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Changing the World's Energy Future

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Data-driven Quasi-static Surrogate Models for Nuclear-powered Integrated Energy Systems

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***Abstract*—The integration of nuclear power into energy systems presents a promising avenue to address the growing global energy demands while minimizing greenhouse gas emissions. In this paper, we introduce a data-driven quasi-static surrogate model for nuclear-powered Integrated Energy Systems (IES) that comprises various components, including a small modular reactor (SMR), steam manifold, balance of plant (BOP), high-temperature steam electrolysis (HTSE), and district heating (DH) system. Traditional physics-based models for these components often entail significant computational resource and time consumption, necessitating the development of efficient surrogate models. The development of a complete surrogate model for the IES involves the creation of individual surrogate models for each component, leveraging machine learning techniques and simulated data. These isolated surrogate models are subsequently integrated, enabling a holistic view of the IES and reducing the computational burden associated with detailed physics-based simulations. This paper outlines the development process, validation, and the performance evaluation of the surrogate models. The exceptional performance, with low root-mean-squared errors and R-squared scores of at least 99.8% across all individual surrogate models, underscores their accuracy and practical applicability. These results demonstrate the potential of these models to expedite the analysis of nuclear-powered IES, offering insights that can shape future research and development efforts.**

***Index Terms*—District heating, integrated energy systems, machine learning, nuclear energy, and surrogate model.**

1. Introduction

The urgency to mitigate carbon emissions across the industrial and residential sectors has underscored the significance of nuclear-powered integrated energy systems (IES). Despite strides in reducing CO_2 emissions in the electric power sector, the industrial and residential sectors remain significant contributors to carbon footprints [1]. With processes like space and process heating accounting for substantial portions of these emissions, the need for decarbonization in these sectors is evident. Nuclear power is a clean and carbon-free energy source capable of providing not only electricity but also thermal energy. However, traditional nuclear power plants, reliant on large light water reactors, face challenges due to safety concerns and economic constraints in the electricity markets [2]. Redirecting excess steam from nuclear plants for alternative applications like desalination, hydrogen production, and district heating becomes crucial, offering promising revenues for reducing carbon emissions. This integration of nuclear energy into renewable energy systems presents a versatile solution to meet diverse energy demands while minimizing environmental impacts and fostering energy resilience.

High-fidelity physics-based models of nuclear-powered IES have been developed to understand and represent the dynamics and interactions among various components of the IES [3]. However, these models, while comprehensive, are burdened by their complexity and computational intensity. Simulating IES with these models involves intricate equations representing different components and their interdependencies, and demands extensive computational resources and time. To minimize computational burden, a viable approach involves constructing a surrogate model for the computationally intensive simulation models [4]. Surrogate models, leveraging machine learning techniques and historical or simulated data, offer a promising alternative. These models, while simplifying the underlying complexity, provide a computationally efficient solution. By encapsulating the behavior of complex systems, surrogate models enable faster insights into system dynamics to support prompt decision-making without compromising accuracy. The development of a surrogate model for IES represents a pivotal step in bridging the gap between the intricacies of physics-based models and the necessity for quick and accurate predictions in real-world applications.

Various types of surrogate and reduced order models have been developed and implemented for different applications in the existing literature. An overview of reduced order modeling techniques has been given in [5], the capabilities and advantages of reduced order models have been emphasized, and the implementation of these models have been shown using examples of multi-physics systems. In [6], a surrogate model based on artificial neural networks has been introduced to quickly evaluate building retrofit solutions, significantly reducing computational time while maintaining accuracy, offering a promising avenue to expedite widespread retrofit analyses for environmental improvements in existing building stocks. In [7], surrogate models, specifically machine learning methods such as k-nearest neighbor and artificial neural networks, have been investigated as efficient replacements for detailed process models in monitoring the evolution of nuclear waste packages, showcasing notable accuracy, especially when incorporating additional internal fuel cask state data in the training set. A machine learning-based surrogate model has been developed in [8] to predict hydrogen production costs from diverse biomass sources and process factors by facilitating early economic analyses. In addition, the study highlighted that integrated heat and electricity systems led to reduced emissions. Notably, during cross-validation, neural networks exhibited higher accuracy compared to other models employed in the analysis. An optimization framework, leveraging machine learning surrogate models trained on annual market simulations, has been introduced in [9] to integrate energy system decisions into market dynamics. This framework surpasses the limitations of traditional "price taker" assumption and significantly improves revenue prediction accuracy compared to standard approaches. Motivated by the aformentioned research works, this paper investigates the development of a data-driven surrogate model for nuclear-powered IES.

