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Original Article

Deep neural network based prediction of burst parameters for Zircaloy-4 fuel cladding during loss-of-coolant accident

Siddharth Suman

Independent Researcher, Patna, 800 020, India

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ABSTRACT

Background: Understanding the behaviour of nuclear fuel claddings by conducting burst test on single cladding tube under simulated loss-of-coolant accident conditions and developing theoretical cum empirical predictive computer codes have been the focus of several investigations. The developed burst criterion (a) assumes symmetrical deformation of cladding tube in contrast to experimental observation (b) interpolates the properties of Zircaloy-4 cladding in mixed $\alpha+\ \beta$ phase (c) does not account for azimuthal temperature variations. In order to overcome all these drawbacks of burst criterion, it is reasoned that artificial intelligence technique may be a better option to predict the burst parameters.
Methods: Artificial neural network models based on feedforward backpropagation algorithm with *logsig* transfer function are developed.
Results: Neural network architecture of 2-4-4-3, that is model with two hidden layers having four nodes in each layer is found to be the most suitable. The mean, maximum, and minimum prediction errors for this optimised model are 0.82%, 19.62%, and 0.004%, respectively.
Conclusion: The burst stress, burst temperature, and burst strain obtained from burst criterion have average deviation of 19%, 12%, and 53% respectively whereas the developed neural network model predicted these parameters with average deviation of 6%, 2%, and 8%, respectively.

1. Introduction

Nuclear fuel cladding is a thin-wall tube that encapsulates pellets of uranium oxide fuel undergoing fission to generate heat [1–3]. The produced heat energy is carried away by pressurised coolant circulating outside of the fuel cladding in light water reactors. In a loss-of-coolant accident (LOCA), there is a decrease in the system pressure outside of the cladding and the heat transfer from the fuel. As the outside coolant pressure drops, internal pressure of cladding becomes higher than the surrounding pressure giving rise to hoop stress while decrease in the heat transfer rate causes a rapid increase in the temperature of the cladding. As a result, the creep deformation or ballooning of the fuel cladding occurs which may eventually cause its bursting. Moreover, ballooning of the fuel cladding may result in a blockage of the coolant sub-channel that in turn may impair the fuel coolability [4].

Understanding the behaviour of nuclear fuel claddings by conducting burst test on single cladding tube under LOCA simulated conditions [5–9] and developing theoretical cum empirical predictive computer codes [10–12] have been the focus of several investigations. Chapman et al. [6] tested Zircaloy-4 cladding having an internal heater to simulate fuel pellet in superheated steam environment. They observed that deformation of Zircaloy-4 cladding is sensitive to even a small temperature difference, and the local temperature variations is a decisive factor for burst parameters. Chung and Kassner [5] performed an extensive burst investigation on Zircaloy-4 cladding in both steam and vacuum environment. It was seen that cladding tube bends during ballooning but before burst, and this phenomenon is more pronounced for burst tests in steam or for pre-oxidised specimens than that in vacuum under otherwise identical conditions. Erbacher et al. [8] conducted burst test on Zircaloy-4 cladding and found that the burst stress depends mainly on the temperature and the oxygen content. A stress based burst criterion, assuming symmetrical deformation of cladding, was proposed based on empirical burst correlation incorporating values of oxygen concentration and burst stress. Sawarn et al. [9] did similar investigation on Zircaloy-4 cladding and proposed the empirical burst stress correlation with different weightage to oxygen concentration. Manngård and

E-mail address: siddharthhuman@gmail.com.

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Massih as well as Suman et al. [10,11] also developed burst criterion to predict the burst parameters of Zircaloy-4 fuel cladding under simulated LOCA conditions. Both studies used empirical burst stress correlation developed by Erbacher et al. [8] and also assumed symmetrical deformation of the cladding.

