Monte Carlo / Thermal-Fluids Coupled Calculations for MHTGR-350MW Benchmark

Matthieu Lemaire[a], Hyunsuk Lee[a], Nam-il Tak[b], Hyun-Chul Lee[c], Deokjung Lee[a*]

[a]*Ulsan National Institute of Science and Technology, 50, UNIST-gil, Ulsan, 689-798, Republic of Korea*
[b]*Korea Atomic Energy Research Institute, 150, Deokjin-dong, Yuseong-gu, Daejeon, 305-353, Republic of Korea*
[c]*Nuclear System Division of Mechanical Engineering Department, Pusan National University (PNU), Busan, Korea*
**Corresponding author: deokjung@unist.ac.kr*

Abstract - *This paper presents coupled neutronics/thermal-fluid results for the steady-state exercise Phase 1 Exercise 3 (P1-Ex3) of the MHTGR-350MW (Modular High-Temperature Gas-Cooled Reactor) benchmark sponsored by the Nuclear Energy Agency of the Organization for Economic Cooperation and Development (OECD/NEA). The results were obtained with the Monte Carlo code MCS developed at UNIST (Ulsan National Institute of Science and Technology) and the thermal-fluid and system transient GAMMA+ code developed by KAERI (Korean Atomic Energy Research Institute). Comparisons between different solutions obtained by benchmark participants, including this solution, will be conducted by the benchmark organizers and first comparison results are expected to be available by end of 2017. The detailed analysis of benchmark solutions is expected to improve the simulation methods for modular prismatic reactors.*

I. INTRODUCTION

The MHTGR-350MW (Modular High-Temperature Gas-Cooled Reactor) is a fourth-generation nuclear reactor design from General Atomics (GA) supported by the US-led Next Generation Nuclear Plant (NGNP) project. In 2012, a numerical benchmark, based on the MHTGR-350MW design and developed by the NGNP project in cooperation with GA, was approved for international participation by the Nuclear Energy Agency of the organization for Economic Cooperation and Development (OECD/NEA) [1]. The purpose of the benchmark is to establish well-defined problems based on a common set of data so as to compare and improve the existing simulation tools for prismatic modular reactors in the field of neutron physics and thermal-fluid simulation.

In this paper, Phase 1 Exercise 3 of the MHTGR-350MW, a steady-state exercise requiring coupled neutronics/thermal-fluids calculations, is tackled with the Monte Carlo code MCS [2] developed at UNIST (Ulsan National Institute of Science and Technology) and the thermal-fluid and system transient GAMMA+ code [3] developed by KAERI (Korean Atomic Energy Research Institute). This work is based on a previous study by KAERI where a steady-state analysis of the PMR-200 (Prismatic Modular Reactor) was conducted with the GAMMA+ code and the deterministic code CAPP [3]. The coupling scheme is adapted so as to use a Monte Carlo code instead of a deterministic code and is applied to the MHTGR-350MW case.

The plan of the paper is as follows. We first provide a brief description of the MHTGR-350MW geometry and present the benchmark exercise. We then introduce the MCS and GAMMA+ codes and explicit the modelling of the MHTGR-350MW in each code. Finally, we detail the coupled-calculation methodology and analyze the obtained results.

II. NEUTRONICS/THERMAL-FLUID STEADY-STATE CALCULATIONS

1. MHTGR-350MW geometry

The axial and radial geometry of MHTGR-350MW are shown in Fig. 1 and Fig. 2 respectively. Main design parameters are summed up in Table I.

The MHTGR-350 features an annular active core (AC) made of hexagonal-shaped fuel blocks and surrounded by an inner reflector (IR) and an outer reflector (OR) made of replaceable solid hexagonal-shaped graphite blocks. The OR is itself surrounded by a permanent reflector (PR) in graphite. Each fuel block contains blinds holes for TRISO (Tristructural Isotropic) fuel compacts, 6 blinds holes for lumped burnable poison and full length channels for helium coolant flow. The annular core consists of 66 fuel columns and the active part of each fuel column is made of 10 fuel blocks stacked vertically. There are 30 channels in the reflector for the insertion of control rods (CR) (boron carbide absorber). Equally, 12 fuel columns contain a large hole for the release of reserve shutdown material: the fuel blocks of those columns are called reserved shutdown control material (RSC) blocks.

