A Physics-Informed Neural Network Approach for Reliable Surrogate Modeling for PWR LOOP Accidents

Fabiano Thulu[1], Zeyun Wu[1], and Yunfei Zhao[2]

[1]Department of Mechanical and Nuclear Engineering, Virginia Commonwealth University, Richmond, VA, USA
thulufg@vcu.edu; zwu@vcu.edu

[2]Department of Mechanical Engineering, University of Maryland, College Park, MD, USA
yzhao111@umd.edu

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INTRODUCTION

The use of modeling and simulations is vital in safety analysis and licensing of the current and next generation of reactors including Small Modular Reactors and Micro-Reactors [1]. One of the most commonly reported transient accidents in nuclear power plants (NPPs) by the U.S Nuclear Regulatory Commission (NRC) is the Loss of Offsite Power (LOOP) accident, which is of a significant safety concern in pressurized water reactors (PWRs), potentially leading to station blackout (SBO) and challenging decay heat removal. Accurate and rapid simulations of this transient is crucial for safety analysis, operation training and emergency preparedness [2].

Highly benchmarked computation codes such as RELAP and MELCOR have been extensively used to understand reactor dynamics in terms of transient and normal operations in NPPs. However, due to limitations these codes pose, such as computational expensive, uncertainty quantification and real-time simulations challenging, researches have been using deep learning and artificial intelligent as surrogates to improve these well-established safety analysis codes [3]. Fast and accurate surrogate models can also be useful for online monitoring, anomaly detection, predictive control and accelerated safety analyses for reactor designs.

Deep Neural Networks (DNN) surrogate model have been used in PWR safety analysis. Radaideh reported DNN gave good forecasting of peak clad temperature and core pressures during the loss of coolant accident [4] . However, purely data driven neural networks (NN), while fast, require a lot of simulation data and may sometimes struggle with generalization to unseen condition or ensure physical consistency [4]. In this work, we have looked at different but most common seen accident scenarios. The research extends to use of Physics Informed Neural Networks (PINN), which inherently embed physical laws, leading to more robust, data efficient, and physical consistent surrogate models [6]. This is particularly important in reactor engineering where data can be scarce and physical accuracy is paramount.

Through the comparative studies on DNN and PINN, this study highlights the advantages of PINN in providing reliable and accurate safety simulations during LOOP. By using physics simulation data, we first trained a purely data-driven DNN surrogate model and subsequently, developed a PINN model that integrates governing physical laws. This dual approach enables rapid, reliable predictions and real-time decision making capabilities in NPPs.

A triple-loop PWR (shown in Fig. 1) model is adopted in this study. It is a type of NPP in which heat generated by the nuclear fission of the fuel in the reactor core is transferred to three separate coolant loops. Each loop contains a steam generator, where thermal energy from the high-pressure primary coolant is transferred to a secondary loot for stem generation. This steam then drives turbines for electricity production.

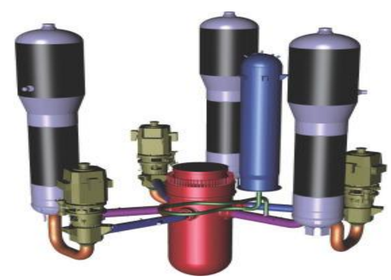

Fig. 1. Schematic view of a triple-loop PWR.

LOOP is associated with the loss of offsite power grid. It can lead to unplanned reactor shutdown, as a precaution measure, since availability of alternating current power is essential for safe operation and accident recovery. Standby diesel generators are required for decay heat removal. Auxiliary feed water system (AFWS) becomes the primary feed water supply. Steam from generators is released into the atmosphere through safety valves [7]

METHODOLOGY

This study applies a phased methodology to systematically develop, train, and evaluate separate models to predict the triple-loop PWR transient behavior under various LOOP accident conditions. The methodology encompasses physics data generation, data preprocessing, and the development & comparative analysis to develop the DNN surrogate and PINN surrogate. Fig. 2 illustrates the comprehensive framework that encompasses all the procedures under the phased methodology.

