Enhancement of RAST-AI Deep Learning Cross-Section Generation Model by Adding Gadolinia Fuel Support

Siarhei Dzianisau, Deokjung Lee*
Department of Nuclear Engineering, Ulsan National Institute of Science and Technology, 50 UNIST-gil, Ulsan, 44919
*Corresponding author: deokjung@unist.ac.kr

1. Introduction

A huge role in accelerating our daily routines belongs to development of Artificial Intelligence as a whole, and Deep Learning in particular. Being quite conservative, the area of Nuclear Engineering is one of the last to introduce Artificial Neural Networks (ANN) into their workflow.

Originally, ANNs in nuclear industry were used for straightforward and well-known tasks such as image recognition, object detection, etc. Over the time, ANNs were found suitable not only for solving abstract problems but also for directly dealing with numerical data. One of promising areas where such approach can be useful is cross-section (XS) processing. In Nuclear Engineering, two types of cross-sections (XS) are known: microscopic XS that characterize each nucleus, and macroscopic XS that describe certain material composition as a macro-system. The physical meaning of those types of XS is also different. Thus, microscopic XS is a measure of probability for a certain nucleus to interact with a neutron of certain energy. Quite differently, macroscopic XS characterize the mean distance that a neutron of certain energy can travel in certain material before interacting with one of material nuclei.

In computer codes for reactor simulation, it is quite common to deal with both of XS types, and to convert one type into another. There are examples of ANN applications for generating or enhancing each of given XS types. Thus, Vicente-Valdez et al [1] suggested a method to tweak and improve the microscopic XS offered by ENDF nuclear data library using a Deep Neural Network (DNN). Whewell et al [2] proposed a way to replace certain macroscopic XS that are used in a neutron transport code by an ANN model, thus reaching reduced memory consumption. Lastly, Li et al [3] proposed using a DNN model paired with a regression tree for homogenized macroscopic XS generation for the purpose of using them in a nodal diffusion code.

The last-mentioned work became the turning point for Dzianisau et al. [4] who expanded the homogenized macroscopic XS approach to supporting a variable Fuel Assembly (FA) geometry and lattice type, thus making it possible to use a trained ANN model as a direct substitute of a lattice physics code STREAM in a two-step code system [5]. As a result, a new hybrid code called RAST-AI was developed. The aim of the current study is to continue the development of RAST-AI by improving the ANN model so that it could support fuel with added Burnable Absorbers (BA).

Hence, this study is organized in the following way. The description of the data management and ANN model design used in this study is presented in Section 2. Then, the main results of the trained model testing, including the results of applying the model in RAST-AI for 3D core-wise problems, are given in Section 3. Finally, the main conclusions and plans for future studies are discussed in Section 4.

2. Methodology

To add the BA fuel support into the model, proper training dataset should be architected and generated. The philosophy behind generating training data in this study follows the previously implemented models in terms of using uniform distribution of pins in a FA.

2.1. Training data preparation

In previous works [4], only fuel containing rods were used in a lattice. In this study, burnable absorber (BA) rods had to be added to further improve the model. Previously, the training data was architected in such a way that each pin location was filled with each type of enrichment equal number of times.

This idea came from a thought experiment in which we imagined that a dataset that consists of all possible pin combinations was generated. Such dataset would have very large size and require enormous hardware and time resources to be produced. However, there is one property of such a complete dataset that would stand true regardless the number of possible combinations or the number of variables (that eventually determines its' size). This property is the uniformity of pin enrichment distribution across all pin locations.

Therefore, we decided to utilize this property of a complete dataset in a much smaller training dataset that is used in this study. The rule of uniformity was proven to be efficient in our previous works, hence, the same rule was applied to the newly generated BA dataset at two different levels. At the outer level, BA pins were marked in the same fashion as fuel pins, and then uniformly distributed across supported FA lattices. Then, at the inner level, the dataset was equally divided into smaller subsets, and a fixed value of Gadolinia (Gd) weight content was set for the entire subset and placed into the designated BA pin positions. Hence, each FA either contained a single type of BA pins or

did not contain any BA pins at all. A schematic that represents the pin mixing philosophy is shown in Fig. 1. A total of 160,000 training samples were generated, including 80,000 samples for 16x16 lattice, and 80,000 samples for 17x17 lattice. These training samples were added to previously generated 99,000 samples with no BA pins [4]. Each FA geometry contained a total of 5 combinations of fuel temperature (TFU), moderator temperature (TMO), and boron concentration (BOR) taken from the list previously presented by Dzianisau et al [6]. The optimization method from the given study was used to determine the overall size of the data.

