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Preliminary Verification of PRAGMA VHTR Module Enhancements for 3D Prismatic VHTR Analysis

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1. Introduction

The prismatic Very High Temperature Reactor (VHTR), has gained attention due to its modular block-type core structure and enhanced passive safety features. Notably, Japan has developed and operated the High-Temperature Engineering Test Reactor (HTTR) [1]. A distinguishing feature of VHTR is the utilization of TRISO particles that are typically fabricated as a fuel compact form in the prismatic VHTR designs. This double heterogeneity makes modeling and a simulation of VHTRs challenging since it requires an accurate self-shielding treatment along with a proper statistical consideration of TRISO particle distribution.

Seoul National University has been developing a GPU-accelerated continuous-energy Monte Carlo (MC) code PRAGMA [2] for advanced reactor analysis [2-4], based on the delta-tracking scheme [5] and OptiX ray tracing library [6]. Recently, the VHTR analysis module was added to PRAGMA and verified for 2D pin and block problems [4]. However, its capability for 3D VHTR simulations remains limited due to the inefficiency in tracking particles in the 3D fuel elements which includes axial stacking of compacts. This study aims to improve and verify the VHTR module capabilities of PRAGMA for the 3D prismatic VHTR analysis. Here, the VHTRs refers specifically to the prismatic-type reactor for brevity, as the pebble-bed type core is not considered in this study. The following sections address the enhancements of PRAGMA in modeling and neutron tracking for accomplishing the practical and efficient simulations of 3D VHTR problems. Then, the preliminary verifications for 3D block problems of VHTR are presented.

2. Geometry Modeling of 3D VHTR in PRAGMA

In PRAGMA, a VHTR core is modeled as a combination of triangular-based meshes and specialized objects for TRISO containers. The unstructured geometry module of PRAGMA primarily utilizes triangular-based meshes [3], preserving volume for most structures. However, TRISO containers require precise modeling due to variations in TRISO distribution. The specialized objects for TRISO containers are superposed onto the triangular-mesh based geometry. The random TRISO distribution is explicitly modeled using the random rejection method or Jodrey-Tory (JT) sphere packing algorithm [7].

In the initial implementation, a container object could represent only a single fuel compact, as the modeling strategy was originally developed specifically for pebbles. Accordingly, each fuel hole in a block is modelled as an individual cylindrical object, while other geometrical components in fuel blocks are explicitly represented using meshes. In a 3D prismatic VHTR core model, cylindrical container objects are stacked axially at each fuel location within the block. As a result, overlapping surfaces occur between the container objects and the block meshes, which inevitably causes neutron trapping due to truncation errors. This approach led to significant degradation in both simulation accuracy and computational efficiency. Additionally, modeling a fuel element with separate cylinders introduced a high computational burden during particle tracking. The geometry modeling strategy has been enhanced to represent a VHTR fuel compact element as a single geometrical entity, incorporating all components, including the sleeve, helium channel, and axially stacked fuel compacts. This approach eliminates the possibility of neutron trapping. By modeling the fuel elements as single cylinders extending through the core, it is expected that neutron trapping is mitigated, and the number of cylindrical objects in particle tracking is significantly reduced. For 3D fuel block modeling, a fuel element is modeled as a single cylinder divided into multiple regions with distinct material compositions, improving both accuracy and computational efficiency.

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3. Tracking Strategies for 3D VHTR

The PRAGMA adopted a localized delta-tracking scheme [8], based on Wood-cock delta-tracking [5], to enhance neutron tracking efficiency in mesh-based geometries. This approach mitigates the high rejection rates caused by heavy absorbers when utilizing the global majorant cross sections. In VHTR simulations, cylinders containing TRISO particles are localized within the delta-tracking scheme. By applying delta-tracking to a cylinder, TRISO distribution can be ignored during neutron tracking, and it is only considered when a neutron undergoes a virtual collision. The exact positions of neutrons within the TRISO distribution are determined using the grid cell search strategy, as described in [9]. Notably, the computational burden of this strategy remains manageable even at high packing fraction of TRISO particles, as the number of neighboring TRISO particles per grid cell is inherently limited.

