# Macroscopic Cross-Section Generation for Nodal Code RAST-K Using Artificial Neural Network

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## 1. Introduction

Artificial Neural Networks (ANN) proved their effectiveness in solving various complex problems in numerous fields of knowledge, including nuclear reactor design and analysis. One of the most popular ways to use ANN in nuclear field is to replace numerically accurate reactor design computer codes with surrogate models that are capable of predicting target output parameters at a much faster speed. The trade-off of using ANN in this case is the uncertainty in the trained model that introduces an error in the final result. However, in some cases the accuracy requirement is not as strict as the requirement to obtain a result quickly. For example, a new reactor design requires many hundreds of human hours in order to find an optimal or nearly optimal fuel design and fuel loading pattern (LP) configuration. An optimal LP search involves numerous trials of possible LP configurations using computationally intensive and time-consuming reactor design codes. Some of those LPs could have been filtered out using ANN prior to running a more accurate computer code.

In our previous writings [1], we discussed the applicability of a convolutional neural network (CNN) to prediction of various core design parameters. Though this approach is quite efficient for predicting various safety and design-related parameters, the trained ANN model is not versatile, i.e. it cannot be used for a different reactor type with a different number of fuel assemblies (FA) or different fuel configuration. To solve this problem, we can use a hybrid approach, which is based on the idea of finding the most computationally demanding parts and replacing them with an ANN model.

In this study, we are working with our in-house nodal diffusion code RAST-K [2]. As explained in the reference, this code is part of a two-step computation system. The first step is to generate macroscopic cross-sections (XS) using some lattice physics code. The second step is to solve a nodal diffusion equation implemented in RAST-K using those XS. The most computationally intensive component in this system is the first – XS generation – part of the process. In addition to that, the core geometry is being specified in the RAST-K part of the two-step code system, which means that we can replace the lattice code with a surrogate ANN model and predict the XS set required for solving a nodal diffusion equation regardless of the target core geometry.

## 2. Model description

The idea of XS generation using ANN is not new. The authors of the ref. [3] applied various machine learning (ML) techniques for predicting XS data for a certain reactor model. However, they are not using some of typical lattice code input parameters (such as fuel enrichment, fuel geometry) for training their models. Though their result shows very small difference with the actual solution, it might be limited by the particular fuel rod arrangement and enrichment that was implicitly built into their training data.

In order to avoid those limitations, we decided to apply the input parameters that are very similar to those used in a typical lattice physics code. However, we introduce our own limitations that we are planning to address in future studies. In particular, we are only modeling XS data for fresh fuel, and we are testing the XS data only for the beginning of cycle (BOC) calculation in our code RAST-K. The training and testing datasets were generated using our in-house deterministic code STREAM [4]. We modelled various fuel enrichments and fuel rod locations in the core as shown in Figure 1. At the same time, we did not model fuel with burnable poisons and control rods in this study. Finally, we did not add the variable fuel rod pitch and fuel pellet thickness as we are planning to address this in our future works.

The ANN model of our choice is a deep neural network (DNN) with 5 fully connected layers. Though we are not using any more complicated techniques such as CNN, we decided to apply the Barcode model [1] for our input data arrangement, listing all fuel rods in one straight line while keeping a strict order of sequence. The FA geometry in our study is a typical 16*16 rectangular FA. In order to address the guide tube input in this geometry, we decided to replace the guide tubes with equivalent fuel rod cells that have no fuel. As a result, our input parameters are listed in one line as follows: temperature of fuel (average), temperature of moderator, boron concentration, and a list of all fuel rod enrichments given in a one-line sequence as they appear in one octant of a FA shown in Figure 1. The output parameters are the following: 2-group diffusion coefficients, 2-group scattering XS, 2-group absorption XS, 2-group fission XS, 2-group nu-fission XS, 2-group kappa-fission XS, $k_{inf}$. After the model was trained, an independent testing set of XS was modelled and predicted, and later used in RAST-K input for comparing the actual outcome of using predicted XS.