In this paper, we develop a data-driven surrogate model for a nuclear-powered IES by integrating individual surrogate models of crucial IES components. Our data is generated by simulating isolated IES components in high-fidelity physics models. We then train our surrogate models with the generated data and evaluate their performance by employing metrics such as root-mean-squared error (RMSE) and R-squared. Ultimately, the individual surrogate models are combined to create an integrated surrogate model for the IES. This integrated model is then validated using a 24-hour simulation dataset derived from a physics-based model developed in Dymola.

The remainder of the paper is organized as follows. Section 2 outlines the structure of the nuclear-powered IES and details its components. Section 3 elaborates on the methodology adopted for the development of surrogate models. The results and discussion are presented in Section 4. Lastly, Section 5 offers concluding remarks and discusses potential future work.

2. Nuclear-powered IES

The nuclear-powered IES discussed in this paper is a complex network of interconnected subsystems designed to efficiently generate both heat and electricity. This system integrates various components, including a small modular reactor (SMR), a steam manifold, balance of plant (BOP), high temperature steam electrolysis (HTSE), a district heating (DH) network, and an electrical grid. Fig. 1 depicts a block diagram of the nuclear-powered IES with the aforementioned components. A more detailed description can be found in [10].

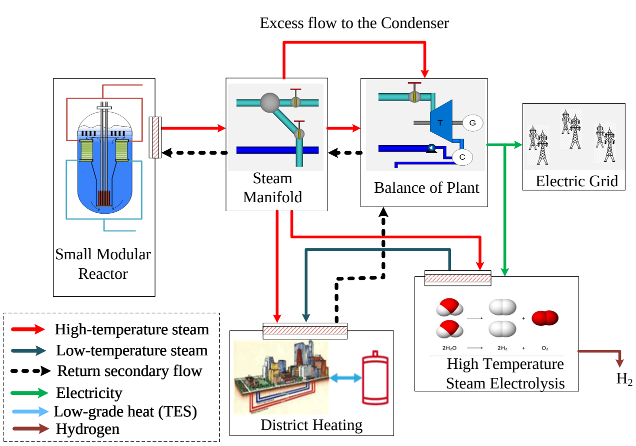

Fig. 1. Block diagram of the nuclear-powered IES [10].

The SMR, fundamentally, serves as the primary energy source, utilizing nuclear fission to produce high-temperature process steam. This steam is then distributed to other components through the steam manifold for electricity generation in BOP, hydrogen production in HTSE, and meeting heating demand of the DH system. The SMR's physics-based model is developed based on NuScale reactor technology, known for its maturity and reliability, to generate high-temperature steam efficiently [11].

The BOP, encompassing a steam turbine and a synchronous generator setup, converts thermal energy from the steam into electricity. Additionally, it includes a turbine control and bypass vales. Based on the electrical demand setpoint provided as an input signal to the BOP control, the turbine valve is operated to regulate the steam flow to the turbine while the bypass valve simultaneously operates to divert excess steam to the condenser. The HTSE process consumes both heat and electricity to produce hydrogen by splitting water within solid oxide electrolyzer cells [12], [13]. This process requires high-temperature steam from the SMR to operate efficiently. HTSE operates in steam control mode in which the steam flow rate is adjusted based on both the physical properties (i.e., pressure and specific enthalpy) of process steam and electrical power supplied to the HTSE. The electrical power supplied to the HTSE is the primary input variable to the HTSE controller.

The DH system supports local heat demand by distributing hot water through insulated pipelines. It utilizes heat from two sources: the first being recovered from the exhaust of HTSE, while the second from the topping steam extracted directly from SMR. It incorporates a thermal energy storage (TES) system to manage surplus or deficient heat during varying demand periods effectively. The TES, a stratified storage tank, stores excess thermal energy when demand is low and releases it when demand peaks.

