M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20, 2017, on USB (2017)

The Verification of Depletion Capabilities in RMC and APOLLO2/COCAGNE Based on KAIST 1A Benchmark

Yuan Yuan[a], Xiao Tang[a], Jingang Liang[b], Xiaotong Shang[a], Kan Wang[a]

[a]*Department of Engineering Physics, Tsinghua University, Beijing, 100084, CHINA*
[b]*Computational Reactor Physics Group, Massachusetts Institute of Technology*
wangkan@tsinghua.edu.cn; yuanyuan15@mails.tsinghua.edu.cn

Abstract - *EDF R&D and the Department of Engineering Physics of Tsinghua University have cooperated to make code to code comparisons for their newly improved codes, APOLLO2/COCAGNE and RMC. As an extension to the previous collaboration on a 3D neutron transport PWR benchmark, the goal of this paper is to validate burnup capabilities in APOLLO2/COCAGNE and RMC based on the KAIST 1A benchmark. Before launching the core depletion calculation, the assembly calculations and the core criticality calculation were performed to identify the discrepancies between these two code systems. The comparisons focus on multiplication factors (Kinf or Keff), flux, reaction rates, power and concentrations of several isotopes. The results of the final core depletion calculation are in good agreement and thus the burnup capability of both APOLLO2/COCAGNE and RMC is stable and reliable*.

I. INTRODUCTION

To validate burnup capabilities in deterministic methods and Monte Carlo methods, EDF R&D and the Department of Engineering Physics of Tsinghua University cooperate to make code to code comparisons on KAIST 1A benchmark for their newly improved codes, APOLLO2/COCAGNE [1] and RMC [2].

APOLLO2, developed by the CEA with the financial support of EDF and AREVA, is a lattice code for assembly calculations and cross-sections library generation. COCAGNE, developed by the EDF R&D, is a deterministic core code which contains a SN solver, named DOMINO, and a SPN solver, named DIABOLO, allowing the user to go from industrial two group diffusion calculation to reference multigroup pin-by-pin simplified transport (SPN) or transport (SN) calculations. RMC, developed by Department of Engineering Physics, Tsinghua University, is a Monte Carlo code for reactor physics calculations.

Previously, extensive verification work has been carried out for APOLLO2/COCAGNE and RMC [3-5]. A. Calloo has validated and compared the two-group diffusion, SPN and SN solvers in COCAGNE for the depletion of KAIST 1A benchmark [6]. APOLLO2/COCAGNE and RMC have been compared using multigroup cross sections based on a 3D PWR full core criticality calculation [7].

In this paper, the code to code comparisons will be extended to depletion capabilities and using continuous energy pointwise cross sections in RMC. Based on KAIST 1A benchmark, we will focus on the results of multiplication factors (Kinf or Keff), flux, reaction rates, power and concentrations of several isotopes and the corresponding discrepancies between RMC and APOLLO2/COCAGNE will be analyzed.

II. KAIST 1A BENCHMARK

The KAIST 1A benchmark [8] is based on a simplified PWR core of small size, which contains 52 assemblies in total and produces 900 MWth at nominal power. It is characterized by high heterogenization and high leakage terms, making it a challenging case for neutronics calculations. In this study, the core was depleted in 2D without coupling to thermal hydraulics calculations. The loading pattern of the core is shown in Fig.1, and the boundaries as symmetric lines are reflective while the rest are vacuum boundary.

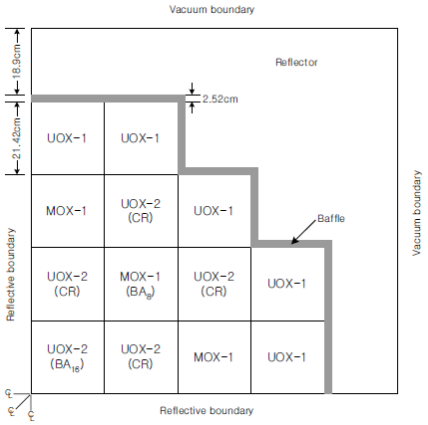


Fig. 1. Core configuration and boundary conditions [8].

There are five types of assemblies in the core. UOX-1 and UOX-2 are UOX assemblies with 2.0% U235 and 3.3% U235 enrichment respectively. UOX-2(BA16) is the UOX assembly enriched at 3.3% U235 with 16 Gd pins in which UO_2 is enriched at 0.711% U235 and the content of gadolinium isotopes is 9%. MOX-1 is the MOX assembly with zoning for plutonium enrichment: 8.7% enrichment in the central zone, 7.0% in in the intermediate zone and 4.3% in the peripheral zone. MOX-1(BA8) is the same as the MOX-1 assembly but with 8 Gd pins.