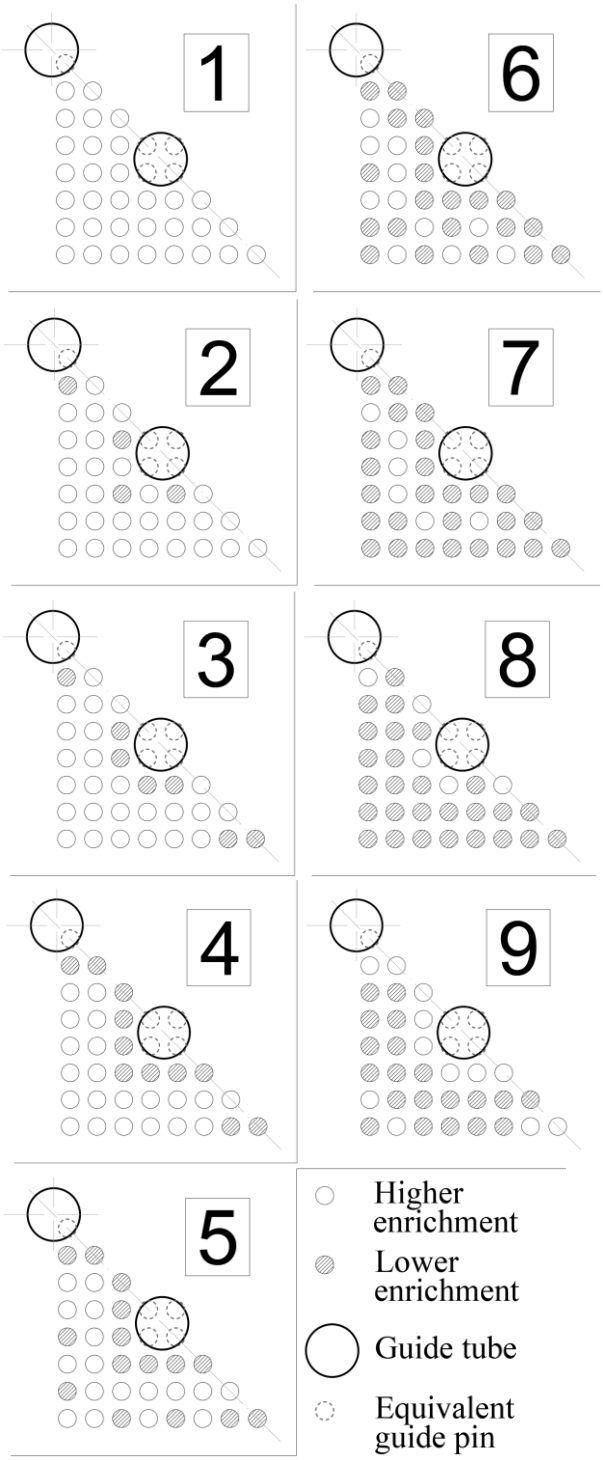


Fig. 1. Geometry of fuel assemblies used in this study.

### 3. Simulation and results

The training dataset consists of 108,000 unique FA samples with non-duplicate input parameters as explained in the previous section. The loss function used in this model is Huber loss [5]. Adam [6] optimizer was chosen for having a dynamically changing learning rate. In order to avoid overfitting, an additional 13,000 sample validation dataset was applied. The best model over 2,000 training epochs was saved based on the lowest value of the loss function for validation dataset.

For testing, an independent unseen dataset consisting of 13,800 FA input/output samples was prepared. For evaluation of the testing prediction results, the values of Mean Relative Error (%) for each predicted parameter were calculated. The entire model was built using TensorFlow [7].

As stated in the previous section, after the XS data was predicted, it was applied to RAST-K input files using automated Python scripts. Two sets of input data were created for each testing sample. RAST-K calculation with pre-defined XS data for BOC takes less than 1 second per input file, which shows the reasoning behind leaving the nodal code calculation instead of making an entire prediction using a more complex ANN. The time of XS prediction was found around 1 second or lower for all 13,800 testing XS sets. At the same time, the XS calculation using a lattice code could take up to a minute for a single set of input parameters, and much longer than that for hundreds or thousands sets of XS (known as branch calculations) required for a nodal code.

For this study, we decided to model a reactor core similar to OPR-1000 core. However, since XS data is generated regardless the reactor core type, we could apply our ANN model for predicting XS for any reactor that is using 16*16 FA type. In future works, we are planning to expand our study on XS generation for burnup calculation as well as to add other types of geometry etc., as was explained in the section 2 of this paper. The RAST-K model geometry used in this study is shown in Figure 2. It consists of FAs of the same type without axial and radial reflectors. The boundary conditions (BC) for the model are: fully reflected for the western and the northern directions, vacuum for all other directions. The results of the XS prediction and RAST-K simulation are shown in Table I.