The localized delta-tracking scheme has been enhanced to incorporate Region-wise Delta-Tracking (RDT) within a cylinder. As multiple material compositions are represented within a single cylindrical model, the number of virtual collisions is expected to increase. Fig. 1 compares the majorant cross sections of materials in a HTTR fuel element. There is a significant disparity between Helium and other materials. In particular, the helium region, especially in cylinders with a large helium fraction, is expected to exhibit a substantial increase in virtual collisions. The RDT scheme mitigates this issue by applying region-specific majorant cross sections, thereby reducing the number of virtual collisions within the cylinder.

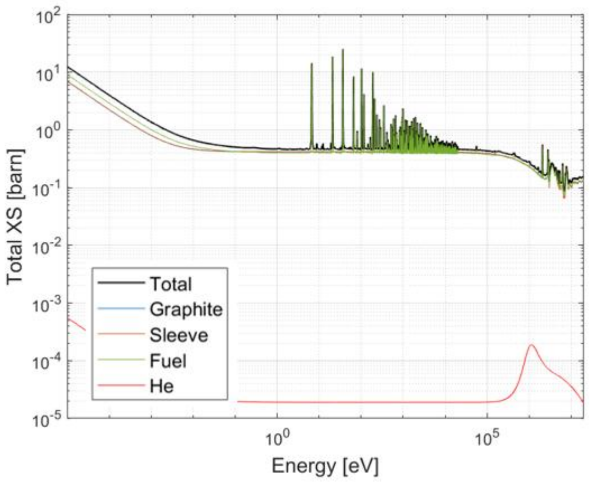

Fig. 1. Comparisons of majorant cross sections in a HTTR fuel element

However, implementing the RDT scheme in a cylinder necessitates additional distance calculations for the surfaces of each region. Although the number of virtual collisions decreases, this can lead to increased computational time due to the additional and potentially unnecessary distance calculations during neutron tracking. Therefore, the effectiveness of the RDT scheme should be assessed regarding its impact on computing time.

4. Problem Description

3D fuel block problems based on the HTTR benchmark [10] are simulated using PRAGMA to verify the VHTR analysis module. HTTR uses an annular fuel compact, as shown in Fig. 2, making it an ideal case for verifying the enhanced geometry modeling and the RDT scheme in PRAGMA.

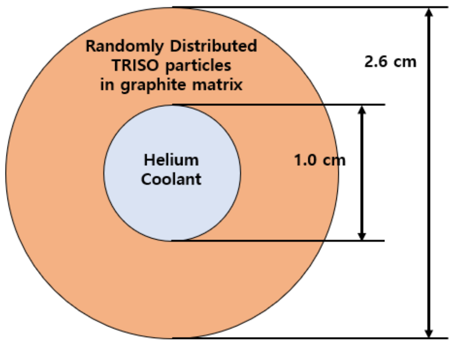

Fig. 2. Horizontal cross-sectional view of HTTR fuel compact

HTTR benchmark includes four types of fuel blocks. Fig. 3 describes the axial configurations of these four fuel blocks. Each block has different axial material compositions, varying in uranium enrichment and natural boron content. Each fuel block consists of nine axial elements, each with a height of 58.0 cm.

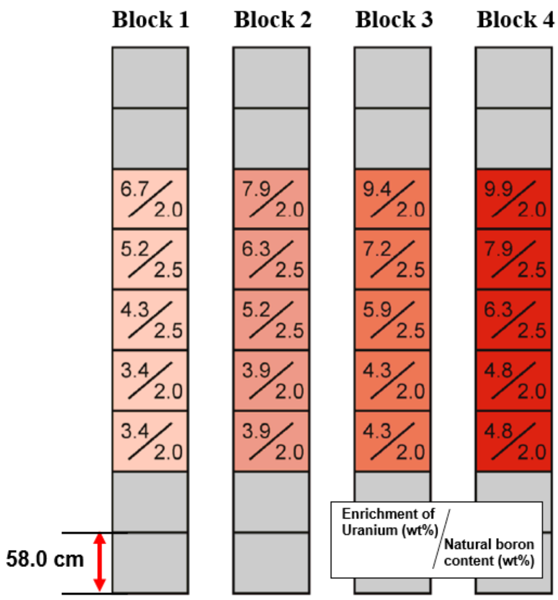

Fig. 3. Axial configurations of HTTR fuel blocks [10]