The last component, the electrical grid, balances electricity production and demand within IES. It is modeled as an infinite source or sink, absorbing surplus electricity and providing additional power if the BOP's production falls short.

High-fidelity physics models of the subsystems are modeled using Modelica within the Dymola environment, leveraging existing transient-process models and introducing new ones for components like the DH system. We use the HYBRID repository developed by the Idaho National Laboratory [3] for the SMR, BOP, and HTSE modules.

3. Surrogate Model Development

Surrogate models offer an efficient alternative to computationally expensive physics-based models, enabling rapid and accurate analysis and prognosis of IES, hence providing better situational awareness of system security, reliability, and resilience [14].

The development of surrogate models in this study follows a structured process and specific steps. The key steps involved in the development process are explained in the following subsections.

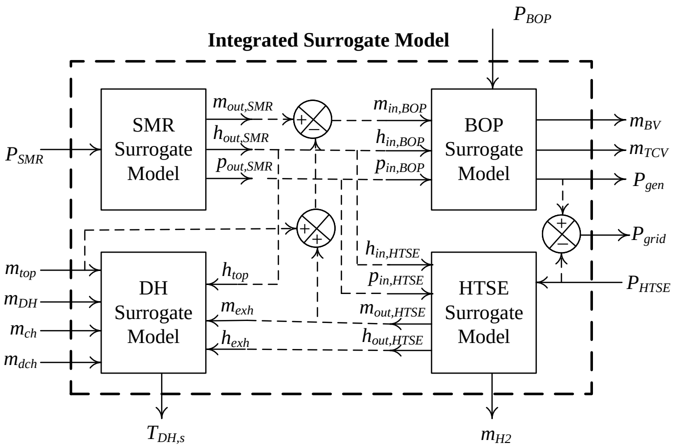

Fig. 2. Block diagram of the integrated surrogate model. Each solid box represents a set of individual models of an IES subsystem, and the dashed box represents an integrated model of the entire IES. Note that arrow directions only represent data flow, not actual energy flow.

A. Data Generation

Extensive data is essential for accurate model development. This step involves data generation through simulation of isolated physics-based high-fidelity models as depicted in Fig. 2 and explained below.

1) Small Modular Reactor: For the SMR, the data collection process involves varying the SMR thermal power demand set point (P_{SMR}) across operating range of 0.2 to 1 per unit (pu) in increments of 0.02 pu. Within this range, properties of the outlet steam, such as mass flow rate ($m_{out,SMR}$), pressure ($p_{out,SMR}$), and specific enthalpy ($h_{out,SMR}$), are recorded. The SMR surrogate model can be expressed as follows:

$$\begin{aligned} m_{out,SMR} &= f_m^{SMR}(P_{SMR}) \\ p_{out,SMR} &= f_p^{SMR}(P_{SMR}) \\ h_{out,SMR} &= f_h^{SMR}(P_{SMR}) \end{aligned} \tag{1}$$

where f_m^{SMR}, f_p^{SMR}, and f_h^{SMR} are functions representing the corresponding input and output variables of SMR.

2) High Temperature Steam Electrolysis: The isolated HTSE models consider the HTSE electrical power demand set point (P_{HTSE}) as well as the pressure ($p_{in,HTSE}$) and the specific enthalpy ($h_{in,HTSE}$) of the process steam at the inlet, as inputs. Data collection involves varying P_{HTSE} from 0.48 to 1 per unit (pu) in increments of 0.02 pu. Additionally, $p_{in,HTSE}$ and $h_{in,HTSE}$ are varied across the entire range of outputs obtained from the SMR for each HTSE demand set point. Within this input range, data is collected for the mass flow rate ($m_{out,HTSE}$) and enthalpy ($h_{out,HTSE}$) of the output steam, as well as the hydrogen production rate (m_{H_2}), which serve as outputs for the HTSE surrogate model. The HTSE surrogate model can be expressed as follows:

$$\begin{aligned} m_{out,HTSE} &= f_m^{HTSE}(P_{HTSE}, p_{in,HTSE}, h_{in,HTSE}) \\ h_{out,HTSE} &= f_h^{HTSE}(P_{HTSE}, p_{in,HTSE}, h_{in,HTSE}) \\ m_{H_2} &= f_{H_2}(P_{HTSE}, p_{in,HTSE}, h_{in,HTSE}) \end{aligned} \tag{2}$$

where f_m^{HTSE}, f_h^{HTSE}, and f_{H_2} are functions representing the corresponding input and output variables of HTSE.