Even single tube burst experiments under simulated LOCA conditions are very complex, tedious, and require dedicated infrastructure. The developed burst criterion in open literature [8,10,11,13] assumes symmetrical deformation of cladding tube which is in contrast to experimental observation of bending of cladding during ballooning of tube before burst [6]. It is worth mentioning that Zircaloy-4 cladding tubes undergo phase transformation from anisotropic α-phase to isotropic β-phase with temperature rise during LOCA. This phase transformation is gradual and there exists a mixed α+β-phase. Different significant thermo-mechanical properties relevant to LOCA such as creep of cladding are not yet well understood for this mixed α+β-phase [8]. Thus, the burst criterion interpolates the properties of Zircaloy-4 cladding in this mixed phase between α-phase and β-phase. Even some arbitrary conditions without any theoretical basis are imposed on strain behaviour of cladding in this phase [8,10,11]. These burst criteria also do not account for azimuthal temperature variations in cladding in spite of the fact that the deformations, in turn burst parameters, are highly sensitive to local temperature of the cladding [6]. Moreover, burst investigation on Zircaloy-4 cladding under simulated LOCA conditions by different researchers [8,9], perhaps owing to different manufacturing route of Zircaloy-4 cladding [14], yielded different empirical parameters in burst correlations. In order to overcome all these drawbacks of burst criterion, it is reasoned that artificial intelligence technique may be a better option to predict the burst parameters of nuclear fuel cladding during LOCA since such technique does not require theoretical understanding of all the occurring phenomena.

Artificial intelligence is science and engineering of making intelligent machines, especially intelligent computer programs to achieve any desired goal. The concept of intelligence refers to certain ability to plan, reason and learn, sense and build certain perception of knowledge. Artificial Neural Network (ANN) is an artificial intelligence technique for building a computer program that learns from data. ANN is the computational model inspired by the animal brain [15]. The neural network model consists of layers, namely input layer, hidden layer, and output layer, and each layer is made up of neurons (also refereed as node). These collection of neurons are created and connected together, allowing them to send messages to each other. Neural network is trained using the available data in iterative manner, each time strengthening the connections that lead to success and diminishing those that lead to failure. In the present article, artificial neural network (ANN) technique has been applied apparently for the first time to predict the burst parameters of Zircaloy-4 nuclear fuel cladding during LOCA. Different neural network architectures have been tested and an optimised deep neural network model has been developed. The performance of the optimised deep neural network has been compared with the experimental results as well as with theoretical cum empirical predictive computer codes usually termed as burst criterion.

2. Data collection

Data collection is a very crucial step prior to development of ANN model. The performance of ANN model is dependent on the accuracy of data used to train such model. Data obtained from single tube burst experiments on Zircaloy-4 fuel cladding under simulated LOCA by Chung and Kassner [5], Chapman et al. [6], Karb et al. [7], and Sawarn et al. [9] are used in the present study to develop neural networks. These studies reported burst experiments in different environments like vacuum or inert or steam environment, with different material conditions like irradiated or non-irradiated cladding but data chosen in this study are only for burst tests conducted on non-irradiated Zircaloy-4 claddings in steam environment.

Chung and Kassner [5] conducted burst tests on the Zircaloy-4 claddings having 10.9 mm outer diameter and 0.635 mm thickness in steam environment for the heating rate and the internal pressure ranging from 3 K/s to 145 K/s and 0.5 MPa–14.5 MPa, respectively. The study was focused on understanding the high-temperature diametrical expansion and rupture behaviour of Zircaloy-4 fuel cladding tubes in vacuum and steam environments under transient-heating conditions that are of interest for LOCA. A high-speed camera was used to record the diametrical and axial changes of the tube during the burst test. Chapman et al. [6] also tested Zircaloy-4 cladding having 10.9 mm outer diameter and 0.635 mm thickness in steam environment under LOCA to determine its deformation behaviour. The heating rate and the internal pressure were varied from 4 K/s to 30 K/s and 0.8 MPa–20 MPa, respectively [6,16]. An analytical expression was deduced for the burst temperature as a function of burst pressure. The experimental results showed excellent correlation between cladding deformation and surface temperature distribution. Deformation was found to be extremely sensitive to even small temperature variations. Sawarn et al. [9] performed transient heating experiments in steam environment on Zircaloy-4 cladding tubes which were internally pressurised using argon gas in the range of 3 bar–70 bar. The heating rate was varied from 5 K/s to 19 K/s. The dimensions of Zircaloy-4 tubes were relevant for Indian pressurised Heavy water reactor with outer diameter of 15.2 mm and thickness of 0.4 mm. Like Erbacher et al. [8], they also found that oxidation or oxygen concentration in cladding tube has very significant effect on the burst stress. Table 1 provides the specifics of all the data used in the present research work.

