VERIFICATION AND VALIDATION OF SUPERMC3.2 WITH HEAVY WATER REACTOR MODEL DCA

by

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The super multi-functional calculation program for nuclear design and safety evaluation is a general, intelligent, accurate and precise simulation software system for the nuclear design and safety evaluations. The heavy water reactor has a much stronger moderation power and much longer diffusion length of the thermalized neutrons. The paper intends to show the verification and validation of SuperMC3.2 with a heavy-water-moderated lattice named the deuterium critical assembly which is very similar to the Canada Deuterium Uranium type reactor and selected from the international reactor physics experiment evaluation project. The calculation results were compared with the reference calculated results and the experimental data from International Reactor Physics Experiment Evaluation Project. The final obtained results proved the accuracy, convenience and universality of SuperMC, and primarily verified the applicability of SuperMC in nuclear analysis of heavy water reactor.

Key words: Monte Carlo, SuperMC, heavy water reactor, verification and validation, deuterium critical assembly

INTRODUCTION

A nuclear power plant is always designed with a conservative approach, which cannot attain the best economic efficiency. The high-fidelity simulation with realistic models can obtain more reliable and precise results, which are very useful for nuclear devices design, construction and operation to improve security and economy. Therefore, the capacity of high-fidelity simulations has become one of the most important assessments of nuclear design codes [1, 2]. For the purpose of ensuring the reliability of the codes, the verification and validation of different applications should be done in sequence using realistic experimental reactor benchmark models.

The Super Multi-functional Calculation Program for Nuclear Design and Safety Evaluation (SuperMC) [3, 4] is a general, intelligent, accurate and precise simulation software system for nuclear design and safety evaluation, which has integrated the automatic geometry and physics modeling module, efficient and accurate particle transport calculation module and intelligent visualization module and been developed by the FDS team [5]. The latest version of SuperMC can accomplish the transport calculation of n, γ, depletion calculation, activation calculation and shutdown dose rate calculation, and can be applied for criticality and shielding design of reactors, medical physics analysis, *etc*. The SuperMC has been verified and validated by more than 2000 benchmark models and experiments, such as the International Criticality Safety Benchmark Evaluation Project (ICSBEP), Shielding Integral Benchmark Archive and Database (SINBAD), and the comprehensive applications from the reactors including the International Thermonuclear Experimental Reactor (ITER), FDS-II, IAEA-BN600, IAEA-ADS, BEAVRS, HM, TCA, *etc*. [6-14]

The heavy water reactor (HWR) has a much stronger moderation power and much longer diffusion length of the thermalized neutrons than PWR on account of using deuterium oxide as a moderator. Furthermore, the HWR can use natural uranium as fuel and generate the plutonium. In order to prove that SuperMC can be applied in the HWR neutronics analysis, the verification and validation (V&V) of SuperMC3.2 with the HWR model is indispensable. In this paper, one heavy-water-moderated lattice was selected from the International Reactor Physics Experiment Evaluation Project (IRPhEP) [15], which is the deuterium critical assembly (DCA) [16]. According to the feature of HWR, the fission reaction of ^{235}U (F25), capture ratio of ^{238}U and epithermal capture ratio of ^{238}U (ρ28) are calculated, and the results are compared with the experimental data and the MCNP5 [17] reference results to prove the accuracy.

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The structure of this paper is as follows: the detailed process of modeling is shown in Section 2, and the calculation results are shown in Section 3. Finally, Section 4 is for the conclusion.

MODEL PROCESS

The DCA model [18] is a tank-type critical assembly with a maximum power of 1 kWth, a heavy-water-moderated, boiling-light-water cooled, and pressure-tube-type reactor developed in Japan. There are ten configurations of the DCA models which have been carried out, varying the lattice-pitch of 22.5 or 25.0 cm and simulating coolant void fractions among 0, 30, 70, 87, and 100 %. In this paper, only the B1-7 core from the report was selected, which is the configuration of the DCA model with the 25.0 cm lattice pitch, 70 % coolant void fraction and the measured coolant level is 102.5 cm. This section will demonstrate the procedure of modeling DCA by SuperMC3.2 with automatic geometry and physics modeling functions.

