Application of MCS/CTF/FRAPCON Multi-physics Coupling Code System in BEAVRS Cycle 1 Depletion Simulation

Jiankai Yu, Hyunsuk Lee, Alexey Cherezov, Hanjoo Kim, Peng Zhang, Deokjung Lee* Department of Nuclear Engineering, Ulsan National Institute of Science and Technology, 50 UNIST-gil, Ulsan, 44919, Republic of Korea *Corresponding author: deokjung@unist.ac.kr

1. Introduction

UNIST developed Monte Carlo code – MCS [1] has been fully coupled with sub-channel thermal/hydraulic code – CTF [2], together with fuel performance prediction code – FRAPCON [3] recently to implement the neutronic, thermal-hydraulic, and fuel performance simulation capability during Monte Carlo neutron transport based depletion analysis. Therefore, MCS can be used as not only reference tools for deterministic codes, but also the whole core pin-by-pin multi-physics analysis tool for the large scale commercial PWRs with high fidelity [4-6].

2. Methodologies

2.1 MCS/CTF/FRAPCON Multi-Physics Coupling

The sub-channel T/H simulation code – CTF, and steady-state fuel performance prediction code – FRAPCON have been fully coupled within MCS source code by the coupling interface, which was written in FORTRAN 2003 language. The diagram of MCS/CTF/FRAPCON coupling scheme can be explained in the following. Thus, CTF and FRAPCON can be easily used as the coupled solver in MCS/CTF/FRAPCON code system.

As shown in Fig. 1, neutron flux and pin-wise power distribution can be tallied in each cycle of MCS neutron transport solver, and then transferred into CTF solver. Thus, CTF will be executed to solve the coolant temperature and coolant density, which will be exchanged back into MCS to update the nuclides number density and target temperature in coolant materials. Meanwhile, the coolant temperature and coolant pressure distribution will be transferred into FRAPCON solver, which can be used as boundary condition for solving heat conduction equation in fuel pellet and cladding and the gap between fuel pellet and cladding. Again, the FRAPCON will feed back fuel temperature distribution into MCS after FRAPCON running. The fuel temperature distribution will be used to update the nuclide target temperature to consider the Doppler broadening effect in fuel materials. Finally, when the update of fuel temperature, coolant temperature and coolant density are ready, the next Monte Carlo neutron transport cycle can be simulated.



Fig. 1. Diagram of MCS/CTF/FARPCON

The data exchange among MCS, CTF, and FRAPCON will be repeated until the power distributions are globally converged.

2.2 New Features

There are some new features can be obtained by this coupling code system. Compared with internal MCS/TH1D coupled code, the cross flow effects among neighbouring sub-channels can be considered accurately in MCS/CTF code. Furthermore, the burnup dependent fuel thermal conductivity and the thermal conductance of gap between fuel pellet and cladding cannot be simulated until the development of MCS/FRAPCON code. However, the cross flow cannot be taken into account in MCS/FRAPCON. Thanks to the fully coupled MCS/CTF/FRAPCON, all those features will be available. By the way, the latest version of steam-table (IAPES-IF97) are used in it.

3. Benchmark Description

3.1 Benchmark description

The BEAVRS benchmark (Benchmark for Evaluation and Validation of Reactor Simulations) presents a typical 4-loop Westinghouse PWR with as much detailed operation information as possible, which has been released by CPRG group at MIT in 2015 [7]. The current release is version 2.0.1, which provides the core loadings and detector signals from the realistic nuclear power plant for the first two cycles of operation [6]. Fig. 1 illustrates the top view and left view of these quarter core modeling layouts. For more details (fabricated fuel assembly loadings, burnable absorber pin layouts, operational histories and control rod positions, and boron concentration), please refer to the manual of this benchmark. The detailed power history of BEAVRS cycle 1 model is shown in Fig. 3. Table I lists the T/H boundary condition of fuel performance feedback through the whole depletion simulation.



Fig. 2. Top view and front view of BEAVRS full core layout.



Fig. 3. Power history of BEAVRS cycle 1

Table I: T/H Boundary Condition

Power (%)	100.00
Outlet Pressure (MPa)	15.513
Inlet mass flow rate (kg/s)	17083.33
Inlet Temperature (°C)	292.70
Gap conductance (W/m-K)	10000.00

3.2 Computational Condition

Multi-cycle technique is used in MCS Monte Carlo neutron transport to ensure that the fissions source distribution reaches converged as quickly as possible. In this simulation, 20 inactive and 40 active multicycles are simulated, each multi-cycle having 300 single cycles, each single cycle including 10,000 histories. Therefore, 1.8 billion histories were used in this simulation, which was performed on a Linux cluster with 65 processes (Intel Xeon E5-2620 @ 3.00 GHz). Finally RMS (Root Mean Square) of pin-wise flux tallied from neutron transport is less than 2 % for the quarter core model. In FRAPCON solver, the criteria used to determine the convergence of gas release in pellet-cladding gap is 1 % in general. FRAPCON feedback are performed every 10 multi-cycle of Mont Carlo neutron transport, which can be guaranteed that the variance of tallied power density for the quarter core between two successive T/H conductions is globally converged.

