

Hybrid Depletion Method for the Light Water Reactor analysis

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Abstract – Monte Carlo (MC) depletion has big obstacle in the full-scale reactor core analysis. It requires a memory usage of terabyte unit. It is thus not allowed to compute with contemporary computer resource. Computation time is another big obstacle in that full-scale reactor core analysis such as BEAVRS 3D core problem. Hybrid depletion method has been introduced by combination in MC code and the Deterministic code. In this work, two codes, MCS and STREAM, are used in implementation of Hybrid method. STREAM code has high accuracy in production of the effective cross-section with pin-based pointwise energy slowing-down method. The hybrid depletion method uses the multi-group flux by tally from the MC code and effective cross-section from the STREAM code. It reduces significantly the memory usage because the massive tallies during MC transport calculation are not needed anymore. It also takes advantage of the reduction of portion of the computation time. In current work, it shows that 10% less computational time and less 30 times of the memory usage are required in the Hybrid depletion method compared to conventional MC depletion method.

I. INTRODUCTION

The Monte Carlo (MC) burnup calculation takes advantages of accurate modeling without any geometry approximation or energy condensation [1-2]. During the MC transport calculation the neutron flux and the reaction rates for nuclides covering in the burnup calculation are tallied. Burnup calculation produces nuclide inventory at next burnup step using information from MC transport calculation. The burnup calculation module has been implemented in the MCS code [3] and it is based on the Chebyshev Rational Approximation method (CRAM) [4] with high accuracy and efficiency. In the MC depletion analysis, several hundreds of nuclides are considered in MC transport simulation and the reaction rates for each nuclide in each burnup region are tallied. Therefore, tremendous amount of computational requirements prohibits the scope from whole core burnup analysis which contains about 50,000 fuel pins. In Kord Smith challenge [5], he suggested that the burnup region is divided by axially 400 regions and radially 10 regions on a fuel pin in the whole core analysis. The depletion calculation generally employs 6 1-group reaction rates, 3-group fission reaction rates which should be tallied during MC transport calculation. Considering normally 300 nuclides on a burnup region in MC depletion calculation, 9 data are tallied for about 300 nuclides in each of the 200 million burnup regions. It requires a memory usage of around 4.5TB regarding the double-precision for tally data. For such computational costs, the MCS code has been developing with hybrid depletion module [6] which uses the resonance treated multi-group (MG) cross section produced by Deterministic method instead of tallying the reaction rates during the MC transport calculation.

Deterministic methodologies on cross section generation are based on in-house MOC code called STREAM [7]. Hybrid depletion method takes account into only the multi-group flux tallies during the transport simulation so that the amount of memory usage is reduced. This paper introduces the preliminary study on the hybrid depletion method and presents the numerical results of hybrid depletion and its applicability for the practical analysis.

II. THE MAIN DRAWBACK OF DEPLETION CALCULATION IN MONTE CARLO AND DETERMINISTIC METHODS

1. Deterministic method

In modern lattice physics codes [7-9], there are still limitations to assure the accuracy in the nuclear reactor analysis. The main limitation comes from the computation of the effective MG cross-sections (XSs). It is not simple to advance the accuracy by utilizing continuous energy cross-sections. One of the main tasks to improve the accuracy is the resonance treatment. STREAM [7], the in-house MOC code, has highly advanced resonance self-shielding method and has been verified with conventional resonance treatment methods and MC codes [10]. However, in the depletion calculation with consideration of several hundreds of nuclides, it is not easy to generate effective MG XSs for all the nuclides corresponding to continuous energy XSs. It will cause discrepancy compared with MC depletion calculation. As shown in Fig. 1, such discrepancy on the multiplication factor with burnup is presented by the comparison between MCS and STREAM for 3.1% UO₂ pin-cell problem, in which both codes use the same depletion module and the

decay data. In order to provide the consistency in the depletion calculation, fixed 1-group flux and 1-group XSs are used. Both MCS and STREAM have performed both the depletion and the transport calculation without calculating of the 1-group flux and reaction rates. In case of STREAM, only the transport calculations on each burnup are performed with the information of the number densities on each burnup from MCS.