3) Balance of Plant: The isolated BOP models consider the power demand set point (P_{BOP}), as well as the mass flow rate ($m_{in,BOP}$), specific enthalpy ($h_{in,BOP}$), and pressure ($p_{in,BOP}$) of the inlet steam, as their inputs. The variable P_{BOP} ranges from 10 to 60 MW in increments of 10 MW, and $m_{in,BOP}$ is varied from 20 to 80 kg/s in increments of 10 kg/s. For each combination of P_{BOP} and $m_{in,BOP}$, the variables $h_{in,BOP}$ and $p_{in,BOP}$ cover the entire range obtained from the SMR. Within this input range, data is collected for the actual generated electrical power (P_{gen}), as well as for the mass flow rates of steam passing through the turbine control valve and the bypass valve, denoted respectively by m_{TCV} and m_{BV}. The BOP surrogate model can be expressed as follows:

$$\begin{aligned} P_{gen} &= f_P(P_{BOP}, m_{in,BOP}, h_{in,BOP}, p_{in,BOP}) \\ m_{TCV} &= f_{TCV}(P_{BOP}, m_{in,BOP}, h_{in,BOP}, p_{in,BOP}) \\ m_{BV} &= f_{BV}(P_{BOP}, m_{in,BOP}, h_{in,BOP}, p_{in,BOP}) \end{aligned} \tag{3}$$

where f_P, f_{TCV}, and f_{BV} are functions representing the corresponding input and output variables of BOP.

4) District Heating: Inputs of the isolated DH models include the mass flow rate (m_{top}) and the specific enthalpy (h_{top}) of the process topping steam from the SMR, the mass flow rate (m_{exh}) and specific enthalpy (h_{exh}) of exhaust steam from the HTSE, the DH demand (m_{DH}) specified in terms of mass flow rate, and the charging (m_{ch}) and discharging (m_{dch}) mass flow rates of hot water in the TES. The variable m_{top} is varied from 0.6 to 1 kg/s at intervals of 0.1 kg/s, while m_{exh} ranges from 4 to 34 kg/s at intervals of 10 kg/s. Additionally, the variable h_{top} varies from 2883 to 3011 kJ/s at intervals of 32 kJ/s, and h_{exh} ranges from 989 to 2549 kJ/s at intervals of 312 kJ/s. Within each combination of these variables, m_{DH} varies from 13.6 to 23.7 kg/s, m_{ch} ranges from 0 to 5.2 kg/s, and m_{dch} ranges from 0 to 7.1 kg/s. Throughout this comprehensive input range, data is collected for the DH supply temperature ($T_{DH,s}$), which serves as the output of the DH surrogate model. The DH surrogate model can be expressed as follows:

$$T_{DH,s} = f_{DH}(m_{top}, h_{top}, m_{exh}, h_{exh}, m_{DH}, m_{ch}, m_{dch}) \tag{4}$$

where f_{DH} is the function representing the input and output variables of DH system.

B. Preprocessing

The collected data undergoes preprocessing which involves identifying and removing outliers, and normalization prior to modeling. Data preprocessing is a critical step to ensure the surrogate models can effectively capture the underlying relationships in the data. The preprocessing prioritizes the extraction of steady-state values for the SMR, BOP, and HTSE components. This deliberate focus aligns with the current research emphasis on developing quasi-static surrogate models. Furthermore, normalization techniques are applied across the dataset. Normalization ensures uniformity in the data distribution by scaling the input variables to a standard range. This standardized form enhances the efficiency of model training and convergence, allowing for more effective learning patterns within the machine learning model [15].

