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Coupled neutronics/thermal-hydraulics analysis of a full PWR core using RMC and CTF

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ABSTRACT

A hybrid coupled strategy was proposed for a coupled neutronics and thermal-hydraulics analysis of a full PWR core, using the continuous-energy Reactor Monte Carlo code (RMC) and the sub-channel code COBRA-TF (CTF). In the code system with hybrid coupling, CTF was invoked and controlled by RMC internally, without external interface. The On-The-Fly cross sections treatment of RMC was used to reduce the complexity of the coupled code as well as to reduce the memory requirement. The domain decomposition parallel technique was developed in CTF to improve the efficiency of full core sub-channel calculations, and the PWR preprocessor of CTF can reduce the complexity of full core modeling establishment. The coupled codes were applied to steady-state simulations of the Benchmark for Evaluation And Validation of Reactor Simulations (BEAVRS) in the hot, full power condition at the full-core level to reveal the effects of the coupling on the full-core power distribution in both axial and radial directions. The influences of other important parameters including the neutron population and the boron concentration were also investigated. The results proved the effectiveness and high fidelity of the coupled system. More systematic and detailed analyses can be performed based on realistic operating conditions of PWR full core with the coupled codes system.

1. Introduction

Reactor physics numerical calculations have been used for reactor design analyses, core power analyses and burn-up calculations, with both deterministic methods and the Monte Carlo method used in these calculations. The Monte Carlo method has the advantages of being a first-principle method and providing high fidelity calculations. The Monte Carlo method can provide high fidelity neutronics analyses of different nuclear reactor designs owing to its flexible geometric modeling and the use of continuous-energy nuclear cross sections. Massively parallel algorithms significantly reduce the computational costs of Monte Carlo codes.

Many factors need to be considered in reactor analyses, such as the fuel pin temperature, coolant temperature and density, and void friction. These thermal parameters that can be predicted by reactor thermal hydraulics codes strongly influence the reactor operations and safety. The single channel method and sub-channel method are two traditional approaches for analyzing the coolant flow and heat transfer in the reactor core with many codes using such models to accurately model the thermal hydraulics process, such as RELAP5 (SCIENTECH Inc., 1998), COBRA-EN (Basile et al., 1999), and CTF (CASL, 2015). Unlike single channel codes, sub-channel codes provide more accurate modeling of the full reactor core or a single assembly taking the mixing flow into account. Detailed pin-by-pin sub-channel modeling of a full core also needs to be run in parallel to reduce the huge computational costs.

The model accuracy requirement for design and safety analyses of current and future nuclear reactors is continuously increasing, so high fidelity numerical reactor simulations are needed that include all the important reactor physics. The interplay between the neutronics and the thermal-hydraulic effects in a nuclear reactor core plays an important role in the reactor design, safety analyses and long term efficiency. To achieve the high fidelity solution with neutronics and thermal-hydraulics (N-TH), the neutronics code can be deterministic code or Monte Carlo code. Compared with the deterministic code, the Monte Carlo code has the greater advantages of accurate geometry and neutron energy treatment, which provides the most important foundation for full-core pin by pin level resolution through one-step direct transport calculations. While traditional deterministic codes based on three-step or two-steps homogenization methods have difficulties to predict the pin level power distributions precisely.

The sub-channel code and the computational fluid dynamics (CFD) code are two kinds of commonly used thermal-hydraulics

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codes. The CFD code can provide high accuracy calculation results but costs too much time especially for full core problems, while the highly efficient sub-channel code can accomplish the pin by pin level sub-channel resolution for full core problem.

There have been many previous studies of N-TH coupling using various combinations of different kinds of coupling codes mentioned above. For example, the deterministic code MPACT (Kochunas et al., 2013) and sub-channel code CTF has been coupled by CASL (Kochunas et al., 2014) in VERA-CS (Clarno et al., 2014). The Karlsruhe Institute of Technology (KIT) in Germany (Hoogenboom et al., 2011) has well achieved the coupling between MCNP (Briesmeister, 2000)/TRIPOLI4 (Brun et al., 2011) Monte Carlo codes and FLICA4 (Aniel et al., 2005)/SubChanFlow (Sanchez et al., 2010) thermal-hydraulics codes. It should be mentioned that the Monte Carlo code RMC (Wang et al., 2015) developed by REAL group of Tsinghua University in China, has been coupled with CFD code CFX (Marchisio et al., 2003) by Li et al. (2012), and Liu et al. (2015) has coupled RMC with the sub-channel code COBRA-EN. Besides, there are still many coupling work between Monte Carlo codes and thermal hydraulics codes being done by different research groups of many countries, which indicates that the N-TH coupling based on Monte Carlo code is an important research trend.

Furthermore, the full-core pin by pin sub-channel resolution is also a great challenge for the traditional thermal-hydraulics codes, but the new generation sub-channel code CTF can well solve the problem by the developed advanced techniques of domain decomposition for parallel computing and preprocessor for simplifying the geometry and power input for users.

Thus, with the great support of the super computer, the Monte Carlo code and sub-channel code CTF can match well for the coupling of full-core pin by pin resolution simulation, and can obtain the high fidelity results with the precise modeling of the full core.

This paper describes a coupled code using the continuous-energy Monte Carlo code RMC, and the sub-channel code CTF. The coupling codes are used to simulate the steady-state BEAVRS benchmark at the hot, full power condition. The temperature dependence of the cross sections in the Monte Carlo code were modeled using the on-the-fly cross section treatment in RMC, which will also be used for the coupled neutronics and thermal-hydraulics analyses in this work.

The simulation results show the necessity of the coupling as well as the significance of key coupled factors, including the neutron population and the boron concentration. The results also show the high efficiency and accuracy of the code. This coupling code provides a powerful tool for coupled steady-state and transient analyses.

This paper is organized as follows: in Section 2, two coupled computer codes are introduced in brief, including the Monte Carlo code RMC and sub-channel code CTF. Section 3 presents the coupling scheme in detail including the proposed hybrid coupling method, the approach to solve the temperature dependence, the principle of mesh mapping and the setting up of convergence criteria. Section 4 describes the modeling details of BEAVRS benchmark and the following coupling results and further discussion about the influence parameters on coupling. Finally, the conclusions and future work are presented in Section 5.

2. Computer codes

2.1. Monte Carlo code RMC

The Monte Carlo transport code, RMC, developed by the Department of Engineering Physics at Tsinghua University, is a continuous-energy Reactor Monte Carlo neutron and photon transport code (Wang et al., 2015). This new generation Monte Carlo code solves reactor analysis problems in complex geometries using continuous energy point-wise cross sections for various materials and temperatures. RMC can now do criticality calculations and burnup calculations with parallel processing using on-the-fly calculations of cross-sections as functions of temperatures with the source convergence acceleration for full-core hybrid calculations (Liu et al., 2017). RMC also has advanced methods to accelerate calculations (Liu et al., 2011; She et al., 2011, 2012).

