## RMC Capability of Multi-cycle HFP Full Core Burnup Simulation

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Abstract - Monte Carlo method is very attractive for high fidelity simulations of nuclear reactors. However, real nuclear reactors are complex systems with multi-physics interacting and coupling. In order to perform the high fidelity multi-physics simulations of real reactors, many advanced methods and capabilities must be developed in new generation Monte Carlo codes, including on-the-fly temperature dependent cross sections treatment, neutronics/ thermal-hydraulics coupling, full-core detailed burnup calculation, critical searching, adjoint-weighted dynamic parameters calculations, equilibrium Xenon method,Monte Carlo refueling capacity, and restart capacity for burnup calculation. In this paper, these mentioned for multiple burnup cycles simulations in Hot Full power condition of PWR full core have been developed in RMC and applied to the two cycles burnup calculations of BEAVRS benchmark. The parameters given in BEAVRS benchmark were calculated and compared with the measured values of BEAVRS benchmark and results of MC21, which show good agreements. This work paves the way for Monte Carlo code in lifecycle simulations of nuclear reactor cores.

## I. INTRODUCTION

With the increasing demands of high fidelity neutronics analysis and the development of computer technology, Monte Carlo method becomes more and more important especially in critical analysis of initial core and shielding calculations, due to its advantages such as flexibility in geometry treatment, the ability to use continuous-energy pointwise cross-sections, the easiness to parallelize and high-fidelity of simulations.

However, nuclear reactors are complex systems with multi-physics interacting and coupling. For examples, nuclides are generated or depleted during the lifecycle of reactors, and thermal-hydraulics has feedbacks on material temperature and density and thus nuclear cross sections. Reactivity control systems such as soluble boron and control rods are adjusted during the operations of reactors to maintain the criticality of power plants. Moreover, when the concentration of soluble boron reach zero, the reactor should be refueled to undergo the next burnup cycle. All of the factors mentioned above should be considered the high fidelity multi-physics simulations of real reactors or benchmarks calculations such as BEAVRS MIT BEAVRS benchmark [1].

In this paper, the abilities mentioned above for multiple burnup cycles simulations in Hot Full power condition of PWR full core have been developed in RMC for multiphysics coupling and lifecycle simulations of nuclear reactors. BEAVRS benchmark was selected as an example and RMC was applied full core two cycles burnup calculation of BEAVRS. The parameters given in BEAVRS benchmark will be calculated and compared with the measured values of BEAVRS benchmark. For other parameters such as pin power distributions, they are compared to the results of MC21.

#### **II. COMPUTATIONAL METHODS**

Some advanced methods have been proposed for PWR full Core two cycles burnup calculation, including the hybrid coupling method with on-the-fly cross sections treatment, layered parallelism based on MPI/OpenMP parallel model for full-core detailed burnup calculation, critical searching for critical boron concentration, adjointweighted dynamic parameters calculations, inline equilibrium Xenon method, Monte Carlo refueling capacity, and restart capacity for burnup calculation.

## **1.** Hybrid coupling method with on-the-fly cross sections treatment

RMC was coupled with sub-channel code COBRA, equipped with on-the-fly temperature-dependent cross section treatment to consider the thermal-hydraulic feedback and temperature effects on nuclides cross sections.

For on-the-fly temperature-dependent cross section treatment, the Target motion sampling (TMS) method based on the ray tracking [2] is used for resolved resonance region and on-the-fly interpolation of thermal scattering data was developed in RMC to consider the thermal scattering and bound effect [3].

For thermal-hydraulic coupling, considered the advantages and disadvantages of external and internal couplings, a new hybrid coupling method is developed.

Hybrid coupling means transforming data via external files of thermal hydraulics code and managing all the useful data by internal memory in neutronics code. The hybrid coupling method can reduce the difficulty of modeling and improve the versatility of coupling by managing all the useful data by internal memory in neutronics code, while making good use of the existing thermal-hydraulics codes. Details of the realizations and advantages of the hybrid internal/external coupling scheme can be referred to references [4, 5].

# 2. Layered parallelism based on MPI/OpenMP parallel model

The huge memory consumption is the bottleneck of full-core detailed burnup calculations of PWR. Therefore, several methods have been proposed to solve the memory problem. such as domain decomposition. data decomposition and layered parallelism based on MPI/OpenMP parallel model. On the other hand, future computer platforms move toward a larger numbers of nodes and processor cores per node coupled with lower memory available, as shown in Fig.1. These new architectures encourage a hybrid parallel algorithm in Monte Carlo simulation. Therefore, layered parallelism based on MPI/OpenMP parallel model was developed [6] and applied to the burnup calculations of BEAVRS, as shown in Fig.2.