In single tube burst tests under LOCA conditions, Zircaloy-4 fuel cladding tubes were internally pressurised and transiently heated to understand their burst or rupture characteristics as well as to evaluate burst parameters, namely burst stress, burst temperature, and total circumferential elongation. In other words, internal pressure and heating rate were input parameters while burst stress, burst temperature, and circumferential strain were output parameters for the single tube burst experiments performed on Zircaloy-4 cladding under LOCA. It is evident from aforementioned experimental details of single tube burst tests under LOCA conditions conducted by different researchers that Zircaloy-4 cladding of different dimensions has been used. In order to develop the ANN model, initial internal pressure p_0 was converted to initial hoop stress σ_0 in order to homogenise the different dimensions of cladding tube using following equations [11]:

$$\sigma_0 = \frac{p_0 r}{s} \tag{1}$$

where p_0 is the internal pressure, r and s are internal radius and thickness of the as-received cladding respectively.

3. Development of artificial neural network model

An Artificial Neural Network (ANN) structure essentially consists of layers and nodes (also known as neurons). Any ANN structure consists of three layers, namely input layer, hidden layer, and output layer. Hidden layer is the layer that establishes the functional relationship among inputs and outputs based on learning by the data. Since the overall ANN architecture affects the

Table 1
Details of experimental data used in the development of ANN model.

Researcher	Cladding dimension		Heating rate	Initial pressure
	Internal diameter	Outer diameter	K/s	MPa
	mm	mm		
Chung and Kassner [5]	10.90	9.63	3–220	0.56–14.50
Chapman et al. [6,16]	10.92	9.65	4.8–30.6	0.8–20.35
Sawarn et al. [9]	15.20	14.40	5–19	0.3–7.10
Karb et al. [7]	10.75	9.30	7–19	2.6–9.40

Table 2
Performance of artificial neural network with different architectures.

ANN architecture	Prediction error		
	mean	maximum	minimum
input-hidden-output	%	%	%
2-1-3	11.60	28.86	0.078
2-2-3	12.39	19.61	0.70
2-4-3	9.56	13.45	0.45
2-5-3	8.96	29.21	1.20
2-1-1-3	12.36	19.44	0.93
2-2-2-3	9.33	14.03	0.63
2-4-4-3	**4.79**	**19.62**	**0.004**
2-5-5-3	6.62	12.27	0.36

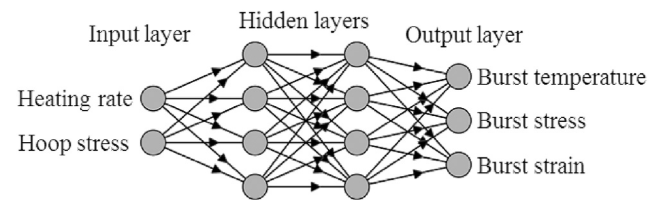

Fig. 1. An optimised back-propagation deep neural network with architecture of 2-4-4-3 used for predicting burst parameters of Zircaloy-4 fuel cladding during LOCA.

predictive response, one of the issues of the present work is to develop an optimal ANN architecture. Some of the factors that can influence the effectiveness of ANN are as follows:

3.1. Network structure

The number of nodes in input layer and output layer are determined on the basis of number of input and output parameters, respectively. However, the number of hidden layers and the nodes in each hidden layer are dependent to the complexity of the input-output mapping, computational memory and time required to achieve the response. Too many hidden layers and nodes result in high computational cost, while too few nodes may not provide optimised results. Thus, the number of hidden layers and number of nodes in each hidden layer is decided on a trial-and-error basis to obtain the best results. Sarkar et al. [17] used ANN with 9-12-1 structure, meaning that it has nine nodes for input layer, one hidden layer with twelve nodes, and one node for output layer, for prediction of in-reactor diametral creep of Zr2·5%Nb pressure tubes. Jin et al. [18] used two hidden layers with 100 and 50 neurons for predicting the onset of radiation-induced void swelling in metals used in nuclear reactors. Cottrell et al. [19] varied the number of hidden layer nodes from 2 to 15 while developing ANN model to predict the ductile-brittle transition temperature of irradiated low-activation martensitic steels. Grzesick and Brol [20] used ANN having 7-72-72-72-7 structure, meaning that it has three hidden layers with seventy-two nodes in each layer for predicting external surface characteristics of machined cylindrical part. In light of randomness of ANN structure used by different researchers to predict different kind of outputs, this study tests and compare the results of different ANN structures selected based on guidelines given by Zhang et al. [21]. They recommended that number of nodes in hidden layer should be n/2, n, 2n, and 2n+1, where n is the number of nodes in input layer. Since number of nodes in input layer is equal to number of input variables, which is two for this study, namely initial hoop stress and heating rate, the number of nodes in the hidden layer should be 1, 2, 4, and 5. Therefore, by limiting the trial-and-error process up to two hidden layers, this study applies eight different network structures, which are 2-1-3, 2-2-3, 2-4-3, 2-5-3, 2-1-1-3, 2-2-2-3, 2-4-4-3, 2-5-5-3.