C. Model Training

The surrogate models undergo training using preprocessed data, optimizing model parameters to minimize the error between predictions and actual component behavior. Training involves three primary steps: dataset segmentation, hyperparameter tuning, and iterative optimization. Dataset segmentation involves partitioning the preprocessed dataset into distinct training and testing subsets. This division allows models to learn from one segment while preserving another for performance evaluation, ensuring their ability to generalize to new data. Hyperparameter tuning involves rigorously exploring diverse configurations, including hidden layer sizes, activation functions, and optimization algorithms, to identify the optimal set of hyperparameters for each IES component. Iterative optimization employs an iterative approach, utilizing the training dataset for learning and the testing dataset for evaluation. Each iteration refines the model, enhancing its ability to accurately capture the intricate dynamics of SMR, BOP, HTSE, and DH components within the IES for robust, high-performance surrogate models.

D. Model Evaluation

The evaluation phase measure the performance and reliability of the optimized surrogate models. The two standard evaluation metrics are employed to gauge the models' predictive accuracy and goodness-of-fit relative to the actual system behaviors, which are explained below.

1) Root Mean Squared Error (RMSE): RMSE is a fundamental metric used to quantify the average magnitude of the errors between predicted and actual values. The RMSE equation is expressed as:

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2} \tag{5}$$

where n represents the total number of data points, y_i and $\hat{y}_i$ denote the actual observations and predictions, respectively.

2) R-squared (R^2) Score: R-squared, also known as the coefficient of determination, assesses the goodness-of-fit of the model by determining the proportion of variance in the dependent variable that is captured by the independent variables. It quantifies the model's ability to explain the variability in the dataset. The R-squared metric is calculated as:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2} \tag{6}$$

where y_i and $\hat{y}_i$ represent the actual observations and predictions, respectively, and $\bar{y}$ denotes the mean of observed values.

E. Validation of the Integrated Surrogate Model

The final step involves integrating the best-performing individual surrogate models of each isolated IES component. This integration results in an integrated surrogate model, complemented by a mathematical representation of the steam manifold responsible for distributing steam from the SMR to other system components. To validate the integrated surrogate model, 24-hour simulation data generated from a physics-based model simulated in Dymola is employed.

4. Results and Discussion

This section presents a comprehensive analysis of the results obtained from the surrogate model development process outlined in Section 3. The surrogate models developed in this paper have been implemented using *Scikit-learn* [16], a widely used Python module for various machine learning tasks.

A. Training, Tuning, and Evaluation of Isolated Surrogate Models

This study develops individual multilayer perceptron (MLP)-based surrogate models for each IES component. The MLP utilized in this study serves as a representative model among various machine learning methods. The training process incorporates data normalization and random partitioning of the original dataset into a training and test set using a splitting ratio of 80:20. Subsequently, a randomized search technique is employed to determine the optimal set of hyperparameters for each output variable of the isolated surrogate models. The search is conducted by randomly sampling from the provided parameter distributions (Table I) and running 1000 iterations to explore various configurations. The search is performed using a three-fold cross-validation strategy, aiming to optimize the model's performance without overfitting. The search is parallelized on a multi-core CPU to speed up the process. The models, configured with the best hyperparameters, are then utilized to predict output variable values using the testing dataset. Evaluation of these predicted values employs two metrics: RMSE and R-squared score. Table II presents the optimal hyperparameters associated with each output variable across the individual surrogate models, indicating high prediction accuracy and goodness-of-fit for each model.

TABLE I
HYPERPARAMETER DISTRIBUTION FOR RANDOMIZED SEARCH.

Hyperparameter	**Values**
Hidden Layer Sizes	(20,), (50,), (100,), (50, 20), (100, 50, 20), (100, 50, 20, 20), (100, 50, 20, 10)
Activation Function	Identity, Sigmoid, Tanh, ReLU
Optimizer	SGD, Adam, L-BFGS

The evaluation metrics RMSE and R-squared scores attest to the robustness and precision of the models. Additionally, representative plots depicting the actual versus predicted values for various outputs are generated. Fig. 3 specifically showcases the actual and predicted values of hydrogen production rates

TABLE II
ISOLATED SURROGATE MODELS EVALUATION RESULTS WITH BEST HYPERPARAMETERS.