Fig. 1 Distributed-shared Memory Parallel NOW Super Computer



Fig. 2 MPI process and OpenMP threads Parallel Model

#### 3. Criticality search

In operation of reactors, the critical boron concentration in coolant keep searching and updating to maintain the critical condition. The criticality search capability based on differential operator method was developed in RMC [7]. The first-order and higher-order derivatives of  $K_{eff}$  are estimated to solve Taylor expansion equation, as shown in Equation 1. The first-order and higher-order derivatives of  $K_{eff}$  are tallied during the neutron

transport. Then the  $\Delta a$  was calculated based on derivatives and  $\Delta k$ . In RMC, the second-order differential operator method was used.

$$\Delta k \Box \frac{dk}{da} \Delta a + \frac{1}{2!} \frac{d^2 k}{da^2} \Delta a^2 \tag{1}$$

#### 4. Inline equilibrium Xenon method

For some weakly coupled systems such as large PWR core, instability problems have been found in burnup calculations such as oscillations in power and flux. The oscillations are mainly caused by xenon. In this paper, the inline equilibrium xenon method [8] was used to deal with the problem of xenon. In this method, the xenon concentration was calculated analytically bases on flux and depletion time.

$$N_{x_{e}}(t) = \frac{(\gamma_{I} + \gamma_{x_{e}}) \sum_{f} \varphi}{\lambda_{x_{e}} + \sigma_{a}^{x_{e}} \phi} \left\{ 1 - \exp\left[-\left(\lambda_{x_{e}} + \sigma_{a}^{x_{e}} \phi\right)t\right] \right\} +$$
(2)  
$$\frac{\gamma_{I} \sum_{f} \phi}{\lambda_{x_{e}} + \sigma_{a}^{x_{e}} \phi - \lambda_{I}} \left\{ \exp\left[-\left(\lambda_{x_{e}} + \sigma_{a}^{x_{e}} \phi\right)t\right] - \exp\left(-\lambda_{I}t\right) \right\}$$
(2)  
$$N_{I}(t) = \frac{\gamma_{I} \sum_{f} \phi}{\lambda_{I}} \left[ 1 - \exp\left(-\lambda_{I}t\right) \right]$$
(3)

#### 5. Monte Carlo refueling capability

The operation of nuclear power plant is a long term process including initial cycle, transition cycles and equilibrium cycles by fuel refueling after each cycle. For example, Fig. 3 is the Cycle 2 refueling pattern of BEAVRS. In the way, the build-in refueling capacity was developed in RMC code [9]. The build-in refueling is realized by building a map between material information, reaction rates tallies, geometry cell, and burnup information in depletion solver. The refueling process was performed automatically through the inner manipulation of RMC once the users have input the refueling scheme. The refueling capability of RMC can handle full core burnup problems with more than millions of burnup regions.



Fig. 3 Cycle 2 refueling pattern of BEAVRS

## **III. RESULTS**

#### 1. Benchmark descriptions

BEAVRS benchmark is specifications and measured results for two cycles of a PWR which was proposed by the MIT Computational Reactor Physics Group. Both the measured data of hot zero power (HZP) and hot full power (HFP) are given in BEAVRS. The geometry model of BEAVRS core was built by RMC, as shown in Fig.4.



Fig. 4 Radial and axial cross section of BEAVRS core

#### 2. Computational model and conditions

For the coupling in HFP conditions, three feedback should be considered, including the temperature of coolant and fuel, the density of coolant and the boron concentration in coolant. To consider the axial distributions of fission power and coolant density, the active core is divided into 10 axial segments. For thermal-hydraulics model in COBRA, only an octant of core has been considered for the 193 fuel assemblies in the full core. Therefore, the grid of 31 channels, each containing an individual fuel assembly, making up the lower triangular region of the quarter-core shown in Fig. 5. Each assembly is divided into 10 axial segments.

