A STUDY ON THE APPLICATION OF ARTIFICIAL NEURAL NETWORK TO PREDICT K-EFF AND PEAKING FACTOR OF A SMALL MODULAR PWR

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Abstract:
Machine learning (ML) using artificial neural network (ANN) methods is being strongly applied in nuclear reactor research. It is used to predict required parameters based on learning from big data sets. The ML models usually give much faster calculation speed while the accuracy is good and can be even better than the normal calculation tools. In this work, a Multi-layer perceptron network was built and trained to predict k-eff and peaking factor of a small modular PWR core. The obtained results are compared with the SRAC2006 code to evaluate the performance of the models. The comparisons show good accuracy and performance of the models.
Keywords: *small modular reactor, machine learning, artificial neuron network, multi-layer perceptron.*

I. INTRODUCTION

Over the past decade, along with the development of computer science and big data, machine learning (ML) has had tremendous development. ML has penetrated almost all human activities such as supporting scientific research, self-driving cars, virtual assistants, image recognition and so on. For nuclear reactor research, ML has also been applied quite a lot to replace simulation tools in predicting necessary parameters in the reactor such as kinetic parameters, power distribution, thermal-hydraulic [1]-[5]. The nuclear reactor is a multi-physics system with complex geometries, so the simulation and calculation of the reactor parameters require complex computationally intensive programs and take a long time to compute. Studies on applying ML show that the program algorithm is simple to predict the necessary parameters with acceptable accuracy, and the calculation speed is also greatly increased.

Research on application of ML, especially artificial neural networks (ANN) to predict parameters, analyze safety, and design nuclear reactors has been vigorously deployed for more than 10 years [6]-[11]. The results show the great potential of ANN in building high-performance precision simulation tools for nuclear reactor. Great support in reactor design, analysis and safety assessment, building digital-twin models to support reactor operation. However, for specific problems, ML models still need to be studied and improved to achieve appropriate accuracy [6]-[8]. In addition, ANN models require relatively large amounts of data to train. Therefore, studying algorithms with high generalizability on a limited data set (especially for experimental data) is also a challenging problem today [12].

This study applies a multi-layer perceptron (MLP) neuron network [13] to predict k-eff and peaking factor for pressurized water-type small modular reactors. The dataset used to train the model is generated by the SRAC2006 code [14], [15]. MLP neural network structure is built and

trained to achieve high accuracy when compared with simulation results. Studying the necessary features to train the model as well as reduce the size of the dataset while ensuring the accuracy of the model is also performed.

II. METHODOLOGY

2.1. Core modeling and data preparation

The analyzed small modular PWR reactor (SMR) is a simplified core that contains 37 shortened PWR fuel assemblies and light water as a reflector. Each assembly consists of 289 rods with 264 fuel rods, 24 control rod guide tubes and 1 instrument tube at the center arranged on a 17x17 grid. The fuel pellets made of UO_2 with three different U-235 enrichment of 2.35%, 3.40% and 4.45% are loaded into three types of assembly named F235, F340 and F445, respectively. The characteristics of the fuel assembly and the SMR core are given in Table 1 [16].

Table 1. Main design parameters for small modular PWR core

Parameters	Values
Reactor thermal power, MW	200
Number of fuel assembly	37
Assembly pitch, cm	21.4173
Assembly height, cm	220
Fuel rod pitch, cm	1.2598
Fuel pellet radius, cm	0.4096
Fuel inner cladding radius, cm	0.4178
Fuel outer cladding radius, cm	0.475
Fuel enrichment, %wt U235	2.35, 3.40, 4.45
Fuel temperature, K	1145
Average coolant temperature, K	583
Operation pressure, MPa	15.5

SRAC2006 is a deterministic code system with many modules used to calculate neutronic characteristics for various types of thermal reactors [14],[15]. It has been validated for core calculations of small modular PWRs through several studies [16], [17].

The advantage of this code is the fast calculation while ensuring accuracy compared to other codes. Therefore, this code is suitable to calculate for a large number of loading patterns (LPs) to create training data for machine learning.