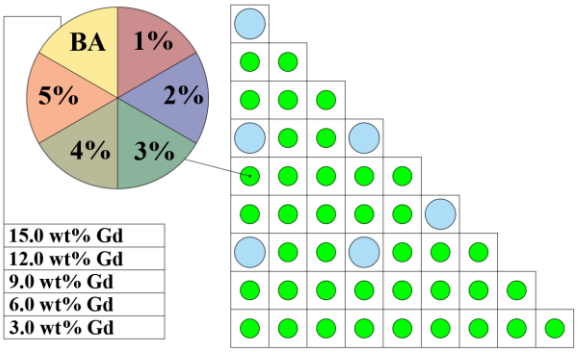

Fig. 1. Frequency of occurrence of each pin type across training samples.

2.2. Testing and validation data

To avoid the problem of having duplicate samples in training and testing data, the validation and testing datasets in this study were designed and generated independently from the training dataset. At the design stage, the datasets were verified to be non-overlapping and to not contain any duplicates. In addition to that, after all the data was generated, a separate code was developed to validate the absence of duplicates in obtained data.

To produce more meaningful testing results, a completely different type of data was designed and generated. This data, called out-range, did not follow any of the training data patterns, such as discrete values of fuel enrichments, TFU, TMO, BOR, and Gd. Instead, those values were taken randomly within the range of the training data (TMO, TFU), or beyond the range of training data (BOR, fuel enrichment, Gd). Such data is very unlikely to be found in real world applications as it clearly violates the intend of having a smooth pin power distribution, as well as utilizing not more than 2 enrichments within each FA. Hence, the out-range data is aimed to provide the highest imaginable complexity to the trained ANN model.

The total size of the validation dataset was 18,000 samples. The size of the in-range testing dataset was 36,000 samples with BA pins, and 36,000 samples without BA pins. The size of the out-range testing dataset was 10,000 samples with BA pins, and 10,000 samples without BA pins. This data includes both 16x16 and 17x17 lattices in equal quantities. Lastly, it is worth emphasizing that the in-range testing data contained only one type of BA pin per each FA, while the out-range testing data consisted random number of non-fixed BA pin types per each FA.

2.3. Neural network model

Once the training data was generated, it was used to train a Convolutional Neural Network (CNN) model that is depicted in Fig. 2. The difference of given CNN