					21	27	
				15	20	26	
			10	14	19	25	31
		6	9	13	18	24	30
	3	5	8	12	17	23	29
1	2	4	7	11	16	22	28

Fig. 5 Radial channels of BEAVRS core (COBRA)

The whole core is divided into 10 axial segments, and each fuel pin and poison pin are treated as single burnup region, summing up to 534880 burnup regions totally. There are no radial rings divisions in each fuel pin. The most burned fuel pin has about 100 isotopes at the end of first cycle, and about 150 isotopes at the end of second cycle. On the basic of neutronics/thermal-hydraulics coupling in HFP condition, the layered parallelism based on MPI/OpenMP was adopted to deal with the memory problem of full-core detailed burnup calculation. The large scale parallelism was performed on Tianhe2 super computer. 70 nodes with 1680 processes were used, each node has 64G memory. The layered parallelism was applied to each node, in which the configuration of 2 MPI × 12 OpenMP/MPI was adopted. This configuration of layered parallelism is consistent with the hardware architecture of calculation nodes of Tianhe2 super computer, which has two CPU and twelve codes per CPU in each node. Through the layered parallelism, the memory footprint of each code in full core detailed burnup calculations can be reduced effectively, so as to meet the requirement of single node in Tianhe-2 super computer (24 cores per node sharing 64G memory).

#### 3. Critical boron concentration comparisons

As the boron concentration in coolant changes in different burnup steps, the capacity of critical search was used to change the boron concentration in each burnup step according to keep the reactor critical. The critical boron concentration calculated by RMC are compared with the benchmark results. For the first cycle, the power is not constant as shown in Fig.6, and the average power is 75% full power. Therefore, the bunrup calculations of 75% and 100% full power are performed. The results are compared with benchmark in Fig.7. The critical boron concentration of 75% power was closer to the benchmark results than full power. After cycle 1, the refueling was carried out. As the power history of cycle 2 was almost in full power, so 100% power was adopted for the burnup calculation. The results are compared with benchmark in Fig.8. The maximum discrepancy of boron concentration is 48 ppm for cycle 1 and 46 ppm for cycle 2.

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Fig. 7 Critical boron concentration of Cycle 1



Fig. 8 Critical boron concentration of Cycle 2

#### 4. Pin power distributions comparisons

Beside the critical boron concentration, the pin power distributions of 1043.0 MWd/tU, 4587 MWd/tU and 12525.6 MWd/tU in cycle 1 was also compared with that of MC21 [10] in Fig.9 & 10. Pin power distributions agree well for both two codes. The pin power distributions of cycle 2 calculated by RMC are shown in Fig.11.



Fig. 9 Pin power distributions at different burnup of RMC



Fig. 10 Pin power distributions at different burnup of MC21



Fig. 11 Pin power distributions of Cycle 2

#### **5.** Detectors responses comparisons

The radial detectors responses in the instrument rod located in the center of some assemblies were also calculated and compared with the benchmark results. The detectors responses at 1043.0 MWd/tU, 4587 MWd/tU and 12525.6 MWd/tU in cycle 1 were compared in Fig. 12  $\sim$ Fig.14. It can be found that the large discrepancies appear in the periphery of core where power was relatively small.



Fig. 14 Comparisons of detectors response at 12525.6 MWd/tU

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The maximum relative errors and Root-mean-square (RMS) errors at three bunrp steps were compared among RMC, MC21 and SIMULATE-3 in Table I and Table II. Noticing that both MC21 and SIMULATE-3 were using the quarter core model for calculations, the relative errors of RMC are in the same level compared with the other two codes.

Table I. Maximum relative errors for three codes						
	1043.0	4587	12525.6			
	MWd/tU	MWd/tU	MWd/tU			
RMC	9.9%	6.7%	7.6%			
MC21	7.7%	3.2%	4.5%			
SIMULATE-3	9.0%	3.5%	3.0%			

Table II. RMS errors for three codes							
	1043.0	4587	12525.6				
	MWd/tU	MWd/tU	MWd/tU				
RMC	2.9%	3.1%	3.8%				
MC21	2.5%	1.2%	2.1%				
SIMULATE-3	2.5%	1.1%	1.1%				

### **IV. CONCLUSIONS**

The multi-physics coupling and lifecycle simulations is crucial for realistic reactors simulations and benchmarks calculations such as MIT BEAVRS benchmark. In order to perform the high fidelity two cycles burnup calculation in hot full power, several advanced techniques were developed in RMC. The results of RMC agree well with the reference values of BEAVRS benchmark and also agree well with those of MC21.

This work proves the feasibility and accuracy of RMC in multi-physics coupling and lifecycle simulations of nuclear reactors.

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