3.2. Number of training and testing data

ANN is conceptually based on learning from data and thus larger the database for training the network, higher probability of better prediction. In material science, data needed to train the ANN is generated from actual experiments. Many constraints such as the availability of material, cost, and time required for conducting the experiments exist for researchers in getting large number data for training. The amount of training and testing data collected by researchers varies from as low as 20 samples of data for training and 10 samples of data for testing during developing ANN models [22]. Zuperl and Cus [23], Cus and Zuperl [24], Kohli and Dixit [25], Al-Ahmari [26], and Davim et al. [27] have obtained accurate results using ANN with total number of data 40, 30, 31, 28, 30, respectively. Thus, the dataset of 322 experiments used in the present study is expected to provide an accurate predictive result for burst parameters using ANN. 10 data from this dataset is excluded for testing of the neural network— these data were chosen in such a way that it covers entire range of heating rate and initial hoop stress. 80% of the remaining data were used for training while 20% were used for validation. Training data are those data that are presented to the network during training, and the network is adjusted iteratively to minimise its error. Validation data are used to measure network generalization, and to halt training when generalization stops improving. Testing data have no effect on training and so provide an independent measure of network performance after the training.

3.3. Network algorithm and its components

Many different ANN algorithms have been proposed by researchers for modelling the response of a system such as Cascade-forward Backpropagation (BP), Time-delay BP, Elman BP, Radial basis, Feedforward BP etc. However, feedforward backpropagation algorithm is mostly applied by researchers for predicting different kind of outputs [17,18,23]. Zuperl and Cus [23] developed ANN model using both feedforward BP and radial basis network algorithm, and it was established that the feedforward BP gave more accurate results. There are also different transfer functions available

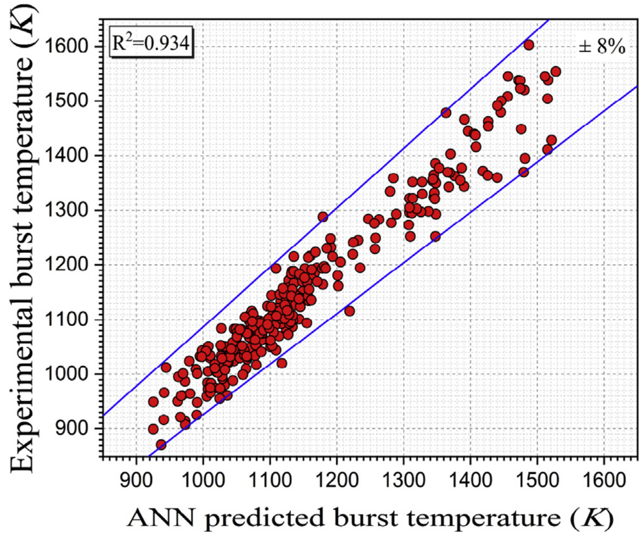

Fig. 2. Comparison of experimental burst temperature with ANN model predicted burst temperature.

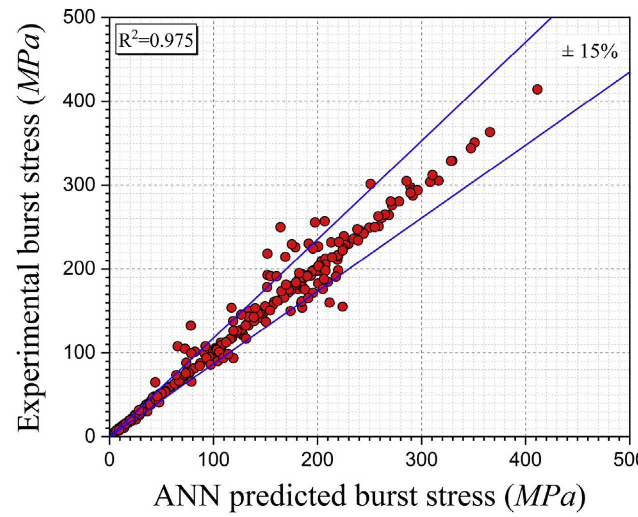

Fig. 3. Comparison of experimental burst stress with ANN model predicted burst stress.