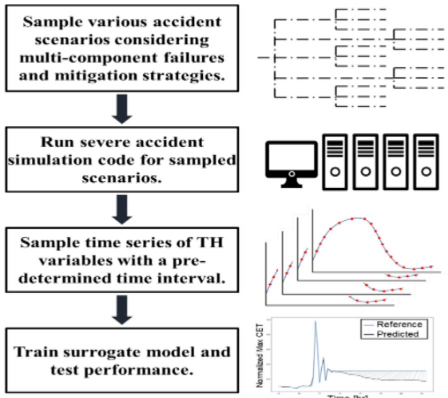

Fig. 2. Framework to construct surrogate models.

The development of both DNN and PINN was carried out in Python, using its ecosystems of scientific computing and machine learning libraries. Both models were trained for a maximum of 500 epochs with a batch size of 64 and 32, respectively. Adam optimizer was used in convergence history, with an initial learning rate of 10^{-4}. 50 epochs were used for monitoring validation loss in DNN and total training loss for PINN models. TensorFlow modules are employed to provide the core capabilities for building, training and optimizing the NN architectures. Pandas library was used for data manipulation and preprocessing. Array handling and scenario splitting was accomplished by tools in NumPy library while Scikit-learn (standardScaler) was employed for feature normalization. One-Hot-Encoder was sufficient to handle categorical variables. Lastly, Matplotlib and Seaborn were used for generating all visualizations.

Data Generation

Dataset was generated using the VCU's 3-loop PWR simulator, which is capable of accurately simulating complex multi-phase, multi-component fluid dynamics, heat transfer and nuclear kinetics relevant to PWR transient analysis [8].

Accident Scenario Matrix

Three types of LOOP cases were examined in this work, namely, Loss of 6900V Auxiliary Buses (A-E), Loss of 120V AC and DC Instrument BUS, and SBO. For each case, the following situations were considered: (1) if the reactor protection system (RPS) and the auxiliary feed-water system (AFWS) function, the End State 1 (OK) is obtained; (2) in the case of RPS functions but AFWS not, End State 2 (F01) is obtained in which decay heat cannot be removed from the reactor; (3) when RPS loses its safety function but AFWS is able to activate, End State 3 (OK) is obtained, and (4) if both RPS and AFWS lose their safety intended functions, worst case scenario is achieved in which reactor is still running but decay heat from the core cannot be removed (F02). Fig. 3 shows the event tree of such an accident case. All these cases were simulated for the three LOOP postulated accident scenarios. Average fuel temperature and primary pressure were recorded for the DNN and PINN surrogate modelling.

Initial Condition Variation

In order to develop a robust surrogate model, twelve varied scenarios with three initial reactor power conditions were considered under this study, making a total of 36 distinct physics simulations. All the 36 simulations ran for 10,000 sec and the first 300 sec being reactor at a steady-state condition.

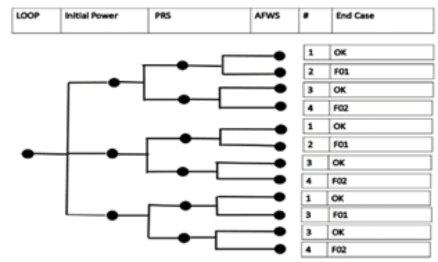

Fig. 3. Event tree of one LOOP simulation case.

Phase 1: DNN Surrogate Model

A supervised DNN was developed to serve as a purely data-driven surrogate model. The DNN consisted of multiple fully connected (dense) hidden layers with a rectified linear unit (ReLU) activation function for nonlinearity. The feedforward DNN architecture was implemented using TensorFlow/Kares. The input features consisted of: scaled time, initial reactor power (numerical scaled), and one-hot encoded categorical variables representing system configurations (accident type, PRS status and AFWS availability). The output layer consists of two neurons with a linear activation function, corresponding to the predicted fuel temperature (T_f) and primary pressure (P_p). The loss function was mean square error (MSE), which is also referred to as standard mean squared error (L_{total}) that can be optimized by the Adam optimizer. Normalized Mean absolute error (NMAE) was also employed as an additional evaluation metric for better interpretability.

$$L_{total} = \frac{1}{N} \sum_{i=1}^{N} \left(\left(\dot{T}_{f,i} - T_{f,i}\right)^2 + \left(\dot{P}_{p,i} - P_{p,i}\right)^2 \right) \qquad (1)$$

where $\dot{T}_{f,i}$ and $\dot{P}_{p,i}$ are the predicted fuel temperature and primary pressure for the data point, and $T_{f,i}$ and $P_{p,i}$ are the corresponding values yielded from the simulations.