The fuel assembly configurations are shown in Fig.2, which are in 17× 17 array and each assembly consists of 264 fuel pins, 24 control rod guide tubes and 1 instrumentation guide tube. Detailed material composition can be found in the benchmark specification [8].

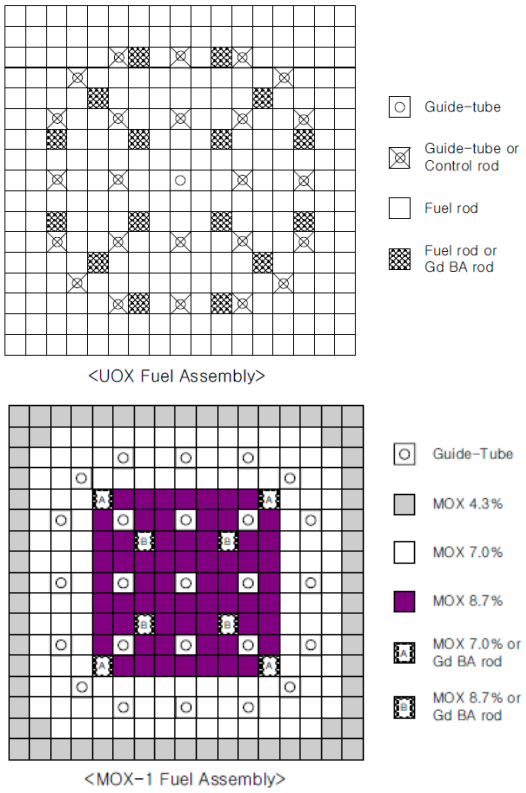


Fig. 2. Fuel Assembly configurations [8].

III. CALCULATION CONDITIONS

The validation work has been divided into three phases to identify the discrepancies between APOLLO2/COCAGNE and RMC, including assembly depletion calculation, core criticality calculation, and core depletion calculation. In this paper, only the results of assembly depletion calculation and core depletion calculation will be presented in the next section since the results of criticality calculation are similar to those of the core depletion calculation at BOC.

Before launching the calculation, both two sides have agreed to modify and simplify some parameters in the benchmark, including ignoring the air gap by using the same isotopes in fuel and dividing the fuel pins into four rings, which cover 50%, 30%, 15% and 5% of the fuel area, respectively. The cross section library used is based on JEFF 3.3.1.

As for the assembly calculation, it is a classical two-step approach with a 281-group self-shielding calculation and the first level flux calculation is done at 281-group with collision probability method to obtain a weighting flux for condensing cross sections to 26 groups, used in the second level MOC calculation. This MOC flux is then used to weight cross sections for the core code COCAGNE. The solver used for COCAGNE calculation is a 26-group Sn calculation.

The burn steps and corresponding critical boron concentrations used for calculations are suggested by EDF. The calculations in RMC are run on the platform of the Inspur TS1000 HPC Server of Tsinghua University with large-scale parallel mode.

IV. RESULTS AND ANALYSIS

1. Assembly Depletion

In the first phase, the UOX-1 assembly and the UOX-2(BA16) assembly were chosen to make assembly depletion calculations. The following parameters have been compared: keff, flux, fission rates, absorption rates, the isotope concentration and distribution of U235, U238, Pu239, Xe135, Sm149, Am241, and Cm244 at different burnup depths. And only some of these comparisons are presented here. For each depletion calculation, 600 cycles of 100000 neutrons/cycle with 200 cycles skipped are used in RMC and the standard deviation of Kinf is about 4pcm.

A. UOX-1 Assembly

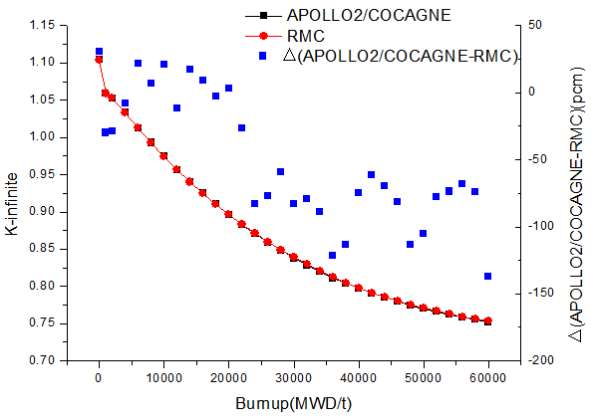


Fig. 3. Discrepancies on Kinf

The Kinfs of APOLLO2/COCAGNE and RMC along burnup are shown in Fig.3, and the largest discrepancy is less than 140pcm. As the U235 enrichment of UOX-1 assembly is only 2%, it can be concluded from the Kinfs burnup curve that the maximum burnup of assembly would be about 20000MWD/t. In addition, the U235 enrichment is only 12% of natural U235 enrichment at 60000MWD/t, which might be a challenge for neutronics simulations and a rare case in practical engineering application. Therefore, the following comparisons are made up to 20000MWD/t and thus the maximum discrepancy of Kinfs is below 31pcm,

which indicates an excellent agreement for Kinfs between APOLLO2/COCAGNE and RMC.