Additionally, block 1 and 2 consist of 33 fuel pins, while block 3 and 4 consists of 31 fuel pins. Fig. 4 shows the radial configurations of the 31-pin and 33-pin fuel blocks. Each block contains an empty pin filled with helium and two burnable poisons at three of its corners

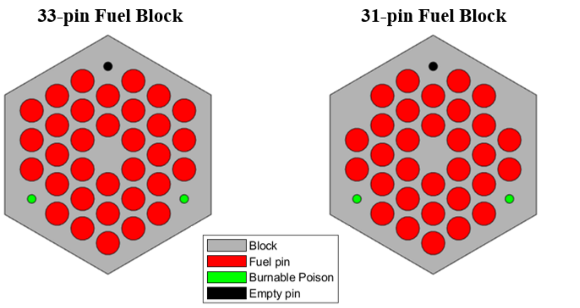

Fig. 4. Radial configurations of 33-pin and 31-pin fuel blocks

5. Results

The PRAGMA VHTR analysis module is verified for the four HTTR fuel blocks with respect to multiplication factors, pin power distribution, and computational time, using the McCARD [11] simulation results as a reference. In this research, McCARD simulations are conducted with 200 MPI processes, while PRAGMA simulations utilize 4 MPI processes. Table I provides the detailed calculation specification for both McCARD and PRAGMA.

Table I. Calculation specifications

Code	McCARD	PRAGMA
# of Processes	200	4
CPU	20×Intel Xeon Silver 420R @ 2.4Hz	2×Intel Xeon E5-2630 v4 @ 2.2Hz
GPU	-	4×NVIDIA GeForce RTX 2080 Ti

The MC simulation conditions of both codes are outlined in Table II. The same number of inactive cycles and total histories in active cycles are used for both McCARD and PRAGMA simulations. For PRAGMA calculations, the Ramp-up scheme [12] is applied during inactive cycles, as a larger number of neutrons are utilized in PRAGMA simulations. To assess the effect of RDT scheme, PRAGMA simulations are conducted both with and without RDT schemes for all cases. Fuel block simulations are performed only for the 300K condition. Note that the uncertainty due to the random TRISO distributions in each fuel compact should be considered in comparisons, as these distributions are generated independently in each code.

Table II. Calculation conditions

Code	McCARD	PRAGMA
Number of Cycles	50 (inactive) / 500 (active)	50 (inactive) / 50 (active)
# of Neutrons / Cycle	1,000,000	10,000,000
XS Library	ENDF/B-VII.1 (300K)	
TSL Library	ENDF/B-VII.1 (296K)	

Table III compares the multiplication factors calculated by McCARD and PRAGMA. The maximum difference is 15 pcm for all cases, which is acceptable given the standard deviation and the uncertainty associated with the random TRISO distribution.

Table III. Comparisons of multiplication factors

Case	McCARD (M)	PRAGMA (P)	Diff. [pcm] (P-M)
Block 1	1.24402 (4)	1.24411 (4)	9
Block 2	1.28472 (3)	1.28480 (3)	8
Block 3	1.32455 (3)	1.32452 (3)	-3
Block 4	1.33958 (3)	1.33973 (4)	15

Fig. 5 presents the normalized pin power distributions in the fuel blocks, as calculated using PRAGMA. Each pin power has a standard deviation of about 0.02%. For each fuel block, the peaking power is observed in the fuel pins adjacent to the empty pin, which is located far from the positions of the burnable poisons. The lowest power is observed in the pins, located between two burnable poison positions.