Besides, the same model has been simulated by different coupling schemes, including MCS/TH1D, MCS/CTF, MCS/FRAPCON, MCS/CTF/FRAPCON as the reference.

4. Results and Discussions

The results of BEAVRS Cycle 1 depletion with fuel performance feedbacks has been collected and analysed in this section. First of all, the computation time spent in different coupling schemes has been compared as shown in Table II.

Coupled Solvers	Time / Days	Time Ratio
MCS/TH1D	6.5	1.00
MCS/CTF	10.0	1.54
MCS/FRAPCON	10.8	1.66
MCS/CTF/FRAPCON	19.3	2.96

Table II. Computation time comparison

It can be seen that MCS/TH1D cost the least simulation time, which costs 6.5 days in the cluster with 65 processors. However, MCS/CTF consumes 10.0 days, about 54 % improvement compared to MCS/TH1D. Since CTF solves the quarter core conservation equation globally, and considers cross flow effects. On other hand, MCS/FRAPCON spends more time than MCS/CTF, which is caused by the incomplete restarting capability in FRAPCON. Therefore, FRAPCON has to restart from zero burnup step at each burnup step fuel performance prediction. However, the improvement of this restarting capability in FRAPCON code is undergoing in our group. Obviously, MCS/CTF/FRAPCON costs the most simulation time, since it need cover all time used in both FRAPCON and CTF solves at each cycle with T/H feedback in all burnup steps.

4.1 CBC Results

The critical boron concentration (CBC) of BEAVRS quarter core model changes with the increase the burnup in this depletion simulation. Meanwhile, the results from MCS code without any fuel performance feedback (actually only TH1D feedback) are also presented as the reference.



Fig. 4. CBC letdown with EFPD.

As shown in Fig. 4, the CBC letdown swings with the increase of the EFPD (Effective Full Power Days), which is the unit of this fuel cycle. It can be seen that the result from MCS/CTF/FRAPCON coupling lies between the Table 24 and Table 25 except at the very beginning of cycle (within 20 EFPD), which agree with them very well. However, the results of MCS code without any T/H coupling are underestimated among the whole fuel cycle 1. Note that Table 24 lists boron letdown data, and Table 25 provides core operating data as a function of exposure, which can be referred in BEAVRS user manual [7].

4.2 Comparison with Measured Data

Additionally, the axially integrated assembly-wise power distribution results are calculated based on the real power level, control rod positions, inlet coolant temperature are listed in Fig. 5. , which can be compared with the measured data at different burnup step of BEAVRS Cycle 1. All these information including power level, control rod positions, and inlet coolant temperature can be referred in BEAVRS user manual. This section just shows the results at the end of cycle 1 (EOC), where measurement condition shown in Table III is used in MCS simulation.

Table III.	Measurement	condition
------------	-------------	-----------

Power (%)	69.86
Calendar days (Day)	573
Burnup (MWD/tHM)	13603.4
Inlet mass flow rate (kg/s)	17083.33
Inlet Temperature (°C)	291.75
ROD A (step)	228
ROD B (step)	228
ROD C (step)	228
ROD D (step)	208

N/A	N/A	1.17	1.05	1.2	1.06	1.2	0.68
1.12	0.99	1.17	1.01	1.22	1.06	1.25	0.69
1.20	1.01	1.22	1.05	1.24	1.08	1.22	0.68
1.10	0.97	1.14	0.99	1.20	1.08	1.22	0.70
1.13	1.05	1.19	1.07	1.22	1.08	1.21	0.70
N/A	1.18	1.03	1.17	1.07	N/A	0.93	0.7
0.98	1.16	1.01	1.19	1.05	1.25	0.92	0.71
1.00	1.21	1.04	1.21	1.07	1.24	0.90	0.71
0.98	1.14	1.00	1.17	1.04	1.22	0.92	0.71
1.04	1.19	1.05	1.20	1.07	1.24	0.93	0.70
1.17	1.03	1.2	1.06	1.23	1.08	1.16	0.66
1.16	1.01	1.15	1.03	1.22	1.07	1.19	0.66
1.21	1.05	1.21	1.06	1.24	1.06	1.19	0.65
1.15	0.99	1.16	1.02	1.23	1.07	1.20	0.67
1.21	1.04	1.19	1.06	1.22	1.07	1.15	0.65
1.05	1.17	1.06	1.24	N/A	1.25	N/A	0.55
1.03	1.18	1.04	1.20	1.05	1.25	0.87	0.53
1.04	1.23	1.06	1.24	1.07	1.24	0.85	0.53
1.00	1.18	1.03	1.22	1.07	1.24	0.88	0.54
1.04	1.20	1.06	1.21	1.07	1.21	0.85	0.51
1.2	1.07	1.23	N/A	1.13	1.11	0.76	
1.21	1.04	1.22	1.07	1.10	1.06	0.75	
1.21	1.07	1.25	1.08	1.14	1.07	0.74	
1.20	1.05	1.22	1.06	1.10	1.07	0.77	
1.22	1.06	1.21	1.07	1.08	1.03	0.73	
1.06	N/A	1.08	1.25	1.11	0.82	0.57	
1.06	1.25	1.06	1.24	1.08	0.80	0.56	
1.06	1.25	1.05	1.24	1.06	0.78	0.55	
1.06	1.25	1.07	1.25	1.09	0.81	0.56	
1.06	1.23	1.06	1.21	1.04	0.77	0.54	
1.26	0.93	1.16	N/A	0.76	0.57		
1.23	0.92	1.17	0.88	0.75	0.55		
1.19	0.89	1.17	0.84	0.74	0.56		
1.20	0.92	1.20	0.88	0.77	0.57		
1.19	0.92	1.15	0.84	0.73	0.53		
0.68	0.7	0.66	0.55			Measured	
0.70	0.71	0.65	0.52			MCS/TH1D	
0.67	0.69	0.65	0.52			MCS/CTF	
0.72	0.72	0.68	0.55			MCS/FRAF	PCON
0.67	0.69	0.64	0.52			MCS/CTF/	FRAPCON