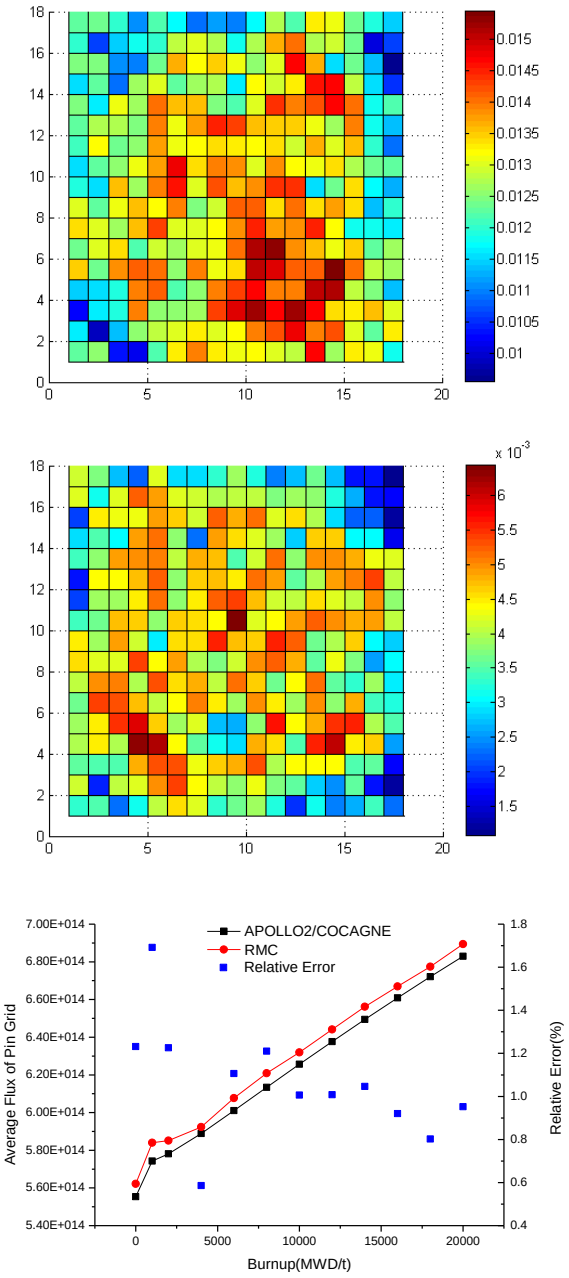


Fig. 4. Discrepancies on flux
(Top: BOC, Middle: 20000MWD/t, Bottom: average flux)

Fig.4. shows the comparison results for flux at BOC and 2000MWD/t and the maximum discrepancies are below 1.6% and 0.7%, respectively. In addition, the flux of RMC is a bit larger than that of APOLLO2/COCAGNE and the relative errors are almost constant, which might be attributed to the normalization factors and thus the different power treatments in two codes. About 1% power in APOLLO2/COCAGNE transfers to water holes as diffusion energy but in RMC all power concentrates in the fuel area. So the discrepancy between RMC and APOLLO2/COCAGNE is about 1% on flux, almost the same as the discrepancy in power distribution.

B. UOX-2(BA16) Assembly

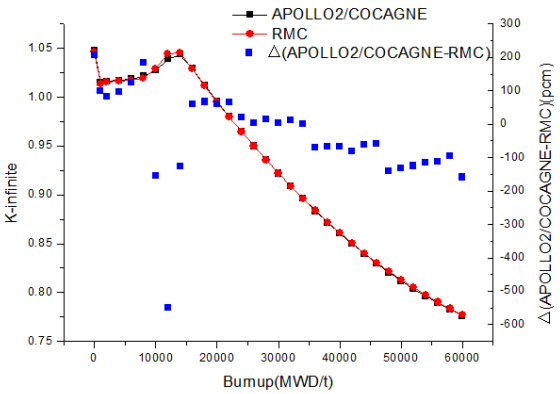
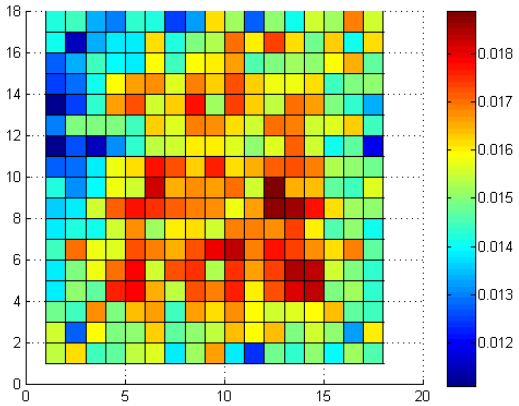