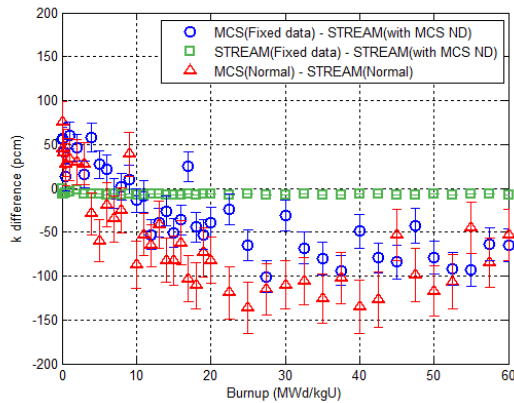


Fig. 1. MCS and STREAM pin-cell depletion results.

The depletion calculations without fixing the data in both MCS and STREAM are also performed. First, the agreement between STREAM depletion results with fixed data (STREAM_FD) and STREAM transport calculation with the number density from MCS (STREAM_MCSND) shows that both codes have the same depletion module. Second, the difference between MCS_FD and STREAM_MCSND represents the error considering overall effects on the Deterministic method excluding the depletion calculation. Finally, the similar behavior on the k difference shows that the error by the transport calculation is more dominant than the error by the depletion calculation modules in both codes. It also implies that 1-group resonance treated XSs can be utilized in the MC depletion with the reduction of the error from the transport calculation.

2. Monte Carlo method

In MCS depletion calculation, 7 reaction types are considered during the depletion calculation, including (n, absorption), (n, γ), (n, α), (n, 2n), (n, 3n), (n, p) and (n, f). MCS tallies the total of 9 reaction rates since 3-group fission reaction rates are needed considering 3-group fission yields. These reaction rates should be tallied for every nuclide in every burnup region. Kord Smith [5] suggested in M&C 2013 conference that 400 axial burnable regions and 10 radial zones for one fuel rod are required for the whole core analysis. Considering normally 300 nuclides in a burnup region in MC transport calculation, it means that 9 data are tallied for about 300 nuclides in 200 million burnup

regions. It requires a memory usage of around 4.5TB regarding the double-precision for tally data. It is not allowed to compute with contemporary computer resource. This is only the consideration from the memory requirement point of view. Computational time is another big obstacle in the scope of whole core analysis.

III. HYBRID DEPLETION METHODS

Hybrid depletion method has been implemented in the in-house code MCS. Hybrid depletion employs resonance treated XSs from multi-group XS generation routine of STREAM instead of using tallied XSs. STREAM has 72 energy group structure to generate multi-group XSs. According to the STREAM's energy group structure, MCS tallies 72-group flux during transport calculation to generate 1-group XSs for depletion calculation which are condensed with 72-group resonance treated XSs. All the processes are performed in the built-in MCS depletion module. Since the reaction rates are not tallied in the transport calculation, it requires only the memory to tally 72-group fluxes. Table I shows a rough comparison of the memory usage required for depletion between the conventional MC depletion method and the hybrid depletion method.

Table I. The comparison of the memory usage between conventional MC depletion and Hybrid depletion

	MC	Hybrid
Reaction type ¹⁾	9	-
Flux ²⁾	1	72
Fuel pin cell	50000	50000
Axial domain	400	400
Radial ring	10	10
Nuclides	300	-
Data type	8 byte	8 byte
Total ³⁾ (Gb)	4321.6	115.2

1) Reaction rates are calculated for every nuclide in every burnup region.

2) Fluxes are calculated in every burnup region.

3) (# of reaction type * # of nuclides + # of flux groups) * # of burnable regions.

The numerical calculations on memory usage of two methods show that Hybrid depletion requires 40 times less memory to tally the information for depletion calculation.

III. RESULTS

Detailed analyses of computational costs and performance for Hybrid depletion method are performed with VERA depletion benchmark suite [11]. Fuel enrichment 3.1% UO₂ fuel pin-cell is used in a pin-cell problem and a 17x17 fuel assembly problem. A plane view and the design parameters are given in Fig. 2 and Table II.