RMC is being used for full core analyses with accurate, efficient results using advanced algorithms together with high performance computing techniques.

2.2. Thermal-hydraulics code CTF

CTF, a thermal–hydraulic simulation code designed for light water reactor (LWR) vessel analysis, is the shortened name given to the version of COBRA-TF (Coolant Boiling in Rod Arrays-Two Fluid) being developed by the Consortium for Advanced Simulation of Light Water Reactors (CASL) and the Reactor Dynamics and Fuel Management Group (RDFMG) at Pennsylvania State University (PSU) (CASL, 2015). CTF uses a two-fluid, three-field modeling approach and can solve detailed full-core models in parallel using the domain decomposition method (Salko et al., 2015). CTF has both sub-channel and 3D Cartesian forms of the 9 conservation equations for LWR modeling.

CTF stems from the original COBRA code, which was developed by Pacific Northwest Laboratory in 1980 and has been used and modified by several institutions, resulting in a series of COBRA codes, such as COBRA-EN and COBRA-IV. In the last decade, CTF has been improved and validated for both pressurized water reactor (PWR) and boiling water reactor (BWR) analyses. Improvements include additional models, enhanced computational efficiency, a PWR preprocessor to simplify the geometry input, and the ability to generate code documentation. CTF has been extensively used throughout the nuclear industry due to its powerful functions and rapid development.

3. Coupling scheme

For the full core pin-by-pin sub-channel calculations coupled with Monte Carlo code, many important aspects and details in the coupling process should be considered. Firstly, the most important aspect is the coupling method, which deals with how the data were transferred in coupling process. The second part introduced how the coupling process takes the advantages of some advanced feathers of CTF, including the domain decomposition and PWR preprocessor. The third part is about the temperature dependence treatment of cross sections developed in RMC. Besides, the mesh mapping strategy and the convergence criteria will also be explained in this section.

3.1. Hybrid coupling method

Traditional neutronics and thermal-hydraulics coupling methods include external or internal coupling. External coupling simply transforms the data in external files produced by the two coupled codes, while internal coupling transforms the data in memory between the two codes. External coupling is easily achieved but is not as versatile and slows the computations. Internal coupling is more versatile but is more complex and needs extensive code changes. Thus, a hybrid coupling method is used here.

The hybrid coupling was introduced in this paper, which transforms the data in the external files of the thermal hydraulics code while managing all the useful data in memory by the neutronics

code (Guo et al., 2016), as shown in Fig. 1. The data of thermal hydraulics code are transferred through external input and output files, while the neutronics code RMC does not need to change and print its input and outputs files. Therefore, the hybrid coupling scheme is a kind of partial external coupling. Therefore, the hybrid coupling is the combination of the external and the internal coupling that has the advantages of good versatility and easy achievement because there is less change work of the neutronics code and the input file. It is worth emphasizing that the CTF PWR preprocessor greatly simplifies the geometry information and power distribution for thermal-hydraulics user input and makes the hybrid coupling more achievable.

In the hybrid coupling of this paper, the neutronics code RMC was used to control the coupling, transfer and store the data internally. Two C++ source codes "read_TH.cpp" and "writepower.cpp" were added to RMC to transfer data. "writepower.cpp" obtains the calculated power distributions from the RMC memory firstly, and then transforms and writes them into the CTF power input file "power.inp". In addition, "read_TH.cpp" reads thermal-hydraulics data from the CTF output files and assigns them to the RMC memory after the CTF calculation.

In RMC, the power distributions were tallied for all the possible fission reactions of all the nuclides which have fission cross sections. Therefore, power tallies in some non-fuel positions such as control rods and burnable poison rods may probably not be zero. However, the CTF code only runs normally if the power source terms in non-fuel rod locations are all zero. Therefore, before transferring the power data from RMC to CTF, the power source terms in non-fuel rod locations must be set to zero, which is also done by "Writepower.cpp". After processing the power data and generating the "power.inp", CTF then runs in parallel. Once the CTF calculation is finished, "Read_TH.cpp" reads fuel pin temperatures and coolant temperatures and densities from CTF output files. These data is stored in RMC as three different three-dimensional matrixes, which will be used as the updated temperatures and densities for new RMC calculations.

Therefore, these two scripts "Writepower.cpp" and "Read_TH.cpp" in RMC act as the data transmission interface in the coupling process. Different from the external coupling, the hybrid coupling uses the neutronics code RMC to transfer data and invoke the sub-channel code CTF.

The algorithm flow diagram is given in Fig. 2 to illustrate the coupling process between RMC and CTF.

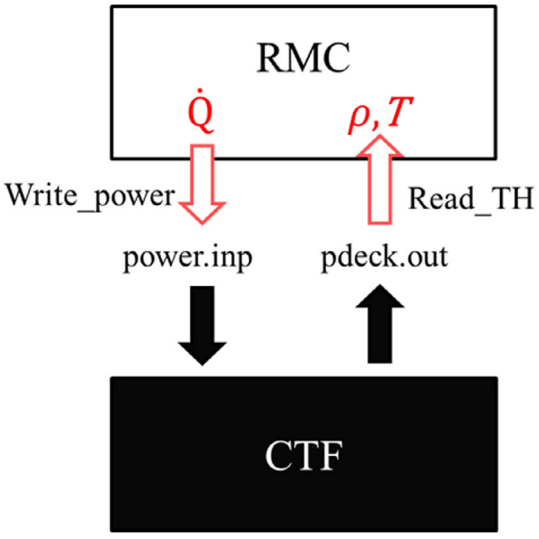

Fig. 1. Schematic diagram of the hybrid coupling.

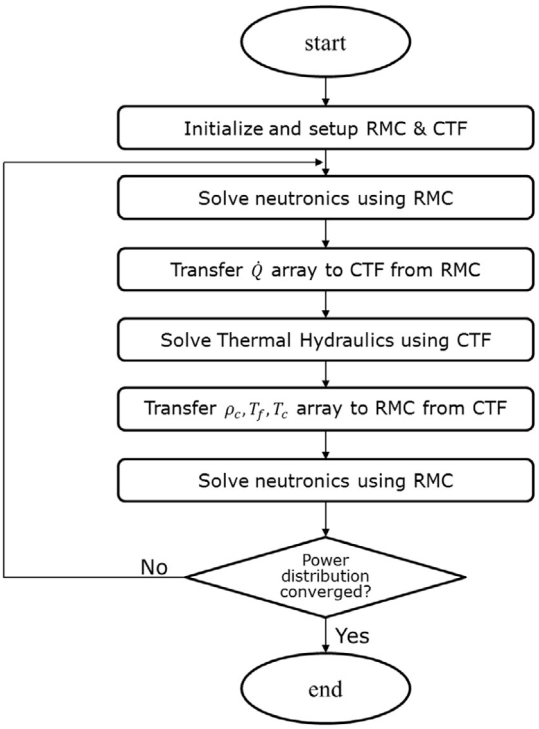

Fig. 2. RMC and CTF coupling algorithm flow chart.