Fig. 5. Discrepancies on Kinfs

UOX-2(BA16) assembly was chosen mainly to investigate the effect of Gd pins. The Kinfs along burnup are shown in Fig.5 and they are almost the same between RMC and APOLLO2/COCAGNE except a few large discrepancy points, which are up to 550 pcm and only appear at around 12000MWD/t. The reason for this peculiar phenomenon will be explained later. Compared to UOX-1 depletion, the UOX-2(BA16) assembly has higher maximum burnup because of higher enrichment and higher discrepancy because of Gd pins. But both cases indicate that the assembly calculated in APOLLO2/COCAGNE burns a little faster than that in RMC.



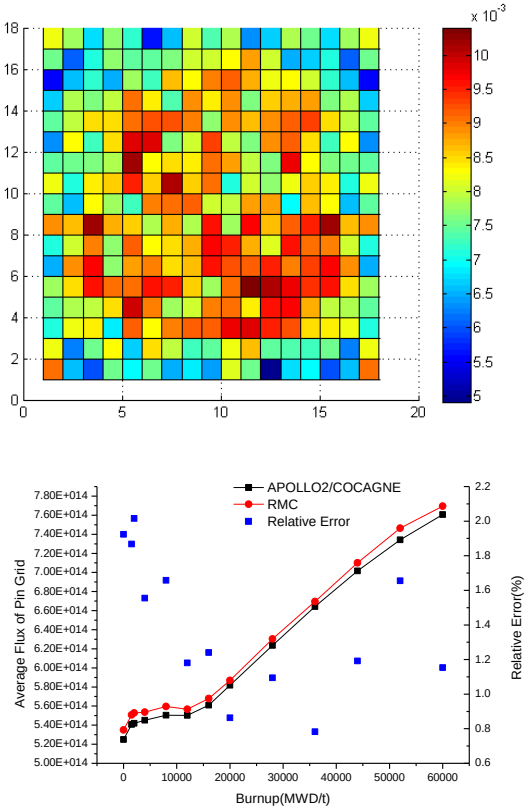


Fig. 6. Discrepancies on flux
(Top: BOC, Middle: EOC, Bottom: average flux)

The discrepancies on flux distributions and average flux of pin grid along burnup are shown in Fig.6. The maximum discrepancies for flux distributions at BOC and EOC are less than 1.9% and 1.1%, respectively. Besides, the flux of RMC is still slightly larger than that of APOLLO2/COCAGNE during the whole depletion due to the different power treatments mentioned before.

Since there are 16 Gd BA pins in UOX-2(BA16) and the U235 enrichment in Gd BA pins is only 0.7% that is close to natural U235 enrichment, power in Gd BA pins is lower and more energy could be transferred away from other fuel pins in APOLLO2/COCAGNE, leading the larger power distribution difference between RMC and APOLLO2/COCAGNE. Therefore the flux discrepancy is larger than that of UOX-1.

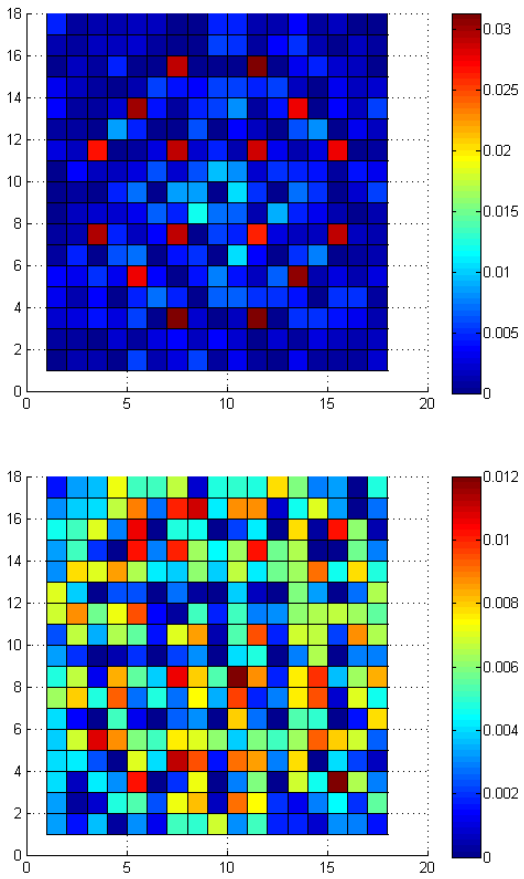


Fig. 7. Discrepancies on fission rates
(Top: BOC, Bottom: EOC)