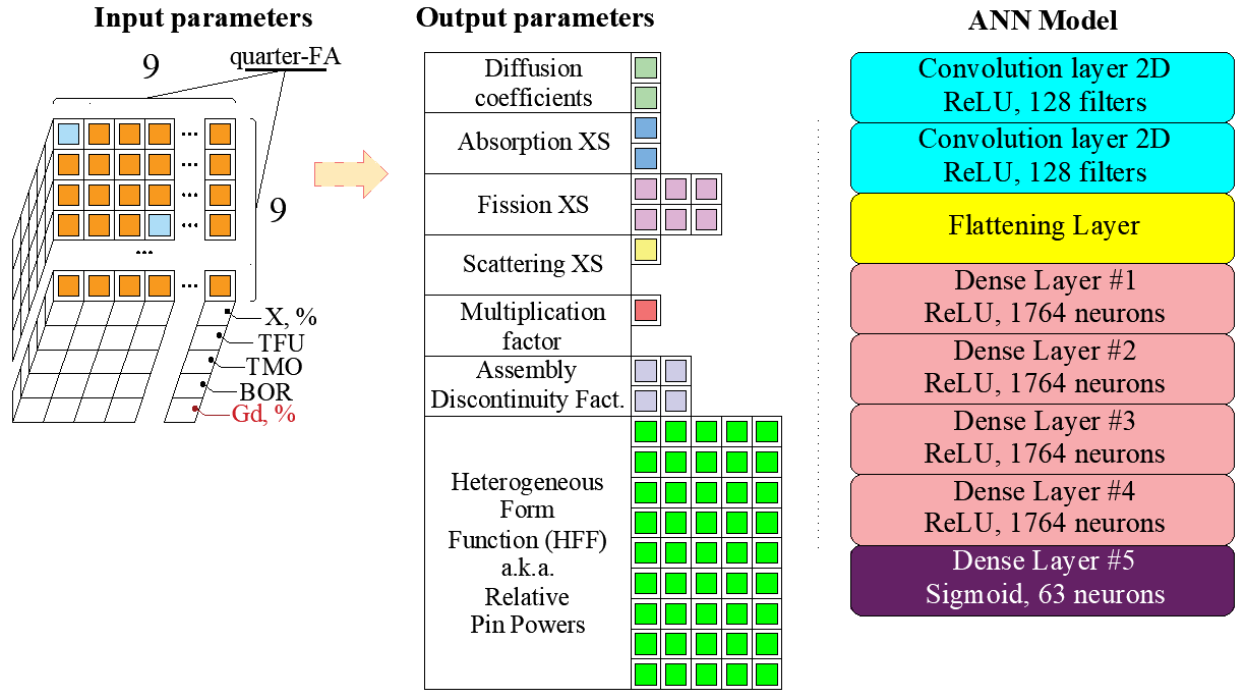

Fig. 2. The structure of input, output, and the neural network model where the input represents a typical quarter of a fuel assembly and has a shape of 9x9x5, 5 being the number of channels per each “pixel”.

model compared to other conventional models is that it does not perform any reduction in size for the input image (using pooling or striding). In fact, given that the input image size is just 9 by 9, it is hard to justify the necessity of size reduction. In addition to that, the input data used in our work has much higher individual significance than a typical pixel data used in image-processing applications of CNN. Therefore, it is within our best interests to retain as much of the input data as possible.

As mentioned above, the input consists of a quarter-FA, 9x9 pin arrangement array, where each pin has 5 channels, thus effectively turning the input shape into a 3D 9x9x5 array. The channels for each pin are the following: pin enrichment (X), takes a normalized value or zero in case it is not a fuel rod but a guide tube; normalized TFU of the target XS set; normalized TMO of the target XS set; normalized BOR of the target XS set; and finally, normalized Gd content, which takes zero values for all but BA rods.

The output consists of a vector that contains target 2-group XS sets, including diffusion coefficients, absorption XS, fission XS and its products, scattering XS. These values are necessary for running a nodal diffusion code and getting core-wise and node-wise results. The output also contains assembly discontinuity factors (ADF) and heterogeneous form function (HFF). ADF and HFF are required for performing pin power reconstruction at the nodal level once the homogenized solution is obtained for the target reactor core geometry.

The model hyperparameters included the following. The chosen batch size was 70, the optimizer was Adam, loss function was Huber loss, total number of epochs for training was 10,000 with early stop tolerance of 2,000 epochs. The model with the lowest validation loss was saved as the best model. Python 3.8 and TensorFlow 2.9.1 were used as an environment for the model.

3. Neural network testing results

The ANN model was trained in accordance with the information provided in the previous section. The total number of epochs before early stop was 7,176, thus yielding the best model recorded at epoch 5,176. Then, the model was tested using previously introduced in-range and out-range testing data. The results are shown in the subsections below.

3.1. In-range testing results

The results of testing HFF distribution for the in-range dataset with BA rods is depicted in Fig. 3. Given that the testing samples without BA rods were shown by Dzianisau et al [4], only the new results obtained for samples that include BA rods are given here.

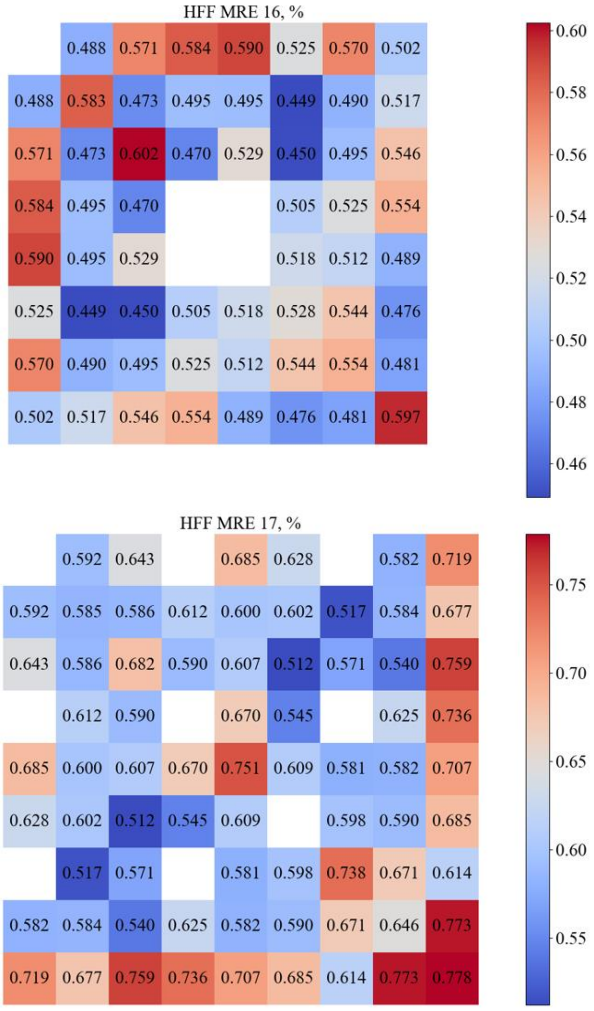

Fig. 3. Mean Relative Differences (in %) of the trained CNN model vs the reference result for in-range testing data with BA rods.