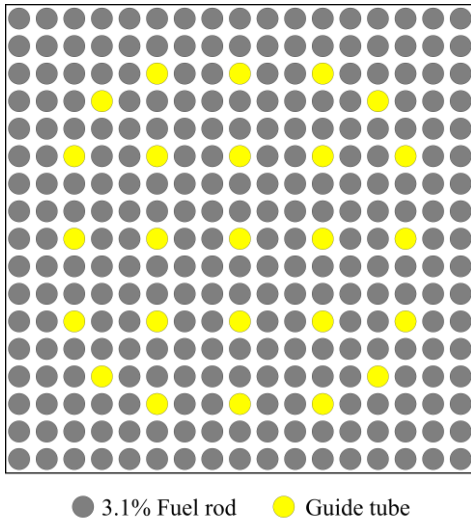


Fig. 2. 17x17 3.1% UO_2 fuel assembly model.

Table II. The fuel assembly design parameters

Parameter	Value
Fuel pellet radius (cm)	0.4096
Gap thickness (cm)	0.0084
Cladding thickness (cm)	0.057
Fuel assembly pitch (cm)	21.5
Number of fuel pins	264
Fuel enrichment	3.1% UO_2
Power density (W/gU)	40.0
Temperature(K)	900/600/600 (Fuel/Gap/Clad)

First, a fuel-pin depletion calculation is performed with STREAM, MCS, and Hybrid method. The cross-section library based on ENDF/B-VII.0 [12] is used in the calculation. The difference of multiplication factors with burnup using three codes are shown in Fig. 3. The results show that Hybrid depletion has good accuracy with differences from MCS depletion to be within 100pcm. After 20 MWd/kgU burnup, STREAM depletion results have a discrepancy of around 100 pcm comparing with MCS result. It confirms the results in Fig. 1 that the resonance treated XSs can generate significantly feasible 1-group XSs for the depletion calculation.

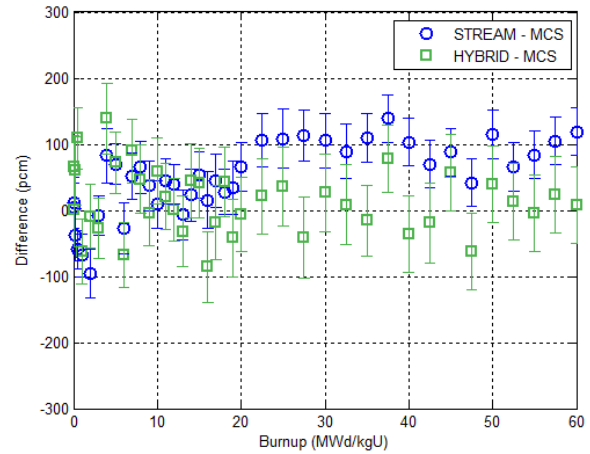


Fig. 3. Multiplication factors with burnup for the fuel pin-cell depletion problem.

Second, the fuel assembly depletion calculations are performed to estimate the practical memory usage. The differences of multiplication factors with burnup agree very well with MCS depletion for both STREAM and Hybrid depletion within 100 pcm as shown in Fig. 4.

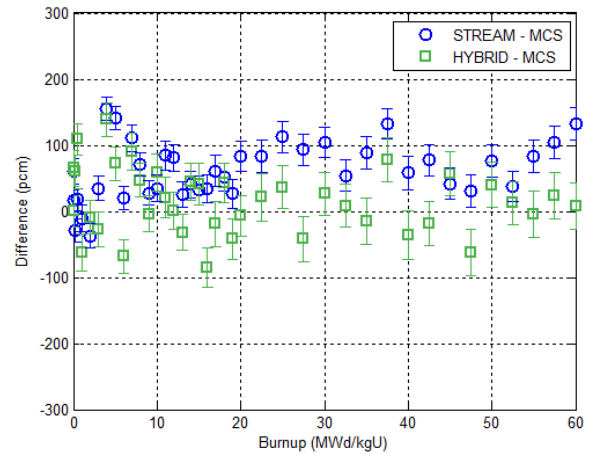


Fig. 4. Multiplication factors with burnup for the fuel assembly depletion problem.

The comparisons of the computational costs are shown in Table III and VI. The memory usage required for hybrid depletion calculation is around 1/2 of the memory required for original MCS depletion as shown in Table III. The reduction of memory usage which is expected in previous study does not involve the requirements of memory for storing the information of the number densities, since MCS depletion has considered 1,374 nuclides in the depletion calculation. Therefore, the number densities of 1,374 nuclides per burnup region should be stored. It takes up

around 60% of total memory. The memory reduction by Hybrid method is achieved only in the portion of the tallied XSs. However, the memory usage for storing the number densities is reduced with the number of the calculation thread, since the information of number densities is divided and distributed by each thread in the parallel depletion. Fig. 5 shows that the memory usage is decreased by the number of calculation threads.

