Proceedings of the Reactor Physics Asia 2023 (RPHA2023) Conference
Gyeongju, Korea, October 24-26, 2023

Multi-Physics Monte Carlo Simulation for a Fuel Pin-Cell with Continuous Temperature and Density

Muhammad Imron and Deokjung Lee *
Department of Nuclear Engineering, Ulsan National Institute of Science and Technology
50 UNIST-gil, Eonyang-eup, Ulju-gun, Ulsan, 44919, Republic of Korea
**Corresponding author: deokjung@unist.ac.kr*

1. Introduction

Multi-physics reactor simulations using the Monte Carlo (MC) method present a distinctive challenge due to the nature of the MC method itself. To obtain proper power distribution and subsequently calculate temperature and coolant density distributions, the problem domain must be discretized into smaller cells, even if the material is uniform. However, this discretization comes at the cost of diminishing the MC method's ability to efficiently handle continuous geometry. Furthermore, this approach requires a substantial number of particles to obtain solutions with reasonable uncertainties. Consequently, a higher level of computational power becomes a necessity, particularly when pursuing enhanced confidence in the results.

In this study, we propose a novel approach by combining Functional Expansion Tally (FET) with Machine Learning (ML) and delta-tracking to address this challenge. In the FET methodology, actual solutions are approximated using a truncated linear combination of polynomials, while Monte Carlo (MC) tallies determine the corresponding coefficients of these polynomials. This unique feature enables FET to generate a continuous representation of reactor power. Additionally, we incorporate on-the-fly ML training during the simulation, utilizing the discrete distribution of fuel temperature and coolant density calculated by a thermal-hydraulics (TH) solver to perform regression. We implemented the proposed method into MCS code [1] to provide preliminary solutions for a fuel pin cell multi-physics problem.

There have been several attempts to address this issue, including localized delta tracking (LTD) [2] and coupled multi-physics approaches using FET in conjunction with modified Continuously Varying Material Tracking (CVMT) [3]. While LTD is capable of handling continuously varying fuel temperature in the radial direction only, the proposed method can manage both radial and axial directions for both fuel temperature and coolant density. The spatially varying coolant density also implies spatially varying boron nuclide density in the coolant. In contrast to employing CVMT, the proposed approach utilizes the well-known delta-tracking to accommodate the continuous variations in temperature and coolant density. Additionally, the proposed method leverages advancements in ML to obtain continuous representations of fuel temperature, as well as coolant temperature and density.

2. Methodology

2.1 Functional Expansion Tally

FET [3,4,5] solutions can be obtained by expanding the tally quantity as a linear combination of polynomials $\psi(\vec{\xi})$ as shown in the Eq. 1

$$f(\vec{\xi}) = \sum_{n=0}^{\infty} \bar{a}_n k_n \psi_n(\vec{\xi}) \tag{1}$$

$$\bar{a}_n = \langle f, \psi_n \rangle = \int_{\Gamma} f(\vec{\xi}) \psi_n(\vec{\xi}) \rho(\vec{\xi}) d\vec{\xi} \tag{2}$$

where $\bar{a}_n$ is the expansion coefficients, $\vec{\xi}$ is the neutron phase space consisting of $(\vec{r}, \vec{\Omega}, E)$, and k_n is the normalization constant which can be calculated according to the choice of the polynomials basis set that is being used.

The calculations of the expansion coefficients in Eq. 2 are easily done in MC simulations with both analog and collision-based estimator. The unbiased collision-based estimator for coefficients $\bar{a}_n$ to reconstruct power (using Eq. 1) is defined in Eq. 3

$$\bar{a}_n = \frac{1}{N} \sum_{i=1}^{N} \sum_{k=1}^{K_i} w_{i,k} \frac{\kappa(\vec{\xi}_{i,k})}{\Sigma_t(\vec{\xi}_{i,k})} \psi_n(\vec{\xi}_{i,k}) \rho(\vec{\xi}_{i,k}) \tag{3}$$

where N is the total number of particles in each batch, K_i is the total number of collisions of particle i, $w_{i,k}$ is particle i weight at collision k, $\kappa(\vec{\xi}_{i,k})$ is the amount of energy released per fission at phase space $\vec{\xi}_{i,k}$, and $\Sigma_t(\vec{\xi}_{i,k})$ is the total macroscopic cross section for reaction x at phase space $\vec{\xi}_{i,k}$.