Overall, Mean Relative Difference (MRD) between the ANN-generated values and the reference values was found below 1% for both tested FA lattices. There are a few outliers such as down-scattering XS (from energy group 1 to energy group 2) or absorption XS for energy group 1, while other MRD values were found below 0.4%. As for the HFF results, both lattices showed decent results with MRD values confidently below 1% for each pin location. Since the trained model supports both of lattice types and was trained with mixed data, it shows higher MRD in the areas where 16x16 and 17x17 FA lattices are most different. Such areas as the peripheral of the 17x17 FA or the large guide tube location of 16x16 FA were found to contain the highest MRD.

3.2. Out-range testing results

Similar to the in-range testing results, the out-range data was tested, the results of HFF generation are shown in Fig. 4. A simple comparison with the in-range results yields higher values of MRD for all output values. At the same time, the results stay well in line with the testing data complexity as discussed in Section 2.

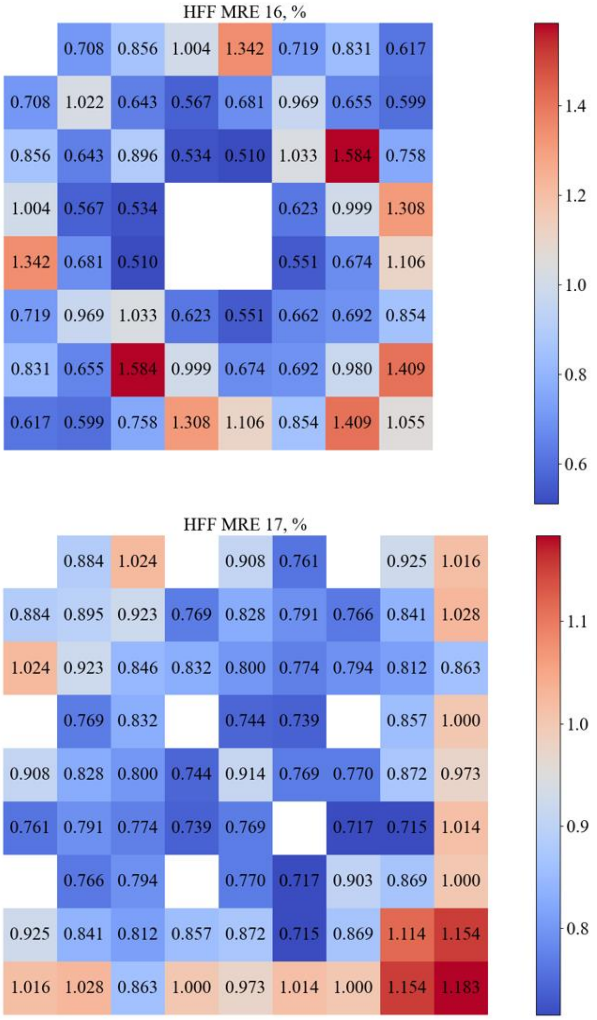

Fig. 4. Mean Relative Differences (in %) of the trained CNN model vs the reference result for out-range testing data with BA rods.

3.3. RAST-AI results

The homogenized macroscopic XS, ADF and HFF were obtained using both a trained CNN and our in-house code STREAM. Then, they were compared using RAST-AI and RAST-K [5] nodal diffusion codes. The reactor models for this test were OPR-1000 [7] and APR-1400 [8] pressurized water reactors that are commercialized in South Korea. The results of the testing are summarized in Table I.