As shown in Fig. 2, after initializing the RMC and CTF codes, RMC calculates the power distribution for the full-core BEAVRS benchmark. After completing the Monte Carlo calculation, RMC transfers the power distribution to CTF. In this process, the power distribution adopts the 1/8 symmetrical treatment, because the RMC statistical deviation can lead to considerable asymmetry after several iterations. CTF then solves the thermal-hydraulics equations and transfers fuel pin temperatures, coolant temperatures and densities to RMC, in which temperatures and densities have no treatment because CTF calculation results have no statistical deviation. After that, RMC runs again. This cycle executes until the convergence criteria are satisfied. The convergence criteria will be described in Sections 3.4 and 4.4.

3.2. Domain decomposition and PWR preprocessor

For the full-core pin level sub-channel resolution problem, the thermal-hydraulics calculation will cost much time if the thermal-hydraulics code runs in serial mode. Moreover, the detailed modeling of geometry relationships and power distributions for a full PWR core is very difficult as the input information is too much. Thus, CTF has developed the domain decomposition parallel approach to promote the calculation speed and the PWR preprocessor to simplify the user input. The details of these two optimization techniques have been illustrated in Ref. Salko et al., 2015. The following part will illustrate how these techniques were used in the coupling process, taking the BEAVRS full core problem as example.

The domain decomposition technique in CTF means dividing the single model into multiple domains. For the reactor full core problem, a feasible domain decomposition strategy is to divide the full reactor core into a collection of all single assemblies. For example, the BEAVRS full core has 193 assemblies with each assembly of 17 × 17 configuration, thus it can be decomposed into 193 domains that can run in parallel.

The PWR preprocessor plays an important role in the parallel domain decomposition technique of CTF. The PWR preprocessor of CTF is developed to simplify the user input of reactor geometry and power information. Take the BEAVRS full core problem in serial mode as example, users only need to write four 300-lines input files that consist of all the parameters needed in the thermal-hydraulics calculation, and the PWR preprocessor executes these four input files to generate the CTF input file that has more than 200,000 lines. On the other hand, in the parallel case, the preprocessor will generate 193 6000-lines domain input files and one 56,000-lines master input file of CTF. It is obvious that the preprocessor has great impact on the input simplification. Compared to serial case, input files of preprocessor for parallel case remain unchanged except for one optional parallel flag, which enable the preprocessor to generate the parallel input files of CTF.

Above all, these two techniques play an important role in the coupling process. The parallel domain decomposition technique enables the code CTF to run in parallel using the number of processors equal to the number of assemblies, which can highly improve the CTF operating efficiency. The PWR preprocessor is developed and optimized to simplify the user input as well as enable the parallel domain decomposition technique. With these techniques developed in CTF, the hybrid coupling between RMC and CTF becomes more flexible and efficient.

3.3. Temperature dependence

Traditionally, the neutron transport for a specific steady state case is calculated using the Monte Carlo method with fixed nuclide temperatures and coolant temperatures and densities. However, these values are distributed in a realistic reactor due to the heat transfer in the core. Generally, the cross sections (especially absorption) and thermal scattering cross sections depend on the fuel pin temperature and the coolant temperature and density. Particularly, resonance absorption changes dramatically with temperatures for the reaction of the target nuclide with the neutrons in specific energy regions. As the nuclide temperatures vary, the cross sections of the resonance absorption change, namely the Doppler-broadening effect, which has negative feedback on reactivity. Thus, the fuel pin temperature strongly influences the reactivity as well as the power distribution. Moreover, the fuel pin temperature also has obvious distribution in the radial direction, and the center temperature is significantly different from the surface temperature. In this coupling, CTF calculates both fuel center and surface temperature. To simplify the distribution situation and save memory, the temperature is considered linearly from the rod center to surface. Besides, the rod temperature is averaged before being transferred, and the treating process is shown as Fig. 3:

As shown in Fig. 3, the radius of the fuel rod is denoted as R. The average fuel rod temperature is calculated by the equation below.

$$T_{\text{fuel}} = \frac{\int_0^R \left(T_{\text{cen}} + \frac{(T_{\text{sur}} - T_{\text{cen}})\cdot r}{R}\right) 2\pi r dr}{\pi R^2} = \frac{1}{3}T_{\text{cen}} + \frac{2}{3}T_{\text{sur}} \quad (1)$$

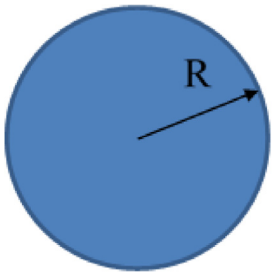

Fig. 3. Fuel rod schematic diagram.

where T_{fuel} represents the averaging fuel rod temperature, T_{cen} and T_{sur} represent the rod center and surface temperature, respectively. The temperature is averaged by the area of the rod cross section.

The coolant temperature has two opposing influences on the reactivity. As the temperature increases, the coolant density and the boron solubility in the coolant decrease, which increases the reactivity due to less absorption. On the other hand, the reduced coolant density reduces the neutron moderation in the coolant and hardens the neutron energy spectrum, which can reduce the reactivity. The boron concentration is normally less than 1400 ppm when the reactor is working normally. In this condition, the first effect has less impact on the reactivity than the second effect. Thus, the coolant temperature has a negative feedback effect with the reactivity decreasing with increasing coolant temperature.

Other parameters, such as the cladding temperature, have little impact on the neutron absorption; thus, only three parameters, the fuel temperature and the coolant temperature and density are taken into consideration in the neutronics and thermal-hydraulics feedback.

Traditional methods create new cross sections files at various temperatures in two ways. One is to create cross sections files for every temperature needed in the simulation, while another is to create cross section files at temperature increments and then interpolate these cross sections to get the correct temperature dependence. Since the coupling may produce any temperature during the calculation, the first method is not practical. The second method usually has cross section files for every 50 K or 100 K, which requires a large number of cross section files that consume much time and take up additional memory.

In RMC, the on-the-fly cross section temperature treatment was developed for both Doppler-broadening effect in resolver resonance region and thermal energy region. For the resolver resonance region, the target motion sampling (TMS) (Liu et al., 2016a) is applied to calculate cross sections for any temperature from 0 K continuous-energy cross sections by taking the thermal motion of the target nuclei into account. For thermal energy regions, the on-the-fly interpolation was used for thermal scattering cross sections (Liu et al., 2016b). Those two methods can accurately predict the absorption cross sections and the thermal scattering cross sections.