for ANN algorithm such as log-sigmoid transfer function (*logsig*), linear transfer function (*purelin*), hyperbolic tangent sigmoid transfer function (*tansig*), and hard limit transfer function (*hardlim*). There is no clear documentation in literature about the selection of transfer function. Nalbant et al. [28] mentioned that the choice of transfer function is dependent on the nature of problem. Kohli and Dixit [25] applied both *logsig* and *tansig* transfer functions in their study, and concluded that both these transfer functions provided almost similar response. However, a number of studies usually applied *logsig* transfer function as it has an advantage that the output cannot grow infinitely large or small. The difference between the experimental output and predicted response of ANN model is error and this error is measure of performance of the model. The error is referred as performance function and there are different performance functions to evaluate an ANN model, for example mean square error (MSE), mean absolute error (MAE), sum of squares for error (SSE), root mean square of error (RMSE), mean absolute percentage error (MAPE) etc. Like the issue of transfer functions, there is no clarity provided by literature regarding the section of performance functions. However, most of the ANN models used for prediction applied mean square error (MSE) performance function.

In light of aforementioned studies performed to predict different outputs using ANN model, this study applied feedforward backpropagation algorithm, *logsig* transfer function, and evaluated the model based on mean square error (MSE) performance function. All ANN models are developed in MATLAB R2018.

4. Results

4.1. Optimisation of neural network architecture

The mean prediction errors in percentage are calculated for each network structure as [29,30]:

$$\%mean\ prediction\ error = \frac{1}{n}\sum_{1}^{n}\left(\frac{|\text{experimental value} - \text{predicted value}|}{\text{experimental value}} \times 100\right) \quad (2)$$

where n is total number of data.

The performance of all the ANN models is provided in Table 2. Based on minimum mean error in the predicted response, the ANN model with two hidden layers having four nodes in each layer, shown in Fig. 1, is found to be the most suitable among all. The mean, maximum, and minimum prediction errors for all the three burst parameters—burst temperature, burst stress, burst strain—obtained from ANN model are 0.82%, 19.62%, and 0.004% respectively. The results of this optimised deep neural network model having 2-4-4-3 structure are only discussed hereafter.

Validation of the optimised neural network

One of the most common problems during the development of ANN is overfitting. Overfitting makes neural network perform excellently on the training data, but it gives very poor results when applied to new dataset or unseen data. This problem is tackled using a validation data set in the present research to see how the model performs to new unseen data.

Fig. 2 shows a comparison between experimentally obtained burst temperature and ANN predicted burst temperature during LOCA tests. The burst temperatures using ANN model has an excellent agreement with experimental value and almost all the values for burst temperature lie within ±8% and the mean error is 2.38%. Linear regression analysis is also performed to evaluate the coefficient of determination R^2 [30] and its value is found to be 0.934. The value of R^2 is very close to unity and thus this ANN model is suitable for the prediction of burst temperature.

The prediction of burst stress also agreed well with the experimental values of burst stress and most of the data lies within ±15% with mean error of 5.50%, as shown in Fig. 3. The coefficient of determination R^2 for burst stress is 0.975.

The circumferential burst strain that gives information regarding ballooning of the cladding tube at burst location is also well predicted by the ANN model. The mean error in burst strain prediction is 9.27% and the coefficient of determination R^2 is 0.953.

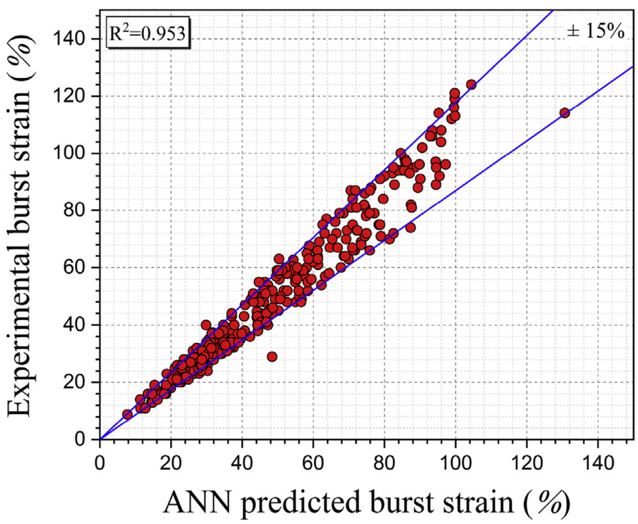

Fig. 4. Comparison of experimental burst strain with ANN model predicted burst strain.