Table I: RAST-AI Compared to STREAM/RAST-K

Parameter	OPR-1000	APR-1400
In-range testing, 16x16 lattice		
Multiplication factor, MAD*, pcm	74.7	76.9
PPF** F_q, MRD, %	0.478	0.459
PPF F_r, MRD, %	0.477	0.459
PPF F_{dH}, MRD, %	0.477	0.459
Restored Pin Power, MRD, %	0.307	0.396
In-range testing, 17x17 lattice		
Multiplication factor, MAD, pcm	67.5	65.6
PPF F_q, MRD, %	0.835	0.938
PPF F_r, MRD, %	0.835	0.938
PPF F_{dH}, MRD, %	0.835	0.938
Restored Pin Power, MRD, %	0.394	0.396
Out-range testing, 16x16 lattice		
Multiplication factor, MAD, pcm	306.2	309.9
PPF F_q, MRD, %	1.316	1.548
PPF F_r, MRD, %	1.315	1.546
PPF F_{dH}, MRD, %	1.315	1.546
Restored Pin Power, MRD, %	0.812	0.882
Out-range testing, 17x17 lattice		
Multiplication factor, MAD, pcm	282.2	282.9
PPF F_q, MRD, %	1.331	1.565
PPF F_r, MRD, %	1.331	1.563
PPF F_{dH}, MRD, %	1.331	1.563
Restored Pin Power, MRD, %	0.848	0.891

* MAD – Mean Absolute Difference
** PPF – Pin Peaking Factor

Based on the results, it could be found that the reactor size does not have a significant impact on the core-wise result. Despite APR-1400 has more FAs, the average pin powers and multiplication factors did not show higher difference with the reference. What did affect the result is the use of out-range data. Given that out-range data violates all possible rules in terms of proper fuel design for reactors as discussed in Section 2, one of the reasons for having a larger difference against the reference could be the limitation of the nodal diffusion method itself. More work should be performed on determining the limitations of the used methods.

4. Conclusions

In this study, a new CNN model was developed to be used in a hybrid nodal diffusion code RAST-AI. The main advantage of the model is the capability to work with Gd fuel, which is the most used type of BA fuel. The model was thoroughly tested using independent in-range and out-range testing datasets. The results of the ANN output compared with the reference show solid performance of the model. In particular, the MRD was

found below 1% across the in-range testing data. The values of MRD for out-range data were found slightly higher compared to the in-range data, thus slightly exceeding the 1% limit of MRD in some cases, such as HFF. However, given that the uncertainty of the 2-step approximation method for pin power reconstruction could reach 5-10% depending on the geometry, the obtained results are still considered reasonable. Since the commercially used FA designs avoid following dangerous patterns presented in out-range testing data, this result should be thought of as an attempt to create the most extreme conditions that challenge not only the ANN model but also the nodal methods themselves.

In our future works, we are planning to introduce further capabilities into the RAST-AI ANN model. There is a plan to develop a model that can work with moving control rods, thus making it possible to simulate transient scenarios. The very final version of RAST-AI should also include the depletion module that could be used for proper assessment of nuclear fuel cycle of studied reactor cores.

Acknowledgement

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT).
(No. NRF-2019M2D2A1A03058371).

REFERENCES

[1] P. Vicente-Valdez, L. Bernstein, M. Fratoni, “233U nuclear data evaluation using machine learning generated cross sections”, Proceedings of American Nuclear Society Mathematics & Computation 2021, pp. 1418-1426, Raleigh, North Carolina, October 3–7, 2021.

[2] B. Whewell, R. G. McClarren, “Reduced models for nuclear data in transport problems”, Proceedings of American Nuclear Society Mathematics & Computation 2021, pp. 1427-1436, Raleigh, North Carolina, October 3–7, 2021.

[3] Z. Li, J. Sun, et al, “Research on the cross-section generating method in HTGR simulator based on machine learning methods”, EPJ Web Conf., 247: 02039, 2021.

[4] S. Dzianisau, F. Setiawan, K. Saeju, J. Park, D. Lee, “RAST-AI: a Standalone Nodal Diffusion/Deep Neural Network Code for Reactor Analysis and Simulation”, Proceedings of PHYSOR2021, Pittsburgh, USA, May 15-20, 2022.

[5] J. Choe, S. Choi, et al, “Verification and validation of STREAM/RAST-K for PWR analysis”, Nucl. Eng. Tech., 51 (2): pp. 356–368, 2019.

[6] S. Dzianisau, K. Saeju, D. Lee, “Optimization of training dataset size for predicting homogenized macroscopic cross-sections using deep neural network”, Transactions of the Korean Nuclear Society Autumn Meeting, Changwon, Korea, October 20-22, 2021.

[7] H. Kim, A. Cherezov, J. Yu, J. Park, D. Lee, “Multi-cycle analysis of OPR1000 using multi-physics coupled codes of RAST-K, CTF and FRAPCON”, Proceedings of American Nuclear Society Mathematics & Computation 2019 Meeting, Portland, Oregon, August 25-29, 2019.

[8] S. Choi, D. Lee, “Preliminary Results for OPR1000/APR1400 Whole-core Analysis with Neutron Transport Code STREAM”, Proceedings of American Nuclear Society Mathematics & Computation 2019, Oregon USA, August 25-29, 2019.