Geometry modeling

Accurate modeling is an extensive task which is the precondition of the high-fidelity simulation. One of the advanced capabilities of SuperMC is automatic and accurate geometry modeling, which can convert the CAD models into the Monte Carlo calculation file with a constructive solid geometry (CSG) representation. Furthermore, the fission reactors always consist of a bulk of repeated structures which are an obstacle for enhancing the modeling system efficiency. Accordingly, a CAD-based hierarchical modeling method was developed to promote the efficiency of modeling the complex hierarchical structures and large-scale models [19]. The new CAD-based method not only creates the detailed models, but also keeps the relations of different components in the reactor. Then the hierarchical structures and repeated structures can be generated and be used for accelerating the geometry navigation in the SuperMC calculations.

Modeling the whole DCA model with the CAD-based Hierarchical Modeling Method to be exact is a top-down detailed procedure, because the DCA model can be divided into several levels such as core assembly pin sub-regions. The DCA model consists of 95 CANDU fuel channel assemblies surrounded by the D2O coolant, and each assembly has three fuel rods rings. The new method supports creating the relations which are the connections of each levels and the arrangements of the components assembled in the whole reactor region. Moreover, the relations are combined with all unique CAD models called *meta-geometry* to represent the whole reactors. Therefore, the method only converts the meta-geometry and then the other geometries can be generated by corresponding relations. This method is sharply reducing the cost of modeling.

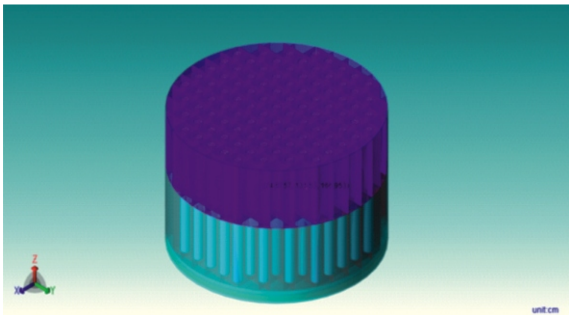

Figure 1. Modeling and visualization of the DCA models in SuperMC3.2

The detailed models of DCA are shown in fig. 1, which are visualized by SuperMC3.2. On the left of the picture is the tree interface that describes the relations between theof levels and different components. The right side of the picture shows the visualization interface in which the models selected by the left trees will be visualized. The left tree interface generated by the relations supports many types of model screens, such as material, level number, universe number and colors. The model screens are convenient for managing the huge scale of models and choosing the models.

SuperMC3.2 supports rapid 2-D section visualization. Figure 2 illustrates the cross-section of the model, visualized by the SuperMC and compares it to the reference models [18]. It can be determined that the visualization results are in good agreement.

Physics modeling

In addition, physical attributes such as materials, source distribution, tallies and calculation conditions (both transport and depletion) can be assigned interactively by the graphical user interface in SuperMC3.2. The DCA core comprises seven types of materials and the fuel cluster is filled by the UO2 (1.2 wt. %) pins which are shown in fig. 3. The DCA case was run in the k-eigenvalue criticality mode which employed 5000 generations with 50,000 neutron histories per generation. Results from the first 100 generations were discarded.

CALCULATION RESULTS AND ANALYSES

After the calculation models of HWR were created, the code to code comparison in criticality calculations has been done between SuperMC3.2 and MCNP5 reference results from the IRPhEP reports. The comparison of calculation results of k_{eff} were