The predicted burst strain is plotted against experiential burst strain in Fig. 4.

5. Discussion

The result of the developed ANN model is compared with burst criterion developed for non-irradiated Zircaloy-4 under loss-of-coolant accident by Manngard et al. [10]. A MATLAB code is written to develop the burst criterion in accordance with governing equations proposed by Manngard et al. [10]. This burst criterion accounts for solid-to-solid phase transformation kinetics, cladding creep deformation, oxidation, and rupture as functions of temperature and time in a unified way during the LOCA transient. Ten different experimental conditions from the collected dataset—testing data as explained in section 2 that covers the entire range of heating rate and initial hoop stress—are used to evaluate the performance of the developed ANN model. The burst parameters for same input parameters are also evaluated using the burst criterion and compared with ANN model predicted outputs. Table 3 presents a comparison of burst parameters, namely burst stress, burst temperature, and burst strain, obtained from the optimised ANN model and burst criterion [10] against the experimental values.

The burst stress, burst temperature, and burst strain obtained

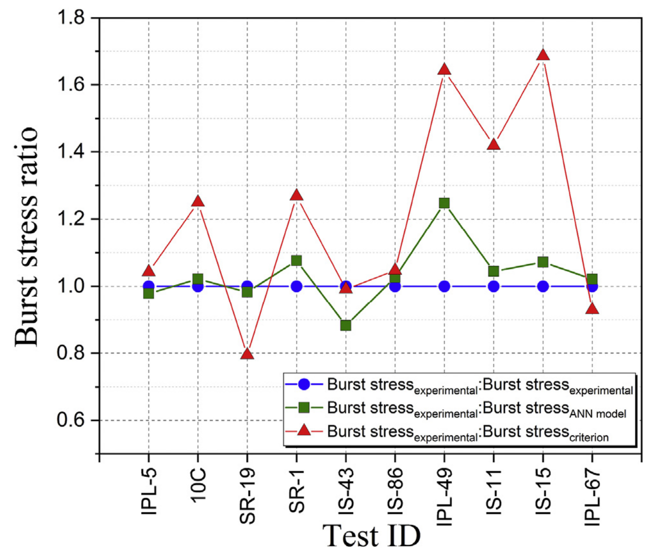

Fig. 5. Comparison of deviation in burst stress obtained from burst criterion and ANN model against the experimental burst stress.

from burst criterion have average deviation of 19%, 12%, and 53% respectively whereas the developed ANN model predicted these parameters with average deviation of 6%, 2%, and 8% respectively. Comparatively huge improvement in accuracy of burst parameters prediction with use of artificial neural network model comes from the facts that the criterion (a) developed on the basis of empirical data of Erbacher et al. [8] which has limited range of heating and internal stress (b) based on ad hoc governing equation for creep behaviour of Zircaloy-4 in mixed $\alpha+\beta$-phase (c) does not account for azimuthal temperature variation. Deviation of same order in outputs of burst criterion has been observed in other reported works [11,31]. All these drawbacks are overcome with the use of neural network since it does not require theoretical or empirical relationship. It learns from data and develop functional relationship and the higher accuracy in its prediction establishes that it outperforms the burst criterion and may be used to study the rupture behaviour of Zircaloy-4 cladding tubes under LOCA transients. To visualise the deviation from experimental values, a ratio of experimental burst stress to burst stress obtained from burst criterion, and a ratio of experimental burst stress to burst stress obtained from optimised ANN model have been obtained. These ratios have been plotted for each test to see deviation from ideal ratio of 1. Similar ratios are also calculated for burst strain. Fig. 5 plots burst

Table 3
Comparison of ANN predicted burst parameters with the output of burst criterion.

