TOWARDS A ROBUST PREDICTION OF MATERIAL PROPERTIES BY ARTIFICIAL INTELLIGENCE AND PROBABILISTIC METHODS

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Abstract

The paper presents the results of a feasibility study aimed at combining probabilistic approaches for dealing with uncertainty with Artificial Intelligence (AI) technology for the prediction of the properties of materials used by the nuclear industry. This allows the AI tools to produce predictions with associated confidence, essential for the application of AI in safety critical systems. More specifically, this work involves predicting the Creep rupture and Tensile properties of a given type of steel material. To do so, a set of Artificial Neural Network (ANN) have been trained from relevant experimental data. However, the collected datasets are characterized by discontinuities and gaps in the data values. Furthermore, no information on its associated uncertainties is provided. To address these problems, a stochastic data-generating method is proposed which is used to enhance the dataset used to train the ANN models. From which, the Adaptive Bayesian Model Selection method is applied to obtain the corresponding probabilistic prediction with its associated confidence bounds. The results are well-validated against the given experimental data where the data is shown to fall within the prediction bounds. The approach has allowed for the improved accuracy of the prediction and making the model robust to bad data.

1. INTRODUCTION

1.1. Research Motivation

Currently, the nuclear sector is faced with 3 key challenges: 1) the need to decommission ageing nuclear reactors; 2) the high costs associated with the construction of new reactors; and 3) the high costs in performing experimental campaigns resulting in the lack of data [1]. Among the 3 challenges, the focus of the research would be on addressing the third challenge. As such, for the work presented in the paper, a general framework combining AI with Uncertainty Quantification (UQ) tools is proposed. This framework is known as project PROMAP – Probabilistic Prediction of Material Properties in Nuclear power plant structures. The objective behind the formulation of such method is to allow for the AI models to yield robust predictions, along with the associated confidence bounds, over a material property of interest under model uncertainty and scarce data.

1.2. Review of Artificial Intelligence in Nuclear

In a recent study, it was found that the AI technology is not widely implemented within the nuclear sector and that the sector is currently lagging behind in the industry 4.0 revolution compared to other industries such as the healthcare, automotive and manufacturing [1]. In addition, the industry seeks to develop new reactor designs for both fusion and fission. These would come in the form of the newer generation Light Water Reactors, Liquid Metal Cooled Reactors, and High-temperature Gas-cooled Reactors which are expected to be more modular and compact in their designs. In this regard, this brings opportunities for the application of AI which can be expected to play an important role in devising new ways to design, construct, operate, and decommission such reactors across the entire project operation duration [5].

The role of AI can be categorised into 2 types [1]: 1) De-centralised decision-making; and 2) Technical assistance. The first category refers to the capability of the AI systems to become autonomous, thereby being able to make simple decisions itself without human intervention. The second category refers to the capability of the AI systems in supporting the decision-making process by human towards problem-solving as well as assisting humans in completing tasks which are too complex and risky for them. These include accident identification, system performance, structural integrity, predictive maintenance, and predicting material properties and behaviours. The focus of the paper is on the technical assistance aspect of AI in the context of material properties prediction.

Over the years, numerous approaches have been implemented to predict material properties in Nuclear applications under scarce data. These include: 1) Shotgun Transfer Learning [2]; 2) Exact Muffin-Tin Orbitals [3]; and 3) Coherent Potential Approximation [3]. For the work presented in the paper, the approach involving Artificial Neural Networks (ANNs) is employed to model and predict nuclear material properties given the following strengths ANNs possess: 1) it provides a fast response in the mapping of the data; and 2) it is able to capture the non-linear behaviour which is a common characteristic of complex systems [4]. These advantages motivated the implementation of ANNs towards the work presented in the paper.

2. PROPOSED METHODOLOGY

The proposed methodology consists of 3 main steps: 1) the enhancement of the existing experimental dataset; 2) training a set of ANNs; and 3) merging the ANN predictions with Bayesian statistics.

The first step involves the implementation of a multi-variate Gaussian Mixture Model (GMM) [6] over the raw experimental data. The assumption is that the measurement error follows that of a zero-mean Normal distribution. In constructing the covariance matrix of the GMM, the following are done: Firstly, the Pearson's correlation coefficients between the features of interest are computed from which the covariance matrix is constructed. This helps to capture the physical relationship between the features, especially in the absence of a physics-based model, ensuring that such relationship is retained in the enhanced dataset. Secondly, the variance of the respective features is set at 1% of their respective nominal value to simulate the given degree of measurement error and variability for this study. This allows for the probabilistic enhancement of the experimental dataset.

