# Deep learning surrogate model for fuel performance analysis

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## 1. Introduction

Nuclear reactor dynamics is a complex phenomenon involving Core Neutronics (CN), Thermal Hydraulics (TH) and Fuel Performance (FP) modeling. Nuclear design requires this Multiphysics analysis to be performed to enhance safety and optimize fuel consumption. CN is responsible for capturing alterations in fuel composition and power distribution within the core. TH, on the other hand, deals with the transfer of heat from the cladding wall to the coolant. The FP analysis delves into the temporal behavior of fuel rods and the heat transfer from the fuel centerline to the outer cladding. Notably, no single code possesses the capacity to comprehensively model all these phenomena.

To tackle these challenges, Multiphysics coupling modules have been devised, allowing for the simultaneous study of various physics phenomena by incorporating insights from other physics models. Of all the various physics models, the FP model stands out as one of the most resource-intensive in terms of both time and memory consumption. Within the Multiphysics framework, it is the FP model that accounts for the dynamic gap heat conductance from the pellet to the cladding. This dynamic gap has a significant impact on a multitude of safety parameters, as it models the mechanical interactions between the pellet and the cladding.

Efforts have been undertaken to introduce surrogate models for FP in the context of depletion and transient analysis [1, 2]. The objective of this research is to develop a deep learning (DL) surrogate model tailored to replace the FP module within the Multi Physics Core (MPCORE) coupling code developed at Ulsan National Institute of Science and Technology (UNIST). Presently, the model is equipped to execute Hot Zero Power (HZP) Rod Ejection Accident (REA) simulations at the Beginning of Cycle (BOC). Notably, the surrogate model's construction does not account for the burnup effect, resulting in improved results due to the uniform initial burnup across all fuel rods.

## 2. Methods and Results

### *2.1 MPCORE Framework*

MPCORE is Multiphysics external coupling framework developed at CORE lab UNIST [3]. The purpose of this framework is to couple codes modeling different physical phenomena and give accurate feedback to other models. Among the coupled codes, CN code is RAST-K (RK) [4], CTH1D and CTF [5] are two TH codes and FRAPTRAN [6] is the only FP code used for transient analysis. FP code FRAPTRAN used for transient analysis calculate the fuel pellet, cladding temperatures, gap width and gap conductance. Among the RK-CTH1D-FP coupled simulation, approximately 70% of the time is taken by FP.

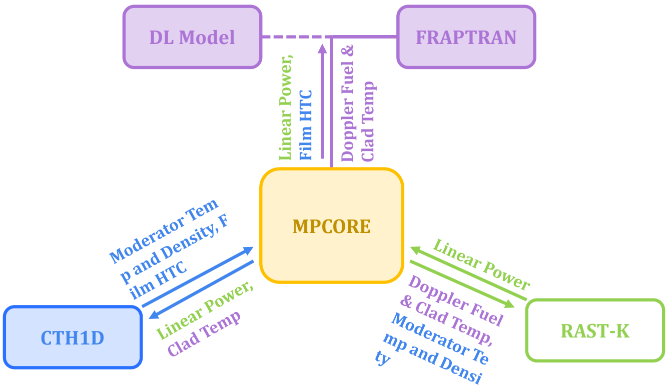



Fig. 1. Proposed MPCORE model replace FRAPTRAN with DL Model.

Deep Learning (DL) trained surrogate model as FP code is proposed in this research for Multiphysics simulations. Fig. 1 illustrates the working of MPCORE. The dotted line show the intended inclusion of DL model in MPCORE.

### *2.2 Reactor Description*

The dataset is prepared for 10 s HZPREA transient analysis at BOC for Watts Bar reactor. Reactor consist of 193 fuel assemblies with 8 different kinds of control rods. It is 17x17 fuel assembly with 25 guide tubes and 264 fuel rods (Westinghouse design). Material specification is given in the benchmark document [7]. D control bank is withdrawn 127 steps to introduce the positive reactivity of $1.2. D bank position and core is octal symmetric. To remove this symmetric effect, data for only 1 octant fuel rods is obtained. Complete core and the octant selected are shown in Fig. 2. Complete reactor core consists of 50952 fuel rods but the selected octant consist of 6447 fuel rods. The data is split into 70% training data (4513 rods), 15% validation data (967 rods) and 15% testing data (967 rods).