Fig.7 shows the discrepancies on fission rates distributions at BOC and EOC, which are mainly caused by the discrepancies on flux. The maximum relative error at BOC is below 3% and that of EOC is below 1.2%. It is obvious that the discrepancies in Gd BA pins are particularly higher than those of surrounding pins. On the one hand, owing to the low U235 enrichment the fission rates in Gd BA pins is much lower than other fuel pins, so the uncertainty in Gd BA pins is also higher. On the other hand, the Gd isotopes are strong neuron absorbers and of great importance for the fission rates in Gd BA pins, so the difference in Gd cross sections can lead to significant discrepancies. In the deterministic method, the self-shielding treatment for resonant nuclides is still a challenging task and more precise multigroup cross section may be desired. At EOC, only the former factor has an effect on discrepancy as the Gd is consumed, and it can be seen that the relative errors in Gd pins tend to be random and similar to those of other pins at EOC.

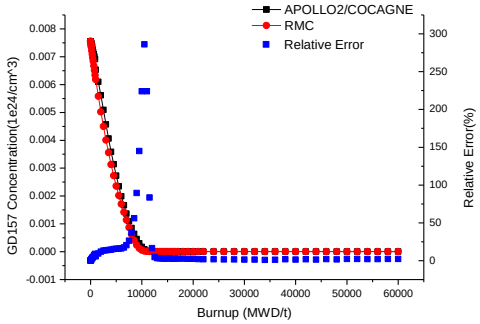


Fig. 8. Discrepancies on Gd157 concentration

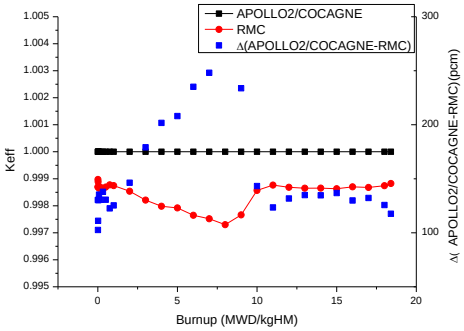


Fig. 9. Keffs along burnup

Since the Kinf is sensitive to Gd concentration, Gd157 concentration along burnup is added to be compared and the results are shown in Fig. 8. It can be found that the Gd157 concentration is almost the same between APOLLO2/COCAGNE and RMC at BOC and EOC and the same goes for Kinfs. In addition, Gd157 burns faster in RMC than that in APOLLO2/COCAGNE, and the relative error accumulates dramatically to 290% around 10000 MWD/t as the Gd157 concentration in RMC is very low. Then the Gd157 concentration is in balance and the relative error drops dramatically to 2%. The change in Gd157 relative error is the same as that of discrepancies on Kinf. The maximum discrepancy in Kinf happens around 12000MWD/t while the discrepancy is slight at BOC and EOC. The Gd BA pins are different from other pins in assembly on cross sections. It may be difficult for deterministic method to deal with burnable absorbers. Gd burnup calculation in deterministic method may need to be more carefully treated and the multigroup cross section for Gd may need to be more precise.

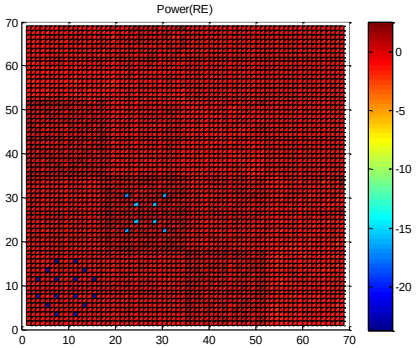
2. Core Depletion

After assembly depletion calculation and core criticality calculation, the calculation model has been carefully checked and improved. The final core depletion calculation was launched and Keff, power distribution, and concentrations of several isotopes are compared.

The Keffs of APOLLO2/COCAGNE and RMC along burnup are shown in Fig.9. With critical search, the Keffs of APOLLO2/COCAGNE are constant one while those of RMC are slightly varied with given critical boron concentrations. The maximum discrepancy is about 270 pcm, which is acceptable for comparisons of the deterministic code and the Monte Carlo code. Regarding statistical error, 800 cycles of 500000 neutrons/cycle with 200 cycles skipped are used in RMC and the standard deviation of keff is about 4pcm.

As with the UOX-2(BA) assembly depletion calculation, the discrepancies of Keffs that increase at first and drop at last might also be owing to those of Gd concentrations.

