High-fidelity coupled neutron transport, thermal-hydraulic and fuel performance simulations using STREAM3D/CTF/FRAPCON

Wonkyeong Kim and Deokjung Lee*
[a]*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

This paper represents one of the recent efforts in the nuclear field to perform high-fidelity simulations of reactor core behavior, including the simulation of neutronics (NX), sub-channel thermal-hydraulics (T/H), and fuel performance (FP). The aim is to achieve precise and sophisticated analysis by using applicable state-of-the-art simulation tools in each physics area and building a coupled system to consider TH and FP feedbacks. STREAM3D [1] is capable of 3D neutron transport calculation. Meanwhile, Cobra-TF (CTF) [2] and FRAPCON [3] have been widely used for high-fidelity numerical simulation of TH and FP, respectively. The coupling of these tools requires a systematic coupling interface and a control driver to enable mutual feedback by physics behavior through data exchange and an established numerical scheme. The paper focuses on how to implement the coupling interface and scheme for the multi-physics reactor analysis system using STREAM3D/CTF/FRAPCON. The effects of feedback in the steady state are investigated, and primary design parameters for a typical pressurized water reactor, including critical boron concentration and pin power distribution, are estimated and compared with stand-alone STREAM3D results and measurements. The applicability to whole-core analysis is also represented.

2. Computational codes for coupled simulations

2.1. 3D neutron transport code STREAM3D

STREAM3D is a 3-dimensional (3D) pin-resolved neutron transport code that employs the Method of Characteristics (MOC) and Diamond/Differencing (DD) [1] scheme to solve the neutron flux distribution throughout the core. The 3D angular flux, scaler flux, and source are approximated with the 2D radial component and the axially linear component, which are then combined to reformulate 3D MOC equation. The solutions are obtained by iteratively sweeping in upward and downward directions to ensure neutron balance in every source region at convergence. The code utilizes a 72 energy group cross section library based on ENDF/B VII.1 data. STREAM3D offers several key capabilities besides solving the transport equation. These include conducting critical boron search and equilibrium boron search, isotopic depletion using the Chebyshev Rational Approximation Method (CRAM), the ability to read and write an isotopic restart file, and the capability to shuffle fuel between cycles and decay isotopes during overhaul. These functions are vital for conducting practical core analysis using STREAM3D.

2.2. Subchannel T/H code CTF

CTF is a sub-channel thermal-hydraulic (T/H) simulation code developed specifically for analysis of Light Water Reactors (LWRs). It provides a range of T/H models that are important for safety analysis such as flow regime-dependent two-phase wall heat transfer, interphase heat transfer and drag droplet breakup, and quench front tracking [2]. CTF uses a two-fluid three-field representation of the two-phase flow to model the liquid film, liquid droplets, and vapor while accounting for mass, axial and lateral momentum, and energy continuity [2]. This allows CTF to simulate cross flow through channels as well as axial flow within each channel [2]. CTF also includes internal models such as spacer grid models for flow mixing and pressure loss, and non-condensable gas mixture handling [2].

2.3. Fuel performance code FRAPCON

FRAPCON [3] is a fuel performance (FP) code that has been developed by Pacific Northwest National Labs, with FRAPCON-4.0 being the current version utilized by this work. The FRAPCON has been extensively validated over the years and is primarily used for analyzing a single fuel rod. The purpose of the code is to calculate the steady-state response of light-water reactor fuel rods during long-term burnup [3]. The FRAPCON takes into account various phenomena such as heat conduction, cladding deformation, fuel-cladding mechanical interaction, fission gas release, and cladding oxidation [3]. It also includes necessary material properties, water properties, and heat-transfer correlations to perform the calculations [3].

3. Coupling methodology

3.1. Geometry model

The radial discretization for each code in the coupling scheme is shown in Fig. 1 for the x-y plane. Hereafter, we use the abbreviated terms NX, T/H, and FP to represent the neutronics, sub-channel thermal-hydraulics, and fuel performance calculations in STREAM3D/CTF/FRAPCON, respectively. The left image in Fig. 1 shows the mesh used for NX

calculations, the center image shows the mesh used for T/H calculations, and the right image shows the mesh used for FP calculations. NX mesh represents the coolant between pins and pins, T/H mesh represents only sub-channels, and FP mesh represents only the pins without sub-channels. Pins usually refers to fuel pins, but the T/H solver treats guide tubes and instrument tubes as pins. These non-fuel pins are simply ignored by the FP solver. The regions outside of the active core (i.e., every structure beyond the baffle, and above and below the fuel) are not modeled by T/H and FP solvers.