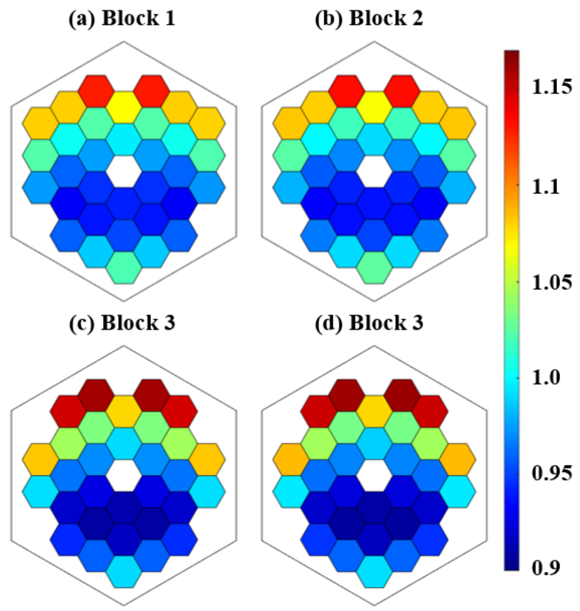

Fig. 5. Normalized pin power distributions in fuel blocks

The maximum and Root Mean Square (RMS) differences between the normalized pin power distribution calculated using McCARD and PRAGMA are less than 0.07 % and 0.01 %, respectively, for all cases, indicating negligible errors.

The computing time for McCARD and PRAGMA are presented in Table IV. When applying the RDT scheme, the computing time of PRAGMA is reduced by about 40 %, which exhibits the effectiveness of RDT scheme. It also shows the GPU-based Monte-Carlo calculation out-performs the CPU-based one for VHTR problems.

Table IV. Comparisons of computing time

Case	McCARD	PRAGMA	
		w/o RDT	w/ RDT
Block 1	4h 43m 28s	48m 53s	35m 29s
Block 2	4h 31m 59s	49m	34m 46s
Block 3	4h 11m 27s	48m 47s	33m 53s
Block 4	4h 7m 14s	49m 47s	33m 46s

6. Conclusions

The PRAGMA VHTR analysis module was enhanced for efficient simulation and modeling of 3D prismatic core problems. For 3D core modeling, a fuel element, including the sleeve, helium channel, and stacked fuel compacts, is represented as a single cylindrical entity during particle tracking, multiple regions having distinct material compositions. The Region-wise Delta-Tracking (RDT) scheme, developed from the localized delta-tracking in PRAGMA, was introduced to address potential computational performance degradation in cylinders with multiple material compositions. The RDT scheme optimizes delta-tracking by reducing unnecessary virtual collisions.

To verify the enhanced geometry modeling and the RDT scheme, four fuel block problems based on the HTTR benchmark were simulated, with McCARD simulation results serving as the reference. The maximum difference in multiplication factors between McCARD and PRAGMA was 15 pcm for all cases, which is acceptable considering the 3 pcm standard deviation and uncertainty of the random TRISO distributions.

The maximum and RMS differences between the normalized pin power distributions were below 0.07% and 0.01%, respectively, for all cases. These results confirm the successful preliminary verification of the PRAGMA VHTR analysis module for 3D block in terms of multiplication factors and pin power distributions. Additionally, the RDT scheme reduced PRAGMA's computing time by approximately 40%, demonstrating both the efficiency of PRAGMA for 3D VHTR simulations and the effectiveness of the RDT scheme.

Extensive verification of The PRAGMA VHTR analysis module will be performed including realistic core problems. Along with further verifications, PRAGMA is planned to include capabilities for the Thermal-Hydraulic (T/H) feedback and depletion calculations to enable complete VHTR simulations. Specifically, PRAGMA is planned to be coupled with other T/H simulation codes, such as SOPHIA [13].

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