In the MCS code, Legendre polynomials are used for rectangular geometry problems, while Zernike polynomials are employed for radial problems. For multi-dimensional FET, such as in the case of fuel pin geometry, the solution is assumed separable. Hence, the reconstructed axial and radial power can be utilized to

represent the multi-dimensional power distribution within the cylindrical fuel pin.

2.2 Machine Learning

After conducting several batches (MCS uses batch system, in which one batch can contain one or more cycles) of MC simulation, power reconstruction both radial and axial directions using FET coefficients is performed within a fuel pin-cell. Subsequently, a thermal-hydraulic (TH) calculation is carried out to determine the two-dimensional fuel temperatures, and one-dimensional coolant temperatures and densities as well as the cladding temperatures for each reconstructed mesh.

The obtained discrete distributions of material properties serve as a dataset for training an Artificial Neural Network (ANN) at each TH calculation. The objective of ANN training is to perform regression, allowing us to obtain continuous representations of fuel temperature, coolant temperature, and coolant densities within the problem geometry. ANN is favored over multi-dimensional interpolation because with ANN, there is no need to store discrete distributions of material properties; instead, only ANN parameters need to be saved. The ANN training is performed on-the-fly during the simulation and independently for each fuel pin. To facilitate ANN training and model prediction during particle tracking, a Fortran library from [6] was employed in this study.

Two ANN architectures are trained at every TH calculation. The first architecture (Fig. 1) is employed to predict the temperature of the fuel pellet. It takes two inputs: radial and axial positions of the given fuel pin. This is because the fuel pellet temperature exhibits significant variations in both the radial and axial directions. The second ANN architecture (Fig. 2) is utilized to determine the temperature and density of the coolant, as well as the temperature of the cladding. It only requires the axial position as input since these material properties vary solely in the axial direction. A fraction of 80% of the dataset was utilized for training purposes, while the remaining 20% was reserved for testing. The maximum acceptable root-mean-squared error for prediction using the testing dataset was set at 3%.

2.3 Delta-tracking

Due to the continuous variation of material properties across the fuel pin, delta-tracking is utilized instead of conventional surface tracking. One of the main challenges in delta-tracking method for continuously varying materials is determining the majorant cross section. The continuous distributions of fuel temperature, coolant density, and, in turn, boron nuclide densities have a significant influence on the cross section (XS) across the pin cell.

The process of determining the majorant XS begins by identifying the maximum microscopic total XS for given majorant energy bins (MEB) for each nuclide. By default, in MCS, the number of MEB is set to 1200 bins, which are distributed across thermal, resonance, and fast regions. To ensure the maximum macroscopic XS is obtained for a given energy bin, the maximum total XS is searched for within overlapping MEB. Once the majorant microscopic XS is determined for each nuclide, it is multiplied by the highest nuclide densities within a given material and then summed to obtain the material-wise macroscopic XS. The subsequent step involves finding the maximum material-wise majorant XS for each MEB in the given delta-tracking region, which is typically set at the assembly level in MCS.

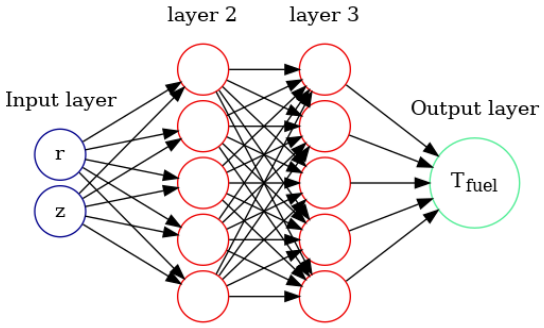

Figure 1. The ANN architecture for fuel pellet temperature prediction

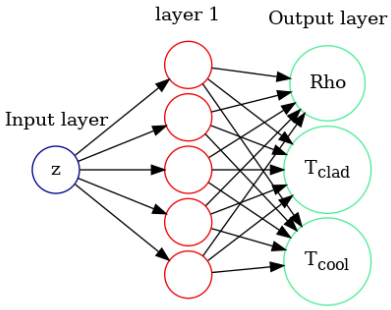

Fig. 2. The ANN architecture for the prediction of the coolant temperature and density, as well as the cladding temperature