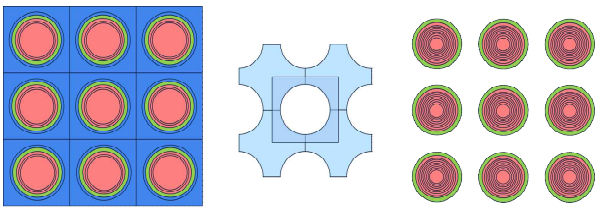

Fig. 1. Radial discretization for coupling scheme.

Regarding the axial discretization, NX solver employs a fine mesh of 3cm or less. while T/H and FP solvers reconstruct the mesh using planes based on the material regions used in calculating macroscopic cross-section in NX solver, with a mesh size ranging from around 5cm to 15cm. As a result, T/H and FP solvers use the same axial mesh scale. The variables exchanged between each solver based on this geometry model are mapped. The pin information is averaged with 4 adjacent sub-channels surrounding each pin as shown in center image in Fig. 1.

3.2. Code coupling

Code coupling is performed through an iterative process using the simple and flexible Picard iteration method. In Picard iteration, one problem is separated into distinct systems of equations representing different physical models, and each system is solved sequentially, one at a time. In this work, NX solver calculates the power distribution at sub-pin level, represented as a linear heat density q, which is then utilized by T/H and FP solvers. Next, T/H solver determines the distribution of coolant temperature T_c, coolant pressure P_c, and cladding heat transfer coefficient h_c, which are passed to FP solver as boundary conditions. Finally, FP solver calculates the distribution of cladding surface temperature T_s, which is provided to T/H solver as a boundary condition. T/H and FP solvers in turn provide the required values for coolant density ρ_c, coolant temperature T_c, and fuel temperature T_f to solve NX problem in the next iteration. This iterative process continues until T_f, T_c and q converge. During this iterative process, the exchange of variables between codes is managed by STREAM3D. Interface modules are added to CTF and FRAPCON to allow for the exchange of variables between codes, and CTF and FRAPCON, including the interface modules, were compiled into DLL format to allow STREAM3D to call subroutines within the interface modules. Therefore, variables between codes can be exchanged directly in memory rather than through writing and reading to files on the hard disk. Figure 2 shows the flow chart of the iterative process.

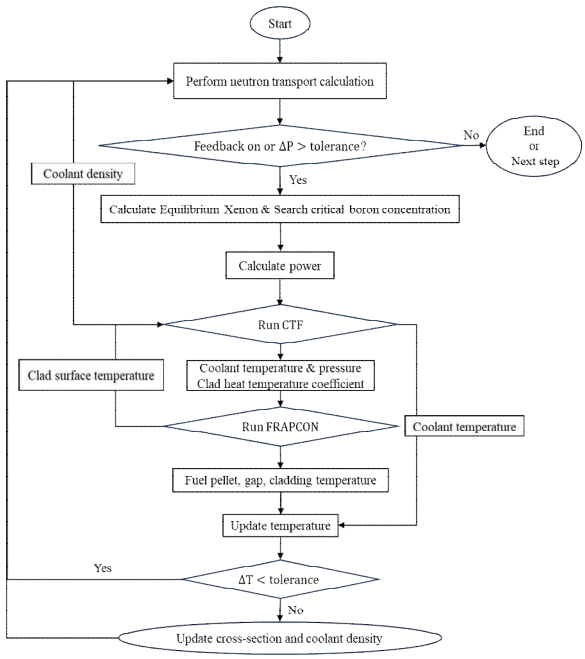

Fig. 2. Flow chart for the coupling algorithm.

3.3. Depletion scheme

To analyze the fuel behavior, the depletion calculation must be included in the coupled calculations. Therefore, a scheme must be designed to accurately reflect or calculate fuel behavior due to fuel burnup in each code. Fuel property changes due to fuel burnup are directly considered in STREAM3D and FRAPCON, while CTF indirectly reflects them based on the power distribution and cladding surface temperature information from STREAM3D and FRAPCON, respectively. STREAM3D performs the depletion calculations at sub-pin level for a given burnup interval and generally uses a prediction-correction like method to improve accuracy. However, since FRAPCON performs continuously the depletion calculation for a given time interval, a backup and loading process of FP calculation information, as shown in Fig. 3, is required to apply the prediction-correction method. The backup and loading of FP calculation information can be performed by calling relevant subroutines in the interface module of FRAPCON. In Fig. 3, N_f is the isotopic inventory, ϕ_f is the flux distribution at the sub-pin level, and q' is the linear power density.