The helium coolant flows through the AC from top to bottom, from the upper plenum to the outlet plenum. A fraction of the coolant flow bypasses the fuel block coolant channels and passes through the CR cooling channels, the gaps between hexagonal columns and the gap between the PR and the core barrel. The helium flowing through the fuel block coolant holes is called the engineered flow and the helium flowing through the CR cooling channels, the gaps between hexagonal columns and the gap between the PR and the core barrel is called the bypass flow.

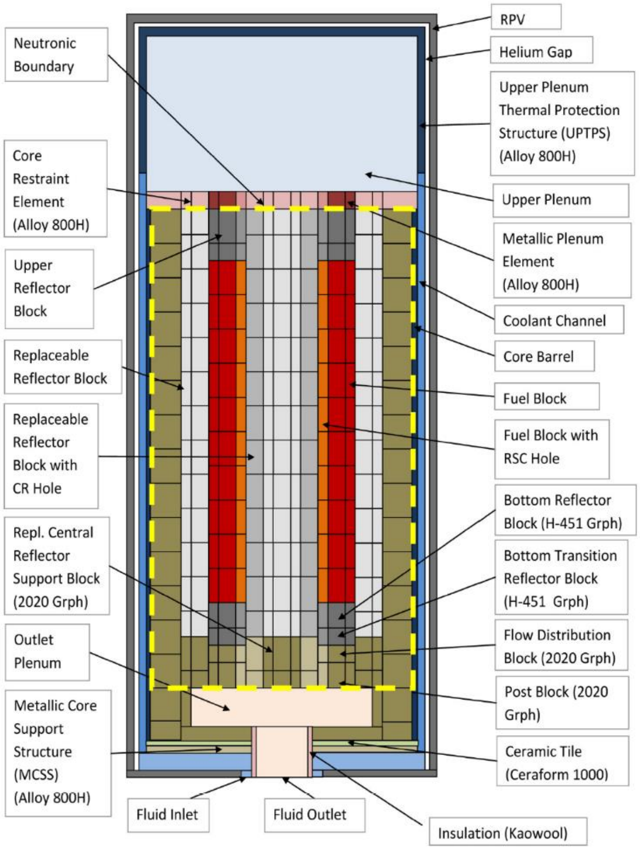

Fig. 1. MHTGR-350MW axial core geometry. [1]

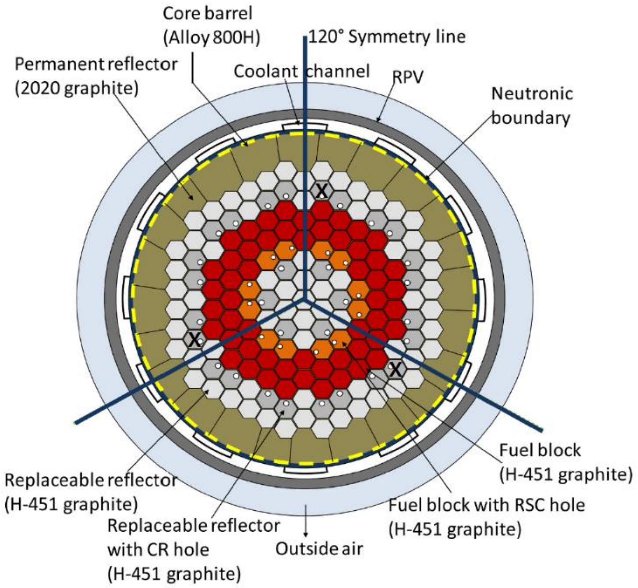

Fig. 2. MHTGR-350MW radial core geometry. [1]

Table I. MHTGR-350MW design parameters [1]

Thermal power (MW)	350
Electrical production capacity (MW)	150
Average power density (MW/m^3)	5.93
Average UO2 enrichment (wt%)	15.5
Packing fraction of TRISO particles	0.35
Moderator	graphite
Primary coolant	helium
Outlet coolant pressure (MPa)	6.39
Total coolant flow rate (kg/s)	157.1
Core inlet temperature (°C)	259
Core outlet temperature (°C)	687
Effective inner diameter of active core (m)	1.65
Effective outer diameter of active core (m)	3.5
Active core height (m)	7.93
Fuel element height (m)	0.793
Number of controls rods in inner reflector	6
Number of control rods in outer reflector	24
Number of RSC channels in core	12

