

Study of Neutronics and Thermal-hydraulics Coupling with RMC/COBRA-EN System

S.C. Liu, J.K. Yu, J.G. Liang and K. Wang

Department of Engineering Physics, Tsinghua University, Beijing, P.R. China
liu-sc13@mails.tsinghua.edu.cn, yjk10@mails.tsinghua.edu.cn,
liangjg06@mails.tsinghua.edu.cn, wangkan@tsinghua.edu.cn

Abstract

Neutronics and Thermal-hydraulics (N-TH) coupling plays an important role in high fidelity multi-physics simulation for nuclear reactor analysis. A coupled N-TH code system based on a continuous-energy Monte Carlo code RMC and the sub-channel code COBRA-EN has been developed. The temperature dependence of nuclear cross sections is handled with the Fast Doppler Broadening (FDB) capability embedded in RMC. This code system has been applied to a PWR fuel pin and a fuel assembly to investigate the effects of N-TH coupling and Doppler broadening. The results show that the coupling system with Doppler broadening is effective for the thermal-hydraulics feedback.

Keywords: Neutronics, Thermal-hydraulics, In-line Doppler Broadening, RMC, COBRA-EN

1. Introduction

With the development of the computer technology, high fidelity numerical reactor simulations including different physics raise wide concern of researchers. High accuracy simulations can reduce design uncertainty, thus enhancing the economic feasibility and safety of nuclear power plants. The interplay between the neutronic and thermal-hydraulic (N-TH) properties of a nuclear reactor core is a fundamental aspect of nuclear core performance. Many previous works related to the coupling of neutronic and thermal-hydraulic codes can be found in References [1, 2 & 3].

Compared to deterministic methods, Monte Carlo methods have the advantages of exact geometry modelling and continuous treatments of neutron energy. Armed with the massively parallel algorithms, the computational cost of Monte Carlo codes can be greatly reduced.

The developed code system in this paper enables the coupling of Monte Carlo code RMC [4] and sub-channel code COBRA-EN [5] for steady-state simulations. In order to deal with the temperature dependence of cross sections for Monte Carlo code, the in-line Doppler Broadening has been developed in RMC. The in-line Doppler Broadening was applied to the N-TH coupling in this work.

2. Coupling codes

2.1 Monte Carlo code RMC

RMC is a continuous-energy Reactor Monte Carlo neutron and photon transport code being developed by Department of Engineering Physics at Tsinghua University, Beijing. The code RMC intends to solve reactor analysis problems, and is able to deal with complex geometry, using continuous energy point-wise cross sections of different materials and temperatures. As one of new generation Monte Carlo codes, RMC is aimed at achieving full core calculations and analysis with high fidelity and efficiency by means of advanced methodologies and algorithms as well as high performance computing techniques.

RMC uses ACE format nuclear cross sections with $S(\alpha, \beta)$ and probability tables treatment in thermal and unresolved resonance energy ranges, adopts constructive solid geometry technique for flexible geometry modelling and employs ray-tracking method as main option for particle transport.

2.2 Thermal-hydraulics code COBRA-EN

COBRA is a sub-channel analysis code which computes the flow and enthalpy distributions in nuclear fuel rod bundles or cores for both steady state and transient conditions. COBRA-EN is an upgraded version of the COBRA-3C/MIT for thermal-hydraulic transient analysis of reactor cores.

2.3 Data exchange tool

The C++ tool has been used to transform the data of two individual codes via external files. The loose coupling scheme is used, in which the coupling between RMC and COBRA is external. Creation of input files for the two codes and data exchanges are managed automatically by the C++ tool.

3. Temperature dependence of cross sections

In pressurized water reactors, the main thermal feedbacks are Doppler effect of microscopic cross sections and the change of moderator density with temperature. In general PWR, the Doppler effect decreases reactivity due to resonance absorption of ^{238}U when temperature increases. The increase of moderator temperature lowers the moderator density, altering the energy spectrum of the core.

