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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 applied to predict required parameters for nuclear reactors based on learning from big data sets. The ML models usually give faster calculation speed while the accuracy is good agreement with physical simulators. In this work, a multi-layer perceptron network was built and trained to predict k-eff and peaking factor of a small modular pressurized water reactor (PWR). The results are compared with those obtained by using a reactor physics code system, i.e. SRAC2006. The comparison shows good agreement accuracy and higher performance of the ML 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 a lot to replace simulation tools in predicting necessary parameters in the reactor such as kinetic parameters, power distribution, and thermal-hydraulic [1]-0 The nuclear reactor is a multi-physics system with complex geometries, thus simulating and calculating reactor parameters necessitates the use of complex, computationally intensive programs and is time-consuming. Meanwhile, studies on applying ML, especially artificial neural networks (ANN) show the great potential in building high-performance precision simulation tools for nuclear reactors with a simple algorithm, acceptable accuracy, and calculation speed is greatly increased. However, for specific problems, ML models still need to be studied and improved to achieve appropriate accuracy 0-0 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 0

This study applies a multi-layer perceptron (MLP) neuron network 0 to predict k-eff and peaking factor for the small modular PWR. The dataset used to train the model is generated by the SRAC2006 code 0, 0. MLP neural network structure is built and trained to achieve good agreement accuracy when compared with simulation results. Studying the necessary features to train the model as well as

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reduce the size of the dataset while ensuring the accuracy of the model are also performed.

II. METHODOLOGY

A. Core modeling and data preparation

The small modular PWR used in the current study is a 200 MW thermal reactor with a simplified core containing 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 central instrument tube arranged on a 17x17 grid. The fuel pellets made of UO_2 with three different U-235 enrichments (2.35 wt%, 3.40 wt%, and 4.45 wt%) are loaded into three types of assemblies named F235, F340, and F445, respectively. The characteristics of the fuel assemblies and the PWR core are given in Table 0.

Table I. Main parameters of the small modular PWR core

Parameters	Values
Reactor thermal power, MW	200
Number of fuel assemblies	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 enrichments, wt%	2.35, 3.40, 4.45
Fuel temperature, K	1145
Average coolant temperature, K	583
Operation pressure, MPa	15.5

To create the training dataset for ML, the neutronic parameters of the reactor core have been calculated by using SRAC2006. This is a deterministic code system with many modules used to calculate various types of thermal reactors 0, 0. It has been validated for core calculations of small modular PWRs through several studies 0, 0. The advantage of this code is fast calculation speed while still ensuring accuracy in comparison with other codes. Therefore, this code is appropriate to calculate a large number of loading patterns (LPs) to create training dataset for ML.

In SRAC2006, the calculations for fuel assemblies are performed by module PIJ with a quadrant symmetry model. Each fuel rod is divided into five annular zones (three fuel zones, one gap zone between fuel and cladding, and one cladding zone). The guide tubes are also divided into 5 zones with four water zones, and one cladding zone. The assembly model is shown in Fig. 1.

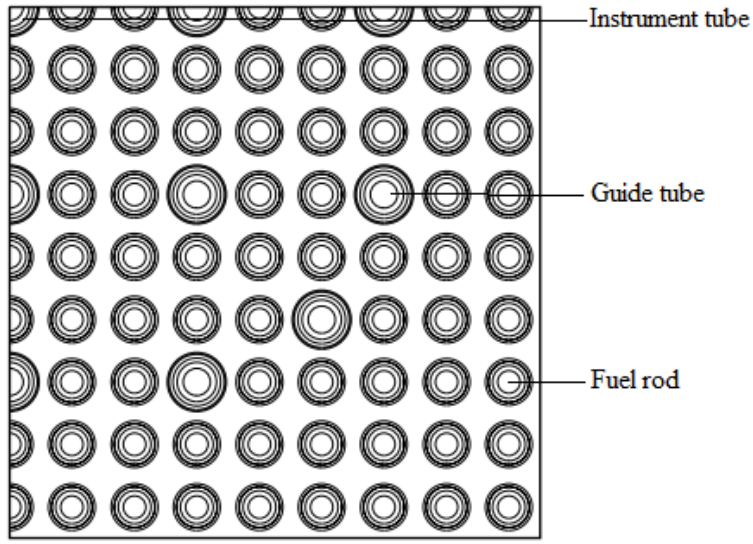


Fig. 1. PWR assembly model (quarter symmetry)

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

Table II. Features of assemblies

Assembly	Index	Enrichment (wt%) U-235	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
F340	2	3.40	1.306	1	1.686E-03	1.577E+00
				2	8.478E-03	8.230E-01
				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 Fig. 2. The core contains 37 fuel assemblies arranged with quadrant symmetry. Thus, at each position of a quarter-core, one of three fuel assembly types is randomly placed to create different LPs. To make the training dataset for the ML 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 cycle. In the following sections, the dataset will be divided into 3 parts including a test set (1000 LPs ~ 0.5 % of dataset), a validation set (3800 LPs ~ 20 % rest of the dataset), and a training set (15200 LPs).