The calculations are performed by module PIJ for fuel assembly and COREBN for 3D core calculations. In PIJ module, the assemblies are modeled according to the ¼-symmetric model. Each fuel rod is divided into 5 zones (3 fuel zones with equal cross-sectional area, 1 zone for gap between fuel and cladding and 1 cladding zone). The guide tubes are also divided into 5 zones with 4 water zone and 1 cladding zone. The assembly model is shown in Figure 1.

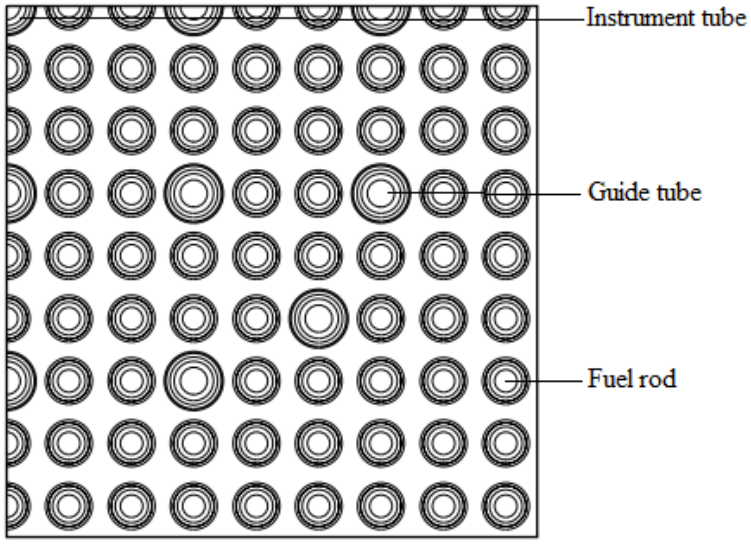

Figure 1. PWR assembly model (quarter symmetry)

The obtained calculation results for three types of assemblies include the infinitive multiplication factor, k-inf, and the homogeneous cross-section (group constants) data at the beginning of cycle for 3 energy groups (Table 2). These data are used as input features for training machine learning models. The burn-up calculations for fuel assemblies were also conducted to make the dataset for core calculation with COREBN code.

Table 2. Features of assemblies

Assembly	Index	Enrichment (%) U235	k-inf	Energy group	Fission XS	Diffusion coefficient
F235	1	2.35	1.221	1	1.467E-03	1.575E+00
				2	5.969E-03	8.274E-01
				3	4.396E-02	3.790E-01
	2	3.40	1.306	1	1.686E-03	1.577E+00
				2	8.478E-03	8.230E-01

F340				3	5.995E-02	3.776E-01
F445	3	4.45	1.356	1	1.902E-03	1.578E+00
				2	1.091E-02	8.189E-01
				3	7.446E-02	3.754E-01

In COREBN, the PWR core is modeled as Figure 2. The core contains 37 fuel assemblies arranged with quarter-core symmetry. So that at each position of a quarter-core, one of the three types of the fuel assembly is randomly placed to create different LPs. To make the training dataset for the machine learning model in this study, 20000 LPs were calculated. The calculated parameters include the effective multiplication factor (k-eff) and the power peaking factor at the beginning of the cycle. In the next sections, the dataset will be divided into 3 parts including test set (1000 LPs ~ 0.5% of dataset), validation set (3800 LPs ~ 20% rest of the dataset) and training set (15200 LPs).