2. **MHTGR-350MW P1-Ex3 benchmark exercise**

P1-Ex3 of MHTGR-350MW benchmark is a steady-state exercise at End-of-Equilibrium-Cycle (EOEC). The benchmark participants must conduct coupled neutronics/thermal-fluids calculations in order to determine full-core spatial distributions of neutron flux, temperatures of fuel, moderator, reflector and coolant, as well as global neutronics and thermal-fluids parameters. P1-Ex3 comprises two subcases, Ex3a and Ex3b. In P1 Ex3a, the bypass flow rate is azimuthally uniform and its value is a constant fixed by the benchmark documentation. In P1 Ex3b, the bypass gaps are explicitly modelled and the bypass flow rate is calculated. The bypass gaps comprise the CR cooling channels, a 2-mm gap between hexagonal blocks and a 3.5-mm gap between the PR and the core barrel.

3. **MCS model of MHTGR-350MW**

MCS is a 3-D continuous-energy and multigroup Monte Carlo code for neutron transport developed by UNIST. Its multigroup analysis capability (used to tackle P1-Ex3) has been verified against C5G7 benchmark [4].

The MCS model of MHTGR350-MW is a full-core model made of hexagonal fuel and reflector blocks. The geometry of the PR is simplified and represented with hexagonal reflector blocks too, as shown in Fig. 3. The core barrel and reactor pressure vessel are not modelled. Radially, there are 271 hexagonal meshes: 19 IR blocks, 66 AC blocks, 78 OR and 108 PR blocks. In the axial direction, there are 14 axial layers: the AC is made of 10 fuel block layers of equal height and 2 layers of reflector blocks are located above and below the AC (top and bottom reflector). For P1-Ex3, 3 control rods (CR) are inserted one AC layer deep at the locations of the black X in Fig. 2 (block 33 in Fig. 3).

All the hexagonal blocks are themselves divided in 6 triangular cells in the MCS model. To each triangular fuel cell is associated a moderator temperature, a fuel temperature and a Xenon135 number density. For P1-Ex3, the MHTGR-350MW benchmark provides a 26-group homogenized neutron cross-section library which must be used by all the benchmark participants. Especially, for the fuel block cross-sections, TRISO fuel particles are homogenized with graphite. Cross-section dependence to fuel/moderator temperatures and Xenon135 number densities is tabulated in the library so that cross-sections can be interpolated linearly from the data in the range [293K; 2000K] for temperatures and [0; 5.10^{-10} #/barn-cm] for Xenon135 concentration. Either hexagonal (at the hexagonal block level) or triangular (1/6th of a hexagonal block) homogenization of cross-sections can be used in the benchmark library. For the MCS model, homogenization of the cross-sections at the triangular level was chosen. This homogenization at the triangular level takes into account the void fraction due to helium-filled CR channels in IR and OR blocks, the void fraction due to RSC holes in RSC fuel blocks and the unbalanced distribution of fuel holes in RSC fuel blocks.

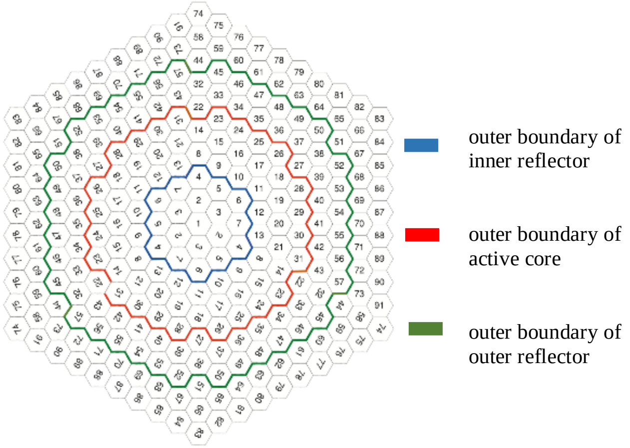

Fig. 3. MCS radial mesh (subdivisions of all the hexagons in 6 triangles is not shown)

4. **GAMMA+ model of MHTGR-350MW**

GAMMA+ is a system/safety analysis code for thermal-fluid and system transient developed by KAERI. The radial nodalization of MHTGR-350MW is presented in Fig. 4. The 120° symmetry of the geometry is taken into account to only model 1/3 of the core. Triangular cells are used to model the fuel blocks and the reflector blocks close to AC, otherwise the IR and OR blocks are modeled with hexagonal cells. The GAMMA+ modelling respects the geometry of the permanent reflector.