The pin by pin power distributions at BOC and EOC are also compared, as shown in Fig.10 and Fig.11. Firstly, it should be noted that the power treatment in two codes is a little different since a small amount of power in APOLLO2/COCAGNE has transferred to water holes while in the current RMC the power only concentrates in the fuel pellet. Hence the power in guide tubes is not zero for APOLLO2/COCAGNE while that is for RMC, and the discrepancies for those pins are neglected in the following comparisons. Filtering the water holes, the discrepancies in Gd pins are much higher than those of other pins at BOC, which may also be attributed to the different power treatments in two codes. Because of the natural enrichment of U235 and the large absorption cross sections of Gd isotopes, the fission power is pretty low in Gd pins and the difference in nonfission capture power may be magnified. As the concentration of Gd decreases rapidly with burnup deepening, the power of Gd pins are close to that of surrounding fuel pins and thus high discrepancies in Gd pins vanish. Therefore the different power treatment should be responsible for the high discrepancy in Gd pins at BOC.



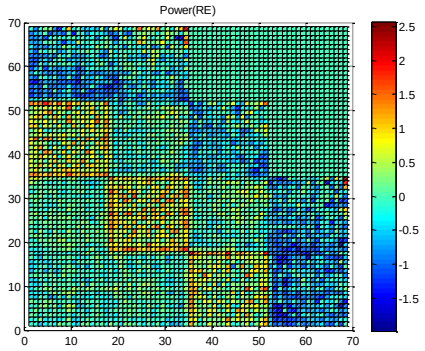


Fig. 10. Discrepancies on power distribution at BOC (Top: filter water holes, Bottom: filter water holes and Gd pins)

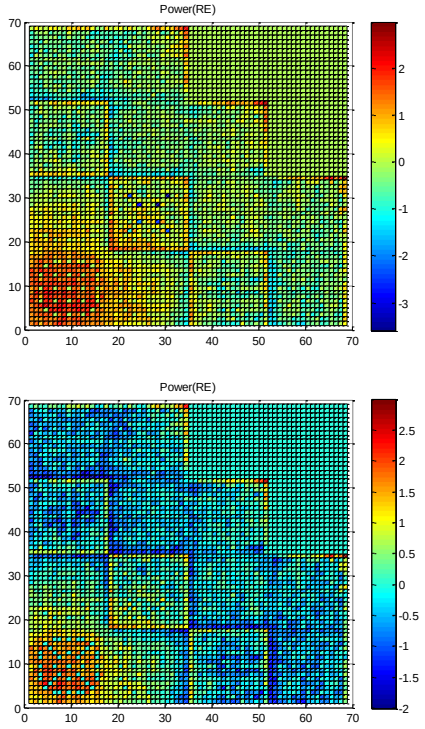
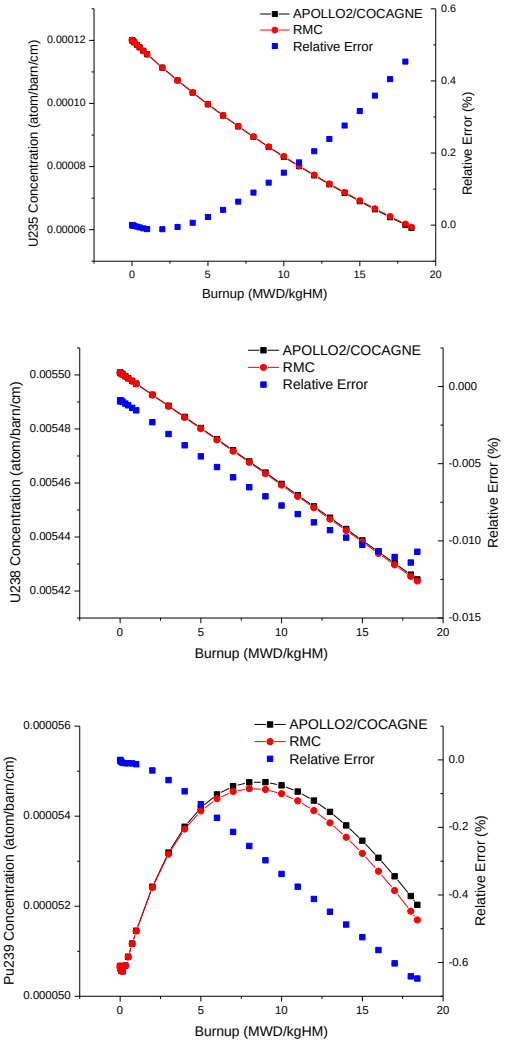


Fig. 11. Discrepancies on power distribution at EOC (Top: filter water holes, Bottom: filter water holes and Gd pins)