In order to consider the Doppler effect of microscopic cross sections, special treatment has to be used for Monte Carlo codes. The ACE-formatted libraries are processed by CSP/RXSP [6] code based on ENDF/B-VII.0. To generate point-wise cross sections at different material temperatures, the in-line Doppler Broadening capability has been developed in RMC [7]. Thus, the memory consumption in Monte Carlo based neutronics simulations can be effectively reduced.

Fast Doppler Broadening (FDB) [6] is a method for Doppler broadening the temperature dependent continuous energy neutron cross sections. In recent work, FDB is coupled into RMC for pre-Doppler broadening cross sections during the neutronics simulations. The Doppler effect of microscopic cross section depends on the energy and temperature. In the broadening, the microscopic cross sections of the specific temperatures were generated in the whole energy range with Fast Doppler broadening before the RMC execution. In this way, abundant cross sections data that cover all the expected temperature range with enough accuracy are no longer needed. The necessary cross sections data are ACE-formatted libraries at zero temperature, which are previously processed by CSP/RXSP code. RMC reads ACE formatted cross section libraries at zero temperature and Doppler broadens them to target temperatures before transport using FDB.

The in-line Doppler Broadening has been applied to the N-TH coupling in this work to take into account the Doppler effect.

4. Coupling process

The coupling between the two codes is performed by data exchange externally. The power distribution in the fuel rod is calculated by RMC, and it is used by COBRA to obtain coolant density and fuel, coolant and cladding temperature. The updated distribution of densities and temperatures is then used in a new RMC input file. The flow chart of the coupling process is shown in Figure 1.

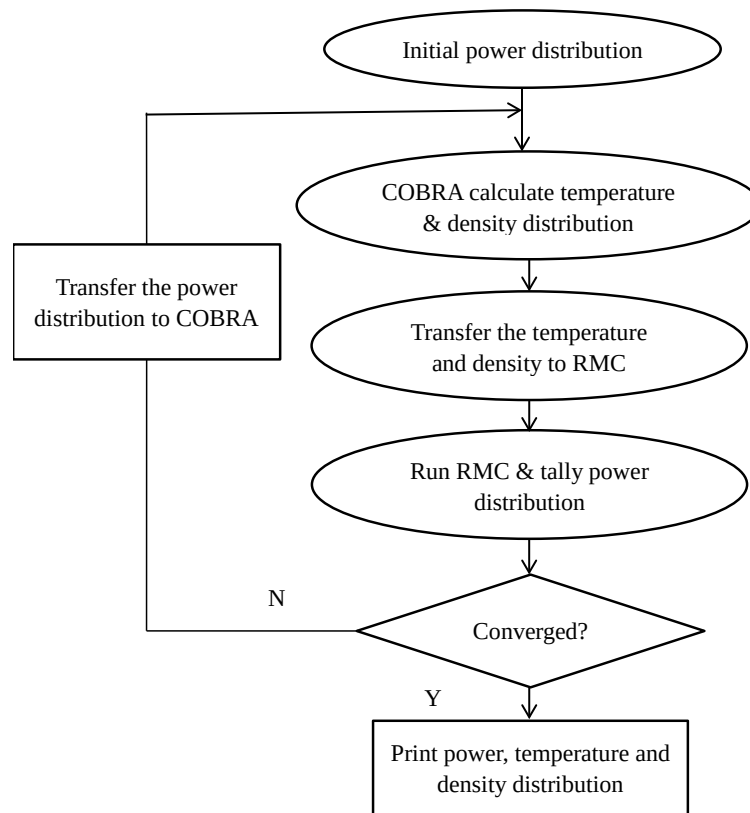


Figure 1 Coupling flow chart

The coupling process can be described as follows:

1. The coupling program starts with initial power distribution;
2. The power distribution is written in the input file of COBRA, and the COBRA calculation is performed. Fuel temperature is computed in each rod, and coolant properties are calculated in the sub-channels;
3. When the COBRA run is finished, the output is read and the distribution of temperatures and density is written in the new input file of RMC;
4. Then RMC is run with the new coolant density in material properties and new temperatures which contributed to the in-line Doppler Broadening;
5. After the executions of RMC, power distributions in each fuel rod are tallied directly;
6. Compare the newly calculated power distribution with the power distribution of previous step to judge the convergence status. If the convergence criterion is reached, output the

distributions of power, temperature and density. Otherwise, go to step 2 until it is converged.

