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CREEP LIFETIME PREDICTION OF LOW-CARBON STEELS WITH ARTIFICIAL NEURAL NETWORKS

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Abstract. *Current energy systems frequently operate under extreme conditions at high pressure and high temperature to increase the overall performance. Materials are often subjected to creep for the aforementioned conditions, which is the tendency of a material to fail due to a constant stress load at an elevated temperature, usually higher than one-third of its melting temperature. Effective creep investigation remains an arduous task, since reproducing high stresses and high temperatures for an extended period of time is not only hard to perform, but also very expensive. In recent years, Artificial Neural Networks have demonstrated the ability to solve complicated problems when a reasonable amount of data is available, predicting unseen situations after being trained with past situations. In the era of big data, where tons of observations are available, a reasonable approach to tackle the creep prediction problem is through a data-driven approach, which consists of gathering a large number of observations from past experiments and developing a unified model for creep prediction. The present work aims to implement an Artificial Neural Network for predicting the creep lifetime of low-carbon steels for high-temperature applications from the chemical composition, thermal treatment performed on the steel and working conditions (stress and temperature). The dataset utilized was created by combining an open-source dataset from the University of Cambridge containing 2,066 observations plus additional 157 observations collected from different publications in the scientific literature. The Neural Network was trained with 85% of the data, and its efficiency was checked on the remaining 15% for an unbiased estimation. The Artificial Neural Network used in this study successfully predicts creep lifetime from chemical composition, thermal treatment and working conditions with an* R^2 *of 88.6%. For few cases, the error is large, which indicates that more observations should be collected for enhancing the algorithm performance. The authors provide the code utilized in the present work for general use.*

Keywords: *Creep Lifetime, Low-Carbon Steels, Artificial Neural Network*

1. INTRODUCTION

Artificial intelligence (henceforth AI) has gained popularity in various fields of science in recent years, and it is becoming increasingly important for scientists, engineers and other professionals who frequently deal with difficult problems where traditional approaches fail to provide good results. Machine Learning (ML), a subfield of AI, is well-known for its ability to solve complicated tasks by learning from experience, allowing the development of quantitative expressions without compromising the known complexity of the problem (Bhadeshia, 2009). That is, when an event lacks a strong theory backing it up but there is a large amount of accessible data, ML approaches should be considered.

Among the many available ML techniques used these days, Artificial Neural Networks (ANNs) are gaining increasing attention for their flexibility and capacity for overcoming puzzling problems that classical ML approaches often fail to properly tackle even for large chunks of data (Tang et al., 2018). ANNs are deep learning techniques that attempt to mimic biological nervous systems (Pollard, 1990). They are being extensively used in different areas of knowledge, such as in medicine, stock market and unmistakably in engineering (Alfonso et al., 2020; Kappen et al., 1993; Silva et al., 2020). In the field of materials science, where there are puzzling problems for which the principles may be known but that are not yet amenable to mathematical treatment (Bhadeshia, 1999), deep learning approaches have greatly helped researchers to properly characterize many uncharacterized materials in the past few years. Singh *et al.* (1998) predicted the yield to tensile strength ratio of hot-rolled steels as a function of carbon and manganese concentrations; Kim *et al.* (2020) created an efficient deep learning method for automatically distinguishing microstructures of low carbon steels; Urda *et al.* (2013) developed a Neural Network to predict pitting corrosion status of stainless steels. From the previous examples, it is clear that ANNs are a powerful tool for solving challenging materials science tasks.

Internal combustion engines, gas power plants and high performance energy systems in general operate under harsh circumstances and regularly approach melting temperatures in order to improve thermodynamic efficiency and minimize costs (Chatzidakis, Alamaniotis and Tsoukalas, 2014). Under the effect of persistent stress and high temperature, materials are prone to creep, undergoing permanent plastic deformation until failure. The prediction of creep lifetime remains an arduous task and often lacks accuracy. Furthermore, experimental investigations are not easily obtained, since it is expensive to reproduce high temperature and high stress conditions and it takes over several weeks or even years until the material fails due to creep (Lim et al., 2004). In that context, the present work aims to create an ANN that can successfully predict with good accuracy the creep lifetime of low-carbon steels and be deployed for real world applications as an attempt to reduce the maintenance frequency of components under creep, increasing energy efficiency and reducing costs.

1.1 Artificial Neural Networks

A typical ANN is represented in Figure 1. The base elements of an ANN are the nodes – also called neurons – and the connections between them. The input layer receives, at each entrance node, one specific feature (a chemical element, one working condition, for instance), which is then multiplied by a random weight ranging from -1 to 1 and summed up all together; this sum is then transformed by an activation function, producing another value that will be passed to the next neuron in the next layer until the process is finished and one (or more) output is obtained. One of the most widely used activation functions is the rectified linear unit (ReLU), which is defined as *max(0,u)*. That is, if the summed input (*u*) is negative, it will return 0, otherwise it returns the summed input itself. The main advantage of using the ReLU activation function over others is that it does not activate all neurons at the same time and usually presents good convergence performance (Gupta, 2020; Krizhevsky et al., 2017). It should be remembered though that it is not guaranteed that the best performance will be obtained applying the ReLU activation function, but for convenience it is often applied for regression problems.

After a series of transformations, the final output (or outputs, if the output layer has more than one node) is then compared to the expected value and, applying a technique known as "backpropagation", the model is refined by adjusting the strength of all previous weights (Buscema, 1998). Depending on how the weights are randomly initialized the algorithm may present different performances (Abed Rouai et al., 2001; Waghmare et al., 2007), but the impact of the weight process tends to be mitigated as the data set grows in size.