3.4. Mesh mapping

The coupling codes were used to model the full core of the BEAVRS benchmark. The BEAVRS benchmark is based on a 1960s PWR design. The benchmark is described in detail in Section 4.1.

The RMC geometry differs from that of CTF, and Fig. 4 shows the relationship between fuel pins and flow channels. RMC uses the rod-centered geometry while CTF uses the channel-centered geometry. In Fig. 4, the circles represent fuel pins while spaces between fuel pins are the coolant channels. RMC models the fuel pin in the interior square surrounding by channels A, B, C and D to predict the power produced in the fuel pin. The fuel pin temperature and the coolant temperature and density are then calculated in CTF using channels A, B, C, and D which adjoin surfaces 1, 2, 3, and 4 in RMC model. Thus, the data input to RMC is the averages of data from the CTF calculation. The data mapping averages the data from the four channels and surfaces as:

$$T_w = \frac{1}{4}(T_{chaA} + T_{chaB} + T_{chaC} + T_{chaD})_w \quad (2)$$

$$T_f = \frac{1}{4}(T_{surf1} + T_{surf2} + T_{surf3} + T_{surf4})_f \quad (3)$$

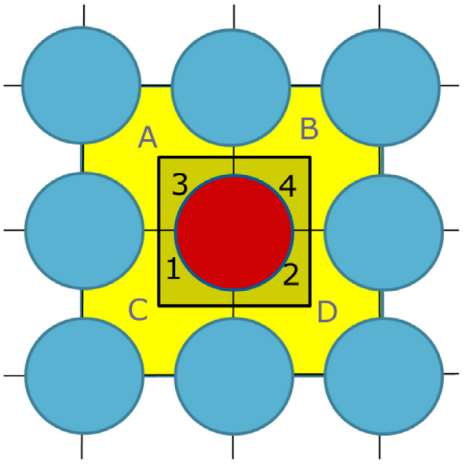

Fig. 4. Mesh mapping of RMC and CTF.

$$\rho_w = \frac{1}{4}(\rho_{chaA} + \rho_{chaB} + \rho_{chaC} + \rho_{chaD})_w \tag{4}$$

where 1, 2, 3, and 4 represent fuel pin surfaces, A, B, C, and D represent flow channels between fuel pins, T_w represents the average coolant water temperature in four channels that were modeled in CTF, $(T_{cha})_w$ is the water temperature in each of the channels, T_f is the average fuel pin surface temperature in the region indicated by the subscript, ρ_{cha} is the average water density in the channels, subscript *f* indicates the fuel pin, and *w* indicates the water.

Thus, all of the conditions used in RMC are the average values calculated from the CTF results.

3.5. Convergence criteria

The Monte Carlo calculations have random variations in the calculations, so the powers calculated by RMC have statistical errors which can be reduced by increasing the number of neutrons and the number of active cycles. In the initial stage of the coupled calculation, the statistical errors in the fuel pin scale at the reactor periphery are larger. The convergence was evaluated based on the relative change in the power levels in each mesh at each iteration given by:

$$\delta_m^n = \left| \frac{P_m^n}{P_m^{n-1}} - 1 \right| \tag{5}$$

where P_m^n is the power in the m_{th} mesh in the n_{th} iteration.

The maximum change was then found as:

$$\delta_{max}^n = max\{\delta_1^n, \delta_2^n, \ldots, \delta_N^n\} \tag{6}$$

This maximum changed significantly each time and did not tend to converge even though the power distribution in the whole reactor changed very little. Thus, the convergence was based on the average change in the power given by:

$$\delta_{ave}^n = \sqrt{\frac{(\delta_1^n)^2 + (\delta_2^n)^2 + \ldots + (\delta_N^n)^2}{N}} \tag{7}$$

This criterion was more reasonable and useful. The threshold of criterion can be depended on the statistical errors in the power tallies of Monte Carlo codes.

4. Results and analysis

4.1. BEAVRS benchmark modeling

BEAVRS is a new benchmark that was based on a 1960s commercial PWR reactor design in the United States with detailed core parameters and operating data developed for use as a reactor analysis verification tool, which was released by the Computational Reactor Physics Group of MIT (Horelik and Herman, 2012). This benchmark is based on a PWR with 193 fuel assemblies, with each assembly having a 17×17 configuration including 264 fuel rods with three different ^{235}U enrichments of 3.1%, 2.4% and 1.6%. As shown in Fig. 5, the 3.1% enriched fuel rods are along the edges of the core with the 2.4% and 1.6% enriched rods configured in a checkerboard pattern in the middle of the reactor core. The coupled simulations also included the eight spacer grids seen in Fig. 6 in the BEAVRS core to include the impact of the additional mixing on the coolant flow which influences the heat transfer between the coolant and cladding and, hence, the power distribution predicted by the RMC calculation.

The full BEAVRS core was modeled in RMC and CTF with the active core divided into 10 axial segments and 255×255 radial meshes. The meshes in the radial direction in the CTF thermal-hydraulics model resolved the geometry to the pin level with each polygon between four rods as a channel. The BEAVRS benchmark geometry then had a total of 56,288 channels over the full core. The data used in the coupled calculations is listed in Tables 1–3.

4.2. Coupled results

4.2.1. Coupled convergence results

The full core CTF model included eight spacer grids and two nozzles in the BEAVRS benchmark. Each RMC transport calculation used 200 inactive cycles and 200 active cycles in the first iteration and 500 active cycles in the following iterations. Each cycle included one million neutrons and a boron concentration of 599 ppm. Since δ_{max}^n given in Eq. (6) was not stable, δ_{ave}^n defined in Eq. (7) was used as the convergence criterion. The average relative statistical error in the power in each fuel pin in RMC for all the meshes was 0.0415, so the convergence criterion was set at 0.0412.

The coupled simulation used 720 parallel cores in the Tianhe-2 super computer for the RMC calculation and 193 cores for the CTF calculation. The variation of the convergence criterion was shown in Fig. 7.

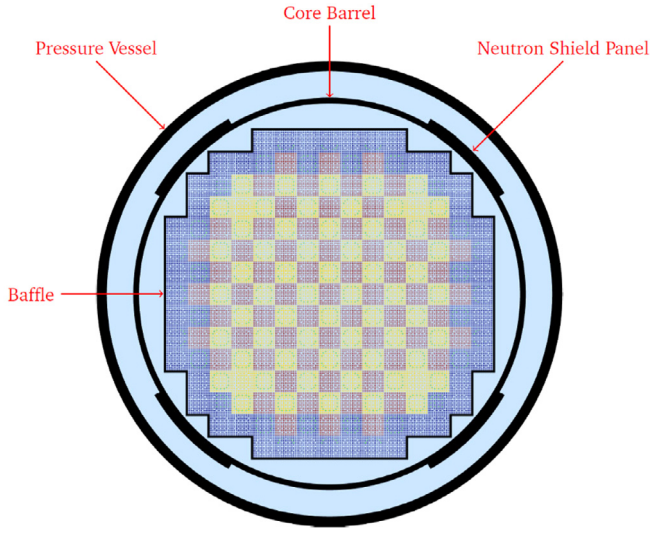

Fig. 5. Radial cross section of the BEAVRS core. The 3.1% enriched assemblies are around the edge with the 2.4% and 1.6% enriched assemblies in the middle.