Sample ID	Input parameters		Output burst parameters								
	Heating rate	Initial hoop stress	Burst hoop stress			Burst temperature			Burst strain		
#	K/s	MPa	MPa			K			%		
			Experiment	Criterion	ANN	Experiment	Criterion	ANN	Experiment	Criterion	ANN
IPL-5	5	19.94	31.23	29.96	31.91	1166	1206	1136	23.09	20.36	27.92
10C	5	105.07	304.80	243.97	298.37	966	748	942	73	42.12	72.26
SR-19	25.9	6.88	9.90	7.81	9.20	1439	1351	1406	26	6.367	28.67
SR-1	24.2	161.73	198	249.03	201.53	961	741	968	16	21.58	17.34
IS-43	50	5.5	5.74	5.79	6.50	1520	1410	1481	32	2.64	32.02
IS-86	51	117.2	213.90	204.27	208.40	983	807	1012	37	27.79	39.87
IPL-49	100	6.71	12.16	7.40	9.75	1448	1454	1476	38	4.89	40.72
IS-11	101	111.54	264.33	186.33	253.13	1053	837	1054	58	25.66	64.42
IS-15	130	5.58	9.86	5.85	9.20	1554	1486	1528	32	2.35	31.37
IPL-67	130	100.23	160.13	172.32	156.79	1068	863	1070	33	27.11	30.77

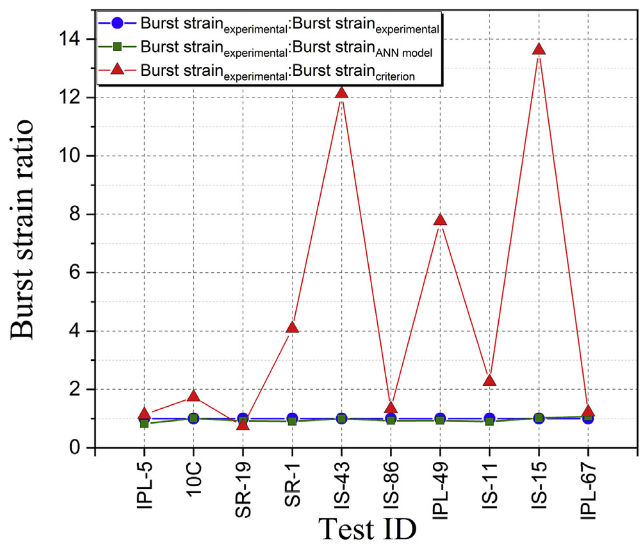

Fig. 6. Comparison of deviation in burst strain obtained from burst criterion and ANN model against the experimental burst strain.

stress ratio for all the testing data tests mentioned in Table 3 while Fig. 6 compares the scatter in burst strain. Burst stress predicted from ANN model has less scatter compared to burst criterion values and it is closer to ratio of 1. ANN model predicts the burst strain in a much superior way compared to burst criterion and the value nearly follows the line of ratio equal to 1 while the burst strain obtained from criterion has scatter too high to be considered reliable.

It may also be inferred from Table 3 that for a given heating rate, a higher initial pressure results in a lower burst temperature. Burst temperatures increase significantly with increase in heating rate for a given internal pressure, that is, higher heating rates produce higher burst temperatures. These phenomena are experientially established by different researchers and well captured by ANN model in the present research. The performance of the developed ANN model is superior to the burst criterion on the unseen experimental burst dataset of different researchers, and it implicates that this ANN model may be utilised for prediction of burst parameters during loss-of-coolant accident experiments. Nevertheless, the focus of the present research is to demonstrate the use of artificial intelligence for predictions of burst parameters during single clad tube burst tests, and to compare its performance against the semi-empirical burst criterion.

6. Conclusions

An artificial neural network has been developed based on data obtained by different researchers from the single tube burst experiments conducted on Zircaloy-4 fuel cladding under simulated loss-of-coolant accident transients. The artificial neural network has been optimised to predict the burst parameters of Zircaloy-4 nuclear fuel cladding during the loss-of-coolant accident transients. The outcomes of the neural network model are in excellent agreement with the experimental results. The results of the developed ANN model are also compared with phenomenological burst criterion developed in literature and it was found that ANN outperforms the burst criterion. The burst stress, burst temperature, and burst strain obtained from burst criterion have average deviation of 19%, 12%, and 53% respectively whereas the developed ANN model predicted these parameters with average deviation of 6%, 2%, and 8% respectively. It is also revealed that for a given heating rate, a higher initial stress results in a lower burst temperature. Burst temperatures increase significantly with increase in heating rate for a given internal pressure, that is, higher heating rates produce higher burst temperatures.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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