Development of BEPU Methodology using Multi-Physics Coupling Code based on RAST-K

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1. Introduction

The conventional approach to nuclear reactor core design and analysis has been a two-step process. A nodal diffusion code called RAST-K v2 [1] has been developed at UNIST CORE Lab to provide high accuracy and computational performance for PWR core analysis and design. This code has been validated with the functioning Korean PWRs without tuning any input and output parameters.

While reactor core analysis technology has been developed worldwide, each physics code is used independently with a one-way coupling algorithm to obtain conservative results. However, the demand for a high-fidelity solution without conservatism has increased due to strengthened safety-related regulations. Therefore, the development of a multi-scale multi-physics code system has emerged as an interest in nuclear research to obtain more accurate solutions by using the two-way coupling method.

Traditional approaches to safety analysis usually rely on a pessimistic hypothesis, which can lead to excessive conservatism. However, with the uncertainty quantification (UQ) and sensitivity analysis (SA) procedure, the best-estimate plus uncertainty (BEPU) approach can be an alternative to traditional conservative approaches in both nuclear industry and regulation.

This paper demonstrates the development of a BEPU methodology using a multi-physics coupling code based on RAST-K. This code system includes a subchannel thermal-hydraulic code and fuel performance code, allowing for the best-estimate solution to be achieved with its uncertainty from stochastic sampling method by perturbing input parameters and nuclear data.

2. Multi-Physics Coupling

In this section, the detail methodology employed in the multi-physics coupling scheme based on RAST-K is explained.

2.1 Coupled Codes

COBRA-TF (CTF) is a simulation code used to analyze thermal-hydraulics in LWR vessels. It can solve both subchannel and 3D Cartesian forms of 9 conservation equations using a two-fluid modeling approach with consideration for three separate independent flow fields. CTF allows multi-channel modeling with consideration of cross-flow and supports parallel calculations using assembly-wise domain decomposition technique. However, CTF uses a simplified heat structure model to calculate fuel temperature, and therefore, requires other physics codes such as fuel performance code for high fidelity core analysis.

FRAPCON and FRAPTRAN are computer codes designed to calculate steady-state and transient performance during long-term burnup and hypothetical reactor accidents for LWR fuel rods. FRAPCON calculates fuel rod performance based on fuel rod power history and coolant boundary conditions, whereas FRAPTRAN calculates fuel performance during transients based on various factors including heat conduction, heat transfer cladding to coolant, elastic-plastic fuel and cladding deformation, cladding oxidation, fission gas release, and fuel rod gas pressure.

FRAPI [2] has been developed to effectively couple external codes such as FRAPCON and FRAPTRAN. It includes features such as code initialization, advancing a time step, data exchanges, fuel rod data saving and loading on the computer memory or binary file, and writing a restart file for FRAPTRAN.

2.2 Coupling Parameters

Fig. 1 illustrates the data exchange process for a multi-physics coupling calculation for both steady and transient state simulations. The RAST-K is the main driver of the coupled code system and calculates the pin-wise power distribution based on given fuel and coolant conditions. The basic reactor core information, such as the geometry and fuel rod composition, is transferred from RAST-K to CTF and FRAPI.

CTF is initialized using the exact pin-wise power and moderator direct heating fraction as the source of heat flux for TH calculation. Since the cladding outer surface temperature is transferred from an external code, the heat structure calculation in CTF is skipped.

Similarly, FRAPI initializes FRAPCON and FRAPTRAN using the basic information of fuel rod. To consider fuel burnup and compositions along the sequential cycle depletion, FRAPI writes and reads the restart file of FRAPCON. The restart file generated from FRAPCON is then assigned to FRAPTRAN to consider the burnup-dependent behavior of fuel performance. The coolant heat convection calculation is skipped in both FRAPCON and FRAPTRAN, as the bulk coolant temperature and the coolant-to-cladding wall heat transfer coefficient are used as the boundary condition. The cladding outer surface temperature is

calculated from the boundary condition and transferred to CTF.

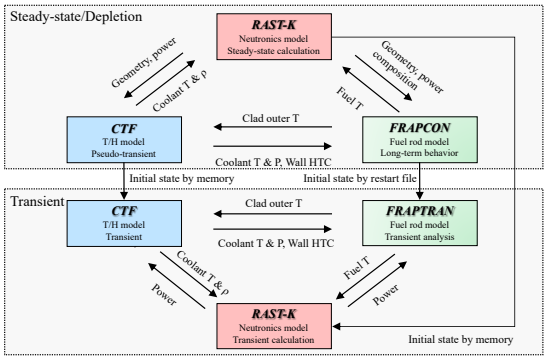

Fig. 1. Data exchange between the coupled codes.