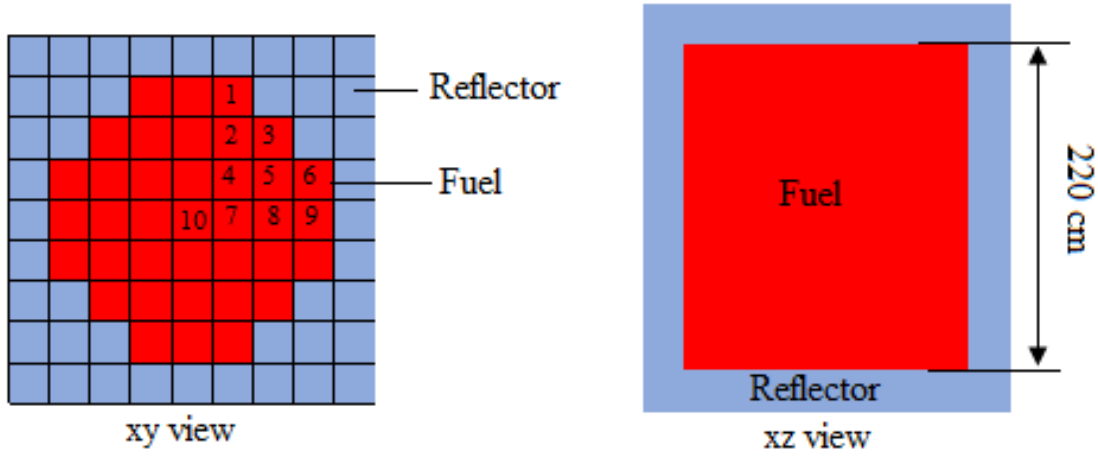


Fig. 2. Core model in CORENBN code

B. Multilayer perceptron neuron network

The multilayer perceptron (MLP) is a type of artificial neural network (ANN) consisting of multiple layers of interconnected artificial neurons or nodes (Fig. 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 input signals received from the previous layer. Introduction of activation functions within these nodes allows for non-linear transformations of the signals, enabling the MLP to model intricate relationships beyond the limitations of linear classifiers.

A perceptron (node) is inspired by structure of neurons, which is illustrated in Fig. 4. The computation in each node is performed in two steps. Firstly, the input data is summed by weight:

$$s = \sum w_i x_i + b \quad (1)$$

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:

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

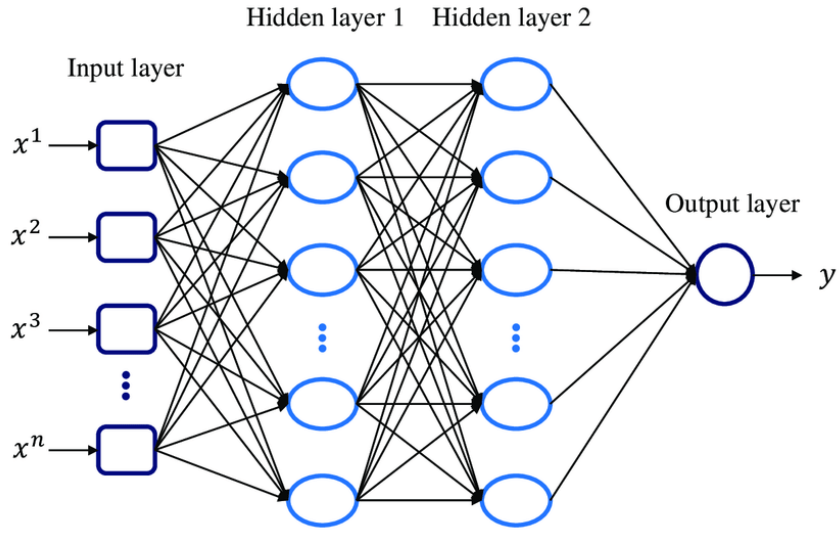


Fig. 3. Multilayer perceptron illustration

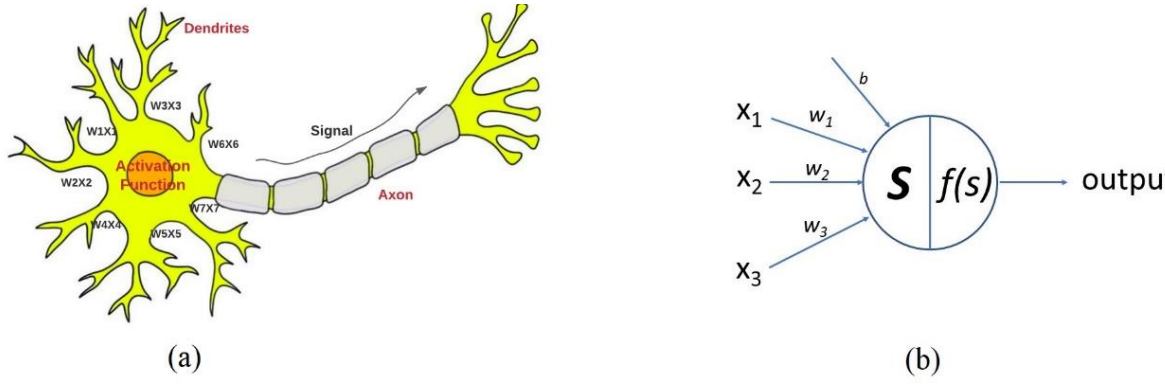


Fig. 4. Neuron (a) and perceptron (b) illustration

In this study, the MLP network structure was built based on some preliminary surveys and experiences of the research team. The number of nodes in the input layer is equal to the number of considered input features. The input features include the arrangement of the fuel assemblies in a quarter core and the neutronic characteristics of the assemblies (these characteristics are calculated by the SRAC2006 code, see Table). Since there are 10 positions in a quarter core, 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 a quarter core, k-inf of the assemblies corresponding to the 10 positions, enrichment of the assemblies corresponding to the 10 positions, combination of the k-inf and the enrichment corresponding to the 10 positions, … Table III 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 III. Samples of input features selections

Number of input features	Case of features	Sample
10	Assemblies index	3, 3, 4, 3, 4, 2, 2, 4, 2, 3
10	Assemblies k-inf	1.306, 1.306, 1.356, 1.306, 1.356, 1.221, 1.221, 1.356, 1.221, 1.306
10	Assemblies 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, and 256 respectively. Dropout classes with 10 % probability was inserted between hidden layers to avoid overfitting during training. The sigmoid function was used as the activation function. The output layer only has one node to predict one type of output (k-eff or peaking factor). Using only one node at the output layer allows the best evaluation of the effectiveness of the ANN in predicting each neutronic characteristic of the reactor. This means that k-eff and peaking factor were predicted by 2 different models. The structure of the MLP network is presented in Table IV.

Table IV. MLP neuron network structure

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

III. RESULTS AND DISCUSSION

A. Survey of number of trained loading patterns

In this section, the effect of number of trained loading patterns on the accuracy of predicted outputs was surveyed. This survey is performed 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, which means that input LPs have 10 features associated with k-inf of assemblies in the 10 positions of a quarter of the core. The number of trained LPs is varied from 1000 to 15000 with a step of 1000. The size of the 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.

Fig. 5 shows the survey results of loss function values and deviation of predicted and real outputs. Minimum of training losses and validation losses of all cases after 200 epochs of training processes have been collected and shown in the sub-figures (a) and (b). In each case, the model with minimal 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 when the number of trained LPs increases. The loss values decrease slowly after 3000 and 6000 trained LPs in the problem of k-eff prediction and peaking factor prediction, respectively. In these numbers of trained LP, the values of maximum absolute deviation of k-eff are 1315 pcm and 912 pcm, 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 simulation codes.

For deep evaluation, the training processes increased to 500 epochs for the two cases in which the input numbers was 3000 and 6000. Table V 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 showed a decrease in 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 (640 pcm and 1.66 %) compared to the predictions for the 1000 test LPs. As it can be seen the prediction results was in anacceptable 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 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.

