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Internal Coupling Scheme in RMC with Thermal-hydraulics Feedback and On-the-fly Doppler-Broadening Method

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Abstract *RMC(Reactor Monte Carlo)[1] is a self-developed Monte Carlo code for nuclear reactor analysis by Reactor Engineering Analysis Lab (REAL), Tsinghua University. On the basis of the self-developed subchannel module (RMC-TH) and Monte Carlo Cell Tally, the internal coupling interface is developed, which combines both input files to one and realizes the fast mesh correspondence process using the cell expansion technology for repeated structure with thermal-hydraulics feedback. It breaks through the bottleneck of geometrical extensibility for coupled code. On-the-fly Doppler broadening method is adopted as the way to consider the temperature effect on microscopic cross section, which only needs the 0 K cross section library so that the memory cost can be apparently reduced. Steady state simulation analysis are performed on PWR fuel pin and 17x17 assembly model, and the results show the feasibility, accuracy and efficiency of the coupling methodology. Therefore, a promising technology roadmap for the large-scale and geometrically universal nuclear reactor in both steady-state and transient conditions with thermal-hydraulic feedback are established. The roadmap can be further applied to neutronics-thermal-hydraulics-depletion coupling in multi-physics simulation process.*

I. INTRODUCTION

The Monte Carlo method is often taken as a benchmark method to validate deterministic methods. Rising attention has been given to it because of its irreplaceable advantages, such as flexibility in geometry treatment, the ability to use continuous-energy point-wise cross-sections, the easiness to parallelize and high-fidelity of simulations.

Nuclear reactors are complex systems with multi-physics interacting and coupling, and the high fidelity simulation of the nuclear reactor behavior should consider three close-interacting processes including neutronics, thermal-hydraulics and depletion. The neutronics calculation gives the neutron flux distributions inside the reactor, which provides the power distribution shape for depletion and thermal-hydraulics calculations. The thermal-hydraulics feedback involves the feedback of void fraction, density distributions of the moderator, and the Doppler effect of heavy nucleus, which leads to the changing of macroscopic cross section, and ultimately effects the power distribution. With the accurate neutron flux distribution, burnup calculation could give the fission and decay products during the life of the reactor, so the total power and material evolution could also be obtained.

RMC already has the embedded burnup modular named DEPTH[5], and one of the on-the-fly Doppler broadening method called TMS based on ray tracking are also implemented in RMC[6]. This method only needs 0K cross section library so that memory requirement in multi-physics simulation can be reduced. In this paper, a subchannel module called RMC-TH has been developed inside RMC which can calculate the thermal-hydraulics behavior. The fast corresponding technology between neutronics and thermal-hydraulics mesh based on cell tally is developed to satisfy the need of fast internal coupling and geometry universality in diverse and large-scale multi-physics simulations.

II. COMPUTATIONAL METHOD

1. Subchannel module RMC-TH

In RMC-TH, a three-equation model for two-phase flow which includes the mixture equations for mass, momentum, and energy balance is implemented, and the pin-level LWR subchannel simulation is supported. The RMC-TH could either be compiled in standalone mode or coupled mode, which means the RMC-TH can run as either a subchannel code independently or a thermal hydraulics module in RMC. SI system of units is used for all of the parameters, and an open source water steam property package named FREESTEAM[4] based on international-standard IAPWS-IF97 is implemented to supply the water property data. The module is coded by C++ with Objective Oriented Programming (OOP) style in order to enhance the maintainability and extensibility.

In traditional subchannel code, take COBRA for example, parameters for every rod and channel and the geometry relationship between rods and channels should be written manually in input file, which becomes a laborious and also an error-prone work, especially for full core problems. In order to overcome the weakness, the freestyle input format and repeated geometry structure just like geometry in Monte Carlo code is adopted in RMC-TH, which greatly simplifies the input content while saving the memory storages. And the index relationship builder will automatically judge the location of rods and channels to guarantee them in the right place. Besides, various kinds of empirical models and correlations including void fraction, subcooling, pressure drop, heat transfer can be chosen, and

the modular style for program design also make the extension of new models fast and convenient.

2. NT-TH Coupling methodology

The main coupled ways could be generally categorized into three types as listed in Fig. 1. The first one named external coupling is the most intuitive way to realize the coupled simulation, which means the information exchange between both modules relies on the external files. Many previous coupling works are based on this method [5, 6]. External coupling has the advantage of little modification and fully using of the existing qualified code, but faces the drawback of poor consistence and universality as well as low data transfer efficient and tail truncation problems. In order to overcome these weaknesses, the data could be transferred through memories rather than files. More importantly, without file writing process there is no need to reconstruct the data structure so that it could be more efficient to realize the universality of the coupled code. In another word, the mesh correspondence method might be automatically realized for various kinds of geometries without any modification to the interface code. However, the coding of internal coupled interface requires the understanding and modification of both source codes, therefore the internal coupling is not available for the "black box" code. The third coupling way called platform coupling is a combination of the previous two. The feature of this kind of coupling is building a uniform I/O platform, inside which the data can be exchanged from either files or memories, and the ideal structure of the platform is to make each module as a "plug and play" device. Multi-physics environments such as MOOSE, ANSYS and COMSOL generally can be classified as platform coupling.