2.3 Coupling Algorithm

RAST-K is the main code of coupling code system by utilizing the dynamic linked library (DLL) of CTF and the source of FRAPI for linking the FRAPCON and FRAPTRAN. The provided version of CTF coupling interface is modified to consider more variables to be exchanged and enable restart capability. FRAPI source code is directly used in RAST-K. Fig. 2 shows the flowchart of coupled code system.

CTF and FRAPCON are initialized during the initialization step of RAST-K. CTF initialization is divided into two steps. The RAST-K generates four basic input files to generate CTF input. The preprocessing module of CTF generates CTF inputs based on the MPI calculation option. Then, CTF is initialized by reading CTF inputs and communication of CTF is set independently with RAST-K. During initialization of FRAPCON, the pin specification is directly transferred through FRAPI. At the initialization step, the restart files of FRAPCON should be prepared and loaded for the restart calculation for cycle depletion.

In the outer iteration of RAST-K, the TH information is updated by calling CTF and FRAPCON. CTF runs iteratively with its own convergence criteria (e.g., mass and energy balance) with given information. After finishing CTF calculation, the pin-wise coolant information is saved in RAST-K. Different from CTF, FRAPCON considers fuel depletion. Therefore, the predictor-corrector step of RAST-K should match that of FRAPCON. After converging gap pressure in FRAPCON, the pin-wise fuel and cladding temperatures are saved. After converging the outer iteration, the calculation result of corresponding step is saved. In this step, the calculation result of CTF is written via intrinsic editing subroutine, and the restart file of the FRAPCON is generated.

For transient-state calculations, FRAPTRAN is added to the coupled algorithm. Due to inconsistency in methodologies used to simulate short and long-term fuel behavior, null transient cannot be achieved. At the initial condition calculation, FRAPTRAN calculation is performed based on the restart file generated from FRAPCON. The fuel temperature information from FRAPTRAN is used for the cross-section feedback. All simulation conditions in each code are stable after converging the initial state, so null transient can be achieved without perturbation. From the transient-state calculation, FRAPCON is deallocated, and only FRAPTRAN is used for fuel performance analysis.

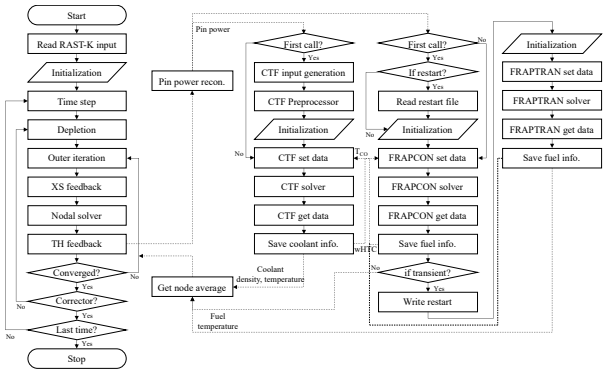

Fig. 2. Flowchart of coupled code system.

3. BEPU Methodology

In this section, the methodology and calculation result results of developed BEPU platform using the multi-physics code is demonstrated.

3.1 Uncertainty Quantification

In the field of nuclear reactor modeling and simulation, there have been several studies aimed at accounting for uncertainty in the input parameters of the models. To achieve this, two popular methods are deterministic and stochastic sampling. The latter involves random sampling of input parameters and statistical analysis of the resulting output responses. Standard statistical analysis is used on the repeated calculations of the output responses, with the assumption that the probability density function of the responses follows a normal distribution. The Shapiro-Wilk test is then used to test if the sample distribution is indeed normal. If the p-value is less than 5%, the null hypothesis is rejected, indicating that the sample distribution is not normal. If the normality assumption is accepted, the confidence bounds of uncertainties in the output responses can be computed.

In the nuclear field, it is common to use a 95th percentile with a confidence level of 95% to set the upper limit for probability. To calculate the uncertainty of output responses accurately with a limited number of code simulations, the appropriate number of simulations must be determined. The one-sided Wilks' non-parametric formula is used to predict how many samples are needed to establish a percentile of the output distribution with a desired confidence [3]. For instance, to establish the third-order one-sided 95th

percentile with a 95% confidence level, 124 samples should be executed.

To observe the uncertainties propagation from basic nuclear data, the stochastic sampling method is employed from the transport lattice calculation. The nuclear data uncertainty is propagated through the lattice calculation to the two-group nodal cross section used in RAST-K. In this research, covariance for scattering, fission, capture, fission spectrum, and number of neutrons per fission are considered by following the method invented by A. Yamamoto [4]. The 72-group covariance matrix for 144 nuclides is generated by using the NJOY-99 based on ENDF/B-VII.1 library.