3. Test Problem

To showcase the capabilities of FET combined with ML in tackling multi-physics problems using MCS, a pin-cell problem was adopted from the VERA benchmark [7]. The pin-cell configuration includes two Inconel spacer grids at the bottom and top, with five zircaloy spacer grids positioned in between. The fuel consists of 2.1 wt.% enrichment with radial reflective

Table 1. Calculation Results

Cases	# of axial/radial discretization	# of particle histories/batch	CBC (ppm)	Max σ on axial power	Running time (CPU-hours)
P1	25/1	$3.0\text{x}10^6$	1810.2±0.8	2.4%	75.3
P2	100/5	$1.2\text{x}10^7$	1814.5±0.7	3.4%	718.0
FET	N/A	$3.0\text{x}10^6$	1817.8±1.0	2.9%	60.6

boundary conditions, while vacuum boundary conditions are applied in the axial direction. The problem involves a critical boron concentration (CBC) search at a full power level which corresponds to 67 kW of thermal power. In the current study, the presence of Xenon is not considered in this test problem.

Three cases were developed for comparison with the proposed method. The first two cases, P1 and P2, use conventional MC coupled multi-physics approach in which the problem domain is discretized into several cells. Each cell has uniform material properties such fuel temperature and coolant density. In the P1 case, the problem is discretized into 25 axial meshes and 1 radial mesh, with a simulation of $3.0\text{x}10^6$ particles per batch. While the P2 case utilizes 100 axial meshes and 5 radial meshes (only for the fuel pellet) to capture smoother distribution of fuel temperature in both radial and axial direction as well as coolant density in axial direction. Note all mesh divisions are equidistant. P2 case employes $1.2\text{x}10^7$ particles per batch to maintain a reasonable uncertainty for given the smaller cells' sizes.

In the FET case, the problem domain discretization is not necessary. At every TH update, the power distribution is reconstructed into 200 equidistant axial meshes and 10 equidistant radial meshes using the tallied FET expansion coefficients. Consequently, there are 2000 data points for training the ANN model to predict fuel temperature that has two-dimensional distribution. Additionally, there are 200 data points for training the ANN model to predict coolant temperature and density, as well as cladding temperature that have one-dimensional distribution. The seventh order of Legendre polynomials and ninth order of Zernike polynomials were used to reconstruct the power in the axial and radial directions respectively.

During the calculation by the TH solver, the radial heat conduction calculations within the fuel pellet were conducted using 10 radial meshes for all cases, while a single mesh was utilized for the gap and cladding regions. Subsequently, the resulting radial fuel temperature distribution was averaged based on the number of radials meshes used in the neutronic calculations. All cases employed a total of 50 batches, with 25 batches designated as active batches. The TH updates were performed every 5 batches of the MC simulation.

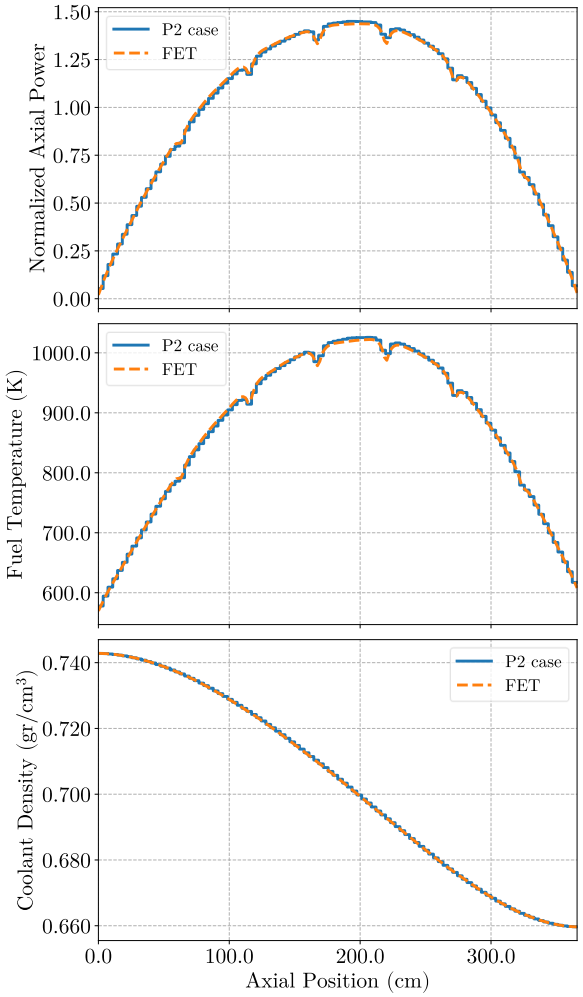

Fig. 3. Axial distributions of normalized power, fuel temperature, and coolant density for P2 and FET cases.