Surrogate Model	**Output Variable**	**Hidden Layer Size**	**Activation**	**Optimizer**	**RMSE**	**R-squared Score**
SMR	$m_{out,SMR}$	(100, 50, 20, 10)	Identity	L-BFGS	0.00002	0.99999
	$h_{out,SMR}$	(100,)	Sigmoid	L-BFGS	0.06911	0.99999
	$p_{out,SMR}$	(100,)	Tanh	L-BFGS	0.00229	0.99999
HTSE	$m_{out,HTSE}$	(100, 50, 20, 20)	Tanh	L-BFGS	0.11324	0.99936
	$h_{out,HTSE}$	(100,)	Sigmoid	L-BFGS	9.48567	0.99898
	m_{H_2}	(50,)	Tanh	L-BFGS	0.00275	0.99829
BOP	P_{gen}	(100, 50, 20)	ReLU	L-BFGS	0.04105	0.99999
	m_{TCV}	(50,)	Sigmoid	L-BFGS	0.05367	0.99999
	m_{BV}	(50, 20)	ReLU	L-BFGS	0.03424	0.99999
DH	T_s^{DH}	(50, 20)	Sigmoid	Adam	0.09521	0.99949

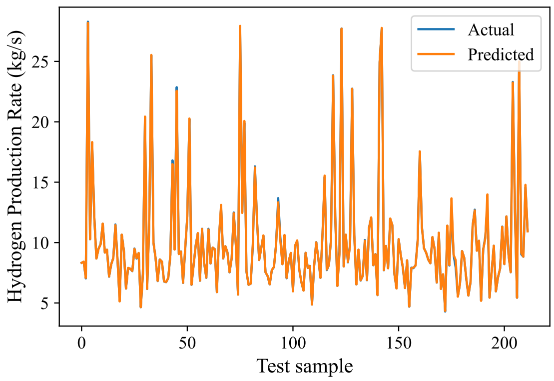

Fig. 3. Actual and predicted values of hydrogen production rates during tests of isolated HTSE surrogate model.

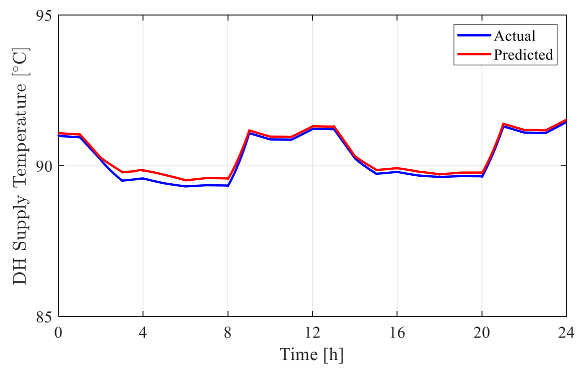

Fig. 4. Actual and predicted temperatures of the supply water of the DH system during the 24-hour simulation.

(m_{H_2}) using the isolated HTSE surrogate model. This visual representation corroborates the evaluation metrics displayed in Table II. For brevity, similar plots for other variables, which exhibit analogous predictive patterns, are omitted.

Our results confirm the high precision and fidelity of the surrogate models in replicating the behaviors of individual IES components. These findings substantiate the efficacy and reliability of the developed surrogate models within the context of nuclear-powered IES.

B. Validation of the Integrated Surrogate Model

The validation process compares the outcomes of the integrated surrogate model with the high-fidelity physics-based model of the nuclear-powered IES. This validation leverages a 24-hour simulation dataset generated through Dymola. For the generation of the 24-hour validation dataset, we considered a case where both the exhaust steam from HTSE and the topping steam coming from SMR through the steam manifold are utilized to meet the demand of the DH system. The TES is utilized to maintain a desired temperature of supply water to the DH system by controlling charging and discharging flows based on our previous work [10].