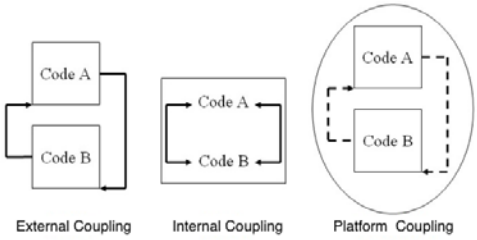


Fig. 1. Coupling methodology

Since RMC-TH is in-house developed, the internal coupling is used as the technology roadmap to couple the NT and TH modules. Cell tally is used to give the neutron flux and the relative power distribution. As shown in Fig. 2, users only need to define the cell which thermal hydraulic feedback effect is applied to, following usual repeat geometry input rules, and then the code will automatically search every bottom cell and find the right temperature and density according to the cell vector index during the particle transport process. The value "1" of option "matfb" in Cell card means only temperature feedback effect is considered, while "2" means both temperature and density feedback effect are considered. This input approach greatly reduces the laborious work of defining different bottom cells which have the same geometric structure but different thermal hydraulic parameters.

```
UNIVERSE 1 lat=1  pitch = 1 1 14.64
    scope = 1  1  25 fill = 2*25

UNIVERSE 2 move = 0.63 0.63 0          // Fuel rod
cell  3   -1      mat = 1  matfb = 1   // Pellet
cell  4   1 & -2  mat = 3              // Air
cell  5   2 & -3  mat = 4              // Cladding
cell  6   3       mat = 5  matfb = 2   // water
```

Fig. 2 Illustration of setting cell with TH feedback

The ideal way of mesh corresponding is to have a bijective mapping between the axial and radial nodalizations of the two parts, so the cell averaged value for fuel temperature (equation 1) was computed using the values T_k in radial positions with local diameter value d_k (d_u denotes the diameter of outer fuel pellet). Then it was correspondingly saved and used during the transport process.

$$T_{ave} = \frac{\sum_k T_k \left(d_k^2 - d_{k-1}^2 \right)}{d_u^2} \tag{1}$$

Generally speaking, mesh tally is more efficient than cell tally because of fast location of particles attributed to regular geometry. However, special technologies including Cell-Mapping method, hash searching and cell level labeling[2] are used in RMC which make the cell tally not less efficient than mesh tally. So cell tallies are adopted in the coupled code considering their benefit on accuracy and flexibility.

Each coupled cycle starts with a subchannel calculation run, assuming a cosine axial power profile and a uniform radial pin power distribution. The relative variation of the volume averaged fuel temperature is used for checking whether the results converge or not. Because the flux calculated by Monte Carlo method will introduce a statistical noise which should also be taken into account, the coupled convergence criterion is improved as (equation 2). The subscript i and j in equation 2 show the sequence of fuel rod mesh in transection and axial direction respectively.

$$\max_{ij} \left| \frac{T_{ij}^{cur} - T_{ij}^{pre} + \xi_{ij}^{cur} - \xi_{ij}^{pre}}{T_{ij}^{pre} + \xi_{ij}^{pre}} \right| \le \varepsilon \tag{2}$$

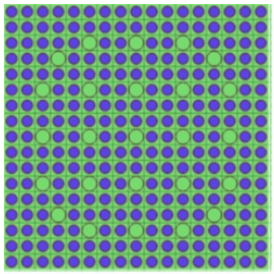
3. On-the-fly cross section update

Due to thermal motion of target nucleus which is known as Doppler effects, special treatments have to be used for cross sections in different temperatures. The traditional approach of pre-generated cross sections has difficulty of memory footprint when the number of temperatures is large. Trumbull[7] studied this issue and suggested that datasets at every 5-10 K would provide the

level of accuracy needed for simple interpolation between temperature points. Considering the range of interest in an operating reactor is between 300K and 3000K, an enormous amount (200-300 GB) of data would be needed.
In order to reduce the memory usage, recently, on-the-fly (OTF) technique has been proposed for detailed temperature modelling in multi-physics calculations. Temperature fitted method was developed in MCNP6 based on series expansions[8]. Becker et al.[9] have used stochastic algorithm for calculating effective Doppler broadening cross sections. The similar method was also developed in RMC by Yang et al.[10]. Another approach named Multipole Representation was used in OpenMC [11]. Viitanen and LEPPÄNEN [12] has also proposed and developed the on-the-fly temperature treatment in Serpent code, known as Target Motion Sampling (TMS) method, which seems elegant and promising. TMS method based on ray tracking has been developed in RMC[3], which has been proved to have high efficiency and accuracy in the cases of PWR and HTGR, no matter the number of nuclides is small or large. In this paper TMS method is adopted as a convenient and efficient way to update the cross section data.