1: Input: $\boldsymbol{N}_{F,0}$
2: **For** burnup point i in 0, 1, 2, … **do**
Predictor step (P)
► Perform coupling calculation ($MP \leftarrow NX, TH, FP$)
3: $\boldsymbol{\phi}_{F,i}^{P}, \boldsymbol{T}_{C}^{P}, \boldsymbol{h}_{C}^{P}, \boldsymbol{P}_{C}^{P} \leftarrow MP(\boldsymbol{N}_{F,i})$
► Perform burnup calculation
4: $\boldsymbol{N}_{F,i}^{P} \leftarrow BU(\boldsymbol{N}_{F,i}, \boldsymbol{\phi}_{F,i}^{P})$
5: Save FRAPCON data for fuel performance information at predictor step
► Perform FP calculation with $\boldsymbol{q}_{i}^{\prime P} \leftarrow \boldsymbol{\phi}_{F,i}^{P}, \boldsymbol{T}_{C}^{P}, \boldsymbol{h}_{C}^{P}, \boldsymbol{P}_{C}^{P}$ and Δt
6: Update fuel status $\leftarrow FP(\boldsymbol{q}_{i}^{\prime P}, \boldsymbol{T}_{C}^{P}, \boldsymbol{h}_{C}^{P}, \boldsymbol{P}_{C}^{P}, \Delta t)$
Corrector step (C)
7: $\boldsymbol{\phi}_{F,i}^{C}, \boldsymbol{T}_{C}^{C}, \boldsymbol{h}_{C}^{C}, \boldsymbol{P}_{C}^{C} \leftarrow MP(\boldsymbol{N}_{F,i}^{P})$
8: $\boldsymbol{N}_{F,i}^{C} \leftarrow BU(\boldsymbol{N}_{F,i}, \boldsymbol{\phi}_{F,i}^{C})$
9: Load FRAPCON data for FP information at predictor step
10: $\boldsymbol{q}_{i+1}^{\prime} \leftarrow 0.5 \times (\boldsymbol{q}_{i}^{\prime P} + \boldsymbol{q}_{i}^{\prime C})$
11: $\boldsymbol{T}_{C} \leftarrow 0.5 \times (\boldsymbol{T}_{C}^{P} + \boldsymbol{T}_{C}^{C}), \boldsymbol{h}_{C} \leftarrow 0.5 \times (\boldsymbol{h}_{C}^{P} + \boldsymbol{h}_{C}^{C}), \boldsymbol{P}_{C} \leftarrow 0.5 \times (\boldsymbol{P}_{C}^{P} + \boldsymbol{P}_{C}^{C})$
12: Update fuel status $\leftarrow FP(\boldsymbol{q}_{i+1}^{\prime}, \boldsymbol{T}_{C}, \boldsymbol{h}_{C}, \boldsymbol{P}_{C}, \Delta t)$
13: $\boldsymbol{N}_{F,i+1} \leftarrow 0.5 \times (\boldsymbol{N}_{F,i}^{P} + \boldsymbol{N}_{F,i}^{C})$

Fig. 3. Depletion algorithm in coupling calculation.

4. Results

4.1. VERA problem #6: 3D single fuel assembly

Problem #6 in the VERA core physics benchmark [4] requires the analysis of a Westinghouse 17×17-type fuel assembly at two different conditions, namely, beginning-of-cycle (BOC) and hot full power (HFP) steady-state conditions. The boron concentration in the assembly is fixed at 1300 ppm. More detailed information is available in the references [4]. Table 1 compares the eigenvalues of STREAM3D/CTF/FRAPCON (ST/CTF/FCN), VERA-CS [5], and MC21/CTF [6]. The results show that the solution from ST/CTF/FCN differs from that of MC21/CTF by 49 pcm, and from that of VERA-CS by 112 pcm.

Table I. Calculated eigenvalues for VERA problem #6

Code	Eigenvalue	Difference (pcm)
MC21/CTF[1)]	1.16424	Reference
VERA-CS[1)]	1.16361	-63
ST/CTF/FCN	1.16473	49
ST/CTF[1)]	1.16513	89
ST/internal-T/H[1)]	1.16495	71
ST/CTF[2)]	1.16719	295
ST/internal-T/H[2)]	1.16710	286

[1)]: Constant gap conductance of 5678.3 W/m^2·K
[2)]: Constant gap conductance of 10000 W/m^2·K

Fig. 4 shows the axially-integrated normalized radial fission rate distributions for ST/CTF/FCN, MC21/CTF, and VERA-CS. The axially-integrated normalized pin powers calculated by ST/CTF/FCN match well with MC21/CTF, with a maximum discrepancy of 0.2% and a minimum discrepancy of -0.2%, and the RMS error is within 0.1%. Similarly, the comparison of sub-channel exit temperature with VERA-CS in Fig. 5 shows good agreement with a maximum discrepancy of 1K, a minimum discrepancy of -0.05K, and an RMS error of 0.7K. The reason for the difference in sub-channel exit temperature is that ST/CTF/FCN represents pin-oriented sub-channel values, which are averaged over four adjacent channels, while the other two codes calculate sub-channel oriented values in CTF to obtain the accurate temperature of the sub-channel.