3. Results and Discussion

Table 1 displays the calculation results for all cases. The coolant's CBC tends to increase as the distribution of material properties becomes smoother. The difference in CBC between the P2 and FET cases is approximately only 3 ppm. It's worth noting that, despite the smaller number of histories in the FET case, the resulting maximum standard deviation in axial power is quite small. The FET case also exhibits the shortest running time, even when compared to P1 case, partly due to its continuous geometry representation without discretization within same material. The FET case has

only four cells for each material in the fuel pellet, gap, cladding and coolant. In contrast, P2 case has 1300 cells (1000 cells for fuel pellet material, and the remaining for gap, cladding and coolant) that deteriorates the MC tracking efficiency.

Fig. 3 shows axial distribution comparisons for normalized power, fuel temperature and coolant density between P2 and FET cases. As illustrated in the figure, the axial distribution of the power, fuel temperature, and coolant densities of the FET case agree very well with the P2 case. To perform direct comparisons and quantitatively assess the accuracy of the FET case, a mesh power tally was done for each case. In the mesh power tally, the power was tallied in 100 bins axially and the relative differences of the FET cases are compared with the other cases in Fig. 4. The figure clearly indicates that axial power of the FET case is closer to the axial power of the P2 case that has smoother fuel temperature and coolant density distributions. This may suggest that as the problem domain discretization is smoother, the solutions would approach FET case's solutions.

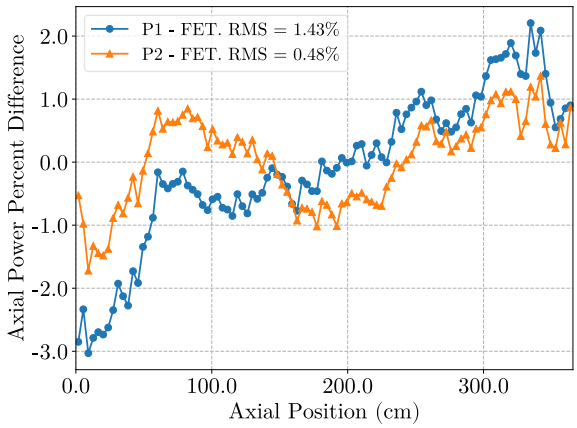

Fig. 4. Percent differences on the axial power (using mesh tally) of the FET case against P1 and P2 cases.

4. Conclusion

The implementation of the FET method combined with the ML technique in MCS has proven to be highly effective for addressing MC coupled multi-physics for pin-cell problems with spacer grids. The approach achieved very good accuracy despite utilizing fewer particle histories. That is largely due to the fewer number of cells used in the presented method. The problem domain discretization into large number of cells diminishes the advantage of the MC method to treat geometry continuously. Moreover, the relative standard deviation of the axial power in the FET case was comparable to that of the P2 case despite smaller number of histories used by the FET case.

Although not discussed in this paper, it is also important to note that the FET approach offers the advantage of requiring smaller computational memory during simulations, especially for whole core problems. This is because, in the proposed method, the fuel pellet is not divided into multiple cells, resulting in only a single material data being saved for each fuel pellet. Additionally, while this study does not employ Computational Fluid Dynamics (CFD) as a TH solver, the proposed method has potential to solve the difficulties in mapping unstructured meshes used in CFD into the meshes used for neutronics calculations.

While the calculation time for the on-the-fly training is a small fraction compared to the tracking time in the pin-cell problem, it is no longer the case for assembly or whole core problems because the training must be done for each pin-cell. Therefore, it is imperative that the training is carried out in parallel and possibly with optimizers. Also, the continuously varying Xenon distribution should be incorporated into the method to broaden its applicability to more realistic reactor problems.

ACKNOWLEDGEMENT

This research has been supported by project L20S089000, funded by Korea Hydro & Nuclear Power Co. Ltd.

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