⁴¹ Pu	7.57E+0 2	2.65E+ 02	-	-	-	-
²⁴² Pu	6.15E+0 0	4.39E+ 02	-	-	-	-
²⁴¹ Am	1.19E+0 1	8.32E+ 02	-	-	-	-

Note : Abs means absorption, Fiss means fission

Table VI Energy integrated reaction rates deviation(C/Average -1) %

	2/2.7 MOX		3/0 UO ₂		4/0 UO ₂	
	Abs	Fiss	Abs	Fiss	Abs	Fiss
²³⁵ U	-0.17	-0.21	-0.20	-0.07	-0.14	-0.11
²³⁸ U	-0.07	0.07	0.08	-0.10	0.20	0.00
²³⁹ Pu	-0.04	0.08	-	-	-	-
²⁴⁰ Pu	-0.13	-0.23	-	-	-	-
²⁴¹ Pu	-0.02	0.00	-	-	-	-
²⁴² Pu	-0.10	-0.52	-	-	-	-
²⁴¹ Am	-0.07	-0.10	-	-	-	-

Note : Abs means absorption, Fiss means fission

4.2 Pin flux of assembly

Neutron flux is the most important physical parameter in nuclear reactor design. To verify the accuracy of neutron flux of COSMC, a typical PWR UO₂ and MOX assembly were adopted. The relative percent differences in flux tallies between COSMC and MCNP for both UO₂ and MOX assembly were performed. As shown in Fig.4 and Fig.5 for UO₂ and MOX assembly, respectively. The largest relative percent differences of neutron flux between COSMC and MCNP is less than 1.6% for the UO₂ assembly and is less than 1.2% for MOX assembly. The largest relative percent differences for UO₂ is larger than MOX due to the gadolinium effect.

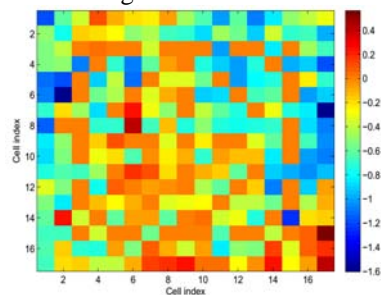


Fig. 4 Relative percent differences of neutron flux between COSMC and MCNP for the UO₂ assembly

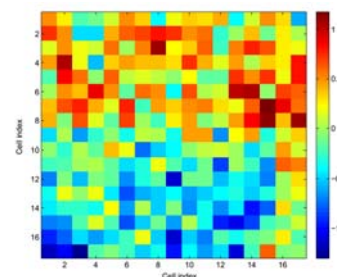


Fig. 5 Relative percent differences of neutron flux between COSMC and MCNP for the MOX assembly

4.3 Effective multiplication factor

The effective multiplication factor and the radial pin-by-pin fission rate distributions are performed by the 3D VENUS-2 core calculation with COSMC code. The VENUS-2 core was modeled explicitly in the three directions. For whole core calculations, 500000 particles per cycle with 1000 cycles (100 are inactive) were used. In the benchmark, the criticality was attained by adjusting the water level. The operating temperature is 23.0°C. However, the temperature of cladding and fuel was not given in the benchmark. If all the temperatures of all the material in the core are assumed as 300K, using the library based on ENDF/B-VII.0, the effective multiplication factor is 1.0025, and the standard deviation is 0.00010, which shows deviation of about 0.25% from the critical state. It is shown that the effective multiplication factor agreed well with MCNP results 1.0020±0.00030 and other institution results calculated by MCNP-4B and deterministic code [4,5].

4.4 Axial distribution for core calculation

The axial fission rate distribution was calculated at six fuel pin positions, i.e., two pins per each fuel region in the core. The average deviation of the C/E (Calculation/Experiment) values for the axial fission rate of the six fuel rods is less than 0.2%. The normalized axial fission rate distribution at two position for the 2/2.7 MOX fuel pin was shown in Fig.6 and the distribution were well expressed in typical cosine shape. The distributions for remaining fuel pins also show a similar tendency. Compared with the experimental data, the COSMC calculation results give a good estimation with the experiment data by considering the calculation uncertainty.

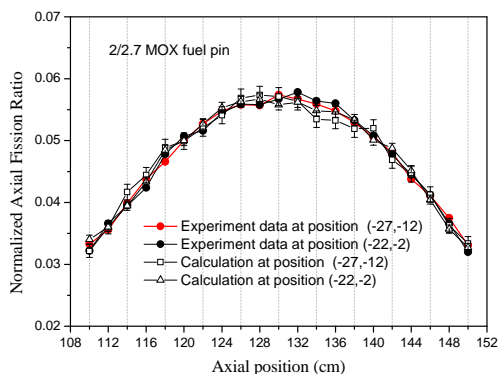


Fig. 6 Normalized axial fission rate distribution in the outermost 2/2.7 MOX fuel pin

4.5 Fission rate distribution in the core

The radial fission rate distribution was calculated for each zone in the z direction and then the average fission rate of each zone in the z direction was used to compare with the experiment data. The COSMC results were in good agreements within maximum error of about 12.7% occurred in the outer 2/2.7 MOX fuel region because of neutron flux difference

5. Conclusion

The 3-D benchmark calculation on the VENUS-2 MOX core measurements were performed. The results show that the consuming time of COSMC is less than that of MCNP, especially for massive tally because of Cell-Mapping method using in COSMC. For the cell calculation, the infinity multiplication factor agreed well with between COSMC and MCNP, large deviation between MCNP, COSMC and benchmark results comes from nuclear library difference. The neutron flux for a typical PWR UO₂ and MOX assembly were also calculated. The largest relative percent differences of neutron flux between COSMC and MCNP for the UO₂ assembly is less than 1.6% and that for the MOX assembly is less than 1.2%. For the core calculation, the K_{eff} agrees well with other code The fission rates in the core distribution are in good agreements within maximum error of about 12.7%. For the axial distribution, the results of COSMC give a good estimation within average of 0.2%. The burnup function

of COSMC would be verified in the future.

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