In order to reduce the computational cost, the coolant and bypass gap channels are grouped. In particular, the coolant channels are grouped in such a way that a single coolant channel is modeled for the triangular region of a fuel column. However, the CR channels are modeled individually.

The modelling of the bypass gaps feature 2-mm bypass gaps between hexagonal columns and a 3.5-mm gap between the PR and the core barrel. Still in order to reduce the computational cost, the bypass gaps are grouped by rings into 16 bypass gaps according to Fig. 5. The 16 bypass rings are then regrouped into 5 components as shown in Table II.

The thermal-fluid properties necessary to the simulation are calculated with the neutron fluence distribution provided by the benchmark. The heat equation is solved at 3 different scales: temperature profile of TRISO particles within a fuel compact, heat exchange between fuel compact and graphite block, heat exchange between wall and coolant. The helium coolant was considered an ideal gas and the multidimensional fluid equations (continuity, momentum and energy conservation) is solved.

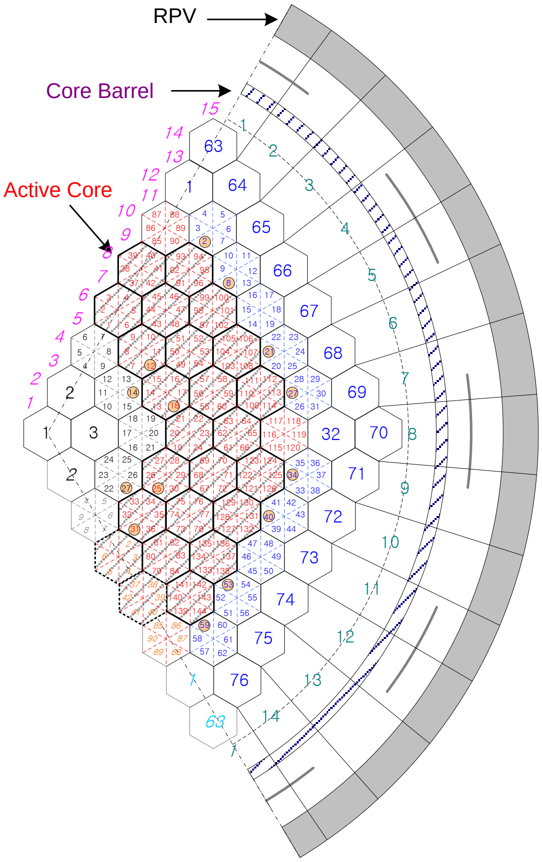

Fig. 4. GAMMA+ radial mesh of MHTGR-350MW.

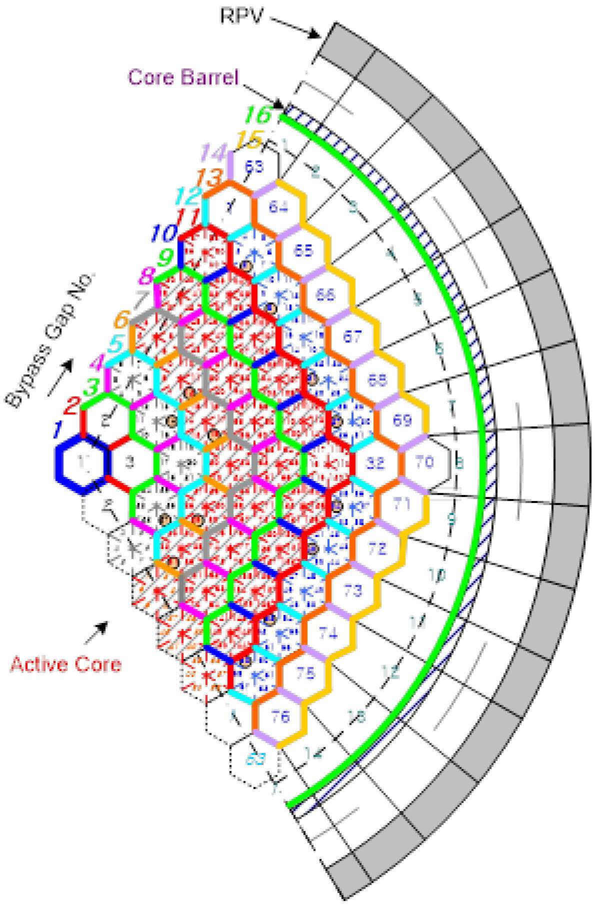

Fig. 5. GAMMA+ grouping of bypass gaps.