5. Results and analyses

This code system has been applied to a PWR fuel pin and a fuel assembly to investigate the effects of N-TH coupling and Doppler broadening. For both fuel pin and fuel assembly, three cases were investigated, i.e. case without N-TH coupling, case without OTF and case with OTF. The case without N-TH coupling means that the coolant density and microscopic cross sections are corresponding to temperature of 293.6K. The case without OTF means that the actual temperature distribution calculated by COBRA is considered for the coolant density, while the microscopic cross sections are corresponding to temperature of 293.6K. The case with OTF means that the coolant density and microscopic cross sections are corresponding to the actual temperature distribution calculated by COBRA. The change of boron density was not considered when the temperature changes.

The operating conditions, fuel properties, clad properties in the two cases are listed in Table 1 to Table 3.

Table 1 Operating conditions

Pressure (MPa)	14.9134
Av. inlet mass flux for fuel channel (kg/m ² /sec)	3.4638×10 ³
Inlet enthalpy (MJ/kg)	1.2994
Av. linear power (W/m)	4.2071×10 ⁴

Table 2 Fuel properties

Conductivity (W/m/K)	3.46
Sp. Heat (J/kg/K)	242.6720
Density (kg/m ³)	10283.9
Diameter (m)	0.0089
Conductivity (W/m/K)	15.22

Table 3 Clad properties

Conductivity (W/m/K)	15.22
Sp. Heat (J/kg/K)	242.6720
Density (kg/m ³)	6487.5
Thick. (m)	2.54×10 ⁻⁴
Gap conductivity (W/m ² /K)	5674.47
Rod diameter (m)	0.0095

5.1 Fuel pin case

In the fuel pin case, the power distribution is one dimensional in the axial direction. The total length of the fuel pin is set as 5m, which is divided into 10 axial intervals. Void boundary conditions are used for upper and bottom surfaces, while the reflective boundary conditions are used for the four surrounding surfaces.

Each transport calculation uses 300 inactive cycles and 1700 active cycles with 1500000 neutrons per cycle, resulting in the standard deviation of 0.000011 for K_{inf} . The max statistic relative deviation of RMC among the 10 axial intervals is 0.0066. Therefore, the convergence criterion is set as 0.005, which means that the convergence is reached once the max relative discrepancy of the axial power among the 10 intervals is smaller than 0.005. The evolution of max relative discrepancy of axial power is shown in Figure 2, and K_{inf} of three cases are listed in Table 4.

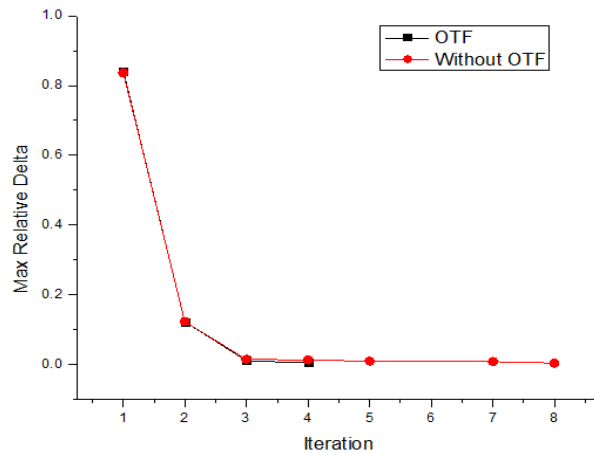


Figure 2 Evolution of max relative discrepancy of axial power

Table 4 K_{inf} of fuel pin case

Without coupling	Without OTF	OTF
1.417542	1.387894	1.378603

From Table 4, it can be found that K_{inf} of “Without coupling” is larger than that “With coupling” which has higher temperature, as the negative temperature coefficients of coolant density is considered. K_{inf} of “Without OTF” is larger than OTF which uses the microscopic cross sections of higher temperature, as the negative temperature coefficient of fuel is considered with OTF. From Figure 2, it can be found that coupling with OTF converges faster than without OTF.

