Neural Network Approach to Model Mixed Oxide Fuel Cycles in Cyclus, a Nuclear Fuel Cycle Simulator

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INTRODUCTION

Nuclear fuel cycle simulators (NFCSs) are fundamental in guiding policy and economic decisions regarding nuclear fuel cycle (NFC) options. This paper introduces a new method to predict the mixed oxide fuel (MOX) criticality value using an artificial neural network (ANN) model, while most current NFCSs use simple MOX fabrication estimations that do not account for burnup effects.

The authors generated over one million depletion simulation results of MOX fuel with varying plutonium vectors and plutonium content to train an ANN network to predict the fuel's Beginning of Cycle (BOC) and End of Cycle (EOC) criticality. Results show that the trained ANN can predict criticality of MOX fuel within 1% error compared with the test data. The trained ANN is implemented into Cyclus, an agent-based NFC, to demonstrate capabilities to model dynamic reactor behavior such as reactor power and incoming plutonium vector variation. This paper concludes with the discussion of the shortcomings of the ANN approach and potential ways to mitigate them.

BACKGROUND AND MOTIVATION

The NFC is a complex system of facilities and material mass flows that are combined to provide nuclear energy for use in society, usually in the form of electricity [1]. NFCSs are system analysis tools used to investigate issues related to the dynamics of a NFC.

Due to their large-scale nature, NFCSs cannot implement high-fidelity physics models since the computational burden becomes excessive. Functionalities in a NFCS are specific models that substitute the behavior of the NFC facility (e.g., reactor, enrichment plant). The functionality highlighted in this paper is mixed fuel fabrication. Functionalities in a NFCS can be divided into two large categories: static and dynamic. Static modeling methods are user inputs that define fixed behavior for a facility model, while dynamic modeling methods use the user's input and facility parameters (e.g., material inventory) to calculate or approximate facility model behavior (Fig. 1).

For once-through fuel cycles, the composition of materials in each stage does not change because the fuel cycle is linear. This makes modeling of the once-through cycle simple, as the material composition in each stage is static. Due to this static nature, simple methods such as fixed depleted compositions, or *recipes*, are good approximations.

However, for a closed NFC, loops created by the reprocessing plant cause the reactor's incoming and outgoing material composition to be dynamic, making simple, static assumptions such as the recipe method a poor approximation [2]. Additionally, the variation in reactor discharge composition changes separated fissile stream composition from the reprocessing plant, which then varies the fissile content in the fuel created by the fuel fabrication facility for a critical fuel. For investigating the state-of-art for these functionalities, three NFCSs are primarily investigated: Cyclus [3], ORION [4], and CLASS [5].

METHODS FOR MOX FUEL FABRICATION

In a NFC, the MOX fuel fabrication plant receives a separated fissile stream such as a plutonium or a transuranic (TRU) stream, as well as a fertile (e.g., depleted uranium) stream. The goal of the MOX fuel fabrication functionality is to find a mixing ratio of the two streams that will make a *fit* MOX fuel.

The *fit*ness of MOX fuel has three layers:

1. Front-end: does the MOX fuel contain enough fissile material?
2. Back-end: does the MOX fuel remain critical after a certain burnup?
3. Core average: does this MOX batch have the criticality required by the reactor?

Methods for modeling MOX fuel fabrication in a NFCS are shown in Table I.

For the recipe-based method, the user enters a fissile fraction, and the NFCS always mixes the fuel to the specified

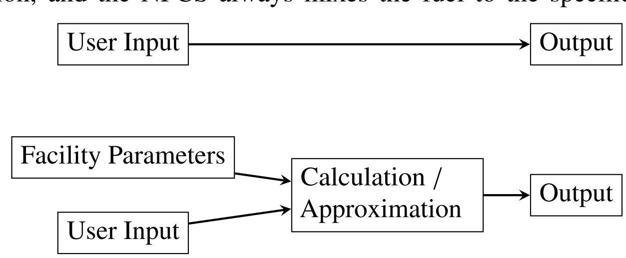

Fig. 1: Logical flow differences between a fixed modeling method (top) and a dynamic modeling method (bottom) for NFCSs.

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fraction. For the equivalent fissile worth method, a cross section library is provided by the user, and the NFCS calculates the mixing ratio to fulfill a certain equivalent fissile threshold. The equivalent fissile value method is used by Cyclus and ORION and is an effective method to take into account the changing plutonium vectors in a NFC simulation. However, there are two shortcomings of the equivalent fissile value method:

1. The equivalent fissile value does not indicate the fuel's criticality, and
2. The equivalent fissile value method does not take into account effects of burnup on the fuel.