The SMR demand set point is maintained at the rated full power condition, i.e., 1 pu, which is equivalent to 60 MWe (200 MWth). Under this rated condition, the SMR produces 84 kg/s of high-temperature steam at 310 °C. The HTSE demand set point is also kept at 1 pu, and the HTSE system receives 7.23 kg/s of high-temperature process steam from the steam manifold and 53.3 MWe of electricity to produce 0.4 kg/s of hydrogen. The topping steam flow supplied to the DH system is maintained at 0.69 kg/s. To match the DH demand profile adopted from our previous work [10], the charging and discharging flows are adjusted to maintain the temperature of the supply water to the DH system at a desired value of 90°C.

Fig. 4 presents a plot of the actual and predicted values for the temperatures of the supply water within the DH system over the 24-hour simulation period. This comparison highlights the alignment between the surrogate model predictions and the physics-based model outputs, affirming the validation robustness of the complete surrogate model. To delve deeper into the predictive accuracy, a detailed analysis of the prediction error during the 24-hour simulation is conducted. The resultant histogram of the surrogate model prediction error portrays the distribution of relative absolute errors (RAEs) across the validation dataset. The RAE of ith data point in percentage is calculated as follows:

$$\text{RAE}_i = \frac{|y_i - \hat{y}_i|}{y_i} \times 100\% \tag{7}$$

where y_i signifies the actual observed value; and $\hat{y}_i$ denotes the predicted value for the corresponding observation.

Fig. 5 depicts the histogram showcasing the RAE distribution. Notably, the analysis reveals that nearly half of the validation data points exhibit RAEs ranging from 0.0525% to 0.1063%. Moreover, approximately 13% of the total data points fall within the maximum error range of 0.2677% to

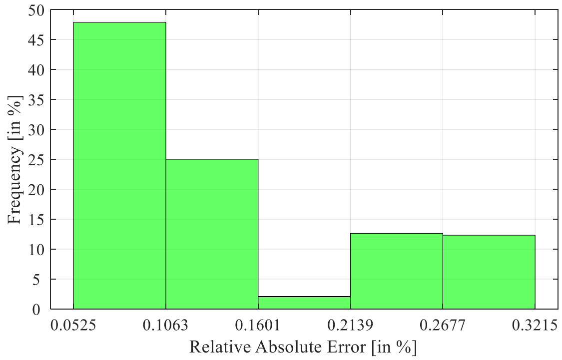

Fig. 5. Histogram of the surrogate model prediction error of DH supply water temperature during the 24-hour simulation.

0.3215%. This statistical analysis substantiates the reliability and accuracy of the integrated surrogate model in replicating the dynamics of the IES during the 24-hour simulation period.

The validation analysis, coupled with the visual representation and statistical insights, underlines the robustness and effectiveness of the complete surrogate model in emulating the behaviors of the nuclear-powered IES. These findings fortify the confidence in utilizing the integrated surrogate model for practical applications within energy system optimization and management.

5. Conclusion and Future Work

This study investigated the development of a simplified, data-driven surrogate model for a nuclear-powered IES by combining individual MLP-based surrogate models representing key components: SMR, HTSE, BOP, and DH. The robustness and accuracy of each isolated model were evaluated using metrics like RMSE and R-squared score, revealing consistently high precision and a strong fit to the data. Subsequently, integrating these individual models resulted in a comprehensive surrogate model for the entire IES, which was further validated against a 24-hour simulation derived from a high-fidelity physics-based model developed in Dymola. The validation confirmed the reliability and accuracy of our surrogate model in mimicking real-world system behaviors.

The development of the surrogate model bears significance in expediting energy system analyses while maintaining accuracy. The models demonstrated the ability to capture the complexities of nuclear-powered IES components, offering insights into their behaviors without the computational overhead associated with traditional physics-based simulations. The alignment between predicted and actual values underscores the robustness and applicability of the approach, paving the way for its practical deployment in optimizing and managing energy systems.

As the future work, the developed surrogate model will be integrated with the optimization tools to expand its capabilities. This future work aims to explore its potential in forecasting additional variables beyond its current scope. By forecasting crucial aspects like hydrogen production rates and potentially more complex variables, we aim to enhance the surrogate model's utility in decision-making processes. Integrating these predictive abilities with optimization frameworks will empower efficient and informed decision-making in energy system management.

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