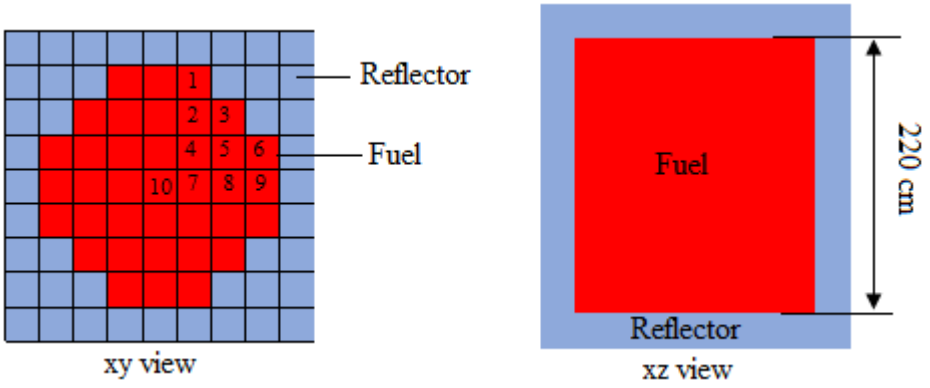

Figure 2. Core model in CORENBN code

2.2. Multilayer perceptron neuron network

The multilayer perceptron (MLP) is a type of artificial neural network (ANN) that consists of multiple layers of interconnected artificial neurons, or nodes (Figure 3). It is a feedforward neural network, meaning that information flows in one direction, from the input layer through the hidden layers to the output layer. The MLP is widely used in various fields for tasks such as classification, regression, and pattern recognition.

The architecture of the MLP consists of an input layer, one or more hidden layers, and an output layer. Each layer is characterized by its nodes, where each node performs a weighted computation on the input signals received from the previous layer. The introduction of activation functions within these nodes allows for non-linear transformations of the data, enabling the MLP to model intricate relationships beyond the limitations of linear classifiers.

A perceptron (node) was inspired by structure of neurons, that is illustrated in Figure 4. The computation in each node is performed in 2 steps. First the input data is summed by weight:

$$s = \sum w_i x_i + b \tag{1}$$

where, w_i are weighting factors, x_i are input signals and b is bias

Then, the output is calculated from the above sum through a nonlinear activation function *f(s)* to be able to build a multi-layer model. The following formula represents the sigmoid activation function:

$$f(s) = \frac{1}{1 + e^{-s}} \tag{2}$$

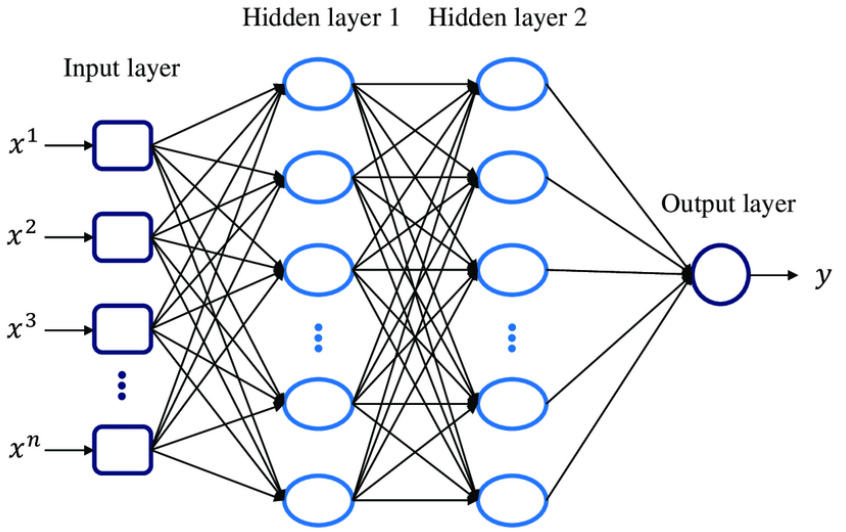

Figure 3. Multilayer perceptron illustration

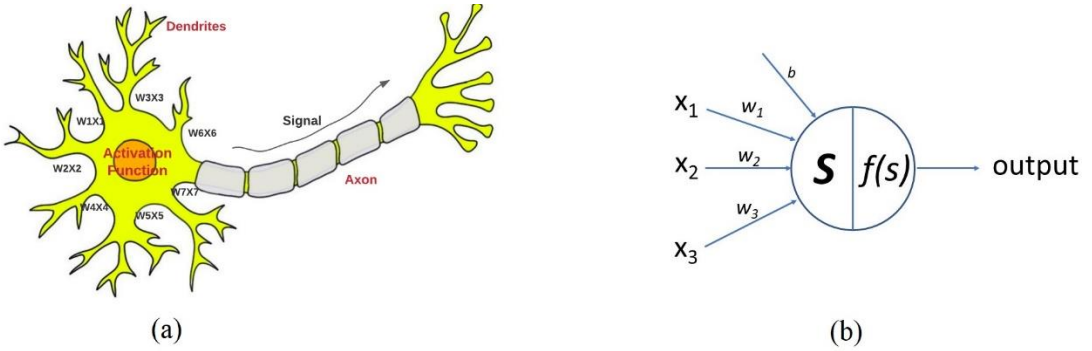

Figure 4. neuron (a) and perceptron (b) illustration

In this study, the MLP network structure is built based on some preliminary surveys and experience of the research team. The number of nodes in the input layer are equal to the number of considered input features. The input features include the arrangement of the fuel assemblies in quarter-core and the neutronic characteristics of the assemblies (these characteristics are calculated by the SRAC code, see Table 2). Since the quarter-core has 10 positions, the number of input

features will be a multiple of 10. There are a variety of ways to select the input features including: fuel assemblies (assemblies index) corresponding to 10 positions in 1/4 core, k-inf of the assemblies corresponding to the 10 position, enrichment of the assemblies corresponding to the 10 position, combination of the k-inf and the enrichment corresponding to the 10 positions, ... Table 3 presents some examples of input features selection. The influence of input features on the prediction results were investigated and shown in Section 3.2.

Table 3. Samples of input features selections

Number of input features	**Case of features**	**Sample**
10	assembly index	3, 3, 4, 3, 4, 2, 2, 4, 2, 3
10	assembly k-inf	1.306, 1.306, 1.356, 1.306, 1.356, 1.221, 1.221, 1.356, 1.221, 1.306
10	assembly enrichment	3.4, 3.4, 4.45, 3.4, 4.45, 2.35, 2.35, 4.45, 2.35, 3.4
20	k-inf and enrichment	1.306, 1.306, 1.356, 1.306, 1.356, 1.221, 1.221, 1.356, 1.221, 1.306 3.4, 3.4, 4.45, 3.4, 4.45, 2.35, 2.35, 4.45, 2.35, 3.4

The MLP network consists of 4 hidden layers with the number of nodes per layer being 256, 512, 512, 256 respectively. Dropout classes with 10% probability are inserted between hidden layers to avoid overfitting during training. The sigmoid function will be used as the activation function. The output layer only has one node to predict one type of output (k-eff or peaking factor). The using only one node at the output layer allows to best evaluate the effectiveness of the ANN for predicting each neutronic characteristic of reactor. This means that k-eff and peaking factor are predicted by 2 different models. The structure of the MLP network is present in Figure 5.

Layer (type)	Output Shape	Param #
dense (Dense)	(None, 256)	2816
dropout (Dropout)	(None, 256)	0
dense_1 (Dense)	(None, 512)	131584
dropout_1 (Dropout)	(None, 512)	0
dense_2 (Dense)	(None, 512)	262656
dropout_2 (Dropout)	(None, 512)	0
dense_3 (Dense)	(None, 256)	131328
dropout_3 (Dropout)	(None, 256)	0
dense_4 (Dense)	(None, 1)	257

Total params: 528,641
Trainable params: 528,641
Non-trainable params: 0

Figure 5. MLP neuron network structure

III. RESULTS AND DISCUSSION

3.1. Survey of number of trained loading patterns

In this section, effect of number of trained loading patterns on the accuracy of predicted outputs was surveyed. This survey is performed in order to determine the minimum suitable number of trained LPs for k-eff and peaking factor prediction problems. The features of input include k-inf of assemblies arranged in one-fourth of LP, it mean that input LPs have 10 features associated with k-inf of assemblies in 10 position of the one-fourth of core. The number of trained LPs is varied from 1000 to 15000 with the step of 1000. Size of validation set and test set are kept as 3800 and 1000, respectively. The number of epochs is 200. In this survey, each case was run three times and the results were averaged.