III. NUMERICAL VALIDATION

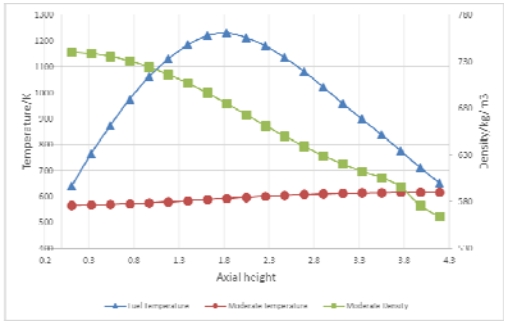
Two cases of PWR single fuel rod and assembly model were used to test the internal coupling method. The geometry parameters and thermal hydraulic boundary conditions are shown in Fig. 3. For the single fuel rod model, the outer boundary is square geometry. There are four materials including fuel (^{235}U, ^{238}U, O), fuel cladding(natural Zirconium), Gas Gap (O) and boracic light water (^{10}B,^{11}B, H,O) used in the models. Inside the fuel rod 9 radial nodes were set up in TH mesh, with 3 radial nodes on outer fuel pin, inner fuel pin and outer pellet respectively. Radially reflective boundary conditions with axially vacuum conditions are implemented in the NT model. The number of histories per cycle was set to 10^5 with 100 inactive and 500 active cycles. Parallel processors were used to significantly reduce the computational time. Every coupled step costs about 7 min with 12 processors for the pin model while 23 min with 24 processors for the FA. Finally the coupled runs stopped until the relative error was less than 0.001.



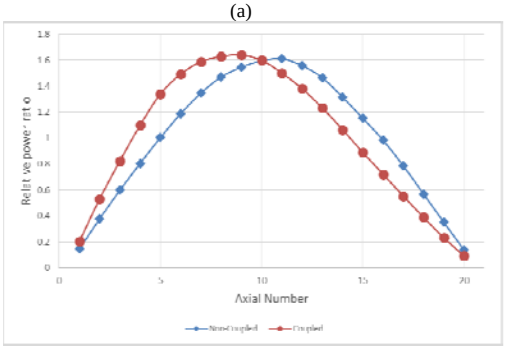
Total length	4.3m
Axial nodes number	20
Radial nodes number	9
Inlet coolant temperature	566.05K
Coolant mass flux	3463.8kg/m2s
Exit pressure	14.91MPa
Pin total power	100kW
FA total power	22.4MW
Pin diameter	9.5mm
Pellet diameter	8.192mm
Gap width	0.082mm
Guide tube diameters	12.294mm

Fig. 3 PWR Pin&FA parameters and TH boundary conditions

Fig. 4 shows the coupled results of the fuel pin model with diluted boron (DB) concentration of 1000 ppm, and the non-coupled results of relative power distribution with a fixed temperature of 293K was also given for comparisons. The results denote that the peak power factor (PPF) increases as the location of the power peak shifts to the bottom, which screwed the cosine-like power distribution of non-coupled profile. The moderator becomes saturated near the top of the channel accompanying by the sharp decrease of the density. The computed outlet void fraction is 0.083, which falls in the reasonable range of PWR.



(a)



(b)

Fig. 4. The results of fuel pin model (DB=1000ppm)

Four cases with different boron concentrations are also studied to further present the effect of thermal hydraulics feedback on axial power distribution, and the results are shown in Table I. The Axial Power Offset (APO) means the ratio of power in lower half to upper half. If the value of APO is more than 1 it denotes the power profile has a bottom prone excursion. From the table we can see that the power profile will distort to the bottom when the boron concentration is relatively low. As the boron concentration increases, the bottom prone distortion will decrease and finally reverse to top prone distortion. This phenomenon can be explained by the two opposite effects of decreasing the moderate density: less moderating capability and less harmful absorption. The TH feedback will cause the power bottom prone distortion when the former one dominates and vice versa. Besides, the effect on the PPF seems to depend on particular conditions. The TH feedback seems beneficial to PPF decreasing only if the distortion is not so big, which

is just the condition of case 3 (DB=1600 ppm). However, it will even increase the PPF if the distortion is serious.