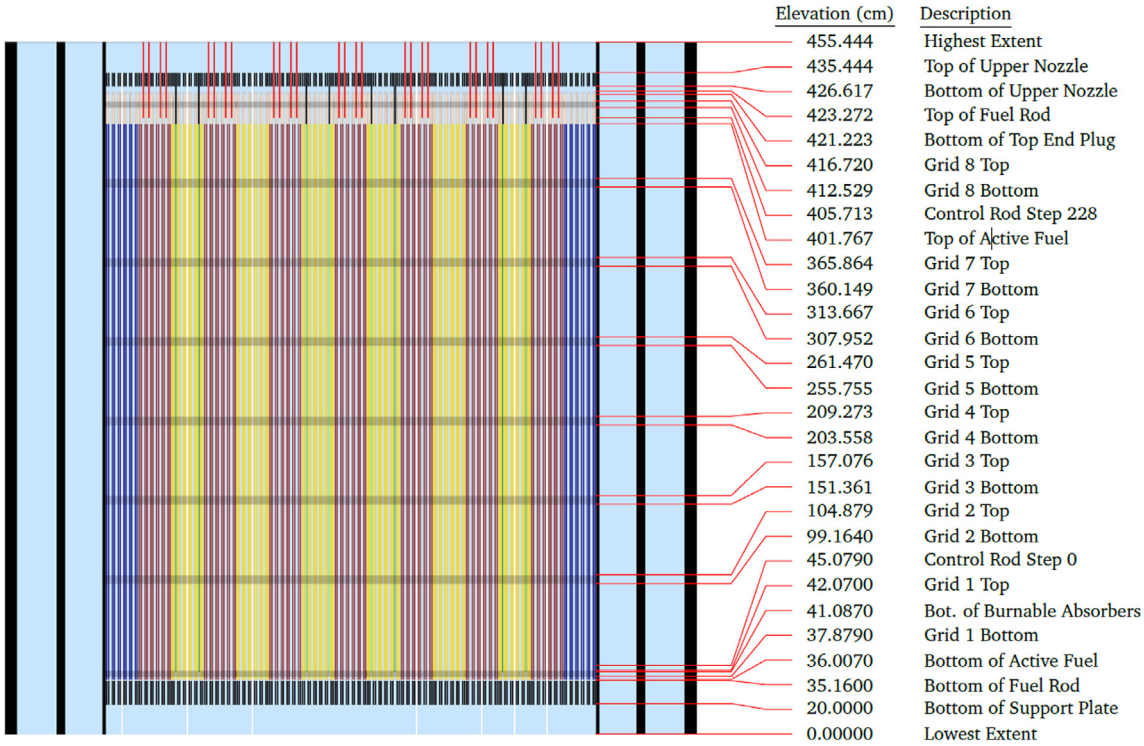

Fig. 6. Axial cross section of the BEAVRS core.

Table 1
Nominal values of the thermal hydraulics conditions.

Item	Value	Units
Total power	3411	MW
Initial mass flow rate	17083	kg/s
Reference pressure	15.517	MPa
Inlet water temperature	292.78	°C
Outlet water temperature	310	°C

Table 2
Assembly geometry.

Item	Size
Number of fuel rods	264
Number of guide tube rods	25
Active length (mm)	3657.6
Bundle pitch (mm)	215.04
Fuel rod diameter (mm)	7.84
Cladding inner diameter (mm)	8.00
Cladding outer diameter (mm)	9.14
Pin pitch (mm)	12.60
Guide tube inner diameter (mm)	11.22
Guide tube outer diameter (mm)	12.04

Table 3
CTF convergence criteria.

Item	Value
Outer Iteration Convergence Criterion	0.001
Maximum Number of Outer Iterations	5
Maximum Number of Inner Iterations	40
Global Energy Balance	0.01%
Global Mass Balance	0.01%
Fluid Energy Storage	0.01%
Solid Energy Storage	0.01%
Mass Storage	0.01%

Fig. 7 shows the change in δ^n_{ave} as the calculation proceeded with δ^n_{ave} smaller than 0.0412 after 8 iterations for 4 hours.

K_{eff} in the coupling process is almost constant after one iteration (Fig. 8). Compared with K_{eff} of the first iteration, the K_{eff} of the other iterations is smaller because of the negative reactivity feedback effect.

Fig. 9 shows the axial power distribution in the vertical direction along the active length during the iterations. After the first three iterations, the power profiles almost overlap, especially after six iterations, which means that the axial power distribution is approaching the convergence criterion.

In this coupling, the calculation time of every part in one iteration is counted accurately, and it is presented in Table 4.

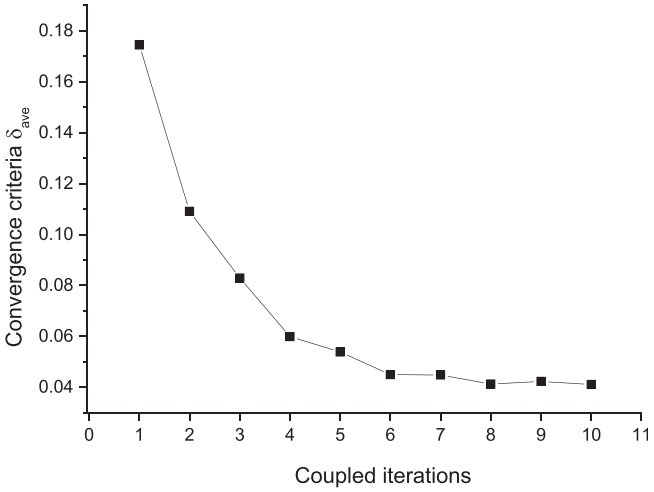

Fig. 7. Convergence of δ^n_{ave}.

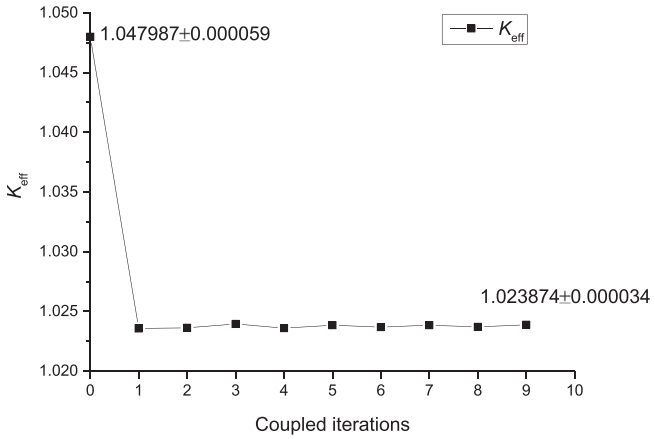

Fig. 8. Variation of K_{eff} during the iterations.