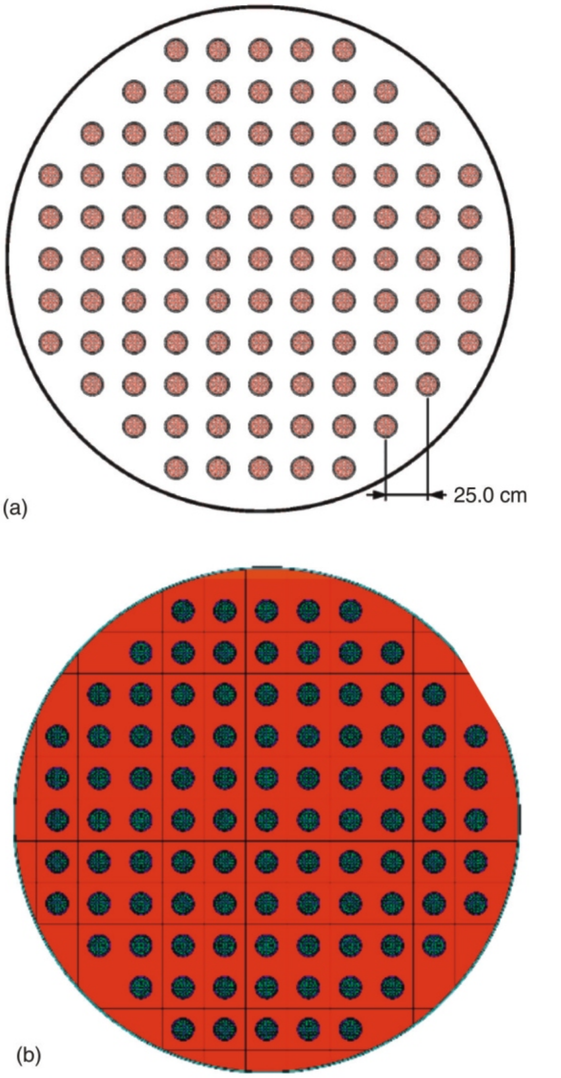

Figure 2. The XY section of the DCA model and comparison with reference models; (a) XY section of the reference model, (b) XY section od DCA models

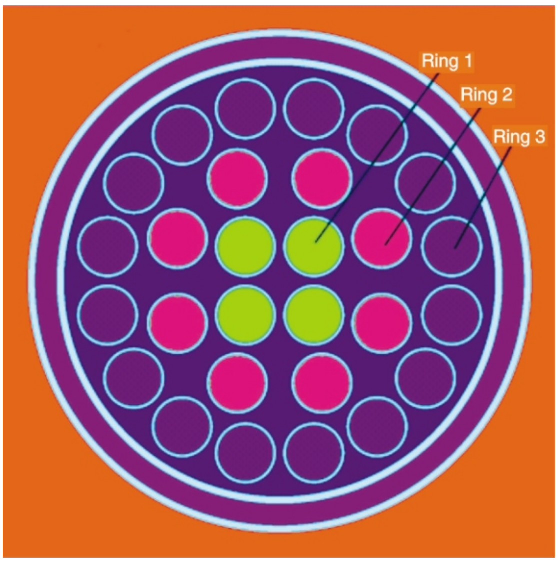

Figure 3. The fuel channel of the DCA reactor

shown in tab. 1. Furthermore, some parts of the results were validated by the experimental data which will be demonstrated as follows. The nuclear data used in the SuperMC calculation is ENDF/B-VI [20].

The DCA fuel channel consists of three concentric rings of fuel pins as shown in fig. 3, where the values of the neutron flux are tallied. Each ring is divided into three parts to meet the experimental situation, where the first part is below 40 cm, the second part is from 40 cm to 60 cm and the last parts is above 60 cm. The code to code comparison results of the fission reaction of ^{235}U (F25) and capture ratio of ^{238}U (C28) are shown in tab. 2. The values of F25 and C28 in each region have good consistence with the MCNP5 reference results. Considering the biggest deviation is less than 0.4 %, it is concluded that the results from SuperMC3.2 are very close to MCNP.

The radius power distributions of each assembly in the DCA model calculated by SuperMC3.2 and compared with MCNP5 reference results were illustrated in fig. 4. The hottest assembly is 38.65 (MeV/g) and the symmetric regions are almost equal. Meanwhile, the code to code comparison results of the power distribution between the SuperMC3.2 and MCNP were depicted in different colors. The max absolute relative error of the two codes is 1.11 %, and the average error is 0.27 %. Therefore, it is can be determined that the SuperMC3.2 obtained the more accurate results in this region and the accuracy of the SuperMC3.2 can be proved.