Figure 6 shows the survey results of loss functions values and deviation of predicted and real outputs. Minimum of training losses and validation losses of the all cases after 200 epochs of training processes have been collected and shown in sub-figures (a) and (b). In each case, the model with minimum of validation loss has been chosen to predict the outputs for 1000 LPs of the test set. The average absolute deviations and the maximum absolute deviations of the 1000 LPs are shown in sub-figures (c) and (d). One can see that the loss values and deviation values decrease as the number of trained LPs increase. The loss values decrease slowly after 3000 and 6000 trained LPs in the problem of k-eff prediction and peaking prediction, respectively. In these numbers of trained LP, the values of maximum absolute deviation of k-eff are 1315pcm and 912pcm, meanwhile the values of maximum absolute deviation of peaking factor are 12.15 and 8.5%. These deviations are much larger than the deviation between core simulations code.

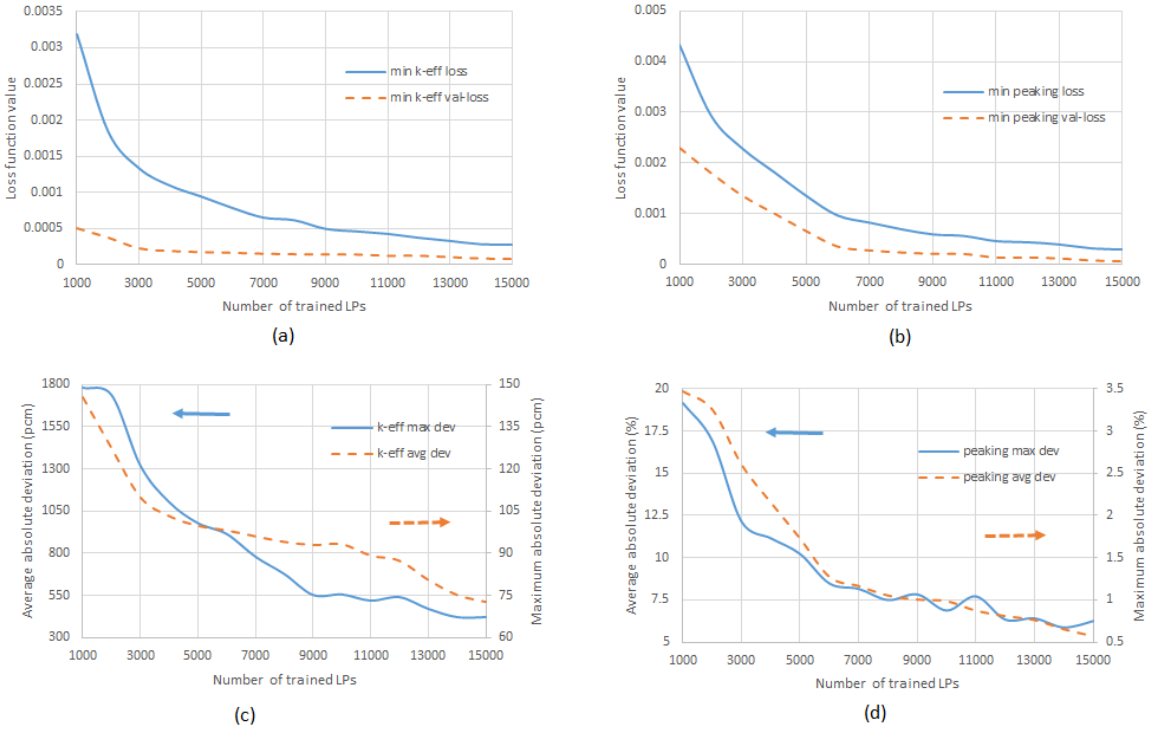

Figure 6. Dependency of loss function values and predicted outputs accuracy on number of trained LPs. Minimum of training loss and validation loss in k-eff prediction (a) and peaking prediction (b); average and absolute deviation in k-eff prediction (c) and peaking prediction (d)