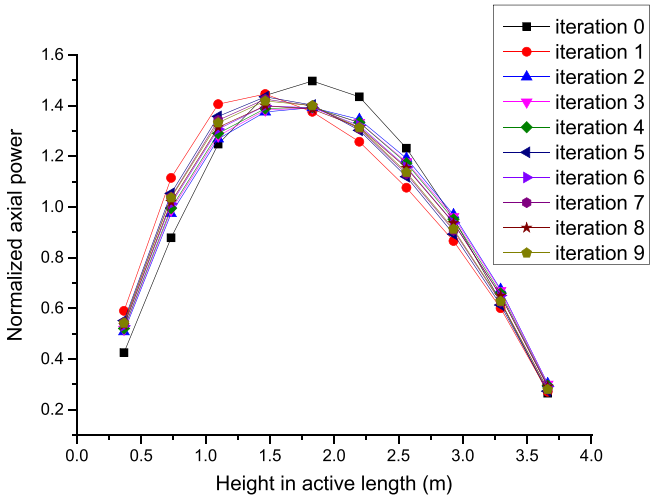

Fig. 9. Full core axial power distribution during the iterations.

The calculation time above belongs to the first iteration, but that of different iterations is almost the same. Therefore, the data in Table 4 can represent the calculation situation for all iterations. "Neutronics calculation" is the neutron transport process by RMC. Besides, "Write power" and "Read TH" represent the data transfer process write power data to "power.inp" and read thermal data from CTF output files, respectively. Moreover, "CTF runtime" is just the CTF calculation time, and "one iteration" is the total calculation time of the first iteration. "Neutronics calculation" and "CTF runtime" account for 94% of the total one iteration time. In contrast, the data transfer processes "Write power" and "Read TH" are only 4% of one iteration time. Therefore, it is the RMC and CTF calculations mainly influence the total runtime.

Table 4
BEAVRS benchmark calculation time of the first iteration.

	Neutronics calculation	Write power	Read TH	CTF runtime	One iteration
Calculation time (min)	14.20	1.28	0.42	11.90	27.80

For the complex BEAVRS full core pin level problem, RMC runs fast with the support of high speed supercomputer Tianhe 2. In addition, CTF is also high-efficient due to the advanced PWR preprocessor and domain decomposition parallel strategy. This coupling code system is efficient consequently.

4.2.2. Coupled effects on the power distribution

The radial power distributions with and without coupling are shown in Fig. 10 with the corresponding radial power peak factors with and without coupling listed in Table 5. The values in Fig. 10 are the sums of all the power generation rates in the vertical location at each radial location.

From the Table 5 and Fig. 10, the neutronics and thermal-hydraulics coupling influences the power distribution and the power peak factor in the radial direction. The temperature feedback given by the coupling makes the axially added radial power distribution more uniform and reduces the radial power peak factor.

The axial power distributions with and without coupling are shown in Fig. 11, where the power at each height is sum of all the power generation rates in the radial direction over the full core.

The coupling increases the power at the bottom of the core and reduces the peak power level (Fig. 11). In the coupled case, the water density decreases with height as the higher water density near the bottom provides better moderation which increases the power in the lower part of the core.

Some of the fuel assemblies in the core had a different tendency, such as for the central assembly as shown in Fig. 12.

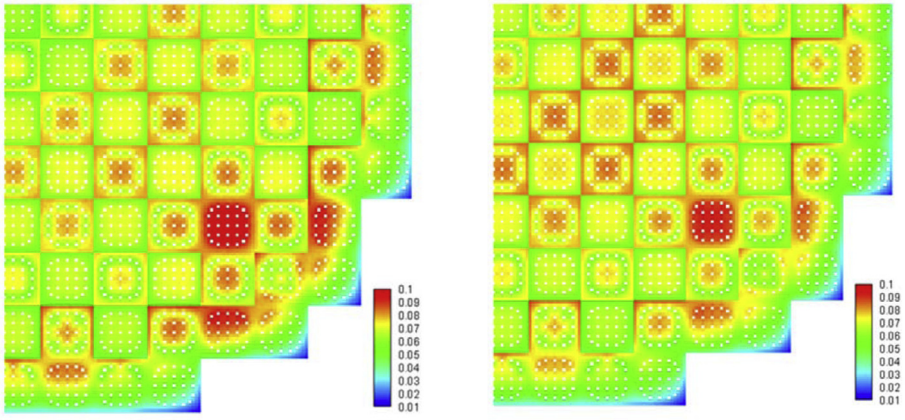

Fig. 10. Radial power distribution in the core.

Table 5
Power peak factors with and without coupling.

	Without coupling	With coupling
Power peak factor	1.49099	1.39556

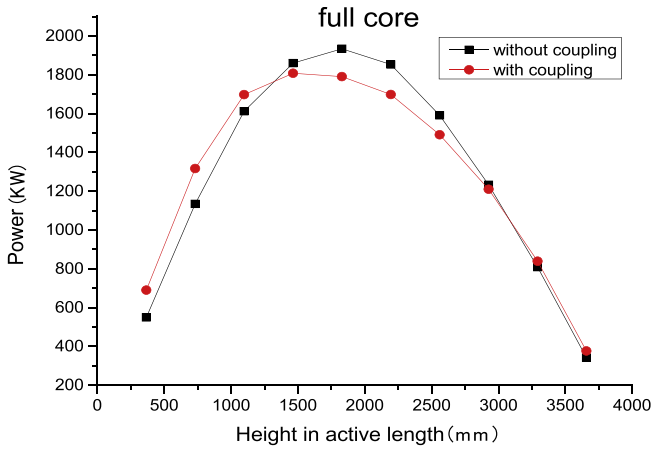

Fig. 11. Axial power distribution.

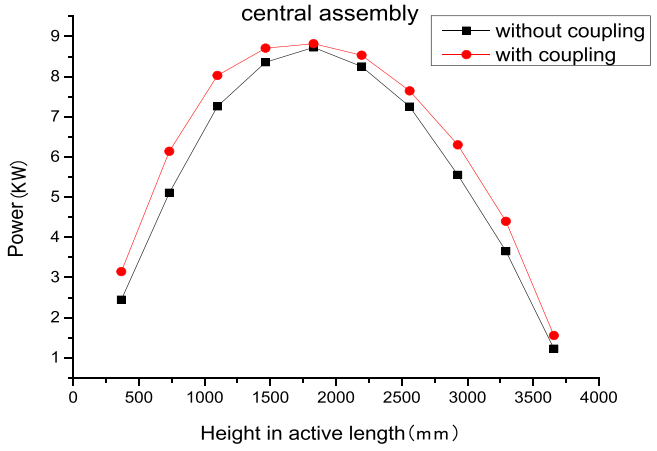

Fig. 12. Axial power distribution in the central fuel assembly.