Based on the tally data, the epithermal capture ratio of ^{238}U (ρ^{28}) and the microscopic thermal fission reaction of ^{235}U (F25) can be calculated to be compared with the experimental data. The ρ^{28} can be defined by the eq. (1) [18]

$$\rho^{28} = \frac{\int_{E_{\mathrm{Cd}}}^{\infty} \sigma_{\mathrm{c}}^{28}(E)\phi(E)\mathrm{d}E}{\int_{0}^{E_{\mathrm{Cd}}} \sigma_{\mathrm{c}}^{28}(E)\phi(E)\mathrm{d}E} \tag{1}$$

where σ_{c}^{28} represents the microscopic cross-section for the ^{238}U capture reaction, and ϕ is the neutron flux. The E_{Cd} – the cadmium (Cd) cutoff energy which is defined as 0.46eV 0.0002. The capture reactions rate of ^{238}U under and above the cutoff energy are tallied separately to calculate the value of ρ^{28}. In the measurement, the Cd cover can capture most of the thermal neutrons, whereas most of the epithermal neutrons can pass through the cover to the inside U foil. Therefore, the measurement of the U foil with the Cd cover can be compared with the U foil without the Cd cover to calculate the value of ρ^{28}. The microscopic thermal fission reactions (F25) in three layers are tallied by reaction of total fission below the energy which is defined as 0.46 eV as well. The calculation results are normalized with the lowest values of layer 1. There were two different tally subdivisions

Table 1. The code to code comparison of the values of k_{eff} with MCNP5 and SuperMC3.2

DCA	MCNP5	SuperMC3.2	Benchmark data	(C-M)/M [%]	(C-E)/E [%]
ID	k_{eff} (M)	k_{eff} (C)	k_{eff} (E)		
B1-7	0.99570 0.00021	0.99579 0.00021	1	0.01	0.42

Table 2. The comparison of F25 and C28 in three layers of the fuel channel

DCA		MCNP5		SuperMC3.2		Comparison results of two codes [%]	
Regions	Sub-regions	Calculation quantities		Calculation quantities			
Height *h* [cm]		F25	C28	F25	C28	F25	C28
Ring 1	$h < 40$	10.8655 0.0003	0.111803 0.0004	10.85915 0.0005	0.112023 0.0007	0.0584	0.1968
	$40 < h < 60$	8.87892 0.0004	0.090493 0.0004	8.87834 0.0006	0.09074 0.0007	0.0065	0.2729
	$h > 60$	13.8843 0.0003	0.14801 0.0004	13.8778 0.0004	0.148538 0.0006	0.0468	0.3567
Ring 2	$h < 40$	13.2418 0.0002	0.124622 0.0002	13.2395 0.0005	0.12493 0.0006	0.0174	0.2471
	$40 < h < 60$	10.8399 0.0002	0.101007 0.0003	10.8379 0.0005	0.101267 0.0007	0.0185	0.2574
	$h > 60$	16.7333 0.0002	0.163673 0.0002	16.7410 0.0004	0.164233 0.0005	0.0460	0.3421
Ring 3	$h < 40$	18.5155 0.0002	0.156496 0.0002	18.5087 0.0004	0.156717 0.0006	0.0367	0.1412
	$40 < h < 60$	15.1886 0.0002	0.127056 0.0002	15.1893 0.0005	0.127292 0.0006	0.0046	0.1857
	$h > 60$	23.2164 0.0001	0.203957 0.0002	23.2195 0.0004	0.204472 0.0005	0.0134	0.2525