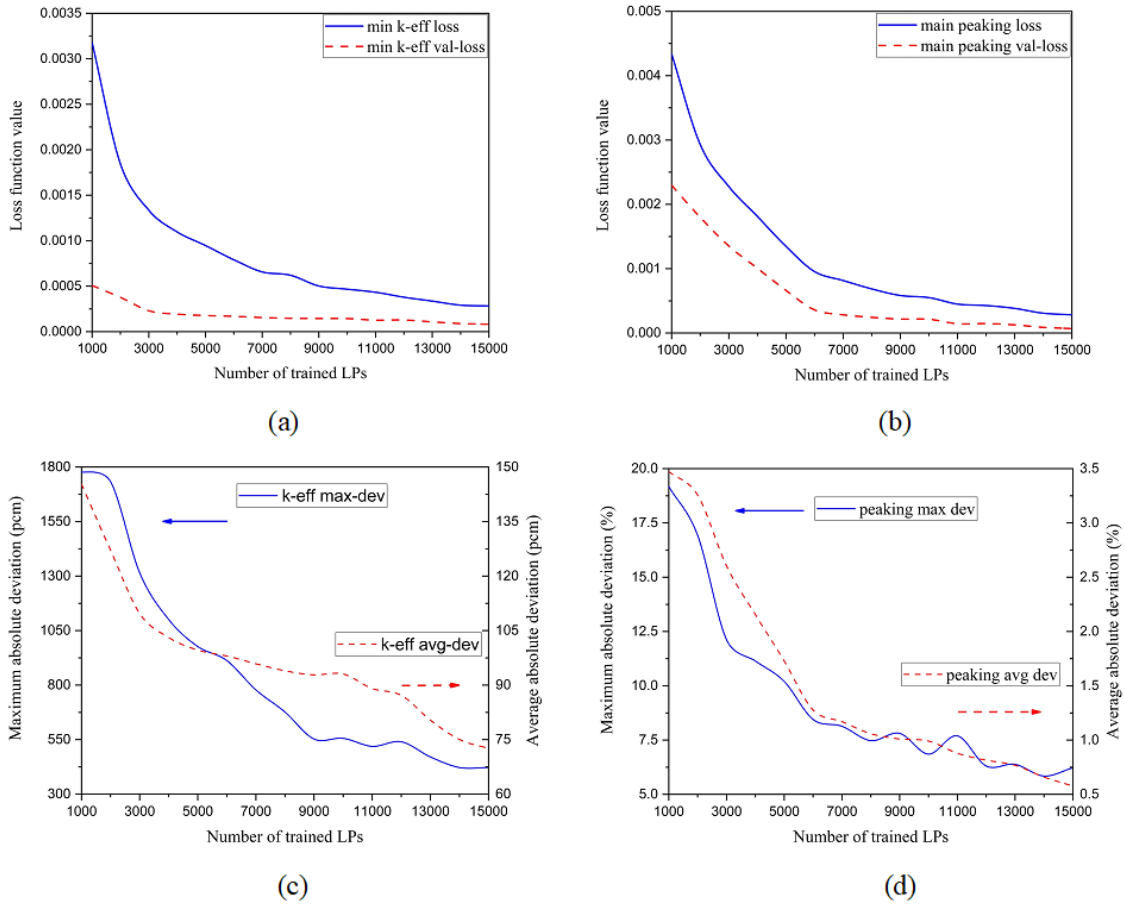


Fig. 5. Dependency of loss function values and predicted output accuracy on number of trained LPs. Minimum of training loss and validation loss in k-eff prediction (a) and peaking prediction (b); average and absolute deviation in k-eff prediction (c) and peaking prediction (d)

Table V. 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

B. Survey of input features

The number of input features also affects to the accuracy of ML models. In this research, each loading pattern includes 10 fuel assembly positions. Each fuel assembly also has many features such as assembly index, k-inf, enrichment, and macroscopic cross-sections, etc. 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 including 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 results. The results are averaged over three runs per case and presented in Table VI. It can be seen that the accuracy of predictions decreases when the number of input features increases. In the cases of one feature per assembly, the 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 II), so it is more difficult to predict based on this feature.

The results of all cases also show good agreement with SRAC2006 in both of average absolute deviation (< 50 pcm in k-eff and < 0.3 % in peaking factor) and maximum absolute deviation (< 300 pcm in k-eff and < 2.5 % in peaking factor). Therefore, the 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 the training speed and accuracy of the model.