The distributions of temperature and density with and without OTF are shown in Figure 3. It can be found that the N-TH coupling taking into account has slight difference with that without OTF. Furthermore, the power distributions of fuel pin are shown in Figure 4. Power Peak Factor (PPF) and Axial offset (AO) are compared, as listed in Table 5. The axial distribution calculated by RMC is asymmetric due to the statistical fluctuation of Monte Carlo methods. However, the distribution is more asymmetric with N-TH coupling, as the coolant

density is smaller at the lower half of the core. PPF with N-TH coupling is larger, so the results are more conservative with N-TH coupling.

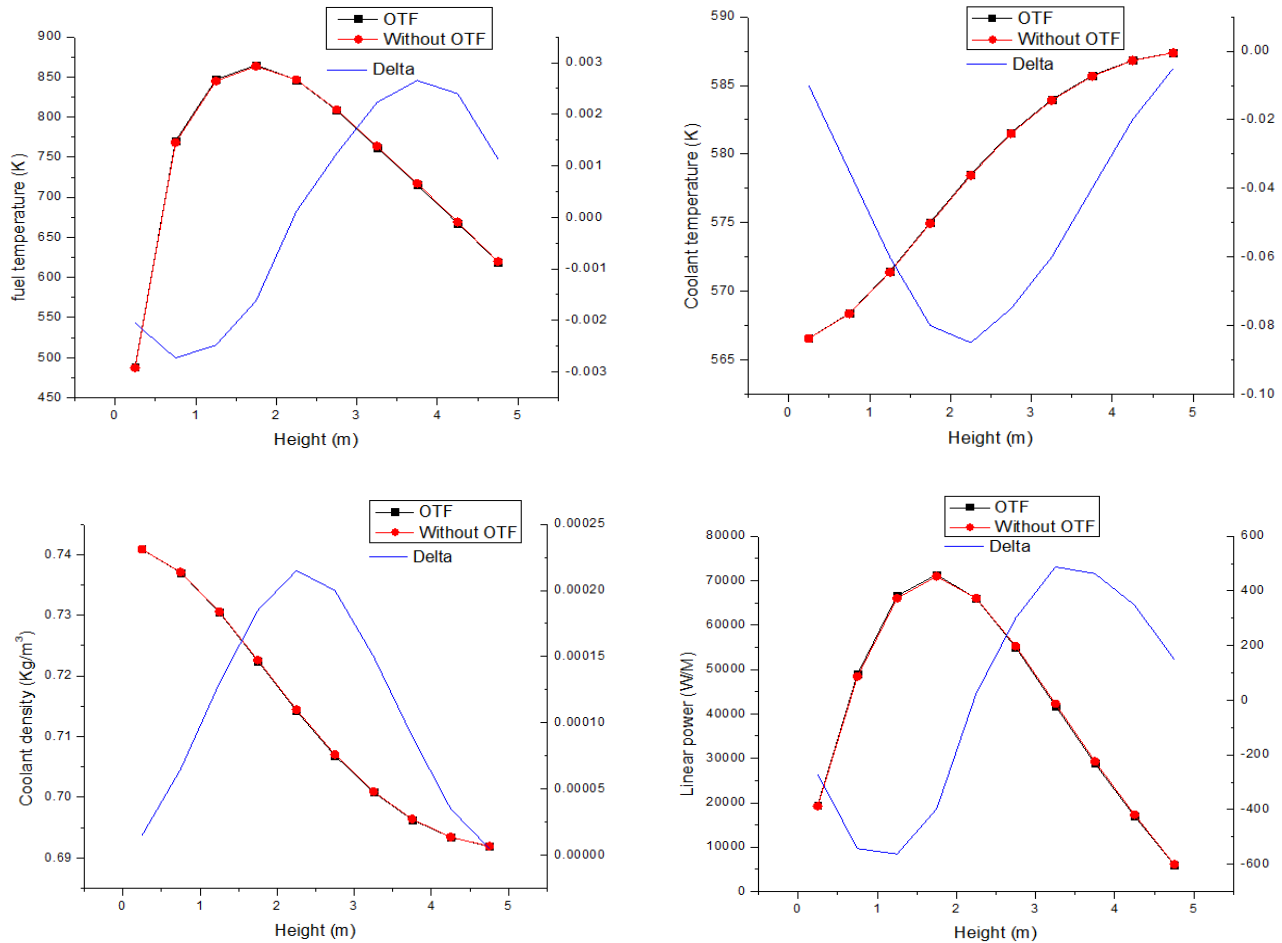


Figure 3 Distributions of temperature and density

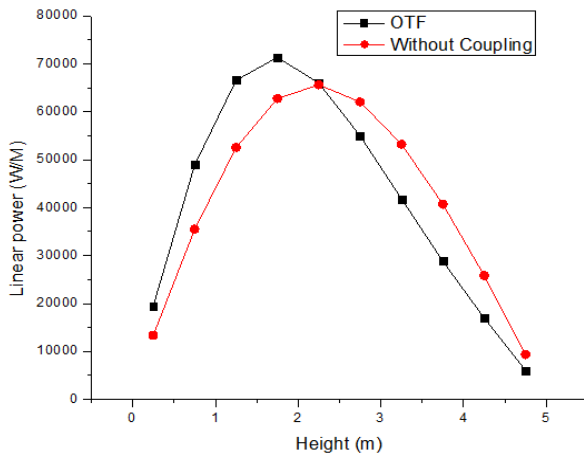


Figure 4 Power distribution of fuel pin

Table 5 PPF & AO of fuel pin case

Case	PPF	AO
Coupling	1.5582	1.2108
Without coupling	1.6866	1.8015
PPF= $P_{\max}/P_{\text{ave}}$ AO= P_L/P_H		