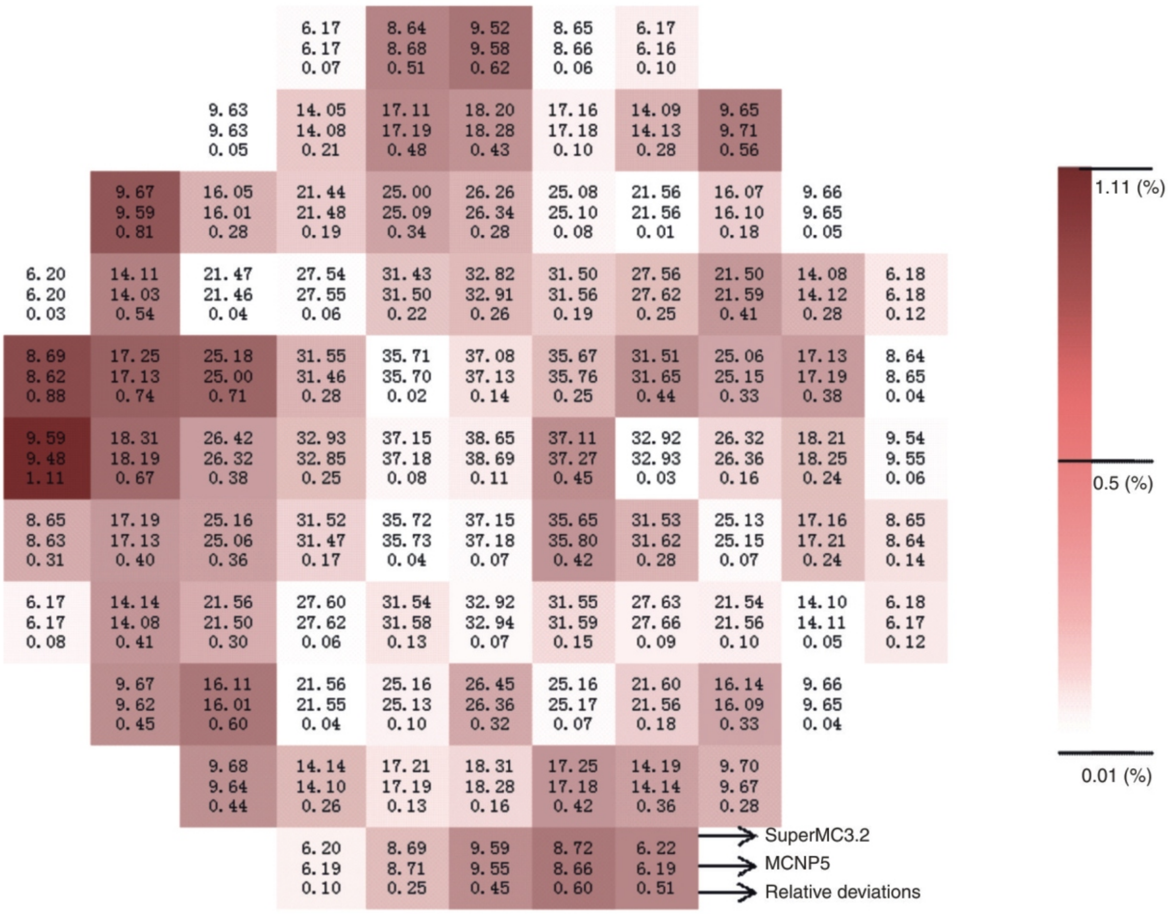

Figure 4. Results and relative deviations in the radial power distribution between SuperMC3.2 and the reference MCNP results

prepared in the IRPhEP reference report, the first is from the 40 cm to 60 cm above the fuel bottom named *standard tally regions* and the second are *large tally regions* which is the entire region under the D^2O level. In this paper, the following results are evaluated with *large tally regions*.

Table 3. Validations of the calculation results ρ^{28} with the experimental data from IRPhEP

Regions	Calculation results (C28)		ρ^{28}		Deviation (C-E)/E) [%]
	$E < 0.46$ eV	0.46 eV $< E < 20$ M eV	Calculation data (C)	Experimental data (E)	
Ring 1	0.144935 0.0005	0.186170 0.0005	1.284507	1.243	+3.3
Ring 2	0.178661 0.0006	0.190503 0.0006	1.066280	1.060	+0.5
Ring 3	0.253101 0.0004	0.210005 0.0004	0.829726	0.893	–7.1

Table 4. Validations of the calculation results F25 with the experimental data from IRPhEP