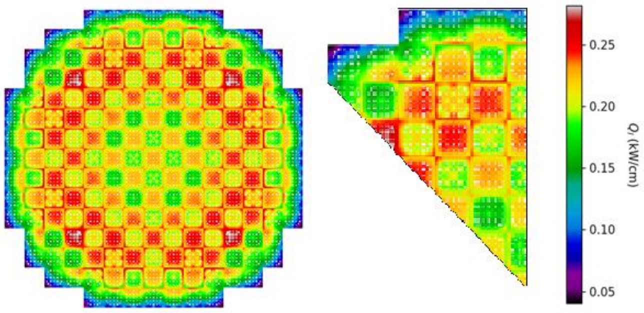



Fig. 2. Complete core and selected octant for fuel rod data.

*2.3 Deep Learning Model*

Single fuel rod is composed of multiple axial meshes (10 considered for this study) that are dependent on each other (spatial sequence). Fuel rod behavior at any time depends on the previous time history of fuel rod (temporal sequence). Convolutional neural network (CNN) is used for spatial sequence prediction and LSTM (Long-Short Term Memory) is used for temporal sequence information. Input data comprises of linear power provided by RK, while film heat transfer coefficient (fHTC), coolant temperature and coolant pressure are provided by TH code. Gap width as predicted by FP code is used as an input for the next step. Gap width is dynamic from the start of transient for uncertainty cases, therefore, it is also used as an input feature. Input data is provided to time distributed layer of CNN. CNN data is further fed to flatten layer before LSTM layer. LSTM works on the convoluted data and find the chronological order between the sequences. The network developed is shown in Fig. 3.

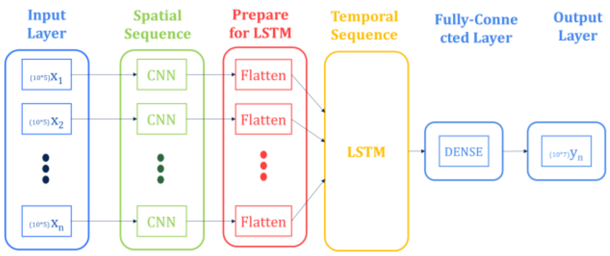



Fig. 3. DL Model trained for FP modeling.

*2.4 Parameters for DL model*

Adam optimizer is used in this study with learning rate of 0.001 and batch size of 32. Mean Squared error (MSE) is taken as the loss metric and Peak Signal to Noise Ratio (PSNR) is taken as evaluation metric. The formula for MSE is given as:

$$MSE = \frac{1}{mn}\sum_{i=0}^{m-1}\sum_{j=0}^{n-1}\left[I(i,j) - K(i,j)\right]^2. \quad (2.1)$$

Where m=92 the number of time steps for 1 fuel rod, n=70 the number of output variables at any time step (7 outputs for each spatial mesh). I(i,j) is the original result as given by the FRAPTRAN code while K(i,j) is the predicted value from DL model.

PSNR is calculated as:

$$PSNR = 10.\log_{10}\left(\frac{MAX_I^2}{MSE}\right). \quad (2.2)$$

$MAX_I$ is the maximum value of any single output variable at any time step. MSE is the one given by (1). Different value of MSE and PSNR values are obtained for each fuel rod.

*2.5 Best model selection*

General architecture of the DL is shown in Fig. 3. The number of layers that can be used for spatial sequence (CNN) or temporal sequence (LSTM) can vary. The type of models and their evaluation metric for 50 epochs is shown in Table I. The table shows the number of layers of each type of neural network.

Table I: Layers selection for best model.

| Model | CNN | LSTM | Dense | PSNR |
|---|---|---|---|---|
| Simple | 2 | 1 | 1 | 48.22 |
| First | 3 | 1 | 1 | 34.36 |
| Second | 2 | 1 | 2 | 19.62 |
| Third | 2 | 2 | 1 | 56.58 |

Best model is obtained for 2 CNN, 2 LSTM and 1 dense layer. 50 epochs were used to test each variant, so the model that performed badly might perform better for more epochs. Testing with more epochs for each variant is not computationally feasible. The best three models obtained from hyper parameter selection search are shown in Table II.

Table II. Hyper parameter optimization.

| Model | Activation | filters/ Units | Learnin g rate | Batch Size | Loss |
|---|---|---|---|---|---|
| First | relu/tanh,re lu/sigmoid | 64/512 | 0.001 | 32 | 2.18e-06 |
| Secon d | relu/tanh/si gmoid | 64/256 | 0.001 | 32 | 2.29e-06 |
| Third | tanh/tanh/ta nh | 64/256 | 0.001 | 16 | 4.06e-06 |

The best model is selected with minimum MSE value.