Table II. GAMMA+ grouping of bypass gaps

Component of bypass flow	Q_i = mass flow rate of bypass number i=1 to 16
AC	$0.5*Q_5 + Q_6 + Q_7 + Q_8 + Q_9 + Q_{10} + 0.5*Q_{11}$
IR	$Q_1 + Q_2 + Q_3 + Q_4 + 0.5*Q_5$
First ring of OR	$0.5*Q_{11} + Q_{12} + 0.5*Q_{13}$
Second ring of OR	$0.5*Q_{13} + Q_{14} + 0.5*Q_{15}$
PR	$0.5*Q_{15} + Q_{16}$

5. **MCS/GAMMA+ coupled system**

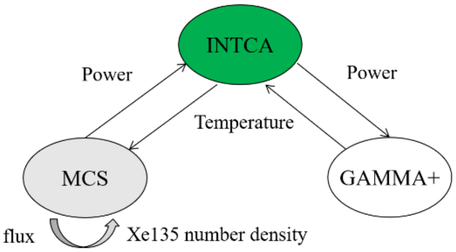

Fig. 6. MCS/GAMMA+ coupled system.

The MCS/GAMMA+ coupled system presented in Fig. 6 allows to conduct loosely-coupled neutronics/thermal-fluids calculations. In this coupled system, MCS and GAMMA+ are separate client codes and a third-party server, INTCA, controls the coupled calculations by receiving requests from the client codes and sending commands to them. Communication between clients and server is conducted through socket connections generated at runtime. More detailed information about the control algorithms of INTCA is available in [3].

A coupled calculation is made of a succession of coupled steps and each coupled step unfolds as follows. On the one hand, MCS simulates the transport of N neutrons, computes the resulting distribution of power densities in the fuel blocks and sends it to GAMMA+. The power density data is used as heat source in GAMMA+. On the other hand, GAMMA+ conducts a null-transient simulation for T seconds (problem time), computes the resulting temperatures of the core components (such as fuel, moderator, and reflector) and sends them to MCS. The temperature data is used to update the multi-group cross-sections used by MCS. Since the meshes of GAMMA+ and MCS are different, both axially and radially, each code uses its own naming convention for the variables. Mapping between the variables of the two codes is conducted by INTCA.

At each coupled step, MCS also calculates the Xenon135 equilibrium number densities in each fuel block by using the Inline Equilibrium Xenon (IEX) method [5]. Using the IEX method is justified as Iodine135 and Xenon135 concentrations have both reached equilibrium in the EOEC MHTGR core. The Xenon135 number densities are used along with the GAMMA+ temperature feedback to update the cross-sections at the end of each coupled step.

For the very first coupled step, in order to generate the neutron cross-sections from the benchmark multi-group library, we assumed an initial uniform temperature distribution for fuel, moderator and graphite (the initial temperature is chosen close to the inlet coolant temperature) and the initial concentration of Xenon135 in the fuel blocks is zero. As for the initialization of the GAMMA+ code, a core power distribution specified in the benchmark documentation is used as initial guess of heat sources in the fuel blocks. The coupled steps are then repeated until convergence of the calculation is reached. Two distinct verifications are performed. First, the convergence of the fission source distribution (FSD) in the MCS Monte Carlo calculation is checked by evaluating the variations of the Shannon entropy and of the center-of-mass of the FSD [6] at each coupled step. Once the FSD has converged, the convergence of the feedback quantities (power densities, xenon number densities, fuel and graphite temperatures) is verified by checking the successive variations of those quantities from step to step. We considered convergence is reached when the variations are below 0.1% for 5 coupled cycles in a row.

III. RESULTS

A number of neutron histories N = 10 million and a null-transient simulation time T = 10s are adopted for MHTGR-350MW coupled calculations. For this choice of parameters, the convergence of the FSD was achieved after 300 cycles. Convergence of the coupled calculation itself was achieved after 200 additional coupled cycles. GAMMA+ runs on a single CPU while MCS calculations are conducted in parallel on 20 CPUs of type "Intel(R) Xeon(R) CPU E5-2690 v2 @ 3.00GHz". For this configuration, the typical computational time for a single coupled step is about 3 minutes and the wall time of a coupled calculation (300 inactive cycles + 200 active cycles) is about 25h.