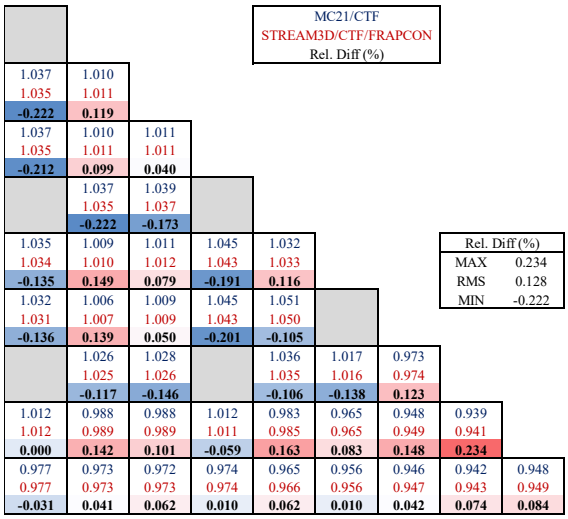

Fig. 4. Comparation of axially-integrated normalized pin fission rates.

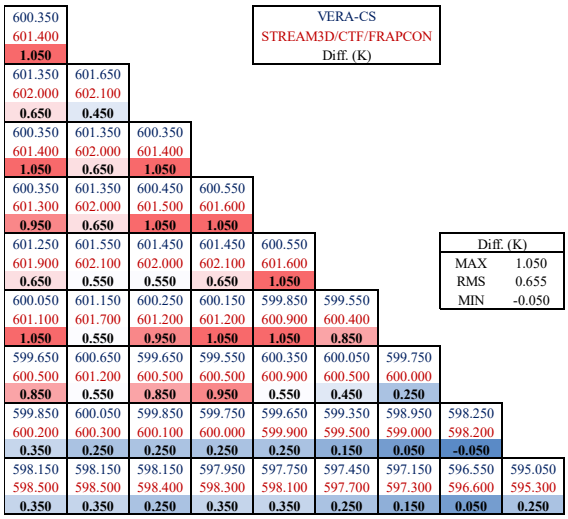

Fig. 5. Comparation of sub-channel exit temperature.

FRAPCON can accurately evaluate gap conductance, which has a significant impact on heat transfer calculations due to burnup, by using coolant temperature, coolant pressure, and clad thermal conductivity as boundary conditions in coupled calculations. Therefore, as shown in Table I, ST/CTF/FPC shows good agreement with the eigenvalue results of MC21/CTF and VERA-CS, which used a fixed gap conductance of 5678.3 W/m^2·K, and calculated a gap conductance value of 5701 W/m^2·K, which is almost consistent with the input values of both codes. As shown in Table I, using a fixed value at the beginning of a cycle resulted in a significant positive reactivity of about 300 pcm compared to using calculated values by FRAPCON. Therefore, this result

suggests that the gap conductance should be considered an important parameter in cycle calculations.

4.2. BEAVRS cycle 1 simulation

ST/CTF/FCN has been used to solve BEAVRS benchmark problem [7] to demonstrate its capability for whole core transport calculation. BEAVRS benchmark is based on a realistic Westinghouse type reactor, and the latest version of the benchmark has been used in the modeling [7]. More detailed information is available in the references [7]. A whole-core cycle 1 simulation is performed with ST/CTF/FCN. The specification provides 24-hours averaged power history, which are relatively prohibitive to simulate. Therefore, there are strategies that use simplified power histories [8] or draw a few power points from the power history [9]. However, in this work, the lower limit of boron letdown is evaluated using both constant 100% power history. It can be seen that the gap conductance is evaluated at 5000 W/m^2·K at the beginning of the cycle and around 20,000-30,000 W/m^2·K or a maximum of 50,000 W/m^2·K on average at the end of the cycle under HFP simulation. Therefore, when using the commonly constant gap conductance of 10,000 W/m^2·K in Figure 6, it can be seen that the reactivity increases at the beginning of the cycle, resulting in a high critical boron concentration (CBC). The CBC calculated by ST/internal-T/H and ST/CTF/FCN becomes similar at 150 EFPD and shows a similar trend thereafter. At 150 EFPD, the gap conductance calculated by ST/CTF/FCN is evaluated at around 10,000 W/m^2·K on average.