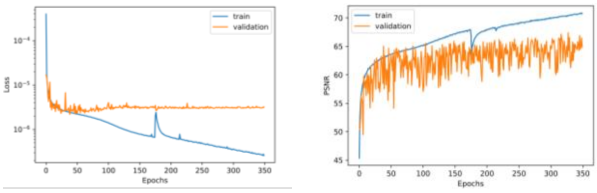
*2.6 Results*

The model is executed for 350 epochs and the best model with minimum loss is obtained at 39 epoch. The results obtained for MSE and PSNR for the model are shown in Table III. PSNR metrics is better metrics to evaluate the image quality. As the value becomes higher the quality of the predicted image closely resembles the original one.

Table III. Results for the best model

| Data | Training | Validation | Testing |
|---|---|---|---|
| MSE | 1.81e-06 | 2.18e-06 | 2.12e-06 |
| PSNR | 65.21 | 65.02 | 64.88 |

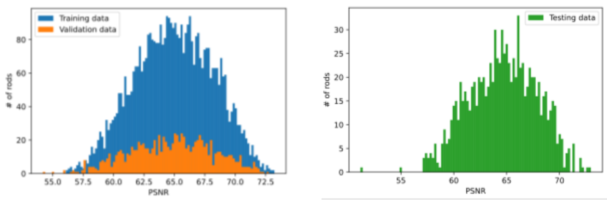
Results obtained for train, test and validation data is in the same range that shows that the model is not over fit for the training data. The loss curve for the training and validation data is shown in Fig. 4. Evaluation metric of PSNR is also plotted with the number of epochs.




(a) (b)

Fig. 4. Fuel rods gap distribution (a) Loss curve MSE with epochs (b) Evaluation metric PSNR.

The best model is selected with the smallest loss value. The histogram of PSNR values for all training, validation and testing fuel rods are shown in Fig 5. Minimum value of PSNR obtained for single fuel rod in training, validation and testing data is 56.08, 54.18 and 51.17 respectively. Maximum value of PSNR obtained for single fuel rod in training, validation and testing data is 73.22, 72.76 and 72.96 respectively.




(a) (b)

Fig. 5. Histogram of PSNR values (a) training and validation data (b) testing data.

The MSE value obtained for all the predicted value is shown in Table IV.

Table IV. MSE value for parameters

| Data | Training | Validation | Testing |
|---|---|---|---|
| Fuel centerline | 3.70e-06 | 2.80e-06 | 4.10e-06 |
| Fuel surface | 3.30e-06 | 1.50e-06 | 3.80e-06 |
| Doppler fuel | 5.60e-06 | 6.20e-06 | 6.70e-06 |
| Clad inner | 2.40e-06 | 3.60e-06 | 2.40e-06 |
| Clad outer | 2.10e-06 | 3.20e-06 | 1.80e-06 |
| gap HTC | 1.10e-06 | 2.30e-06 | 2.50e-06 |
| Gap width | 2.20e-07 | 2.30e-07 | 3.50e-07 |

Uniform distribution of gap width is used during the data generation step, but the power is not following the uniform distribution. More rapid change in power is observed near the rod withdrawal assemblies. Uniform distribution in all the input parameters may further increase the PSNR. Quantile or power transformation can be used at the preprocessing step for uniform distribution of all input parameters. At present, the input is only scaled between 0-1. Power transformation may be applied in future to increase the model accuracy.

The linear power input and output trends for 1 sample rod, PSNR value of 68.0, is shown in Fig. 8. Gap width slightly increases in the start for some cases due to densification and will keep on decreasing for rest of the transient time. The output shows the actual (solid line) and predicted (dashed line) results for each axial mesh from 1 (bottom of fuel rod) to 10 (top of the fuel rod).