Unlike the average for the entire core, the power in the central assembly with coupling is always higher than that without coupling (Fig. 12). This is because the power in the central fuel assembly is relatively small, the negative temperature feedback will increase the total power of this assembly to make power distribution more uniform, keeping the total reactor power constant.

Therefore, the coupling has different influence on the radial and axial power distribution as well as the temperature and density distribution. This proves the effectiveness of the neutronics and thermal-hydraulics coupling between RMC and CTF.

4.3. Parameters which influence the coupling effects

4.3.1. Number of neutrons

The influence of the number of neutrons used per cycle on the coupled results was analyzed by running cases with $5x10^5$ and $2x10^5$ neutrons while keeping the other conditions the same. The convergence of δ^n_{ave} for the different numbers of neutrons is shown in Fig. 13.

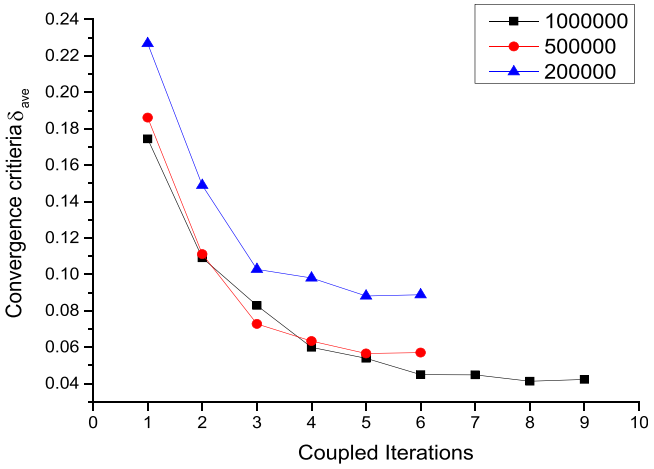

Fig. 13. Convergence with different numbers of neutrons.

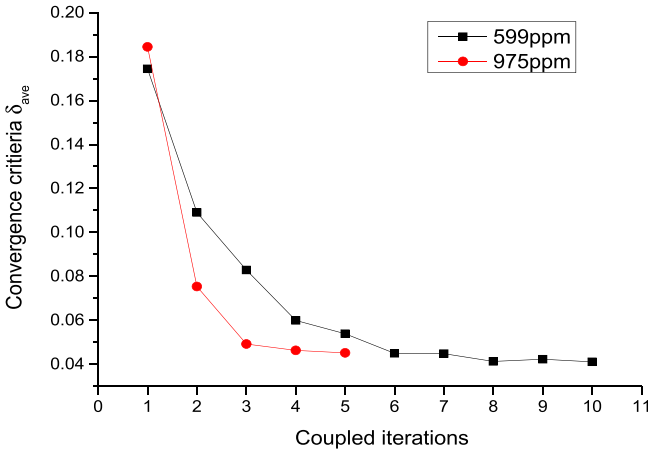

Fig. 14. Convergence with different boron concentrations.

Fig. 13 show that as the number of neutrons decreases, the relative change in the power predicted by the Monte Carlo calculation, δ^n_{ave}, increases. Thus, the convergence is better with a larger number of neutrons by increasing a few from 5×10^5 to 1×10^6 neutrons.

4.3.2. Boron concentration

The influence of the boron concentration on the coupled results was investigated for a boron concentration of 975 ppm with the other conditions the same. The convergence of δ^n_{ave} for the two cases with different boron concentrations is shown in Fig. 14. The power peak factors and the K_{eff} for the two boron concentrations with and without coupling are listed in Table 6.

Fig. 14 shows that the 975 ppm curve converges faster than the 599 ppm curve because the boron number density in the water decreases as the water temperature increases, so there is less neutron absorption which gives a positive feedback. Therefore, the increased boron concentration somewhat compensates for the negative temperature reactivity feedback, so the power peak factor is larger than with the lower boron concentration and converges faster.

Moreover, the data in Table 6 says that the increased boron concentration reduces K_{eff}, and the reductions of K_{eff} from without coupling to with coupling is also smaller for 975 ppm than 599 ppm.

Table 6
Power peak factor and K_{eff} with different boron concentrations.

Boron concentration (ppm)	Power peak factor		K_{eff}	
	Without coupling	With coupling	Without coupling	With coupling
599	1.49099	1.39556	1.047987	1.023839
975	1.59336	1.44235	0.998544	0.977435

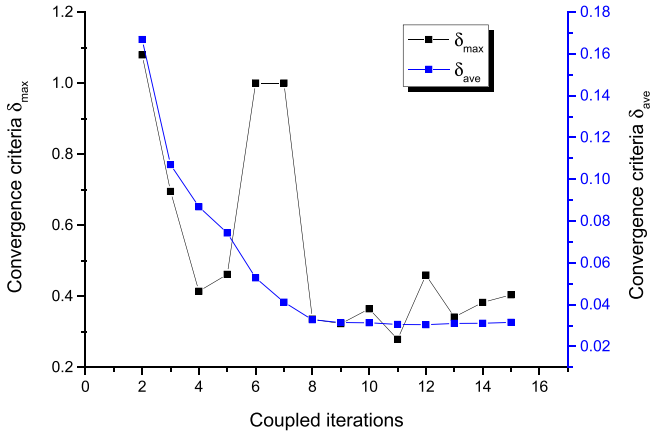

Fig. 15. Convergence of the original criteria (δ^n_{max} and δ^n_{ave}) for the full reactor core.

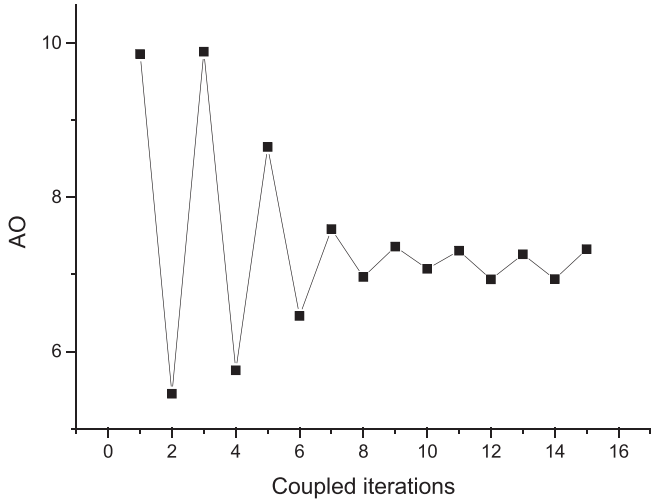

Fig. 16. Convergence of AO for the full reactor core.