For each subcase of P1-Ex3, 3 coupled calculations are conducted: one with nominal CR position and two to compute the CR worth, with CR all-in position and CR all-out position. For the CR worth calculation, only the thermal-fluid coupling with GAMMA+ is used: the IEX coupling is deactivated and the Xenon135 distribution is taken constant throughout the coupled calculations, equal to the distribution determined for a CR at nominal position

The convergence of P1-Ex3b is illustrated on Fig. 7, which displays the variations during 500 coupled cycles of the Shannon entropy and of the axial offset (defined as the fission power generated on the top 5 AC layers minus the fission power generated by the bottom 5 AC layers, divided by the total fission power). Both parameters reach an asymptote after approximately 200 inactive cycles. The center-of-mass of the FSD also becomes stationary after about 200 inactive cycles: its cycle-to-cycle motions never exceed a few millimeters after 200 inactive cycles.

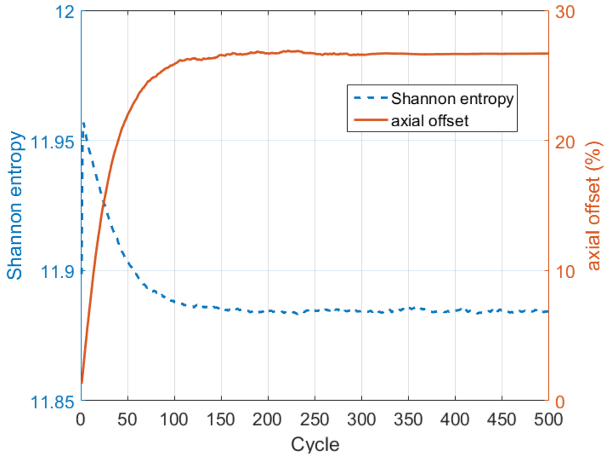

Fig. 7. Evolution of axial profile of power densities.

The convergence for P1-Ex3b of the axial profile of fuel power densities and fuel temperatures from the 10th coupled cycle to the 500th and last coupled cycle are presented in Fig. 8 and Fig. 9 respectively (1 = bottom AC layer, 10 = top AC layer; coolant flows from top layer 10 to bottom layer 1). The profiles are similar for both Ex3a and Ex3b. As the coupled calculation goes, the axial profile of power density becomes more and more skewed towards the top of the core. The maximum fission power is obtained in AC layer 8 when convergence is reached. The fact that the maximum fission power is axially located in the AC layer 8 results from a balance between the presence of 3 CR in AC layer 10 and the large difference in fuel temperatures (about 350°C) between AC layer 10 and AC layer 1. The large fuel temperature difference between the top and bottom layers (which is induced by the top-bottom coolant flow) causes the power densities to be higher in general in the top AC layers than in the bottom AC layers.

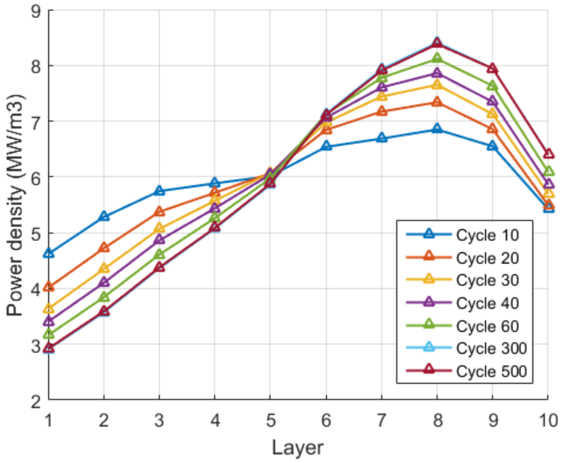

Fig. 8. Evolution of axial profile of power densities.