Table I. The effect on axial power distribution with different Boron concentration

	Axial PPF		APO	
DB/ppm	Non-coupled	Coupled	Non-coupled	Coupled
600	1.637	1.757	0.895	2.048
1000	1.611	1.639	1.015	1.527
1600	1.610	1.599	0.826	0.857
2000	1.619	1.631	1.011	0.675

Fig. 5 shows the power distribution result of FA with thermal hydraulics feedback. Considering the density and temperature variation along the axial as well as the radial directions, the PPF decreases to 1.0716 from 1.0866, which further confirms the capability of power flattening effect by coupled calculation.

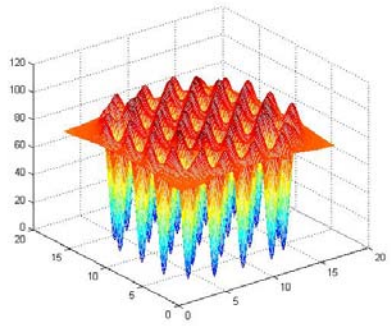


Fig. 5. The power distribution of FA with TH feedback

IV. CONCLUSIONS

The paper describes the subchannel module RMC-TH developed for NT-TH coupled simulation, and proves the fidelity of the internal coupled Monte Carlo/thermal-hydraulics calculating capability for RMC. Uniform I/O file layout is designed, and the cell expansion technology for repeated structure combined with internal fast mesh correspondence method base on cell vector are developed to break the bottleneck of the universality for coupled code and making the input writing procedure more convenient. On-the-fly Doppler broadening method is adopted to consider the temperature feedback for the microscopic cross section, which only needs 0K cross section library so that the memory cost in NT-TH coupled simulation is greatly reduced. The numerical validation are performed with PWR fuel pin and 17x17 assembly models in steady state condition. The results show the effect of diluted Boron concentration on the power distribution and the capability of power flattening with the thermal hydraulics feedback, which confirms the feasibility, accuracy and efficiency of the coupling methodology. A promising roadmap for further Monte Carlo based transient coupling and NT-TH-depletion multi-physics simulation are also established.

REFERENCES

1. K. WANG, Z. LI, D. SHE, J. G. LIANG, Q. XU, Y. QIU, J. YU, J. SUN, X. FAN, AND G. YU, “RMC – A Monte Carlo code for reactor core analysis,” Annals of Nuclear Energy, vol. 82, pp. 121-129 (2014).
2. D. SHE, Y. LIU, K. WANG, G. YU, B. FORGET, P. K. ROMANO, AND K. SMITH, “Development of burnup methods and capabilities in Monte Carlo code RMC,” Annals of Nuclear Energy, vol. 51, pp. 289-294 (2013).
3. S. LIU, Y. YUAN, J. YU, AND K. WANG, “Development of on-the-fly temperature-dependent cross-sections treatment in RMC code,” Annals of Nuclear Energy, vol. 94, pp. 144-149 (2016).
4. OHN PYE. "Freesteam 2.0", URL: http://freesteam.sourceforge.net.
5. [F. P. ESPEL, M. N. AVRAMOVA, K. N. IVANOV, AND S. MISU, “New developments of the MCNP/CTF/NEM/NJOY code system – Monte Carlo based coupled code for high accuracy modeling,” Annals of Nuclear Energy, vol. 51, pp. 18-26 (2013)
6. M. VAZQUEZ, H. TSIGE-TAMIRAT, L. AMMIRABILE, AND F. MARTIN-FUERTES, “Coupled neutronics thermal-hydraulics analysis using Monte Carlo and sub-channel codes,” Nuclear Engineering and Design, vol. 250, pp 403-411 (2012).
7. T. H. TRUMBULL, “Treatment of nuclear data for transport problems containing detailed temperature distributions,” Nuclear technology, vol. 156, pp. 75-86 (2006).
8. G. YESILYURT, W. R. MARTIN, AND F. B. BROWN, “On-the-fly Doppler broadening for Monte Carlo codes,” Nuclear Science and Engineering, vol. 171, pp. 239-257 (2012).
9. B. BECKER, R. DAGAN, C. BROEDERS, AND G. LOHNERT, "An alternative stochastic doppler broadening algorithm." Proc. M&C 2009, Saratoga Springs, New York, May 3-7, 2009, American Nuclear Society (2009).
10. F. YANG, J. LIANG, G. YU, AND K. WANG, "Research on on-the-fly doppler broadening based on the stochastic algorithm." Proc. 2015 ANS Annual Meeting, San Antonio, TX, June 7-11, 2015, American Nuclear Society (2015).
11. B. FORGET, S. XU, AND K. SMITH, “Direct Doppler broadening in Monte Carlo simulations using the multipole representation,” Annals of Nuclear Energy, vol. 64, pp. 78-85 (2014).
12. T. VIITANEN, AND J. LEPPÄNEN, “Explicit treatment of thermal motion in continuous-energy

Monte Carlo tracking routines," Nuclear Science and Engineering, vol. 171, no. 2, pp. 165-173 (2012).