Table 1: Statistical data for power distribution

power		MAX	MIN	RMS
BOC	Filter water holes	2.6%	-23.7%	1.9%
	Filter water holes and Gd pins	2.6%	-2.0%	0.6%
EOC	Filter water holes	3.2%	-3.7%	0.7%
	Filter water holes and Gd pins	3.0%	-2.0%	0.7%

Filtering water holes and Gd pins, the relative errors for most pins at BOC and EOC are below 2% except pins that are next to the corner of the baffle or at the boundary of UOX and MOX assemblies in which the discrepancy is up to 3%. It may be explained by the higher flux gradient and local heterogeneities in these zones and the homogenization process in deterministic methods. In general, considering the fact that the root mean square of discrepancies shown is Table 1 is less than 2%, power distributions from two codes mostly are in good agreement.



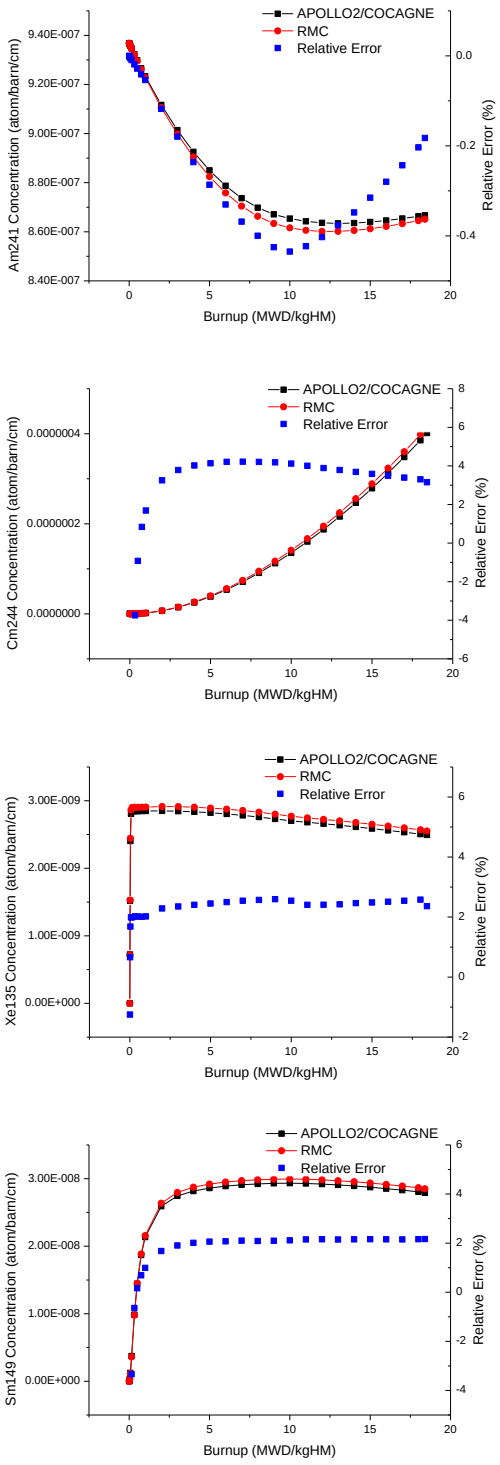


Fig. 12. Discrepancies on isotopes concentrations

Furthermore, concentrations of several isotopes such as U235, U238, Pu239, Am241, Cm244, Xe135 and Sm149 have also been compared. The discrepancies of these isotopes concentrations integrated over the core along burnup are shown in Fig.12, and these at EOC are 0.51%, 0.01%, 0.60%, 0.18%, 3.15%, 2.36%, 2.17%, respectively, which can be regarded as acceptable.

The discrepancies of U235 and Pu239 that are important isotopes for fission reactions are within 0.5%. The concentrations of poison isotopes like Xe135 and Sm149 are a little larger in RMC than that in APOLLO2/COCAGNE, which may contribute to the fact that the Keff is lower in RMC.

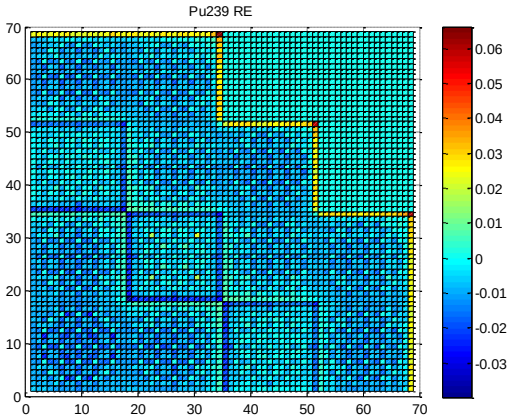


Fig. 13. Discrepancies on Pu239 concentration at EOC

The discrepancies of Pu239 concentration distribution at EOC are shown in Fig.13. Obviously, the discrepancies for pins which are near the reflector or at the boundary of UOX and MOX assemblies are higher than those for surrounding pins. This phenomenon resembles that for pin power distribution, indicating that the homogenization process and treatment for regions with high flux gradient and local heterogeneity are the main source for the discrepancies.