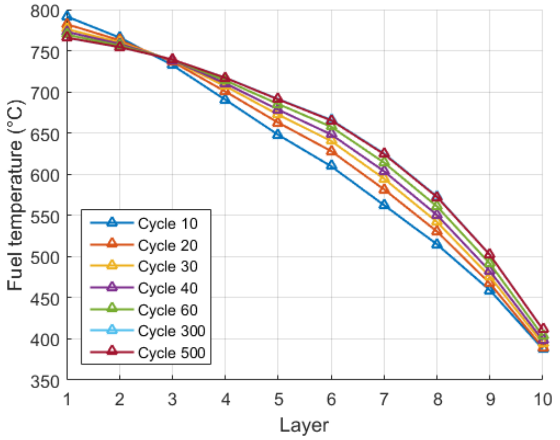

Fig. 9. Evolution of axial profile of fuel temperatures.

The distribution of bypass flow rates between P1-Ex3a and P1-Ex3b is presented in Table III. There are large differences in the bypass flow distribution between P1-Ex3a (standard values determined by GA) and P1-Ex3b (values calculated by MCS/GAMMA+), especially for the bypass CR cooling in IR and the AC region, even though the total bypass flow rates are close to each other in both cases. The difference in the bypass flow distribution may be due to differences in the form loss coefficients as the form loss coefficients used by GA to generate P1-Ex3a bypass flow rates are not specified in the benchmark documentation.

For P1-Ex3a and P1-Ex3b, the global neutronics parameters (with uncertainty at one standard deviation) are presented in Table IV and the global thermal-fluid parameters in Table V. The global parameters are almost the same between the two subcases. The only difference between the two subcases P1-Ex3a and P1-Ex3b is the modelling of the bypass gaps, but the resulting difference in the bypass flow distribution has barely an impact on the global parameters.

Table III. Bypass flow rate distribution for P1-Ex3

Mass flow rate (kg/s)	Ex3a	Ex3b
AC	2.36	3.34
IR	0.79	0.87
CR cooling in IR	1.89	0.71
CR cooling in OR	2.83	3.33
First ring of OR	2.17	1.88
Second ring of OR	2.55	2.19
PR	4.71	5.61
Total bypass flow	17.28	17.93

Table IV. Global neutronics parameters P1-Ex3

	Keff CR nominal	CR worth	Axial offset
Ex3a	1.05906 ± 2.10^{-5}	1138 ± 3	26.7%
Ex3b	1.05923 ± 2.10^{-5}	1145 ± 3	26.7%

Table V. Global thermal-fluids parameters P1-Ex3

All temperatures in °C	Ex3a	Ex3b
Maximum fuel temperature	1162	1166
Average fuel temperature	643	641
Average moderator temperature	636	635
Average reflector temperature	382	387
Average coolant temperature	550	549
Maximum core barrel temperature	328	329

The radial distribution of power density, axially averaged along the 10 AC layers, is similar for both Ex3a and Ex3b and is shown in Figure 10. The highest power densities are found close to the IR and, to a lesser extent, to the OR, due to the increased thermalization of neutrons from the reflectors. The hottest triangular fuel column is indicated with a black cross, with an axially-averaged power density of 10.6 MW/m3. It is possible to distinguish the 4 triangular fuel cells hosting a RSC hole as their axially-averaged power density (about ~2.5 MW/m3) is very low compared to the rest of the core.

The radial temperature profile in the bottom AC layer is also similar for both Ex3a and Ex3b and is shown in Figure 11 (the fuel temperature is plotted in the AC region while the graphite temperature is plotted in the reflector region). The bottom AC layer is the layer where the fuel temperatures are the highest and where the maximum fuel temperature is reached. It is possible to observe triangular hot spots in the fuel block areas closest to the IR, where thermal neutron flux is the most intense. In the 1/3rd core representation, 3 once-burned fuel blocks and 3 twice-burned fuel blocks are directly facing the IR. The fuel temperatures are higher in the 3 once-burned fuel blocks than in the 3 twice-burned fuel blocks, which is logical because of the greater fission rates in the once-burned fuel.