There is additional memory usage which has to be considered in Hybrid depletion. Multi-group XSs processing routine takes up significant memory usage of about 2.3Gb. It is due to the pre-generated library for advanced MG XSs processing which implemented in STREAM. Multi-group XS processing routine is managed and executed in independent data server from computing server which performs the MC simulation. Therefore, such memory usage and computational time for multi-group XSs processing are separately managed as shown in Fig. 6.

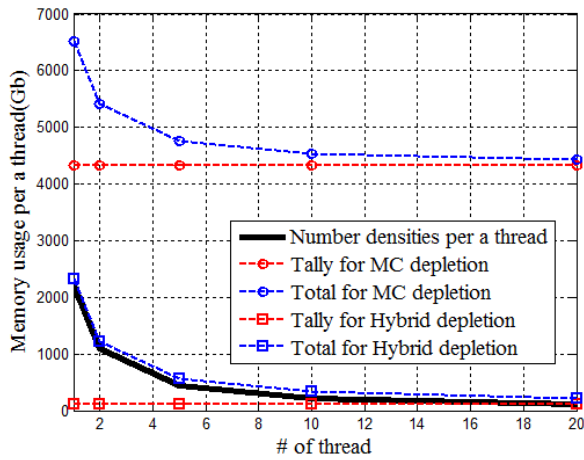


Fig. 5. The memory usage for MC and Hybrid depletion.

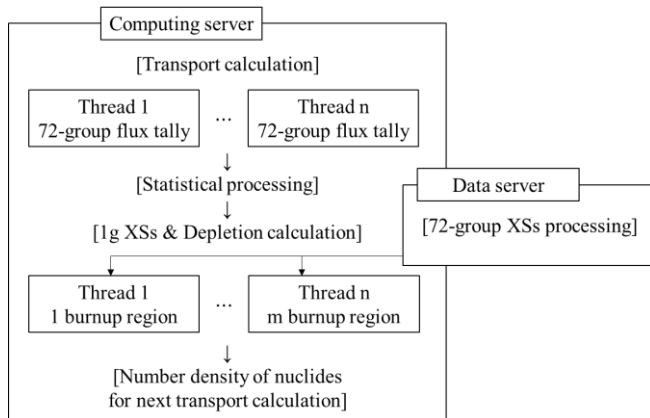


Fig. 6. Flow scheme for parallel hybrid depletion.

Table III. The memory usage for the fuel assembly depletion calculation problem.

Unit(Kb)	MCS	Hybrid
Geometry	6.6	6.6
Tracking	193.4	193.4
Indexing	6.6	6.6
Read ACE XSs	5.1Gb	5.1Gb
Material	4734.9	4738.3
Depletion	24887.3	11787.1
MG XSs*	0	2.26Gb

* The memory for multi-group XS generation is only taken by the data server.

In the hybrid depletion, only 72-group fluxes per burnup region are tallied during the transport calculation. Therefore, computational burden would be significantly reduced comparing to original depletion method. Hybrid depletion takes 10% less computational time in the transport calculation compared with original method.

Table IV. The computational times for the fuel assembly depletion calculation problem.

Unit(Sec)	MCS	Hybrid
Transport	163886	147640
Read ACE XSs	252	258
Read Input	0.1	0.6
Depletion	771	678
MG XSs*	0	21679

* MG XSs generation is processed during transport calculation in independent data server.

IV. CONCLUSIONS

Hybrid depletion method has been implemented in MCS code in conjunction with the Deterministic code, STREAM code. The accuracy and the performance of the hybrid depletion method has been demonstrated with the VERA fuel assembly model. The resonance treated XSs with high accuracy which is comparable to the continuous energy XSs of MC code are applied in the Hybrid depletion. It reduces the computational resources by massive tally in MC depletion. In terms of the calculation time, it takes advantage 10% less computational time reducing the tally burden. Especially, the memory usage in the Hybrid depletion is reduced with the increase of the number of calculation threads. The Hybrid method then requires less 30 times of the memory usage compared to conventional MC depletion method.

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