In the second step, a set of ANN models of varying architectures is constructed to predict each target feature of the steel type being studied. This is to introduce the element of model uncertainty and loosens the assumption of the choice of model to describe the relationship between the input and corresponding target feature. For this study, the ANNs are trained using the synthetic data generated in the first step and are then validated using the experimental data. To quantify the strength of validation by the ANN, the R^2-score is computed for each model. Detailed conceptual and mathematical descriptions to ANNs can be found in [7].

In the third step, the Adaptive Bayesian Model Selection (ABMS) method is implemented to incorporate the elements of Bayesian statistics to the ANN predictions under model uncertainty [8]. The concept behind the ABMS algorithm is based on Bayesian inference to account for the posterior probability across the set of ANN models used to predict a given target feature. From there, a robust prediction on the target feature of interest is obtained, along with the 95% confidence interval as determined by the posterior distribution across the ANN models (i.e. Bayesian model averaging) [9, 10, 11]. While implementing the ABMS method, the synthetic data generated in the first step is used to calibrate the set of ANNs used for the prediction and is then validated with the experimental data. It will be assumed apriori that all ANN models in the set are equally likely and a Uniform distribution is used as the prior. On the other hand, a GMM is used to approximate the posterior for the computation of the confidence intervals. Mathematical details behind the ABMS method and its procedures can be found in [9, 13].

To summarise the above steps presented in the section, an illustrative flow-chart is provided in Fig. 1.

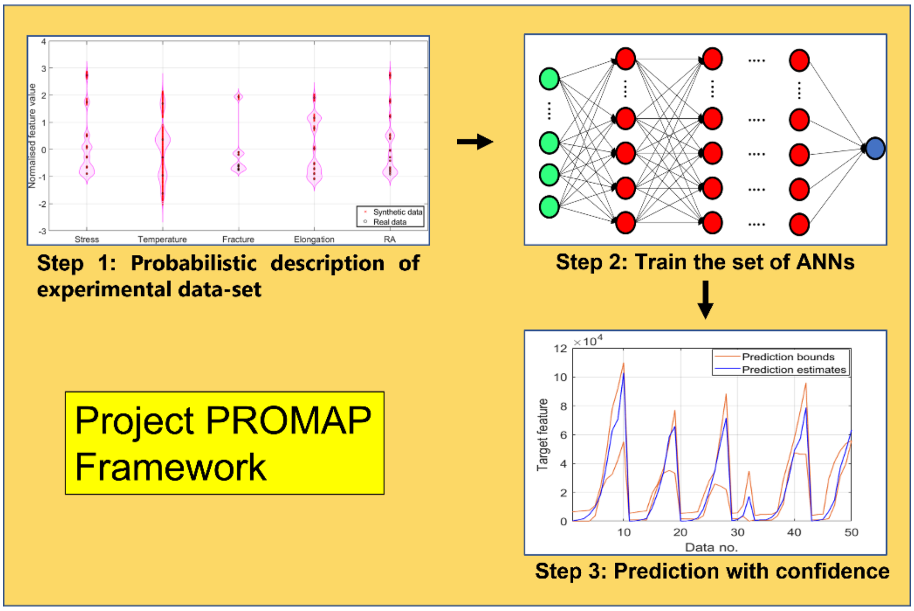

FIG. 1. Flow-chart illustrating the proposed methodology which constitutes the framework for Project PROMAP.

3. CASE STUDY

3.1. Experimental Data

The database of the material properties used in this work is based m a previous experiment campaign under the Material Properties Predictor for Power Plant Steels (M4PS) project [1, 12]. The database contained the properties of 58 type of steel and the material properties of interest are: 1) Creep rupture properties; and 2) Tensile properties. For each of these properties, their corresponding identified key input and target features are summarised in Table 1 and Table 2 respectively [12].

TABLE 1. INPUT AND TARGET FEATURES FOR CREEP RUPTURE PROPERTIES PREDICTION.

Input features	Target features
Material code	Fracture time (FT)
Cast code	Elongation
Stress	Reduction of Area (RA)
Temperature	
Composition (19 components)	

TABLE 2. INPUT AND TARGET FEATURES FOR TENSILE PROPERTIES PREDICTION.