5.2 Fuel assembly case

In the fuel assembly case, the power distribution is two-dimensional in the radial direction. The fuel assembly model is simplified because of 1/8 symmetry of 17×17 PWR fuel assembly. The total length of the fuel pin is set as 0.1m with one axial interval. Reflective boundary conditions are used for the six surrounding surfaces.

Each transport calculation uses 300 inactive cycles and 1700 active cycles with 100000 neutrons per cycle, resulting in the standard deviation of 0.00004 for K_{inf} . The max statistic relative deviation of RMC among the 45radial meshes is 0.0011. Moreover, the actual statistic relative deviation will be smaller due to the 1/8 symmetry. Therefore, the convergence criterion is set as 0.001. The evolution of max relative discrepancy of axial power is shown in Figure 5, and K_{inf} are listed in Table 6.

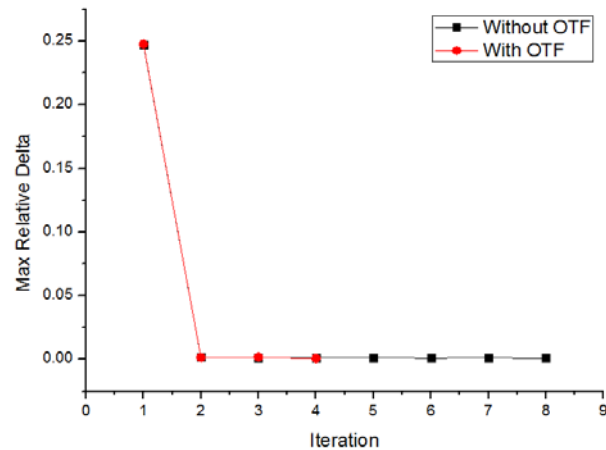
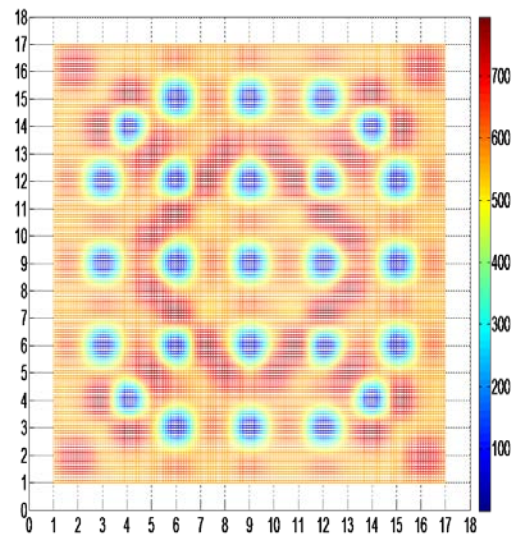
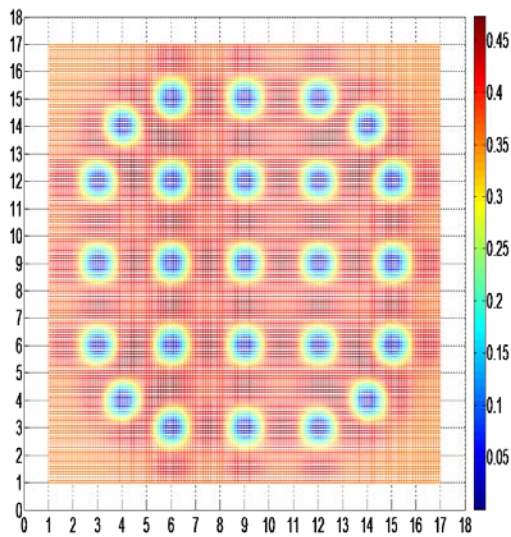