The multi-physics code is used to simulate a high-fidelity model, so that the detailed technological and operation data are required as an input data. By considering the uncertainty from input data such as manufacturing, geometry, boundary conditions, and core conditions, the impact of input parameter uncertainty propagation on output response can be quantified. For example, the input parameters of CTF include boundary conditions such as inlet temperature and system pressure, geometry to model the subchannel and spacer grid, and factor to model physical phenomenon. The detail information for modeling the geometry and composition of fuel pellet is used in FRAPCON and FRAPTRAN. The uncertainty of each input parameter is referred from the previous works done by expert of each physics. The input parameter perturbation is performed on-the-fly during calculation based on Latin hypercube sampling method.

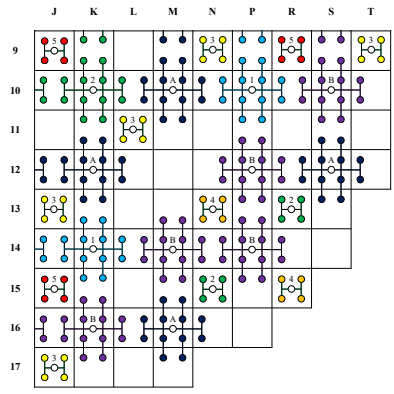

Fig. 3. Configuration of control rod assembly in APR1400.

3.2 Rod Ejection Accident

In this study, the multi-physics coupled code based on RAST-K was used to simulate a rod ejection accident (REA) in the third-cycle of an APR1400 reactor. The full core model of the reactor is used for the simulation, and the configuration of the control rod assembly is shown in Fig. 3. To ensure a significant power increase, the control rod worth was corrected to allow for a power increment even with the withdrawal of a single rod. During the simulation, one control element assembly (CEA) is withdrawn in the hot zero power (HZP) condition at the end of the cycle (EOC). A reactivity of 1.18 $ was injected, causing the power to rise to approximately 90%. The transient began with the full withdrawal of one R4 bank located at N-14 within 0.05 seconds. The time step size for the transient calculation was set to 0.01 seconds for 0 to 2 seconds, and it increased to 0.1 seconds for 2 to 4 seconds. The initial core power was 1E-5% and the inlet temperature was set to 295 C.

3.3 Reactor Safety Parameters

UQ is conducted for several key parameters, including core power, reactivity, peak fuel centerline temperature, fuel enthalpy, fuel enthalpy-rise, and minimum departure of nucleate boiling ratio (MDNBR). Fig. 4 presents the changes in core power and reactivity during the transient. It is observed that after the control rod is fully withdrawn, the core reactivity reaches its peak at approximately 0.15 seconds. The minimum and maximum core reactivities correspond to the minimum and maximum core power levels, which are 1.151$ and 1.248$, and 79.8% and 168.4%, respectively. The peak core power is 68.7% higher than the nominal case due to the additional reactivity insertion. Since the negative temperature effect on reactivity affects the peak time points of all samples differently, the peak time points are not directly used as safety parameters.

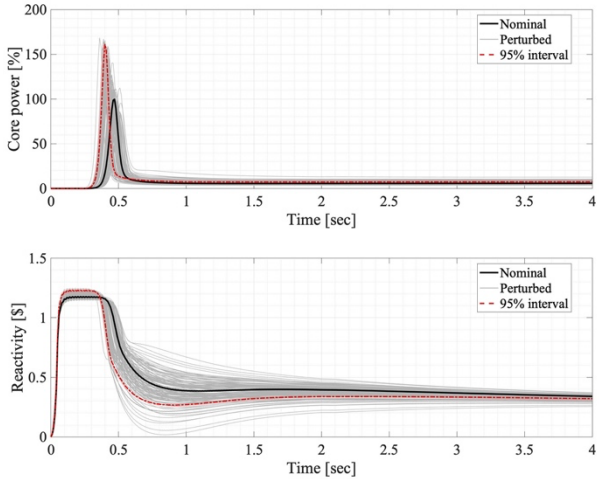

Fig. 4. Core power and reactivity change during transient.

The 95th percentile of the distribution is calculated among all perturbed cases to establish a tolerance limit with a 95% confidence level. In other words, there is a 95% confidence that the true peak value is below the 95th percentile interval, which is shown in the red line in Fig. 4. Although core power and reactivity are not directly used as safety parameters, their 95% tolerance limits are also quantified.