Input features	Target features
Material code	Ultimate Tensile Strength (UTS)
Cast code	Elongation
Temperature	0.2% Proof Stress (PS02)
Composition (19 components)	Reduction of Area (RA)

To study the profile of the experimental data, a series of scatterplot diagrams are generated for both Creep rupture and Tensile properties data. These diagrams are presented in Fig. 2 and Fig. 3, respectively. From the figures, it can be observed that there is significant unevenness in the distribution as well as significant gaps between the data points. In addition, it can also be seen that some data points are grouped about discrete values as seen in the plot for Elongation vs Temperature in Fig. 1 and that for RA vs Temperature in Fig. 2. This leads to significant loss of information as the data points do not explore the entire domain of the experimental input values. Such issue of having only limited data points can be attributed to the high costs associated with performing an experiment campaign [1]. Hence, to keep costs low, experiments can only be done with selected input parameter values.

Another problem faced is the lack of uncertainty quantification over the experimental data points. The measured data obtained does not include any information on its confidence bounds or measurement error. In addition, due to the limited experimental campaigns conducted, the inherent variability associated with the experimental data (i.e. the aleatory uncertainty [8]) is not captured as well.

Hence, there are 2 main problems that PROMAP seeks to address: 1) How to enhance the existing dataset without having to perform additional experiment campaigns; and 2) How to propagate the uncertainties in predicting the material property of interest using AI tools. For this study, the Chromium-Nickel-Carbon steel type is studied for Creep rupture properties prediction, while the Chromium-Nickel-Molybdenum steep type is studied for Tensile properties prediction under scarce data. These respective steep types are chosen due to their relatively small data size available for the corresponding material properties which are relevant for this study.

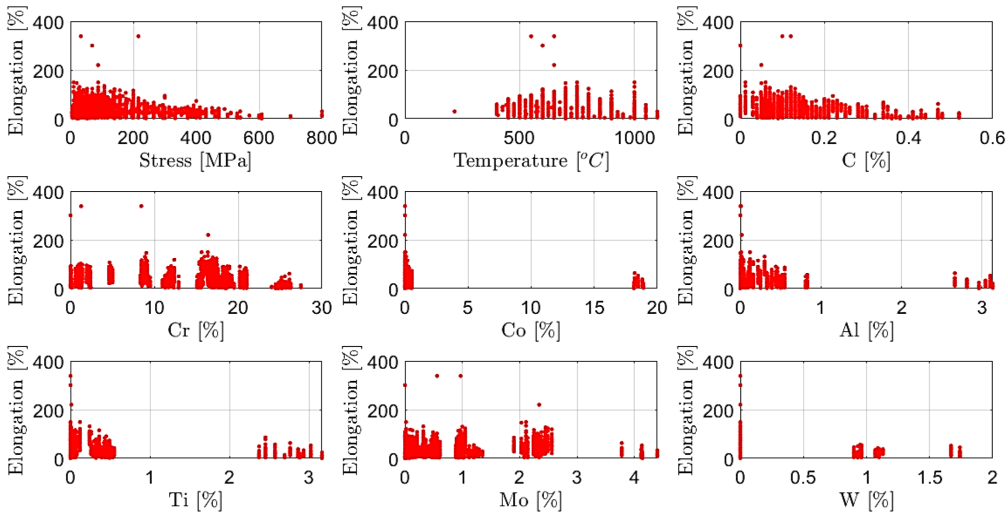

FIG. 2. Scatterplot diagrams illustrating the experimental data of the selected input features for Creep rupture properties against the target feature of Elongation.