Therefore, the equivalent method only partially addresses the first layer of the *fit*-ness of MOX.

Database interpolations methods employ a large database of MOX data to find the appropriate mixing ratio. This method can be effective, but the accuracy depends on the scope of the database and lacks in flexibility.

Surrogate Method Approach

A surrogate method approach for MOX fabrication employs a surrogate model (regression model) for approximating the appropriate mixing ratio for MOX fuel.

Leniau et al. [6] developed an ANN to predict the required plutonium content and to predict depleted MOX fuel compositions in CLASS. Leniau et al. trained the model to predict the plutonium content in fresh fuel, given the plutonium vector, uranium stream enrichment, and maximum burnup (Fig. 2). The model predicts a plutonium content for the MOX fuel that remains critical after the maximum burnup, satisfying the second layer of the *fit*-ness of MOX. However, the ANN architecture is designed so that the EOC criticality criteria are hard-coded into the ANN, so the ANN is specific about its question and thus is not flexible in its implementation to the NFCS.

The method herein aims to implement similar capabilities, with improvements in flexibility and robustness—mainly to increase the implementation flexibility of the trained ANN model by making the ANN architecture less problem-specific. The ANN architecture in this work is set up so that the model predicts the BOC and EOC k_{inf} values of the MOX, with high-resolution burnup steps (Fig. 3). This modification to the ANN design allows flexible implementation of the ANN to address the third layer of the *fit*-ness of MOX.

METHOD

The workflow for this effort is as follows:

1. Generate data with SCALE/TRITON [7]
2. Perform data curation
3. ANN Perform training and testing
4. Implement into Cyclus

TABLE I: Methods for MOX fuel fabrication in an NFCS.

Static Modeling	Dynamic Modeling
· Fixed fraction	· Cross section + equivalent fissile worth · Database interpolation · **Surrogate models**

Cyclus is used for implementation of the created ANN since its source code is freely available on Github.

Data Generation and Curation

In this effort, 200,000 SCALE TRITON cases were run on MOX assemblies with constrained, randomly generated plutonium vectors with random plutonium content in the MOX (Fig. 4). The process began from a separated plutonium vector with an isotopic composition randomly sampled. Then the ^{241}Pu vector was decayed for a time between 0 to 9 years (randomly sampled uniformly) to obtain the final plutonium vector for MOX fabrication. The randomly generated plutonium vector is mixed with depleted uranium for varying plutonium content (4% to 10%). For each MOX assembly composition, a SCALE/TRITON input file was created and run. Twenty-five burnup steps, up to 72 GWd/MTHM, were used per input, making 5 million data points. A python script parsed all the output files for the k eigenvalues (Fig. 5) and the depleted compositions.

ANN Training and Testing

The neural network is trained with the Keras python package [8]. The first ANN was designed to predict the criticality of a MOX assembly before and after irradiation (Fig. 3). For the ANN model, a separate hyperparameter optimization was run to optimize the number of hidden layers, neurons per layer, and activation functions. The data were split 60-20-20, where 60 is the training set, and the other two sets are for hyperparameter search and final model testing (Table II). The workflow is as

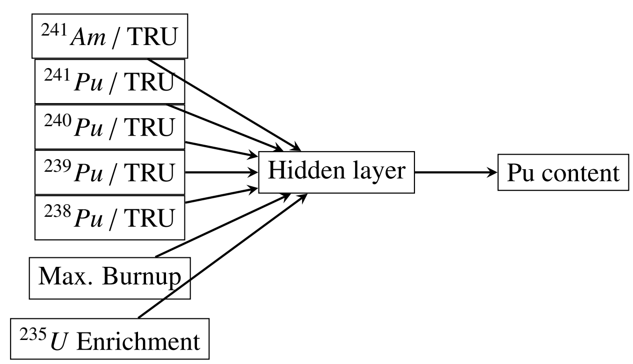

Fig. 2: ANN architecture used to predict plutonium content in fresh fuel, by Leniau et al. [6]

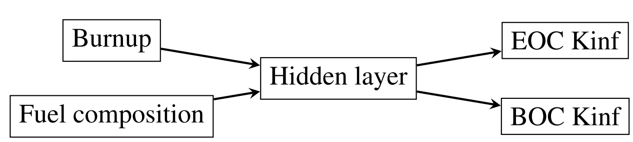

Fig. 3: ANN architecture used in this work.

follows:

1. Neural network is trained on the training set (60% of data).
2. Prediction error is measured with the validation set (20% of data).
3. A hyperparameter set with the lowest prediction error is selected.
4. Test set is used to test final model.

For the criticality prediction, over 97% of predictions have errors less than 0.5% compared with the test data (97% for EOC, 99% for BOC).