Phase 2: PINN Surrogate Model

Building upon the DNN, a PINN surrogate was developed to enhance the physical fidelity of the surrogate models. It incorporated the underlying physics equations for PWR thermal-hydraulics directly into its training objective, aiming to achieve superior generalization and physical consistency. The PINN architect consisted of a fully connected model with an input vector comprising scaled time and one hot encoded scenario parameters. Four connected NN hidden layers were used, each layer having 128 neurons and using tanh activation function. Scaled fuel temperature and primary pressure were the output layers.

The total loss function minimized during the training was

$$L_{total} = w_{data}L_{data} + w_{physics}L_{physics} + w_{IC}L_{IC} \qquad (2)$$

where L_{data} = MSE between PINN predicted value and corresponding simulation data, $L_{physics}$ = MSE of the residuals of governing equations that describe the reactors thermal-hydraulic behavior. The specific lumped-parameter equations govern the fuel energy balance, primary coolant energy balance, and primary pressure evolution, respectively,

$$\rho_f c_p V_f \frac{dT_f}{dt} = Q_{gen} - U_{fc}A_{fc}(T_f - T_c) \qquad (3)$$

$$\rho_f c_{p,c} V_c \frac{dT_c}{dt} = U_{fc}A_{fc}(T_f - T_c) - Q_{AFWS} - Q_{loss} \qquad (4)$$

$$\frac{dP_p}{dt} = K_p \frac{dT_c}{dt} \qquad (5)$$

where Q_{gen} (heat generation) is determined by the RPS status (decay heat if scrammed, nominal power if failed RPS) and Q_{AFWS} (AFWS heat removal) is active if AFWS is operational, otherwise zero. L_{IC} = the initial condition loss, which penalizes deviation of the PINN's predictions from the true simulation data at the transient initiation time (t = 300 sec). The importance of these loss components is controlled by their respective weights ($w_{data}, w_{physics}, w_{IC}$) which are hyper parameters tuned during the training process to optimism convergence and accuracy. All the physical constants including $\rho_f, c_p, V_f, V_c, U_{fc}, A_{fc}, K_p, Q_{loss}, m_{AFWS}$ were set to realist triple-loop PWR design values.

For both DNN and PINN, out of 36 datasets, 29 was allocated to the training set and the remaining 7 set was reserves for test set. For the final PINN model, the comprehensive test set served as the ultimate verification for evaluating the models generalization capabilities after training was complete.

RESULTS

Performance of the DNN Surrogate

The constructed DNN demonstrated a good predictability for both average fuel temperature and primary pressure dynamics across the entire reactor transient period. The model offers significant computational speed-up for real-time analysis. As shown in Figs. 4 and 5, the predicated pressure and temperature trends closely matched the primary truth data. While minor discrepancies are observed during abrupt temperature transients (rapid cool or heating) the DNN model follows the general trajectory of physics simulation data. This indicates a successful learning of dominant thermal behavior. Also, despite some under-or over-shooting during sharp pressure reversal, the model maintains the correct phase and magnitude trends during transient.

For fuel temperature, the DNN achieved an NMAE approximately 3.1%, indicating the model maintains tight tracking of thermal response. For primary pressure, NMAE of around 2.4% was observed. This was much influence by sharp transient and recovery spikes during rapid depressurization or depressurization events. By error distribution, the highest discrepancies occurred during the early post-accident periods, when system responses are most nonlinear. Beyond this phase, prediction errors remain low.

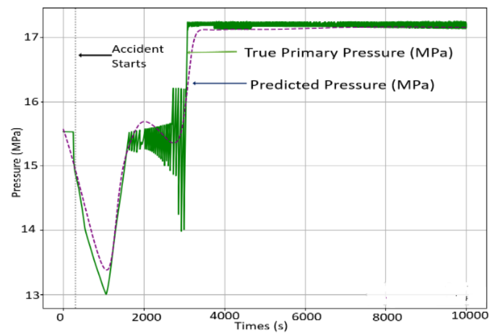

Fig. 4. Pressure for Loss of 6900V with the end case F01.