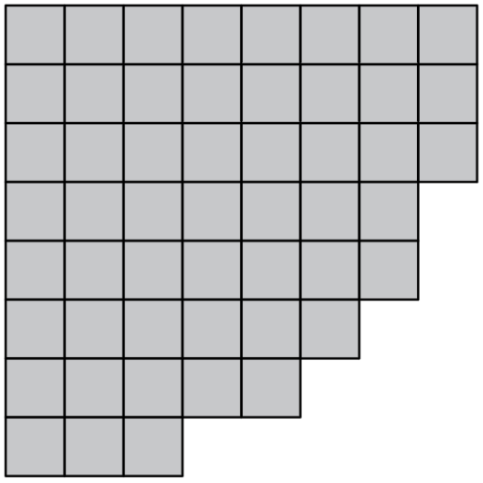

Fig. 2. A quarter-core OPR-1000 input geometry for RAST-K. All used fuel assemblies are of the same type.

Table I: Results of DNN XS prediction and RAST-K simulation.

| Parameter | MRE, % |
|---|---|
| XS data prediction – DNN vs STREAM | |
| Diffusion coefficient $D_1$ | 0.184 |
| Diffusion coefficient $D_2$ | 0.092 |
| Macroscopic absorption XS group 1 | 0.111 |
| Macroscopic absorption XS group 2 | 0.156 |
| Macroscopic scattering XS group 1 | 0.141 |
| Macroscopic fission XS group 1 | 0.113 |
| Macroscopic fission XS group 2 | 0.087 |
| nu*Macroscopic fission XS group 1 | 0.062 |
| nu*Macroscopic fission XS group 2 | 0.181 |
| kappa*Macroscopic fission XS group 1 | 0.139 |
| kappa*Macroscopic fission XS group 2 | 0.258 |
| Infinity multiplication factor $k_{inf}$ | 0.063 |
| RAST-K Simulation – comparison of XS | |
| Multiplication factor $k_{eff}$ | 0.203 |
| Excess reactivity rho | 0.016 |

As shown in Table I, the results of XS prediction stay way below 1%. The result of RAST-K simulation also stays close to the reference obtained using XS generated in lattice code. Finally, the values of power distribution were determined during RAST-K calculation. The relative difference in power distribution for the case with the highest $k_{eff}$ difference is shown in Figure 3.

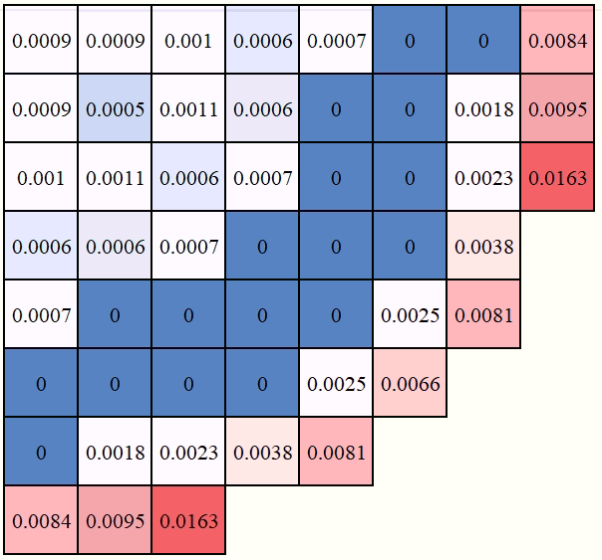


Fig. 3. Relative difference (%) in power distribution calculated using RAST-K for the XS sets based on the STREAM-generated XS vs the ANN-generated XS.

The values of power distribution indicate much lower difference than the previously determined values of $k_{eff}$.

All in all, the results demonstrate that it is possible to use XS data generated using ANN for calculations that need to be done quickly and do not require an accurate result. Our nearest goal for future works is to add variable FA geometry and to expand our XS prediction model for predicting XS for various burnup points.

## 4. Conclusions

In this study, we performed a preliminary study on generating macroscopic XS data for our nodal code RAST-K using a DNN model. We found that XS data could be predicted using a simple ANN model and input parameters common for a lattice physics code. The advantage of using ANN is the speed of XS prediction, which is noticeably faster than a comparable calculation using a deterministic code. The mean relative difference of predicted XS data against the calculated XS data was found much below 1%, and the eigenvalue calculation using the predicted data showed the difference below 1% compared to the eigenvalue calculated with the actual XS data. The relative difference for the power distribution values was found noticeably lower than the one for the eigenvalue calculation. This result could be appealing for some purposes, as we discussed in the Introduction of this paper.

In our future studies, we are planning to add other types of FAs, burnable poison rods/Gadolinia rods, control rods, and improve our neural network model so that it could generate XS data for burnup and transient calculations.

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