Table I presents the results of an uncertainty quantification analysis of safety parameters obtained

from a REA simulation. The mean values of peak core power, reactivity, and fuel centerline temperature are found to be larger than their nominal values. This may be due to the higher core power inducing a higher reactivity defect by temperature feedback. The sample mean of peak core power should be larger than the nominal value because the fuel enthalpy represents the integration of power over time. Thus, the sample mean is not biased from the nominal case. The predicted peak fuel centerline temperature obtained from the best-estimated calculation is 527.95 C. When using the best-estimated plus uncertainty approach, an additional 88.86 C of 95% confidence is obtained. This indicates that the current BEPU approach reduces the margin to the peak fuel temperature by 100.26 C when compared with the nominal value. Although the predicted minimum value of MDNBR among all simulations is smaller than the typical value of DNBR limit for PWR, which is 1.30, the 95% tolerance limit of MDNBR is 1.380. The predicted MDNBR decreases to 1.477 from the nominal value of best-estimate calculation. It is expected that this methodology can provide more margin to the conservative case.

Table I: Safety parameters with its uncertainties

Parameter	Nominal	Mean ± Rel. STD	95% Limit
Peak power (%)	99.73	117.69 ± 21.3%	161.03
Peak reactivity ($)	1.177	1.194 ± 1.9%	1.231
Peak fuel centerline temperature (C)	516.55	527.95 ± 8.4%	616.81
Peak fuel enthalpy (cal/g)	26.95	27.99 ± 6.1%	31.13
Peak fuel enthalpy-rise (cal/g)	9.58	10.65 ± 16.5%	14.16
MDNBR (-)	1.517	1.477 ± 7.3%	1.380

In addition to the uncertainty quantification results from the REA simulation, similar calculations are performed using RAST-K standalone and point kinetic equation (PKE) methods. Fig. 5 summarizes the best-estimate safety parameters and their 95% confidence tolerance limits from both methods. The peak fuel centerline temperature, fuel enthalpy, fuel enthalpy-rise, and MDNBR calculated using PKE were closer to the safety limit than those calculated using RAST-K MP. This indicates that the BEPU approach provides more safety margin than the conservative method, as demonstrated by the PKE results. While the 95% confidence tolerance limit of MDNBR from RAST-K MP is 1.380, the corresponding value from PKE is smaller than 1.0.

4. Conclusions

The coupling of RAST-K, CTF, FRAPCON, and FRAPTRAN is performed for multi-physics simulation of LWR fuel rod performance, including steady-state and transient responses. The details on the individual codes and the coupling algorithm, including data exchange and initialization steps are provided. In this study, uncertainty quantification is performed for a reactor core modeling and simulation of a rod ejection accident using stochastic sampling methods. The resulting output responses are analyzed using standard statistical analysis, and the confidence bounds of uncertainties of output responses are computed. The safety parameters of interest including core power, reactivity, peak fuel centerline temperature, fuel enthalpy, fuel enthalpy rise, and MDNBR are also quantified, and the 95% tolerance limits were established with 95% confidence. By comparing the best-estimated solution from MP code with conservative solution from PKE, the safety margin can be increased. Therefore, the BEPU approach should be required to get more safety margin, and it will probably allow higher operational flexibility of the reactor.

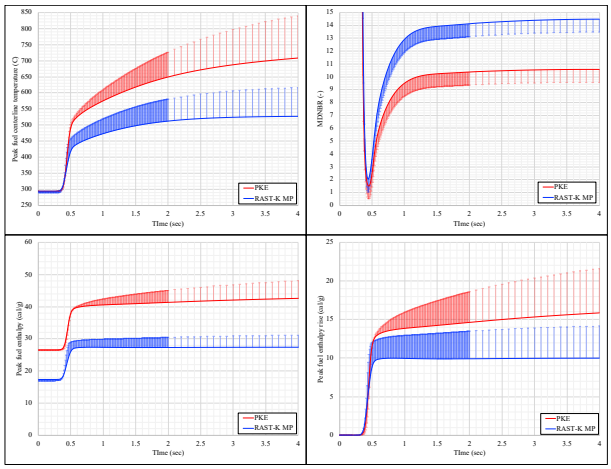

Fig. 5. Comparison of best-estimate and conservative solutions of safety parameters.

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REFERENCES

[1] J. Park, et al., “RAST-K v2-Three Dimensional Nodal Diffusion Code for Pressurized Water Reactor Core Analysis,” Energies, 13(23), 6324 (2020).
[2] A. Cherezov, J Park, H. Kim, D. Lee, Fuel rod analysis program interface for tightly coupled multi-physics system, In Proceeding of the ANS Winter Meeting, Nov.16-19, 2020, Chicago, IL.
[3] I. S. Hong, et al., Generic Application of Wilks’ Tolerance Limit Evaluation Approach to Nuclear Safety, Nuclear Energy Agency, 2013.
[4] A. Yamamoto, K. Kinoshita, T. Watanabe, T. Endo, “Uncertainty quantification of LWR core characteristics using random sampling method,” Nuclear Science and Engineering, 181, 160-174 (2015).