For deeply evaluation, the training processes were increased to 500 epochs for the two cases in which the input numbers are 3000 and 6000. Table 4 shows the comparison of the two cases of 3000 and 6000 trained LPs and the case of all trained LPs (15200 LPs). The minimum loss function values are average of three runs for each case and the deviations are aggregated from predictions for the 1000 test LPs. The results show a decrease of the loss functions and the deviations when increasing the number of trained LPs. In all cases, the average deviations of k-eff and peaking factor are comparable with other reactor core simulators. In the case of 3000 trained LPs, however, the maximum deviation of k-eff and peaking factor are quite large (640pcm and 1.66%) when compare the predictions for the 1000 test LPs). One can see that the prediction results are acceptable agreement with SRAC2006 when the number of trained LPs is at least 6000 LPs. In other words, MLP models can be trained well with at least 6000 LPs in this problem. Nevertheless, the following chapters will present the results of the model trained with the entire training set (15200 LPs) so that the best performance of the model can be seen.

Table 4. Comparison of cases with different number of trained LPs

Parameters	**k-eff**			**Peaking factor**		
Number of trained LPs	3000	6000	15200	3000	6000	15200
Minimum of training loss function	5.8E-04	2.7E-04	1.5E-04	7.4E-04	2.9E-04	1.0E-04

Minimum of validation loss function	1.5E-04	7.8E-05	4.4E-05	2.7E-04	7.0E-05	1.7E-05
Average of absolute deviations (%)	0.095	0.069	0.054	1.185	0.565	0.280
Maximum absolute deviations (%)	0.640	0.269	0.208	7.665	5.651	2.444

3.2. Survey of input features

The number of input features also affect to the accuracy of machine learning models. In this research, each loading pattern includes 10 positions of fuel assemblies. Each fuel assembly also have many features such as assembly index, k-inf, enrichment, macroscopic cross-sections,... Therefore, the number of input features can be chosen is a multiple of 10, depending on the number of features of fuel assemblies that we want to use for the prediction. The previous calculations only used k-inf of the assemblies as the input features. In this section, a survey of input features is performed to evaluate the influence of input features on the prediction results.

The calculations have been performed for five cases included three cases of one feature per assembly (assembly index, k-inf, enrichment), one case of two features per assembly (k-inf and enrichment) and one case of all features of assemblies (k-inf, enrichment, group constants). Number of epochs is set to 500 and number of trained LPs is 15200 to ensure the best prediction resutls. The results are averaged over three runs per case and presented in Table 5. It can be seen that the accuracy of predictions decreases when the number of input features increase. In the cases of one feature per assembly, k-inf input feature gives worse prediction results than the index and enrichment features. This may be because the k-inf of the assemblies are not so different (see Table 2) that it is more difficult to predict based on this feature.

The results of all cases also show good agreement with SRAC2006 in the both of average absolute deviation (< 50pcm in k-eff and < 0.3% in peaking factor) and maximum absolute deviation (< 300pcm in k-eff and < 2.5% in peaking factor). Therefore, MLP neuron network can be used to predict well k-eff and peaking factor based on one or more features of the fuel assemblies (even using only the fuel assembly index). In the next section, the two features k-inf and enrichment of the assemblies will be used to build the MLP models for predicting k-eff and peaking factor of the reactor. This choice ensures both training speed and accuracy of the model.