4.4. Different convergence criteria

The effect of the convergence criterion on the result was investigated by defining different convergence criteria. The previous results showed that the coupling changes the power distributions in the radial and axial directions in the core, so the effect of the power partitioning between the upper and lower parts of the core was monitored by defining:

$$\mathrm{AO} = \frac{P_{upper} + P_{bottom}}{P_{upper} - P_{bottom}} \tag{8}$$

where P_{upper} and P_{bottom} represent the total power produced in the upper and lower halves of the core. The average relative changes in the power produced by defining $\delta^n_{\sigma,\max}$ and $\delta^n_{\sigma,\mathrm{ave}}$ to represent the maximum and average changes in the power produced in each meshes relative to the average relative power variation in the meshes:

$$\delta^{\mathrm{m,n}}_{\sigma} = \frac{\left|\frac{P^n_m}{P^{n-1}_m} - 1\right|}{\sigma^n_m} \tag{9}$$

$$\delta^n_{\sigma,\max} = \max\{\delta^{1,\mathrm{n}}_{\sigma}, \delta^{2,\mathrm{n}}_{\sigma}, \ldots, \delta^{\mathrm{m,n}}_{\sigma}\} \tag{10}$$

$$\delta^n_{\sigma,\mathrm{ave}} = \sqrt{\frac{(\delta^n_{\sigma 1})^2 + (\delta^n_{\sigma 2})^2 + \cdots + (\delta^n_{\sigma N})^2}{N}} \tag{11}$$

where P^n_m is the power in the $\mathrm{m_{th}}$ mesh in the $\mathrm{n_{th}}$ iteration and σ^n_m is the statistic relative power variation in the $\mathrm{m_{th}}$ mesh in the $\mathrm{n_{th}}$ iteration which was obtained directly from the tally file produced by RMC.

AO, $\delta^n_{\sigma,\max}$ and $\delta^n_{\sigma,\mathrm{ave}}$ were then used in new calculations with 1.5×10^6 neutrons, a total of 700 cycles with 200 inactive cycles and a boron concentration of 599 ppm. These coupled simulations used 480 parallel cores in the Tianhe-2 super computer for the RMC calculation and 193 cores for the CTF calculation. Convergence data for 15 iterations which took about 15 h with the convergence data presented in Figs. 15–17.

All the convergence criteria except for δ^n_{max} became almost stable after the eighth iteration with the curves of δ^n_{ave} and $\delta^n_{\sigma,\mathrm{ave}}$ agreeing well with each other. AO had small, stable oscillations after the eighth iteration that also indicate convergence; thus, the coupled calculations were converged after eight iterations.

Thus, AO and $\delta^n_{\sigma,\mathrm{ave}}$ can also be used as convergence criteria together with δ^n_{ave} for these coupled calculations.

5. Conclusions and future work

This paper presents a coupled RMC/CTF code that uses a hybrid coupling technique which combines the advantages of external and internal couplings. The hybrid coupling method both simplifies the modeling and enhances the versatility of the code system through using the neutronics code memory. The TMS cross sections method developed by RMC, which uses temperature dependent cross sections that are calculated on-the-fly, is used to simplify the cross section calculations as well as to reduce the memory requirement.

This coupled code system is then used for steady-state, full core simulations of the BEAVRS benchmark in the hot full power condition. The results show the effects of the coupling on the full-core power distribution in both the radial and axial directions. The coupling caused Doppler-broadening effect of the target nucleus cross sections reduces the power peak factor in the radial direction, so the coupling homogenizes the radial power distribution. In the axial direction, the power peak is reduced by the negative reactivity feedback with the power in the lower part increasing as the coolant density increases in the lower part of the reactor core. The coupled software package was also used to study the effects of key parameters on the convergence including the neutron population and the boron concentration. The results show that larger numbers of neutrons and higher boron concentrations improve the convergence because the higher boron concentration compen-

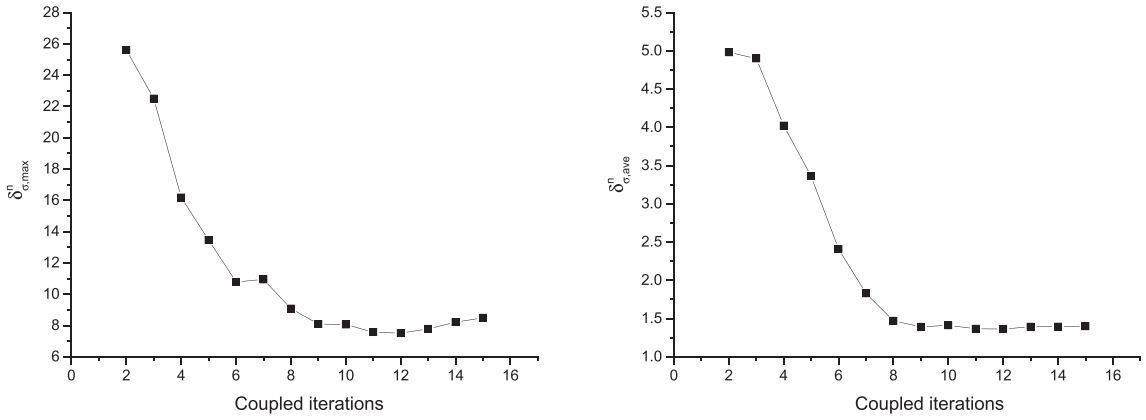

Fig. 17. Convergence of $\delta^n_{\sigma,\max}$ and $\delta^n_{\sigma,\text{ave}}$ for the full reactor core.

sates for the negative temperature reactivity coefficient. Various convergence criteria were also evaluated with AO defined by Eq. (8), which reflects the vertical power difference in the core, and $\delta^n_{\sigma,ave}$ defined by Eq. (11), which reflects the statistical variations in the power produced in each mesh, vary in the same trend as the power variations described by δ^n_{ave}, so these two criteria can be also used as convergence criteria.

The coupled neutronics/thermal-hydraulics code is effective and high-fidelity, which verifies the feasibility and capability of this hybrid coupled codes system. This codes system provides versatile and flexible coupling of the RMC and CTF codes.

There are many possible extensions of the coupled RMC and CTF code for future studies. One possible extension is to develop a more versatile coupled system through the HDF5 file. HDF5 uses a hierarchical data storage structure in which the data can be obtained from the HDF5 file straight-forwardly by a C++ script. Compared with the traditional text file, HDF5 file provides easier way to handle the data when coupling, which can reduce the limitations and complexity of the multi-physics coupling.

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