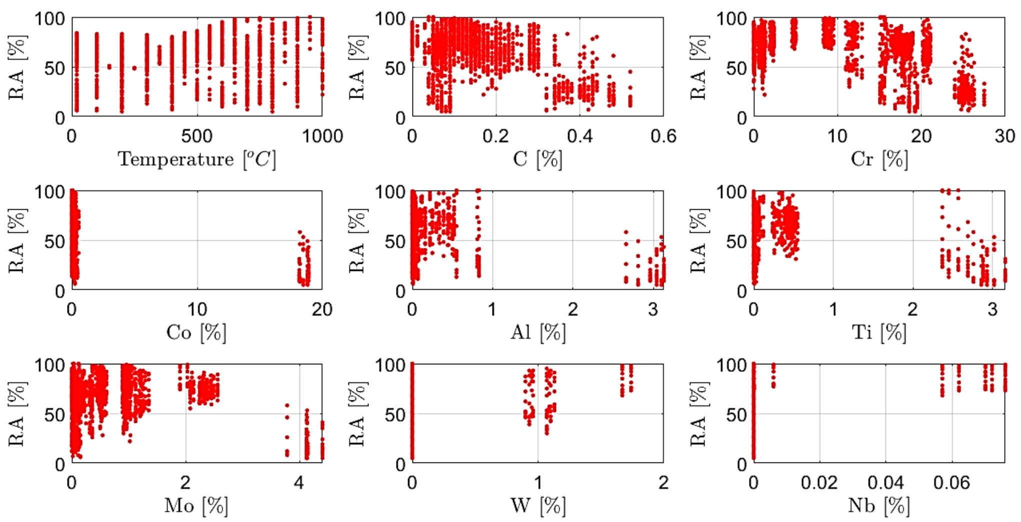

FIG. 3. Scatterplot diagrams illustrating the experimental data of the selected input features for Tensile properties against the target feature of Reduction of Area (RA).

3.2. Dataset Enhancement

Using the data enhancement approach described in Section 2, for the case of the Creep rupture data, the Pearson's correlation is computed between the features: Stress, Temperature, FT, Elongation, and RA. Next, the multi-variate GMM is constructed over the experimental data from which, 10000 synthetic data is generated in a stochastic matter. This procedure is repeated for the Tensile data for the following features: Temperature, PS02, UTS, Elongation, and RA. The resulting enhanced data for both the Creep rupture and Tensile properties data are presented in Fig. 4.

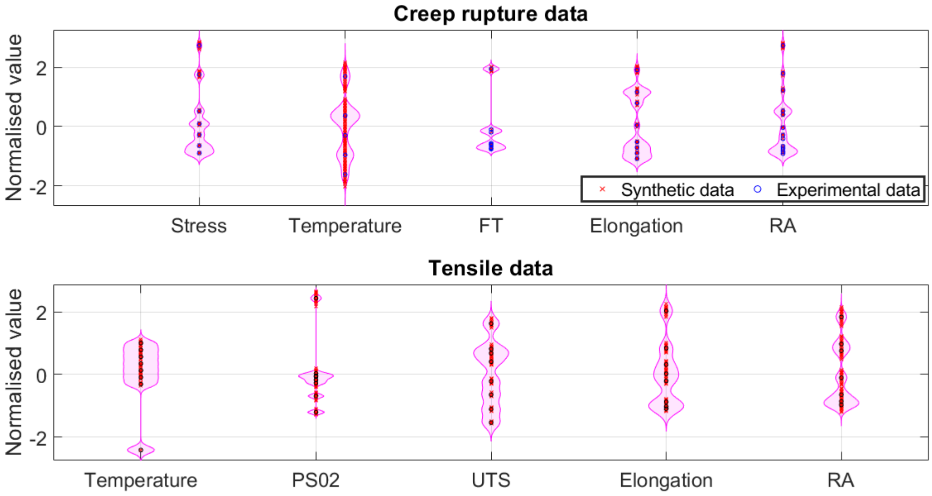

FIG. 4. Violin plots of the synthetic data along with the experiment data for both the Creep rupture data and Tensile data presented in the (standard) normal scale for fair comparison.

4. RESULTS AND DISCUSSIONS

4.1. Artificial Neural Network Training

For each of the target features, 5 ANN models are constructed and trained to which their corresponding R^2-scores in the prediction performance of the Creep rupture and Tensile properties are presented in Table 3 and Table 4 respectively. The training times for the ANN models range between 1.63s to 1534.80s and is dependent on the number of hidden-layers and hidden-nodes.

Based on the results in Table 3 and Table 4, the R^2-scores are at least 92.91% which indicates a strong degree of validation against the experimental data as well as the effectiveness of using the synthetic data as the training data. However, it needs to be highlighted as well that such high R^2-scores is due to the small experimental dataset and that such scores may potentially be lower with the increased size of the experimental dataset used for validation.

TABLE 3. R^2-SCORES OF THE RESPECTIVE ANN MODEL FOR THE TARGET FEATURES FOR CREEP RUPTURE PROPERTIES PREDICTION.