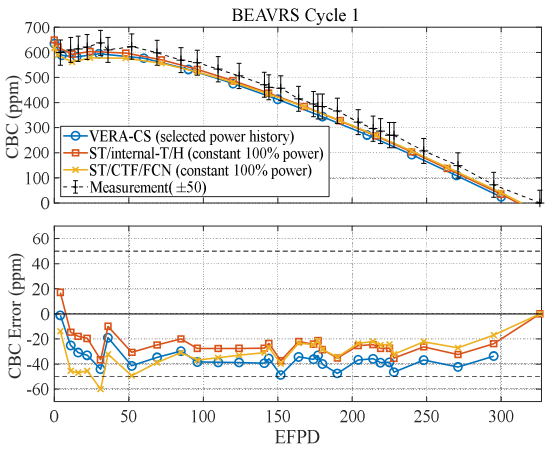

Fig. 6. Comparation of cycle 1 boron letdown curve.

ST/CTF/FCN and ST/internal-T/H both showed lower CBC values, which can be explained by the fact that the average power level over cycle 1 is 57%. If the decreased power level in each calculation is used, the CBC and cycle length would increase. When the calculation was performed with a constant power level of 75%, the CBC was increased by about 40 ppm in other study [8].

5. Conclusions

In conclusion, this paper presents a systematic coupling interface and a numerical scheme for multi-physics reactor analysis using ST/CTF/FPC. The coupling of these tools was achieved by developing an iterative process using the Picard method, and exchange of variables between the codes was managed by STREAM3D. The effects of feedback in the steady state were investigated, and primary design parameters for a typical pressurized water reactor were estimated and compared with stand-alone STREAM3D results and measurements. The depletion scheme was also presented, and its accuracy was demonstrated by applying it to Problem #6 in the VERA core physics benchmark. This work also contributes to providing results of BEAVRS whole-core simulation with various physical phenomena using a multi-physics coupled code system and quantitatively evaluating the effect of accurate gap conductance prediction on the reactivity of cycle calculation.

ACKNOWLEDGEMENT

This study was sponsored by the Korea Hydro & Nuclear Power Co.'s affiliated Central Research Institute (KHNP-CRI).

REFERENCES

[1] S. Choi, W. Kim, J. Choe, W. Lee, H. Kim, B. Ebiwonjumi, E. Jeong, H. Lee, D. Yun, D. Lee, Development of High-Fidelity Neutron Transport Code STREAM, Comput. Phys. Commun., 264:107915, 2021.
[2] M.N. Avramova, R.K. Salko, CTF–A Thermal Hydraulics Subchannel Code for LWRs Transient Analyses, User's manual, CASL-U-2015-0055-000, March 10, 2015.
[3] K. J. Geelhood, et al., FRAPCON-4.0: A Computer Code for the Calculation of Steady-State, Thermal-Mechanical Behavior of Oxide Fuel Rods for High Burnup, PNNL-19418, Vol. 1, Rev. 2, September 2015.
[4] A.T. Godfrey, VERA Core Physics Benchmark Progression Problem Specifications, Consortium for Advanced Simulation of LWRs, CASL-U-2012-0131-004, 2014.
[5] M. Sieger, VERA 3.3 release notes, CASL-U-2015-0042-000, 2015.
[6] D. J. Kelly, A. E. Kelly, B. N. Aviles, A. T. Godfrey, R. K. Salko and B. S. Collins, MC21/CTF and VERA multiphysics solutions to VERA core physics benchmark problem 6 and 7, Nucl. Eng. and Tech., Vol. 49, p.1326, 2017.
[7] N. Horelik, B. Herman, M Ellis, S. Kumar, J. Liang, B. Forget, K. Smith, Benchmark for Evaluation and Validation of Reactor Simulations, BEAVRS, V3.0.1, MIT, 2019, https://github.com/mit-crpg/BEAVRS,.
[8] M. Ryu, Solution of the BEAVRS Benchmark Using the nTRACER Direct Whole Core Calculation Code, J. Nucl. Sci. Technol., Vol. 52, 7-8, 961, 2015
[9] B. Collins, A. Godfrey, S. Stimpson, S. Palmtag, Simulation of the BEAVRS benchmark using VERA, Annals of Nuclear Energy, Vol. 145, 107602, 2020.