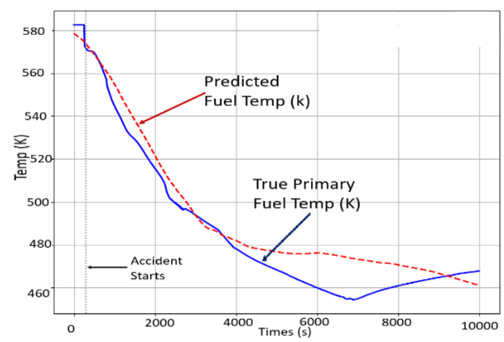

Fig. 5. Fuel temp. for Loss of 6900V with the end case F01.

Performance of the PINN Surrogate

Upon completion of training, the PINN's predictive accuracy was evaluated on the held-out test set. The model achieved NMAE of 2.3% and primary pressure of 1.6%. Numerically, these results place the PINN's overall data-fitting performance as comparable better to DNN baseline, as shown in Figs. 6 and 7 for the same accident case. Visual inspection of PINN's predictions for individual test accident cases show a nuanced picture, demonstrating a significant disparity in performance for temperature outputs. This is summarily to what was reported by Antonello et al., 2023 where PINN's did not actually predicted the true date set correctly. They also suggested that PINN models are not good for lager data sets [9].

Inasmuch that the model did not precisely replicate the high frequency oscillations characteristics of the true transients, it successfully captures the initial pressure drop, subsequent recovery, and the general trajectory towards a stable operating plateau. This suggest that even the simplified pressure ODE, coupled with the network's learning, provide sufficient physical guidance to model the pressure evolution better than the data driven approach.

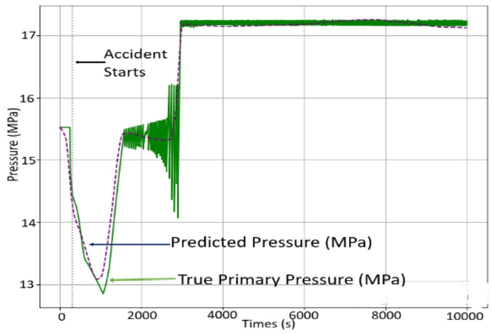

Fig. 6. Pressure for Loss of 6900V with the end case F01.

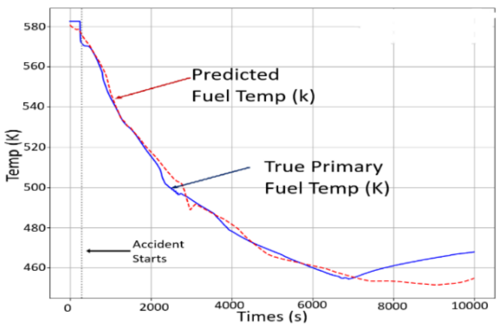

Fig. 7. Fuel temp. for Loss of 6900V with the end case F01.

CONCLUSIONS & FUTURE WORK

This study aimed at developing and evaluating data-driven surrogate models capable of emulating complex triple-loop PWR transient responses, starting with a purely data driven DNN and following by PINN. The initial calculations using DNN surrogate model, trained, verified and tested on 36 physics simulations of the LOOP transient, have shown some limitations. The DNN model indeed captures the intricate, non-linear, and oscillatory dynamics of the reactor conditions in time, but qualitative analysis of predictions against true transient profiles indicates a gap in physical fidelity. This might lead to the model failure in reproducing critical trends, particularly in severe accident progression when rapid pressure and temperature changes occur.

The PINN surrogate was formulated to address the challenges faced by DNN. The PINN model was designed to predict fuel temperature, average primary coolant temperature (as internal state variable) and primary pressure. PINN's unique training objective minimized a multiple component loss function, combining data driven errors with physics-based residual derived from governing equations for fuel energy balance, primary coolant energy balance and primary pressure evolution, alongside with initial conditions.

The current PINN implementation has demonstrated a partial success, most notable in its ability to predict the overall transient and magnitude of primary pressure for a long time. This presents a significant step forward from purely data-driven approaches. With the model struggling to capture fuel temperature and inability to capture high frequency pressure oscillations, future work will focus on developing more sophisticated lumped-parameter higher-fidelity physics model, coupling with higher order PDEs. Primary coolant temperature will also be investigated. The insights gained from this work underscores both the immense potential and inherent complexities of deploying PINN as reliable surrogate model for complex accident cases.

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