ANN Configuration	R^2-scores [%]		
	FT	Elongation	RA
23-18-1	99.85	99.98	99.98
23-32-1	-	99.94	99.95
23-18-9-1	99.99	99.99	99.99
23-27-18-9-1	99.99	99.99	99.99
23-64-32-8-1	99.99	-	-
23-64-32-16-1	99.99	99.99	99.99

TABLE 4. R^2-SCORES OF THE RESPECTIVE ANN MODEL FOR THE TARGET FEATURES FOR TENSILE PROPERTIES PREDICTION.

ANN Configuration	R^2-scores [%]			
	UTS	Elongation	PS02	RA
22-18-1	94.68	99.88	96.60	94.58
22-32-1	-	-	96.59	-
22-64-1	99.99	99.99	-	94.58
22-18-9-1	99.84	99.88	92.91	94.55
22-27-18-9-1	99.97	99.99	92.94	94.82
22-64-32-16-1	99.99	100.00	99.98	99.95

4.2. Robust Probabilistic Predictions

The results to the probabilistic predictions to the target features corresponding to the creep rupture and tensile properties of the steel being studied are presented in Fig. 6 and Fig. 7 respectively. For each of the plot, the robust estimates and the 95% confidence interval are plotted against the corresponding validation data point (i.e. Data no.). From the figures, it can be observed that the 95% confidence interval of the estimates generally enclose the experimental data points which indicates a strong degree of validation of the probabilistic estimates by the ABMS method. In addition, despite the small number of experimental data points, the 95% confidence intervals across the target features are not as wide. This is attributed to the large number of calibration data (i.e. the 10000 synthetic data points) used to train the set of ANNs and the strong R^2-scores achieved by the surrogate models as reflected in Section 4.1. The result is a high degree of precision and accuracy on the estimates of the target features of interest.

However, it is also observed that the 95% confidence interval bounds for the tensile properties target features Elongation and RA are significantly wider than those for the corresponding target features for the creep rupture properties. This is due to the relatively poor R^2-scores achieved by the ANNs used to predict these tensile properties compared to those achieved the ANNs used to predict the creep rupture properties. As a result, the uncertainty in the estimates is greater in the case of the aforementioned target features for tensile properties compared to those for the creep rupture properties.

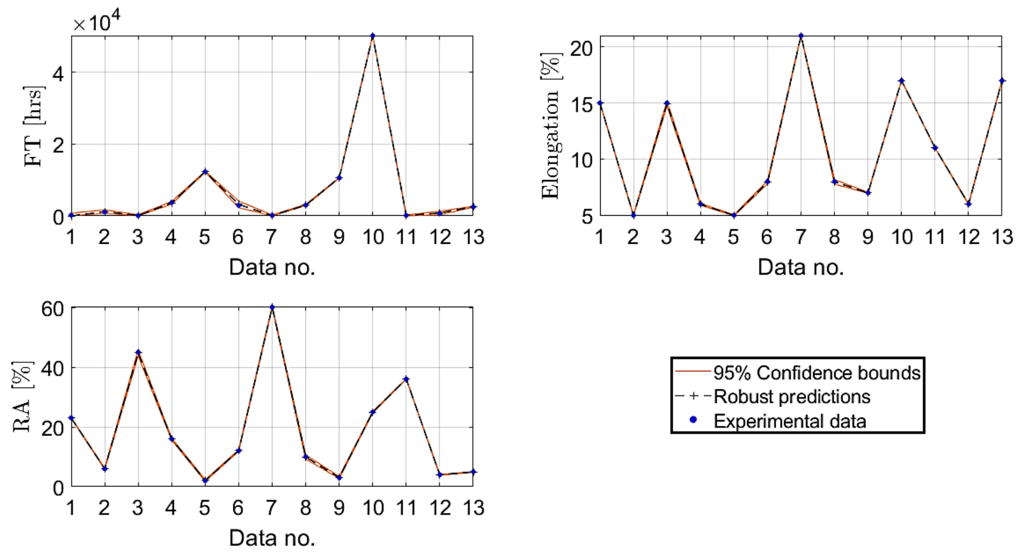

FIG. 6. Results of the robust estimates by the ABMS method over the target features for the steel's creep rupture properties.