Table VI. Comparison of number of input features

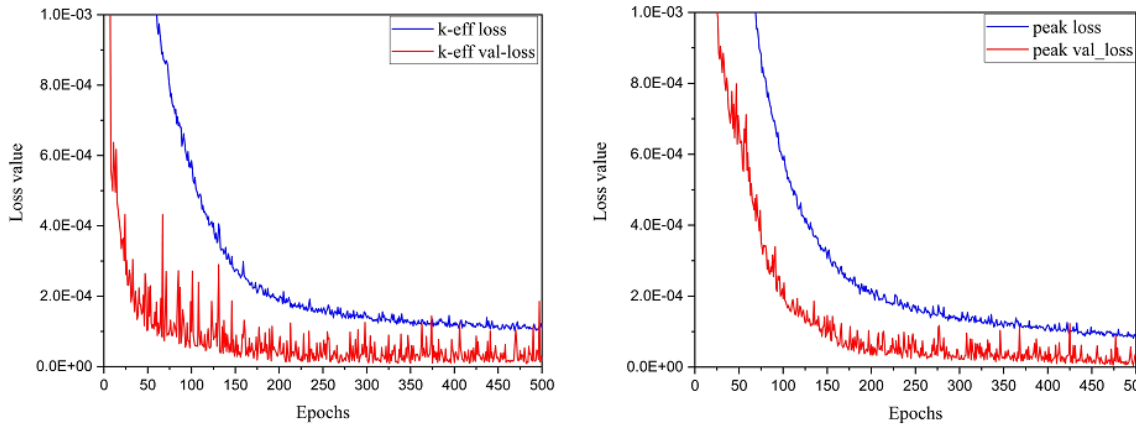
Output	Parameter	Input features				
		Index	k-inf	enrichment	k-inf, enrichment	all
k-eff	Minimum of training loss function	1.14E-04	1.43E-04	1.12E-04	9.78E-05	6.33E-05
	Minimum of validation loss function	1.34E-05	4.15E-05	1.33E-05	8.73E-06	8.87E-06
	Average of absolute deviations (%)	0.028	0.049	0.027	0.024	0.022
	Maximum absolute deviations (%)	0.153	0.290	0.181	0.227	0.284
Peaking factor	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

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

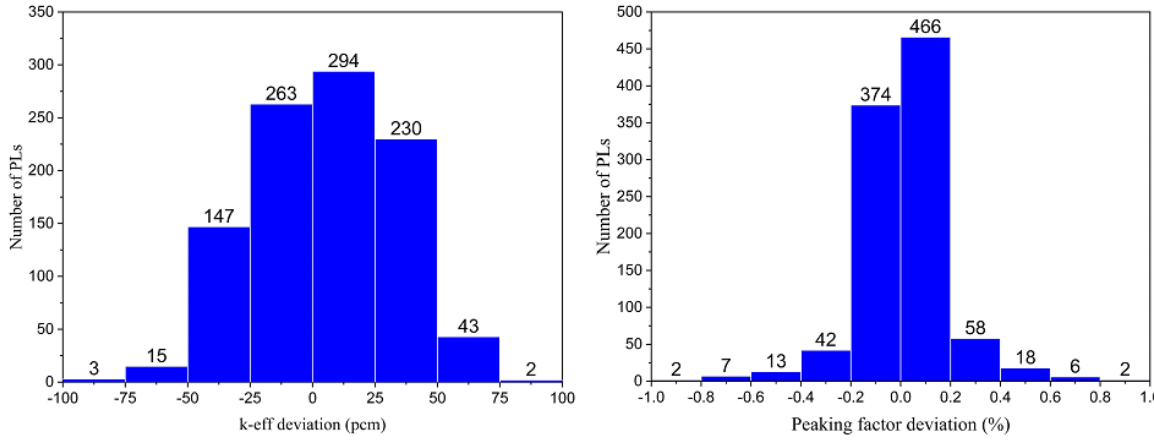
This section shows the training process and prediction results of the two best models including the k-eff prediction model and the peaking factor prediction model. The input features include k-inf and enrichment of assemblies. The models were trained in 500 epochs and the values of loss and validation loss functions during the training process are shown in Fig. 6. 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 were not used in training and validating processes). The results of the comparison with SRAC2006 code are presented in Fig. 7 and Table VII. It can be seen that the deviations of k-eff are mostly between -50 pcm to 50 pcm and the deviations of peaking factor are mostly between -0.4 % to 0.4 % (Fig. 8). The average deviations for k-eff and the peaking factor are 0.024 pcm and 0.135%, respectively, while their maximum deviations are 268 pcm and 1.764% (Table 7). These results show good agreement between the MLP models and SRAC2006 code. In addition, MLP models only need about five seconds to compute for 1000 LPs, while the time required for SRAC2006 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.



(a) (b)

Fig. 6. Loss and validation loss functions during training process of k-eff prediction model (a) and peaking factor prediction model (b).



(a) (b)

Fig. 7. Deviation distribution of k-eff prediction (a) and peaking factor prediction (b) predicted by the best models

Table VII. Summary results of the best models

Parameters	k-eff	peaking
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 predict k-eff and peaking factor of the small modular PWR core. 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 traning 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 24 pcm and 268 pcm, respectively, and the average and maximum deviations of peaking factor are 0.135 % and 1.764 %, respectively. These show great promise for applying machine learning models to nuclear reactor research, design, and operation.

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