Table 5. Comparison of number of input features

output	**Parameter**	**input features**				
		Index	**k-inf**	**enrichment**	**k-inf, enrichment**	**all**
k-eff	Minimum of training loss function	1.14E-04	1.43E-04	1.12E-04	9.78E-05	6.33E-05
	Minimum of validation loss function	1.34E-05	4.15E-05	1.33E-05	8.73E-06	8.87E-06

	Average of absolute deviations (%)	0.028	0.049	0.027	0.024	0.022
	Maximum absolute deviations (%)	0.153	0.290	0.181	0.227	0.284
peaking	Minimum of training loss function	9.85E-05	1.00E-04	1.00E-04	8.15E-05	5.99E-05
	Minimum of validation loss function	1.27E-05	1.60E-05	1.46E-05	4.16E-06	2.91E-06
	Average of absolute deviations (%)	0.274	0.285	0.269	0.127	0.091
	Maximum absolute deviations (%)	2.004	2.419	1.811	1.996	1.885

3.3. Predicting k-eff and peaking factor using MLP neuron network

This section shows the training process and prediction results of the two best models including the k-eff prediction model and the peaking factor prediction model. The input features include k-inf and enrichment of assemblies. The models were trained in 500 epochs and the values of loss and validation loss functions during the training process are shown in Figure 7. The best models are the ones with the smallest validation loss functions. Both training processes of k-eff and peaking factor converge after 450 epochs. In the figure, overfittings do not occur due to the large amount of training data and the dropout algorithm in the MLP neuron network architecture.

After 500 epochs, two models with the lowest validation loss value were chosen as the best models. The two best models were used to predict k-eff and peaking factor of 1000 test LPs (the LPs did not use in training and validating processes). The results of comparison with SRAC2006 code are presented in Figure 8 and Table 6. It can be seen that the deviations of k-eff are mostly between -50pcm to 50pcm and the deviations of peaking factor are mostly between -0.4% to 0.4%. The maximum deviation of k-eff and peaking factor are 268pcm and 1.764%, respectively. These results show good agreement between the MLP models and SRAC2006 code. In addition, MLP models only need about 5 seconds to compute for 1000 LPs, while the time required for SRAR is about 1 hour. Therefore, it can be seen that when there are enough data for training, MLP models are able to predict k-eff and peaking factor of nuclear reactor accurately and at high speed.

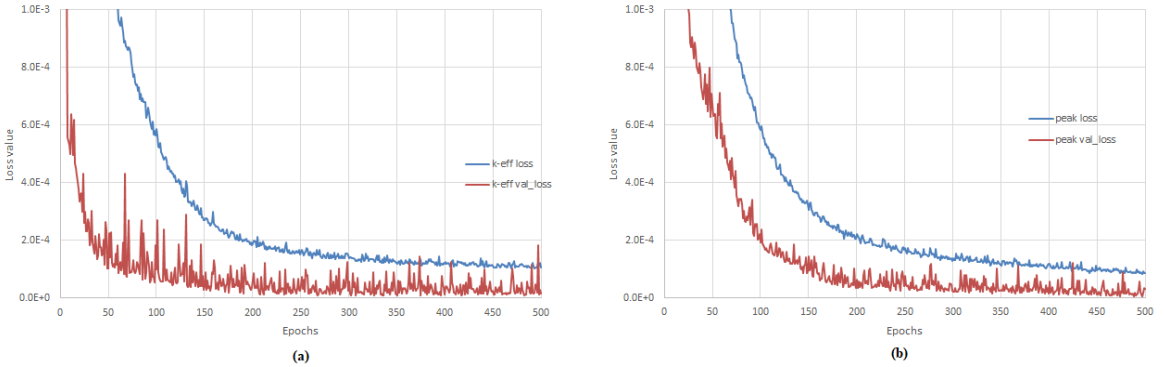

Figure 7. Loss and validation loss functions during training process of k-eff prediction model (a) and peaking factor prediction model (b).