RESULTS

The fuel fabrication and reactor models are implemented into Cyclus, and the capabilities are demonstrated for a three-batch reactor (Table III) with a given plutonium fissile stream (Table IV). The burnup of the fuel is grouped by batches. This reactor burns fuel to

$$\frac{3000\text{MWth} * (18 * 3 * 30)\text{days}}{(24 * 3)\text{MTHM}} = 67,500\frac{\text{MWth} \cdot d}{MTHM}.$$

The reactor parameters and plutonium stream were varied in the tests to show the adaptability of the dynamic MOX fabrication model.

The reactor's power output was varied from 800 to 1,200 MWe to demonstrate the effect of different reactor power rates on MOX fuel demand and criticality over a cycle (Fig. 6). The decrease in criticality by burnup is followed by a sudden increase, which is by refueling. At the refueling time, the reactors require a fuel with a k_{inf} value to reach the objective core-averaged k value. Therefore, higher power reactors require MOX fuel with higher TRU content (Fig. 7). The abnormal behavior for 600 MWe at timestep 54 is due to the model underestimating the EOC k_{inf} of the MOX assemblies, thereby requesting a high k_{inf} batch. Varying the cycle length would have the same effect, as a longer cycle length increases TRU content in the incoming MOX fuel. Different fuels have dif-

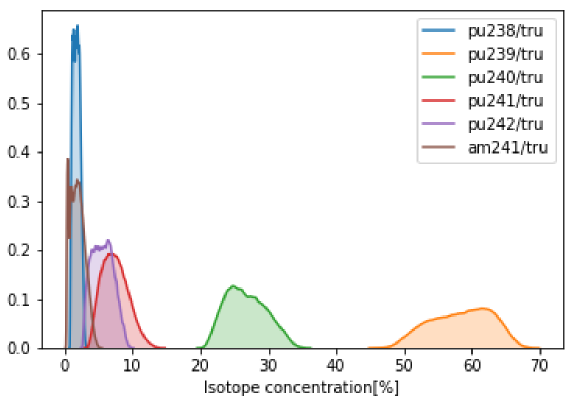

Fig. 4: Histogram of plutonium vector distribution. Differences in shape are due to the different ranges of potential compositions.

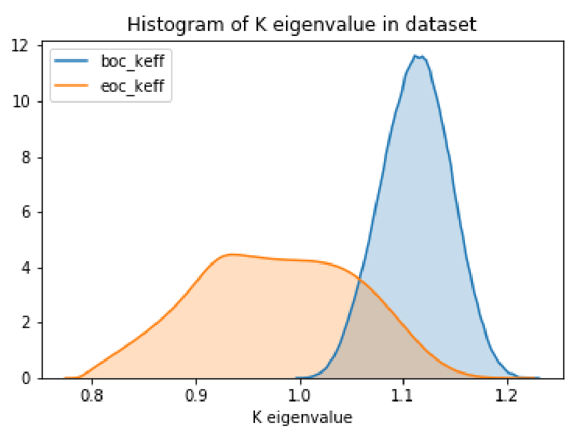

Fig. 5: BOC and EOC k eigenvalue distribution in the data

TABLE II: Input, Hidden, and Output Layer of the ANN Used for MOX Fabrication Modeling in This Work.

Input Layer	Hidden Layers	Output Layer
^{235}U ^{238}U ^{238}Pu ^{239}Pu ^{240}Pu ^{241}Pu ^{242}Pu ^{241}Am Burnup	3 Hidden Layers (Dense) X 27 Neurons per Layer (activation fcn. RELU)	BOC k_{inf} EOC k_{inf}

TABLE III: Reactor Parameters Used for Testing

Parameter	Units	Value
No. Batches		3
Batch Mass	MTHM	24
Reactor Power	MWe	1,000
Efficiency	%	33.3
Cycle Time	months	18
Refuel Time	months	0
Target k_{inf}		1.10

TABLE IV: Plutonium Vector Used for Testing

Isotope	Composition [%]
^{238}Pu	1.83
^{239}Pu	48.57
^{240}Pu	31.85
^{241}Pu	9.14
^{242}Pu	8.13
^{241}Am	0.48

ferent sensitivities to burnup ($\frac{\delta k}{\delta BU}$), which causes dips in TRU content.

A fundamental function of a fuel fabrication model is to account for the change in the plutonium vector to adjust TRU content in the MOX fuel. In a modeled scenario in which the incoming plutonium stream increased in ^{239}Pu and decreased in ^{240}Pu with time, the fuel fabrication output MOX fuel with lower TRU content, with higher fissile quality of the incoming plutonium stream (Fig. 8).