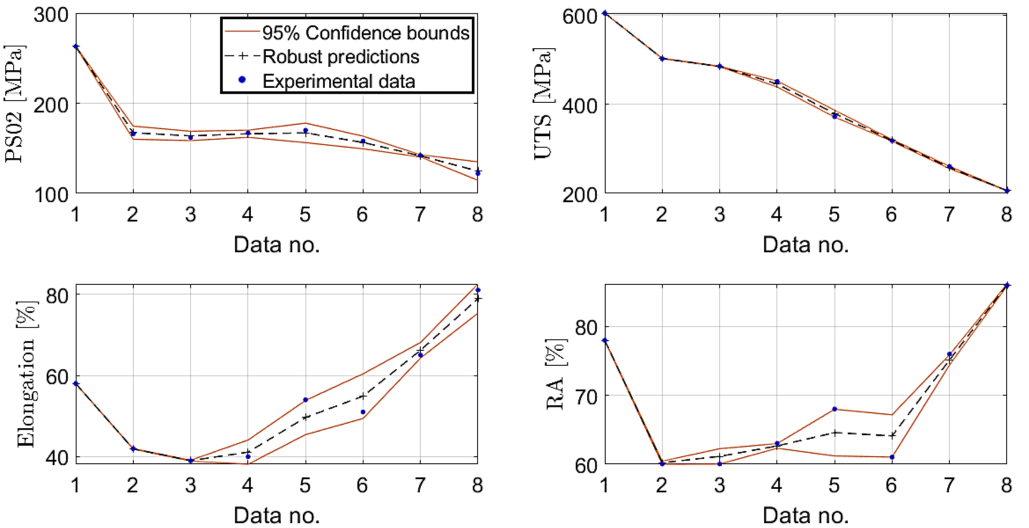

FIG. 7. Results of the robust estimates by the ABMS method over the target features for the steel's tensile properties.

4.3. Computational Times

The resulting computation times taken by the ABMS algorithm to generate robust estimates of the corresponding target features are presented in Table 5. Based on the resulting times in Table 5, it can be observed that the computation time by the ABMS in predicting the target features for the steel's Creep rupture properties is significantly longer compared to that for Tensile properties. This is because there are 13 validation data points for the case of the Creep rupture properties data while there are only 8 validation data points for the case of the Tensile properties data. Thus, it takes more time for the ABMS algorithm to generate the robust estimates and the 95% confidence interval bounds in the case of the target features for the Creep rupture properties.

TABLE 5. COMPUTATIONAL TIMES BY THE ABMS ALGORITHM FOR THE RESPECTIVE TARGET FEATURE.

Material property	Target feature	Time elapsed [s]
Creep rupture	FT	6.33
	Elongation	4.51
	RA	5.38
Tensile	PS02	2.69
	UTS	2.36
	Elongation	2.01
	RA	2.71

5. CONCLUSION

Project PROMAP presents a novel framework merging Artificial Intelligence with Uncertainty Quantification tools to provide a probabilistic prediction over the nuclear material properties. This involves the training of a set of ANN models and the subsequent implementation of the Adaptive Bayesian Model Selection method to generate robust predictions and its associated 95% confidence intervals over the target feature of interest. The latter whose results are validated against experimental data. Based on the resulting training performance of the ANN models, the R^2-scores are at least 92.91% when validated against the experimental data across all models constructed which indicates a strong degree of accuracy in the model prediction by the individual ANN relative to the experimental data. From the results of the probabilistic robust predictions by the Adaptive Bayesian Model Selection method, it can be observed that not only the robust estimates show a strong degree of agreement with the experimental data, its 95% confidence intervals also enclose the experimental data without any leaving any outlier. This also demonstrates the high degree of accuracy and precision achieved by the Adaptive Bayesian Model Selection method.

There are 4 key benefits which PROMAP seeks to provide: 1) by providing a probabilistic prediction instead of a deterministic one, the uncertainty of the estimates is accounted for. This allows for the users to determine the level of confidence on the predictions as well as make an informative risk-based decision on the choice of materials to use in the design of new nuclear reactors; 2) the proposed framework accounts for the uncertainty associated with the choice of the ANN models used for the prediction of the material properties; 3) the stochastic data-enhancement method involving the Gaussian Mixture Model, along with the information on the correlation between the features of interest, is used to generate synthetic data from the experimental data whilst ensuring that he physical relationship between the features is retained in the absence of a physics-based model; and 4) this framework can help reduce the need to run multiple experimental campaigns, thereby saving costs. More details to Project PROMAP and the results obtained can be found in [13].

For the users' interest, the MATLAB codes written to generate the results presented in the paper are made available on OpenCOSSAN [14] via: https://github.com/cossan-working-group

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