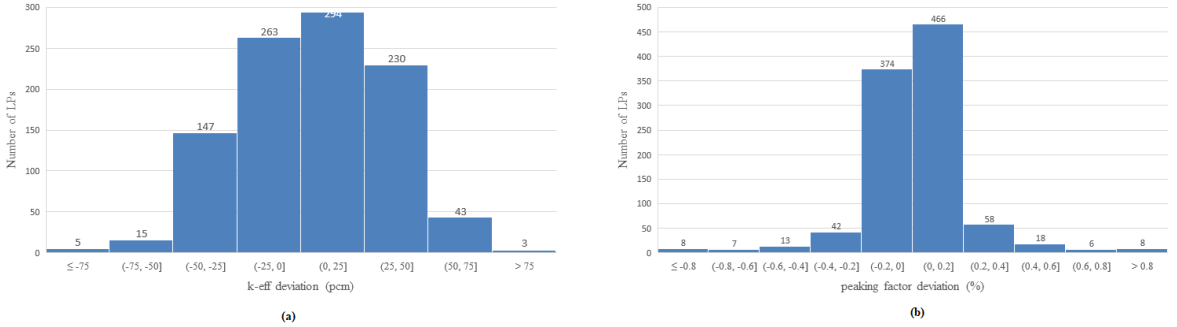

Figure 8. Deviation distribution of k-eff prediction (a) and peaking factor prediction (b) predicted by the best models

Table 6. Summary results of the best models

Parameters	k-eff	peaking
Loss function of the best models	1.01E-04	8.15E-05
Validation loss function of the best models	8.73E-06	4.16E-06
Average of absolute deviations (%)	0.024	0.135
Maximum absolute deviations (%)	0.268	1.764

IV. CONCLUSIONS

This study has built a MLP network structure to apply to predict k-eff and peaking factor of SMR reactor. The MLP network consists of more than 500000 parameters with 1 input layer, 4 hidden layers and 1 output layer with 1 output. A dataset of 20000 LPs and necessary features has been calculated by SRAC2006 code to train the MLP network. The dataset was divided into test set (1000 LPs), validation set (3800 LPs) and test set (15200 LPs). The trained model was used to predict the k-eff and peaking factor of the test set and compared with the results of SRAC2006 to evaluate the accuracy of the models.

The survey results show that it takes about 6000 LPs to train MLP models with acceptable accuracy. When there is enough training data, models can use only 1 or more features of the fuel assembly to train the model while maintaining accuracy. The best MLP models show a good agreement with SRAC2006 code. Calculations for 1000 test LPs show that the average and maximum deviations of k-eff are 24pcm and 268pcm, respectively, and the average and maximum deviations of peaking factor are 0.135% and 1.764%, respectively. In addition, the calculation speed of MLP models outperform SRAC2006 code (5 seconds vs 3600 seconds for 1000 LPs). These show great promise for applying machine learning models to nuclear reactor research, design and operation.

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NGHIÊN CỨU ÁP DỤNG MẠNG THẦN KINH NHÂN TẠO ĐỂ DỰ ĐOÁN K-EFF VÀ HỆ SỐ ĐỈNH CÔNG SUẤT CỦA LÒ PHẢN ỨNG MÔ ĐUN NHỎ LOẠI NƯỚC ÁP LỰC

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Tóm tắt: Học máy (ML) sử dụng các phương pháp mạng thần kinh nhân tạo đang được ứng dụng mạnh mẽ trong nghiên cứu lò phản ứng hạt nhân. Nó được sử dụng để dự đoán các tham số cần thiết dựa trên việc học hỏi từ các bộ dữ liệu lớn có trước. Các mô hình ML cho tốc độ tính toán nhanh hơn rất nhiều trong khi độ chính xác tốt và thậm chí có thể tốt hơn các công cụ tính toán thông thường. Do đó, trong nghiên cứu này, một mạng Perceptron nhiều lớp được xây dựng để dự đoán k-eff và hệ số đỉnh công suất của vùng hoạt lò phản ứng mô đun nhỏ loại PWR. Kết quả thu được được so sánh với chương trình SRAC2006 để đánh giá hiệu suất của mô hình học máy. Kết quả tính toán cho thấy độ chính xác và hiệu suất cao của các mô hình học máy.

KEYWORDS: *lò mô đun nhỏ, học máy, mạng thần kinh nhân tạo, mạng Perceptron nhiều lớp*