In addition, it should be noted that RMC uses a detailed complicated chain containing 1487 isotopes while COCAGNE uses a reduced chain with 40 isotopes, consisting of the main fuel isotopes, as well as some for minor actinides and neutron absorbers. The difference in depletion chains may also contribute to the discrepancy of isotope concentrations.

V. CONCLUSIONS

To validate burnup capabilities in deterministic methods and Monte Carlo methods, EDF R&D and the Department of Engineering Physics of Tsinghua University cooperate to make code to code comparisons on KAIST 1A benchmark for their newly improved codes, APOLLO2/COCAGNE and RMC. Before launching core depletion calculation, assembly calculation and core criticality calculation were performed to identify the discrepancies between these two codes. All results between RMC and APOLLO2/COCAGNE are in good agreement, and the discrepancies are almost all within acceptable range.

In the final core depletion calculation, the maximum discrepancy of Keff along burnup between APOLLO2/COCAGNE and RMC is about 270 pcm. The relative errors for most pins at BOC and EOC are below 2% except pins that are next to the corner of the baffle in which the discrepancy is up to 3%. More importantly, high discrepancies occur in the water holes and Gd BA pins due to the different power treatment in two codes. In addition, as indicated by assembly calculation, the cross section processing of Gd may also play an important part in Gd burnup and Kinf since RMC uses ACE format continuous energy pointwise cross sections while APOLLO2/COCAGNE uses multigroup cross sections. For isotope concentrations comparison, the discrepancies of U235, U238, Pu239, Am241, Cm244, Xe135, Sm149 concentration at EOC are 0.51%, 0.01%,0.60%, 0.18%, 3.15%, 2.36%, 2.17%, respectively. Furthermore, the homogenization process and treatment for regions with high flux gradient and local heterogeneity are another main source for the discrepancies.

To sum up, EDF R&D and the Department of Engineering Physics of Tsinghua University use their own developed codes with different methods and solvers (Determinism and Monte Carlo) to launch the depletion calculations respectively and the results are in good agreement with each other. It can be concluded that both APOLLO2/COCAGNE and RMC are suited to provide accurate depletion solutions for PWR core depletion calculations.

ACKNOWLEDGMENTS

This work is partial supported by funding from EDF R&D and National Science and Technology Major Project of Large Advanced PWR Nuclear Power Plant in China (2011ZX06004-024). The support by the Tsinghua High Performance Computational Platform “Inspur TS10000” HPC Server is also appreciated.

The authors would like to thank our cooperators in EDF R&D, Ansar Calloo, Hadrien Leroyer and Marie Hypolite for their kind help and useful discussions.

REFERENCES

1. L. Plagne and A. Ponçot, “Generic Programming for Deterministic Neutron Transport Codes”, Proceeding of Mathematics and Computation, Supercomputing, Reactor Physicsand Nuclear and Biological Applications, M&C 2005. Palais des Papes, Avignon, France (2005).
2. Kan WANG, LI Zeguang, SHE Ding, et al. RMC-A Monte Carlo code for reactor physics analysis[C]. Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo (SNA + MC), 2013, Paris, France.
3. Qiu, Yishu, et al. "3D Neutron Transport PWR Full-core Calculation with RMC code." SNA + MC 2013 - Joint International Conference on Supercomputing in Nuclear Applications + Monte Carlo 2014.
4. She, Ding, et al. "Development of burnup methods and capabilities in Monte Carlo code RMC." Annals of Nuclear Energy 51(2013):289-294.
5. She, Ding, et al. "2D full-core Monte Carlo pin-by-pin burnup calculations with the RMC code." Annals of Nuclear Energy 64.64(2014):201-205.
6. Calloo, Ansar, et al. "Validation of the SPn depletion schemes of the EDF Gabv2-Cocagne tools using the KAIST 1A benchmark." PHYSOR 2016.
7. Shichang LIU, et al.” Comparisons of 3D Heterogeneous PWR Full-core Transport Calculations by RMC and the SN DOMINO Solver from COCAGNE Platform Using Multigroup Cross sections.” Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo (SNA + MC), 2015.
8. Benchmark specification: http://nurapt.kaist.ac.kr/benchmark/kaist_ben1a.pdf