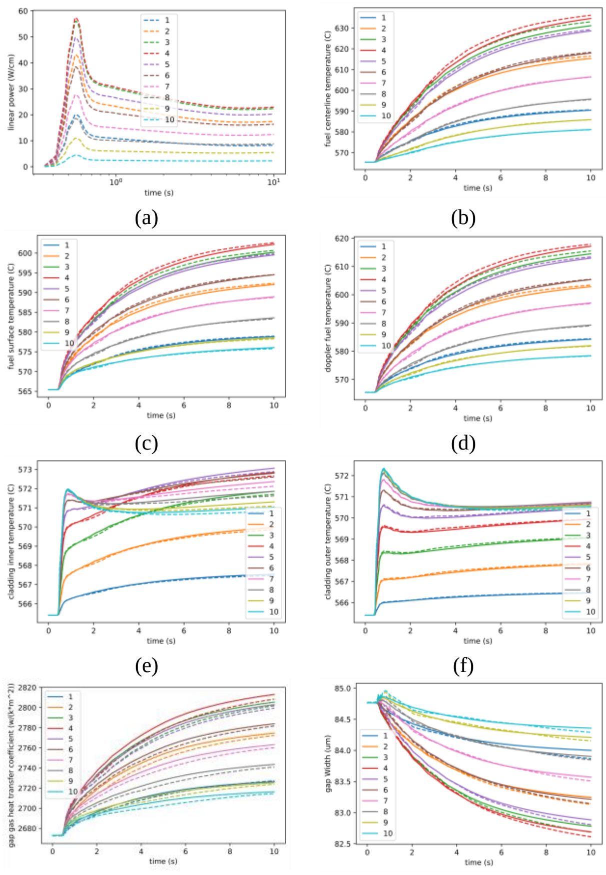



Fig. 6. Qualitative result for single fuel rods gap distribution; Input feature (dotted: actual) {(a) linear power}; Output features (solid line: actual, dotted line: predicted) {(b) – fuel centerline temperature (c) fuel surface temperature (d) doppler fuel temperature (e) cladding inner surface temperature (f) cladding outer surface temperature (g) gap heat transfer coefficient (h) gap width}

Gap HTC keep on increasing with time as the gap closes. Fuel temperatures (centerline, doppler, surface) also keep on increasing with time. The axial meshes are numbered from bottom to top. Cladding outer temperature is provided to TH module while doppler fuel temperature is provided to CN module. Other parameters are used in next step modeling and output comparison. Thus, the present surrogate model will completely replace the FP module of MPCORE.

Most of the parameter values are in well agreement with the actual rod results. Gap width is different for each rod in the start. All the temperature values start from 565$^{o}$C because REA is starting from HZP. In HFP, the initial temperature for all the rods may be different as well. This model is trained for HZP REA transient so it cannot be used for HFP REA transient.

## 3. Discussion

It is evident from the results mentioned above that the neural network can perform all the tasks of FP code. Earlier researchers use surrogate models for gap conductance prediction. But in this research, one DL model taking the spatial and temporal sequence information and performed all tasks of FP (temperature, gap conductance, and gap width prediction). The safety parameters like fuel centerline temperature that were predicted by FP code can now be predicted accurately with DL model. For robust training of DL model, variable gap width is assumed for each fuel rod.

In actual coupled analysis, linear power is dependent on FP code outputs. Coolant characteristics are also dependent on the gap conductance and cladding temperatures. Including surrogate model in MPCORE code will affect the output of CN and TH module. The change in RK and TH code will affect the behavior of surrogate model. So, the actual test of the DL trained surrogate model lies in the final inclusion of DL model in MPCORE.

## 4. Conclusion

The surrogate model in place of complex FP code is proposed in this research. Current MPCORE framework couples CN-TH-FP code, in which the FP code takes the highest computation time. This framework is not feasible for application of uncertainty propagation. This surrogate model can speed up the Multiphysics coupling methodology and UQ results can be obtained in reasonable time. The results obtained by the surrogate model is in close agreement with the actual results of FRAPTRAN FP code. BEPU approach requires the use of dynamic gap conductance with CN and TH codes. Surrogate model fulfils the criteria for BEPU in very less execution time. The trained model has well predicted the temperatures and gap characteristics for fuel rod.

FP code used for training the DL model is 1.5D code. The code itself has some limitations and 3D codes (like BISON) can yield better results. DL trained model can, at best, be the replacement of 1.5D code. It means that DL models trained with higher dimensionality codes can easily surpass the accuracy of low dimensional codes in terms of accuracy. The time requirement of DL model is negligible as compared to the actual FP code.

Many prospects open following this work. One of future work can be to replace the TH module in MPCORE with DL model. Using CNN2D and LSTM in place of whole core subchannel TH code may speedup the work manifolds. The resultant product will take similar time for Multiphysics modeling as taken by simple CN module.

## ACKNOWLEDGEMENTS

This research was supported by the project(L20S089000) by Korea Hydro & Nuclear Power Co. Ltd..

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