Figure 5 Evolution of max relative discrepancy of axial power

Table 6 K_{inf} of fuel assembly case

Without OTF	OTF
1.407486	1.396452

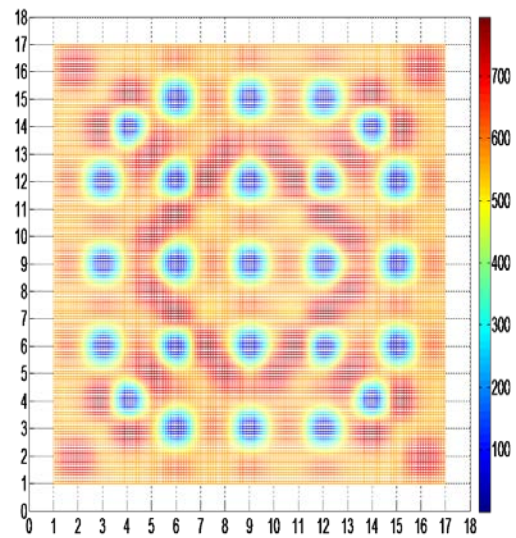
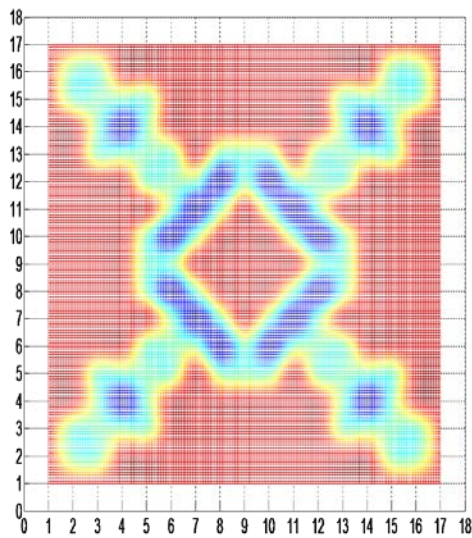
From Table 6, it can be found that K_{inf} of “Without OTF” is larger than OTF, as the negative temperature coefficient of fuel is considered with OTF. From Figure 5, it can be found that coupling with OTF converges faster than without OTF. The distributions of power and fuel temperature are shown in Figure 6, and the distributions of coolant density and temperature are shown in Figure 7. Furthermore, power distribution without coupling is shown in Figure 8. It can be found that the N-TH coupling taking into account has slight difference with that without OTF. Power Peak Factors (PPF) of three cases are also compared, as listed in Table 7. It can be found that PPF with N-TH coupling is smaller, which is closer to the real conditions. Therefore, the margin of safety can be reduced, so as to increase the benefit of power plants.