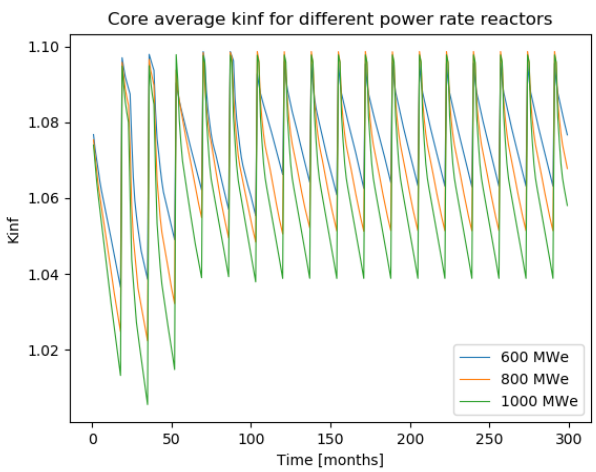

Fig. 6: Core average k_{inf} value for reactor with 800, 1,000, and 1,200 MWe power rates. Lower power rates lead to lower k_{inf} value demands for new MOX fuel.

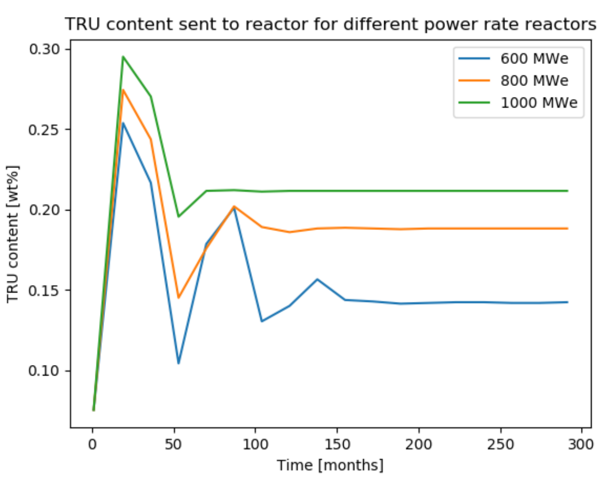

Fig. 7: TRU content of incoming MOX fuel for reactor with 800, 1,000, and 1,200 MWe power rates. Lower power rates lead to a lower k_{inf} value demand, resulting in a lower TRU content for incoming MOX fuel.

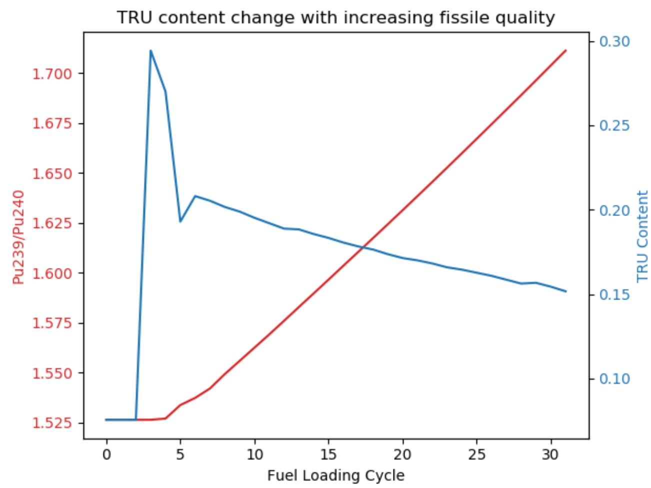

Fig. 8: The Pu vector is varied to have more ^{239}Pu and less ^{240}Pu to demonstrate the impact of higher fissile quality Pu in fuel fabrication. Higher fissile quality of incoming Pu stream leads to lower TRU content.

DISCUSSION

This work demonstrates a rapid and effective method to model a MOX fabrication and reactor in a large-scale fuel cycle simulator. Implementing an ANN model to predict BOC and EOC kinf from an initial composition vector allows the fabrication plant to adjust the criticality of the outgoing MOX batch to fulfill the varying need of the reactor. This approach improves upon the previously existing equivalence models by being able to reflect the MOX reactors' varying power rates (burnup rates) and the varying batch-wise MOX criticality demand.

Improvements can be made by generating more data on MOX criticality calculations that span a wider range of potential plutonium vectors and TRU content in MOX fuel. A physics-informed cost function can also be implemented during the training of data to prevent the model from making unnatural calculations. Also, non-deep learning algorithms such as linear regressions can be implemented to make predictions for unfamiliar data. Finally, the dimensionality reduction method can be employed to reduce the complexity of the ANN.

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