Neural Network Surrogates for Predicting Core Characteristics throughout the Equilibrium Cycle

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1. Introduction

In recent years, loading pattern (LP) optimization research has focused on the application of artificial intelligence, which can reduce the computational cost of the optimization or search improved loading patterns that the conventional optimization procedures have difficulty to find. Since the number of possible LPs is extremely large and the evaluation of each candidate requires expensive core physics calculations, neural network surrogate models have been widely employed as fast evaluation tools in the optimization frameworks.

Most of the previous core surrogate models represent a fuel assembly with its composition or instantaneous state data such as the assembly averaged enrichment and the number of burnable absorber rods [1,2] or the few-group homogenized cross sections evaluated at the beginning of cycle (BOC) [3]. These inputs lack information on the neutronic characteristics that vary with burnup; thus, it may be difficult for a single model to predict the core characteristics at every burnup step. Consequently, the previous studies either made the prediction only at BOC or trained separate models at each burnup point.

In an equilibrium cycle core, the once and twice burnt assemblies are loaded together with the fresh ones, so the burnup information is essential for the prediction. In this work, the burnup dependent infinite multiplication factor (k_∞) curve and the pin power form function of each assembly, which are obtained from the lattice calculation, are used as the inputs of the core surrogate model to provide the burnup information. The two-step procedure is performed with DeCART2D and MASTER, and the convolutional neural network (CNN) based surrogate models are developed for both steps. This is intended to reduce the computational cost of the entire procedure, and at the same time, the core characteristics of the equilibrium cycle are predicted at every burnup step by a single model. The framework is demonstrated for an APR-1400 core loaded with LEU+ fuels of up to 7.0 wt.% enrichment.

2. Lattice Surrogate Model

2.1 Network architecture

The lattice surrogate developed in this work replaces the DeCART2D calculation in the two-step procedure and provides the k_∞ curve and the burnup-dependent pin power form function required by the core surrogate. The two quantities are predicted by two convolutional neural networks with task-specific structures, as illustrated in **Fig. 1**. The input is a set of 8×8 pin map channels in which each pin position is characterized by its U-235 enrichment and its Gd_2O_3 content. The design variables of **Table I**, together with the derived quantities such as the assembly average enrichment and the total Gd loading, form a separate condition vector. This vector is encoded by a small fully connected network and injected into every convolution block through the feature wise linear modulation (FiLM) layers [4], which scale and shift the convolutional feature maps so that a single network covers the whole range of the design variables.

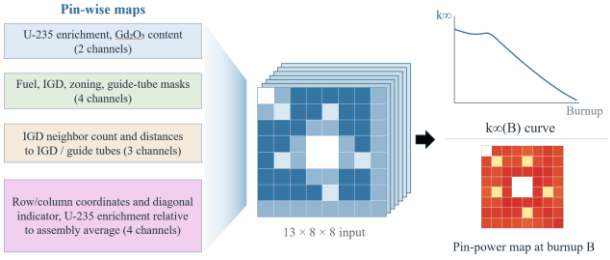


Fig. 1 Pin-wise input encoding and outputs of the lattice surrogate model

Table I. Sampling ranges of the design variables

Design variable	Range / values
Fuel enrichment (wt.%)	5.0–7.0
Enrichment difference of zoned pins (wt.%)	0.4–0.8
IGD U enrichment (wt.%)	3.0–4.3
Gd_2O_3 content (wt.%)	6–10
Number of IGD	12 / 16 / 20 / 24
Zoning pattern	2 types

2.2 Training data

The training data is comprised of 1,022 DeCART2D calculations sampled by the Latin hypercube method over the design variable ranges summarized in **Table I**. The 1,022 assemblies are split into 862 training and 160 validation cases, and the outputs from this lattice surrogate model are the k_∞ and pin power distribution for 62 burnup points.

2.3 Validation results

Table II summarizes the prediction accuracy over the 160 validation assemblies, each evaluated at 62 burnup points, which gives 9,920 assembly and burnup point samples. **Figs. 2 and 3** show the corresponding error distributions. The k_∞ error is 11.6 pcm on average and remains below 60 pcm at the 99th percentile, and the error of the peak pin power is of the order of 10^{-4} in the normalized power unit.

Table II. Lattice surrogate validation accuracy

Parameter	Mean	P95	P99	Max
$\|\Delta k\infty\|$ (pcm)	11.6	35.2	59.6	128.0
Peak pin power difference	0.0001	0.00028	0.00045	0.0014