Relative power distribution with coupling

Fuel temperature/K

Figure 6 Distributions of power and fuel temperature



Coolant density/ (Kg/m³)

Coolant temperature/K

Figure 7 Distributions of coolant density and temperature

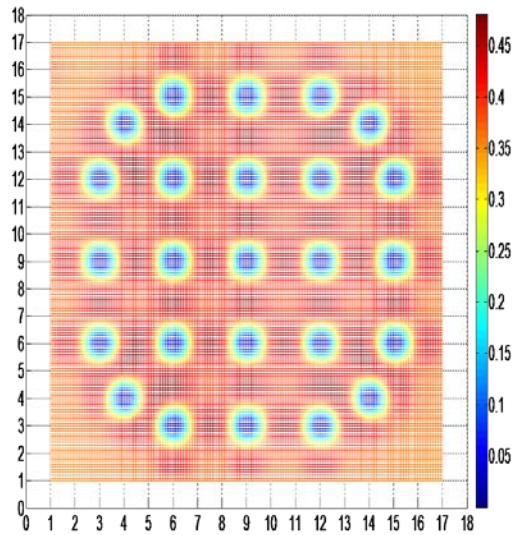


Figure 8 Relative power distribution without coupling

Table 7 PPF & AO of fuel pin case

Case	PPF
Coupling without OTF	1.08123
Coupling with OTF	1.08165
Without coupling	1.094077

6. Conclusion

A computational tool has been developed for the neutronics and thermal-hydraulics coupling between RMC and COBRA-EN. A special effort has been made to deal with the temperature dependence of cross section. The in-line Doppler Broadening was developed in RMC to generate point-wise cross section at different material temperature.

With the analysis of the PWR fuel pin and assembly cases, the feasibility of the coupling system has been demonstrated. Results show that the coupling system with Doppler broadening is effective for the thermal-hydraulics feedback. OTF has noticeable influences on the effective multiplication factor, while with slight influences on the converged power and temperature distribution. Moreover, coupling with OTF converges faster than without OTF.

The advantages of N-TH coupling have also been discussed. For the axial power distribution of fuel pin, PPF with N-TH coupling is larger, which is more realistic and conservative as it is closer to the safety margin. For the radial power distribution of fuel assembly, PPF with N-TH coupling is smaller, which is closer to the real conditions, taking into account the heat exchange. Therefore, the margin of safety can be reduced, so as to increase the benefit of power plants.

The coupling system introduced in this paper is the first step toward more comprehensive tool capable to perform full core coupling calculation and transient calculations.

7. References

- [1] M. Vazquez, H. Tsige-Tamirat, L. Ammirabile, et al. “Coupled neutronics thermal-hydraulics analysis using Monte Carlo and sub-channel codes”. Nuclear Engineering and Design, 2012, 250: pp. 403-411.
- [2] A. Nuttin, N. Capellan, S. David, et al. “Facing Challenges for Monte Carlo Analysis of Full PWR Cores: Towards Optimal Detail Level for Coupled Neutronics and Proper Diffusion Data for Nodal Kinetics”, SNA+ MC 2013-Joint International Conference on Supercomputing in Nuclear Applications+ Monte Carlo, Paris, France, 2014, October 27-31.
- [3] J. E. Hoogenboom, A. Ivanov, V. Sanchez, et al. “A flexible coupling scheme for Monte Carlo and thermal-hydraulics codes”, International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering, Rio de Janeiro, RJ, Brazil, 2011, May 8-12.
- [4] K. Wang, et al. “RMC – A Monte Carlo code for reactor core analysis”. Ann. Nucl. Energy, 2014, <http://dx.doi.org/10.1016/j.anucene.2014.08.048>
- [5] “COBRA-EN: Code System for Thermal-Hydraulic Transient Analysis of Light Water Reactor Fuel Assemblies and Cores”, PSR-507, 2001.
- [6] J.K. Yu, et al. “The Development and Validation of Nuclear Cross Section Processing Code for Reactor-RXSP”. Nuclear Power Engineering, 2013, Vol.s1,pp 10-13. (In Chinese)
- [7] J.K. Yu, J.G. Liang, K. Wang. “Development of In-Line Temperature Dependent Cross Sections Processing Capability in RMC Code”. 2015 ANS Annual Meeting, San Antonio, TX, 2015, June 7-11.