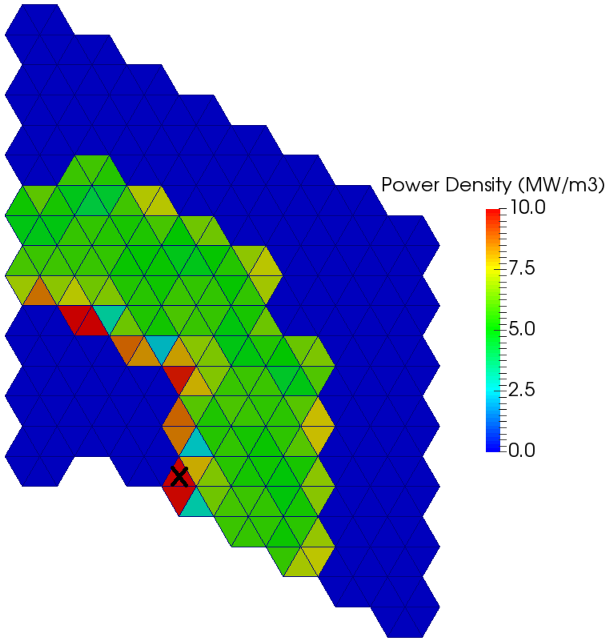

Fig. 10. Axially-averaged power density distribution.

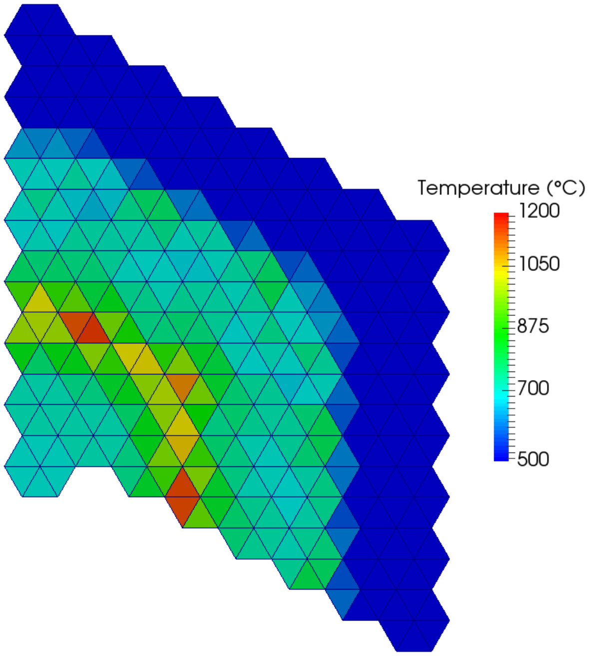

Fig. 11. Radial temperature profile in bottom AC layer.

IV. CONCLUSIONS

In this paper, coupled steady-state results for the OECD/NEA MHTGR-350MW neutronics/thermal-fluids benchmark problems were obtained with the Monte Carlo code MCS developed at UNIST and the thermal-fluids code GAMMA+ developed by KAERI. The results obtained for P1-Ex3a and P1-Ex3b are very close, including the total bypass flow which only varies by 3% between Ex3a and Ex3b, despite large differences in the bypass flow distribution itself. The similarity between the results of Ex3a and Ex3b seems to indicate a lesser sensitivity of the GAMMA+ physical model of MHTGR-350MW to the bypass flow distribution.

Reasonable results are obtained in terms of power density, neutron flux and temperature distributions. It is found that the top-to-bottom coolant flow of MHTGR-350MW induces fuel temperatures which are much higher at the bottom than at the top of the core, with a 350°C difference in average between bottom and top fuel temperatures. The higher fuel temperatures induce lower power densities at the bottom than at the top because of the increased fuel absorption due to Doppler broadening. The axial power density profile is strongly top-skewed as a result in the EOEC core, as burnable poison cannot flatten the power distribution any more. The AC layer with the highest power densities is the 8th AC layer, which results from a balance between the presence of 3CR in the top AC layer and the decreasing fuel temperature profile from bottom to top. The maximum fuel temperatures are predicted in the bottom AC layer, in the triangular once-burned fuel cells directly facing the IR, a zone of intense thermal neutron flux. It is interesting to notice that the zones of maximum fuel temperatures (bottom AC layer) do not correspond to the zones of maximum power densities (8th AC layer).

Results for P1-Ex3 using the MCS/GAMMA+ coupled code system were submitted to the MHTGR benchmark committee. The final code-to-code comparison of solutions between benchmark participants is expected to provide advanced understanding of the physics of prismatic modular reactors and to allow for improved modelling of such reactors in simulation codes. First comparison results are expected to be available for end of 2017.

NOMENCLATURE

AC = active core
CR = control rod
FSD = fission source distribution
GA = General Atomics
IEX = inline equilibrium xenon
IR = internal reflector
OR = outer reflector
P1-Ex3 = Phase 1 Exercise 3
PR = permanent reflector
RSC = reserve shutdown control

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