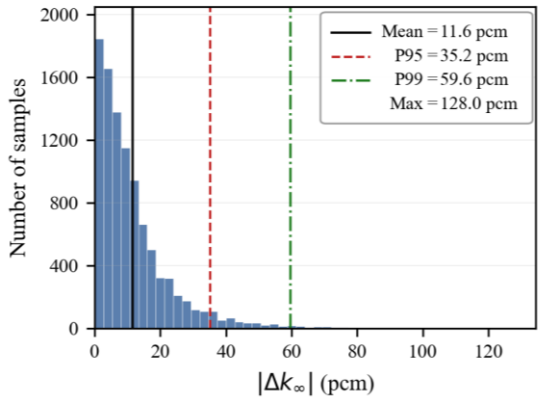


Fig. 2 k_∞ prediction error distribution

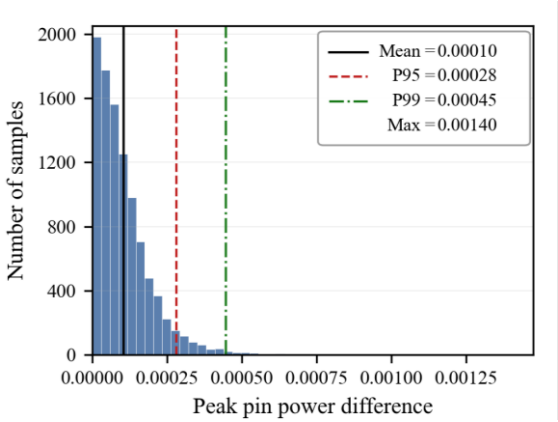


Fig. 3 Peak pin power prediction error distribution

3. Core Surrogate Model

The core surrogate replaces the MASTER calculation. It receives the burnup-dependent lattice responses supplied by either the lattice surrogate or DeCART2D and predicts the radial power peaking factor (F_r) and the cycle length throughout the equilibrium cycle.

3.1 Overall prediction procedure

For the equilibrium cycle core, the BOC burnup is zero for fresh assemblies, whereas once and twice burnt assemblies retain the burnup accumulated during their previous cycles. The BOC burnup of each loaded assembly is therefore required to evaluate the burnup-dependent core characteristics. However, this burnup distribution is determined by the power history and shuffling history of the assemblies and is not available for a newly proposed equilibrium loading pattern.

The prediction begins with an approximate BOC burnup map constructed from the shuffling history. A first-stage BOC burnup network corrects this initial map, which is then refined through a fixed-point iteration. At an iteration m, the normalized power of each assembly is predicted at every burnup step and integrated over the cycle to calculate its burnup. For a reloaded assembly, the BOC burnup for the next iteration is calculated as

$$B_i^{(m+1)} = B_{src(i)}^{(m)} + G_{src(i)}^{(m)} \quad (1)$$

where src(i) denotes the previous-cycle location of the assembly loaded at node i, and $B_{src(i)}$ and $G_{src(i)}$ are its BOC burnup and predicted cycle burnup gain at that location, respectively. The BOC burnup of a fresh assembly remains zero. Each iteration therefore represents one approximate equilibrium cycle calculation followed by assembly shuffling. In this validation, four fixed-point updates were used, giving a BOC burnup RMSE of approximately 0.4 GWd/MTU.

The refined BOC burnup map is used to construct the burnup-dependent inputs at each burnup step. Using the input representation and network architecture described in **Section 3.2**, the core surrogate predicts the maximum F_r at each step and the cycle length in EFPD. **Figure 4** summarizes the overall procedure of the core surrogate model.

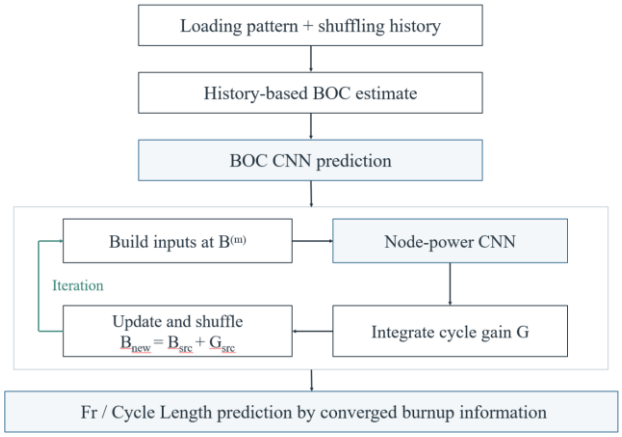


Fig. 4 Overall core surrogate prediction procedure

3.2 Input encoding and network architecture

An LP at burnup step s is encoded as a 9×9 quarter core map with 40 channels per node, as shown in Fig. 5. The first 11 channels are obtained by interpolating the assembly k_∞ curve at ten burnup points offset by {−24, −12, −6, −3, 0, +3, +6, +12, +24, +48} GWd/MTU from the current burnup in **Eq. (1)**, together with the value of the same curve at zero burnup, which identifies the assembly design. The next 11 channels contain the corresponding samples of the pin-power form function. A further 11 channels provide the k_∞ samples associated with the previous-cycle location, and the remaining 7 channels describe the shuffling history and core geometry.

The prediction models use the fully convolutional residual architecture described in **Fig. 5**. A 3×3 convolutional stem expands the 40 input channels to 96 feature channels, followed by five residual blocks with squeeze-and-excitation channel attention [5] and a prediction task (i.e. F_r, EFPD) specific 1×1 convolutional layer. Separate networks are trained for BOC burnup, assembly power, F_r, and cycle-length prediction, with approximately 0.9 million trainable parameters per network.