Fig. 5. Axially integrated detector signal at the EOC

The comparison of axially integrated detector signal between calculated results and measured data has been performed in Fig. 5. The overall relative errors with different coupled solvers to measured data are listed in Table IV, including maximum (MAX), minimum (MIN) and the root mean square (RMS).

Table IV. Relative error with different coupled solvers

Coupled Solvers	MAX	MIN	RMS
	[%]	[%]	[%]
MCS/TH1D	3.85	-5.78	2.12
MCS/CTF	4.98	-5.89	2.70
MCS/FRAPCON	5.22	-6.18	2.45
MCS/CTF/FRAPCON	3.62	-7.53	2.86

Table IV shows the RMS of relative errors of simulated results to measured data with different coupling scheme. The similar RMS can be obtained by MCS/TH1D, MCS/CTF, MCS/FRAPCON, and the fully coupled MCS/CTF/FRAPCON. The range of RMS shows very good performance of MCS based coupling code system in the whole BEAVRS cycle 1 depletion analysis.

4.3 Other Distributions

Furthermore, some important distribution can be obtained by the MCS/CTF/FRAPCON coupling code system, for instance, the hoop stress in Fig. 6, gap conductance in Fig. 7, ZrO2 thickness in Fig. 8, and et .cl.



Fig. 6. Hoop stress distribution at EOC



Fig. 7. Gap conductance distribution at EOC



Fig. 8. ZrO₂ thickness distribution at EOC

5. Conclusions

The BEAVRS Benchmark cycle 1 depletion with multi-physics coupling feedback has been performed by the fully coupled MCS/CTF/FRAPCON code system. Firstly, the CBC letdown with 100% power level was compared with the measured values shown in Table 24 and Table 25 of the manual, which shows a very good agreement between MCS results and measurement. Besides, the axially integrated power distribution at

EOC calculated from the real power level, control rod position, inlet coolant temperature was compared with measured data, which also shows the good accuracy of this coupling code system. Afterwards, the detailed distributions, such as the distributions for hoop stress, gap thickness, gap conductance and ZrO₂ thickness have been displayed in the paper. These unique quantities which can be only simulated by MCS/CTF/FRAPCON code system are illustrated to performance the multi-physics coupling capability of MCS code.

5. Acknowledgement

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT). (No.NRF-2017M2B2A9A02049916)

REFERENCES

[1] H. LEE, "Development Status of Monte Carlo Code at UNIST," KNS Spring Meeting, Jeju, Korea, May 12-13, (2016).

[2] R. SALKO, "CTF Theory Manual," Reactor Dynamics and Fuel Management Group, Pennsylvania State University, 2014.

[3] K.J. GEELHOOD, "FRAPCON-4.0: A computer code for the calculation of steady-state, thermal-mechanical behavior of oxide fuel rods for high burnup", Pacific Northwest National Laboratory, (2015)

[4] J. Yu, "Preliminary Validation of MCS Multi-Physics Coupling Capability with CTF", *Proceedings of the Reactor Physics Asia 2017* (*RPHA17*) Conference, Chengdu, China, August. 24-25, (2017).

[5] J. Yu, "Fuel Performance Coupling of FRAPCON within MCS", *Transactions of 2017 ANS Winter Meeting*, Washington, D.C., Oct. 29 - Nov. 2, (2017).

[6] H. LEE, "Preliminary Simulation Results of BEAVRS Three-dimensional Cycle 1 Wholecore Depletion by UNIST Monte Carlo Code MCS", *M&C* 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20, (2017)

[7] N. Horelik, "MIT benchmark for evaluation and validation of reactor simulations (BEAVRS), Version 2.0", MIT Computational Reactor Physics Group, MIT, (2016).