Regions	Fission reaction (<0.46 eV)		F25 distribution (normalized by Ring 1)			Deviation	
	MCNP5	SuperMC 3.2	MCNP5 (C_M)	SuperMC 3.2(C_S)	Experimental data (E)	(C_M-E)/E [%]	(C_S-E)/E [%]
Ring 1	29.2683	29.2541	1	1	1	–	–
Ring 2	36.2343	36.2375	1.238	1.239	1.208	+2.5	+2.6

The ρ^{28} of rings 1-3 is calculated by the eq. (1) and listed in the tab. 3. The biggest deviation occurred in ring 3 at 7.1 % with 3.7 % of experimental uncertainty. Ring 2 achieved the best agreement with the experimental data with the 0.5 % deviation, which was much lower than the 4.0 % uncertainty. It was better than that of ring 1, where the relative deviation was 3.3 % with the 4.3 % experimental uncertainty. Table 4 shows the comparison of F25 values among the MCNP5, SuperMC3.2 and experimental data. The results which were obtained almost equal between the two MC codes. The max deviation between the simulation and experiment is under 3 % which can be considered as an acceptable result. Based on the calculation results from SuperMC3.2 we can concluded that they are in good agreement with the experimental data, considering the almost same deviations of the MCNP5 results and experimental data.

From the aforementioned results, it can be determined that the edge regions of the fuel cluster have a higher proportion of thermalized neutrons because of the much longer diffusion length. Meanwhile, the proportion of fission neutron escape to the capture of ^{238}U in the edge regions is higher than in the center regions. The fuel rods in ring 3 contribute more power to the core than other regions in one fuel cluster. However, the power distribution of the whole core conforms to the common rule that it is the hottest in the middle and low on all sides.

CONCLUSION

An HWR model selected from IRPhEP named DCA was applied in the V&V procedure of the SuperMC code. The DCA pin-by-pin models were created by the advanced automatically modeling system of SuperMC. Because the HWR has a much stronger moderation power and much longer diffusion length of the thermalized neutrons, the fission reaction of ^{235}U, capture ratio of ^{238}U and epithermal capture ratio of ^{238}U are calculated and validated by the experimental data. Furthermore, the power distributions of the core were calculated and compared with the reference results from the MCNP5 code. The final obtained results have shown that the results from SuperMC agree well with the experimental data and other reference results. The works which is shown in the paper has completed a series of tests of SuperMC3.2 and has proved the accuracy, convenience and universality of SuperMC and that the preliminary application of HWR nuclear analysis can be trusted.

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AUTHORS' CONTRIBUTIONS

Q. GAN is the first author of the paper, and he is the main implementers and one of the thought contributors of the research. P. Long is the corresponding author of the paper, and he is the main thought contributors of the research. The other authors are all the supporters of the research.

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ВЕРИФИКАЦИЈА И ВАЛИДАЦИЈА СуперМЦ3.2 ПРОГРАМА НА МОДЕЛУ ТЕШКОВОДЕНОГ РЕАКТОРА СА КРИТИЧНИМ ДЕУТЕРИЈУМСКИМ СКЛОПОМ

Супер мултифункционални програм СуперМЦ3.2, за прорачун нуклеарног дизајна и процене сигурности представља општи, интелигентан, тачан и прецизан симулациони софтверски систем за нуклеарни дизајн и сигурносне процене. Тешководни реактор има мног јачу моћ успоравања и много већу дужину дифузије термичких неутрона. Намера је овде да се прикаже верификација и валидација СуперМЦ3.2 програма са решетком која је модерирана тешком водом, названом деутеријум критични склоп. Склоп је врло сличан канадском реактору типа деутеријум уранијум који је изабрана из Међународног пројекта евалуације експерименталне реакторске физике, IRPhEP. Резултати израчунавања упоређени су са референтним израчунатим резултатима и експерименталним подацима из IRPhEP. Коначни добијени резултати доказали су тачност, практичност и универзалност СуперМЦ програма и првенствено потврдили применљивост овог програма у нуклеарној анализи тешководних реактора.

Кључне речи: Монте Карло, СуперМЦ, тешководни реактор, верификација, валидација, деутеријумски критичан склоп