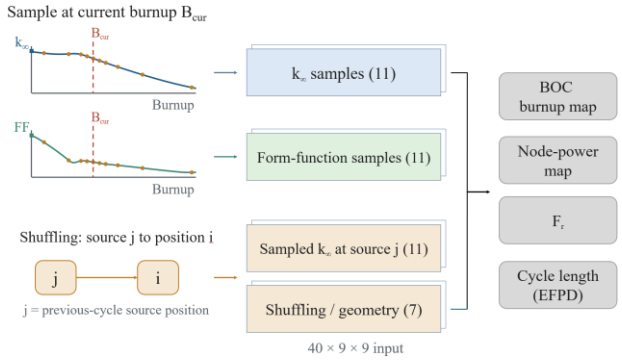


Fig. 5 Burnup-dependent input encoding and outputs of the core surrogate models

3.3 Training procedure

Training data comprise 20,740 equilibrium-cycle LPs evaluated with MASTER during surrogate-assisted genetic algorithm optimization of the core loading pattern, corresponding to 550,415 burnup-step samples. The data were split 90/10 at the LP level so that the accuracy of the core surrogate could be evaluated on unseen LPs.

The networks are trained with AdamW under smooth L1 loss functions. During training of the final prediction networks, Gaussian noise with a standard deviation of 2 GWd/MTU was added to the true BOC burnup of the once and twice burnt assemblies to reduce sensitivity to residual errors in the estimated BOC burnup. The dataset is expanded through active learning, and the models are retrained when new assembly types are introduced.

4. Results

4.1 Prediction accuracy

Table III compares the prediction errors obtained using the BOC burnup map converged through the fixed-point iteration with those obtained using the true BOC burnup from MASTER. The comparable errors under the two conditions show that the residual error in the estimated BOC burnup has small effect on the F_r and cycle length predictions. The LPs are composed of the assembly types of **Table I** that appear in the training dataset, with F_r and cycle lengths within the trained range of 1.50 to 1.60 and 550 to 700 EFPD (1,455 LPs) respectively.

Table III. Core surrogate validation accuracy

Parameter	BU	Mean	P95	P99	Max
$\|\Delta F_r\|$	Fixed-point	0.006	0.021	0.044	0.068
	True	0.006	0.021	0.044	0.060
|ΔEFPD|	Fixed-point	0.6	3.1	5.2	6.0
	True	0.6	3.0	5.2	6.0

4.2 Comparison of Input Representation

Three input representations were compared to examine their influence on the accuracy of the core surrogate. The first consists of the k_∞ depletion curves and pin-power form functions described in **Section 3.2**. The second consists of the assembly compositions, including the fuel enrichments, number of IGD, and Gd_2O_3 content. The third consists of two group homogenized cross sections interpolated at the current burnup of each node. The same training data, LP level split, network body, and training conditions were used for all three models.

Table IV compares the F_r and cycle length errors of the three input representations using the true BOC burnup obtained from MASTER. The k_∞ curve and cross section inputs give nearly the same F_r errors, while the

composition input gives a larger error. The three inputs give comparable cycle-length errors. The k_∞ depletion curves and pin power form functions are used in the present model because they are directly generated and validated by the lattice surrogate described in **Section 2**.

Table IV. Comparison of input representations

Core parameter	k_∞	Composition	Cross sections
$\lvert\Delta F_r\rvert$	0.0060	0.0101	0.0071
$\lvert\Delta$EFPD$\rvert$	0.50	0.61	0.42

5. Conclusion

This study developed convolutional neural network surrogate models for the DeCART2D/MASTER two-step procedure. The core surrogate predicts the equilibrium cycle core characteristics at every burnup step from the burnup dependent k_∞ curves and pin power form functions of the loaded assemblies, rather than from the composition alone or from the lattice information evaluated at a single burnup point. The BOC burnup map of the once and twice burnt assemblies is first estimated from the shuffling history and then refined through an equilibrium cycle iteration. This procedure enables the core surrogate to evaluate a new LP without requiring the true BOC burnup distribution from a preceding MASTER calculation.

The lattice surrogate predicts k∞ with a mean absolute error of approximately 12 pcm. Using BOC burnup estimated with the fixed point iteration, the core surrogate predicts F_r and cycle length with mean absolute errors of 0.006 and 0.6 EFPD, respectively. Three input representations were compared using the true BOC burnup. The k_∞ curve and homogenized cross section inputs gave similar F_r errors, whereas the composition input showed less accurate predictions. These results indicate that burnup dependent lattice information is more suitable than composition alone for predicting the equilibrium cycle behavior. Since the k_∞ curves and pin power form functions are directly generated by the lattice surrogate, they provide a consistent interface between the lattice and core models. In conclusion, it is expected that the proposed surrogate system can effectively replace the lattice and core calculations using computer codes in LP optimization studies, in which a large number of candidates must be evaluated.

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