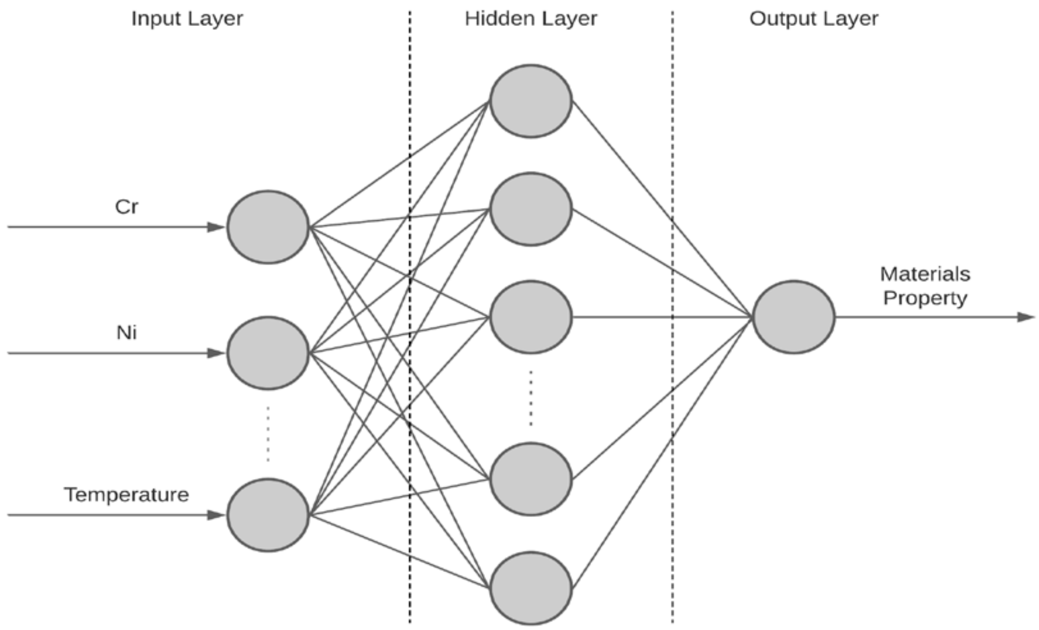

Figure 1. Schematic representation of an Artificial Neural Network.

The number of hidden layers, number of neurons per hidden layer and the activation function in each hidden layer are all hyperparameters that should be found through trial and error by tuning the model. There are other tunable parameters as well that should be considered when dealing with an ANN, and some of them are represented in Table 1. To find the best combination of hyperparameters for an ANN, the most usual approach is to resort to a technique known as "Cross-Validation". This method splits the training data set into k-folds, where (k-1) folds are used for training the ANN and the remaining fold is used to assess the accuracy of the model as a validation set. The k-fold Cross-Validation constantly changes the validation set, making use of all the data, not squandering it (Misraa, 2017). One can apply statistical tests while using Cross-Validation to compare the error distributions and carry out a stability analysis, however all statistical tests in this scenario should be viewed as heuristic tests instead of rigorously correct methods due to the violation of the independence assumption, since the training and validation sets overlap (Dietterich, 1998).

Table 1. Some of Artificial Neural Network hyperparameters that can be tunned

Hyperparameter	**Function**
Learning rate	How fast the model moves towards the minimum of a loss function
Epochs	How many times the ANN sees the same data during training
Batch size	How many samples will be seen before the weights are updated

After performing a Cross-Validation and selecting the model that has the highest performance on average, the model should be retuned with the whole training set and its performance assessed once more on unseen data to verify the robustness of the model. Usually, the original dataset is split into a training set, which will be cross-validated, and a test set, which will be used to assess the unbiased performance of the final model. Ideally, one should not leave too many observations on the test set since it would harm the performance of the final model, which will be trained with less data, but if too few observations are left on the test set it will not hold statistical significance, not fulfilling its purpose. In the scientific literature, it is common practice to have a training set and test set ratio equal to 80:20, but the ratios of 85:15 and even 90:10 are not uncommon.

2. MATERIALS AND METHODS

A survey on the scientific literature was performed in order to make a data set containing the chemical composition of low-carbon steels, the thermal treatment conditions and working conditions. A total of 2,223 points were gathered, 2,066 from a Cambridge open-source project in (Yoshida et al., 1999) and 157 from different sources in the literature (Abe et al., 1992; Fedoseeva et al., 2020; Fujita et al., 1980; Klueh, 1980; Li et al., 1999; Mazaheri et al., 2010; Strang et al., 1997; Vivas et al., 2020; Wang et al., 2016). The dataset is described as follows:

- Chemical Composition: Carbon (C), Silicon (Si), Manganese (Mn), Phosphorus (P), Sulphur (S), Chromium (Cr), Molybdenum (Mo), Tungsten (W), Nickel (Ni) Copper (Cu), Vanadium (V), Niobium (Nb), Nitrogen (N), Aluminium (Al), Boron (B), Cobalt (Co), Tantalum (Ta), Oxygen (O) and Rhenium (Re).
- Thermal Treatment Conditions: Normalising temperature and time, cooling rate of normalisation, tempering temperature and time, cooling rate of tempering, annealing temperature and time, cooling rate of annealing.
- Working conditions: Stress, temperature and creep lifetime.

The chemical elements are in w.t.%. If the presence of an element was not informed, it was considered as zero. The normalising, tempering and annealing temperatures are in Kelvin. If not informed, it was considered as 293 K. The normalising, tempering and annealing times are in hours. If not informed, it was considered as zero. For all cases, both the heat treatment temperature and time were informed simultaneously or none was informed. The cooling rate of normalisation, tempering and annealing are furnace cooling, air cooling, oil quench or water quench. If not informed, it was considered that the material was air cooled. The stress is in MPa. The working temperature in Kelvin. The creep rupture lifetime is in hours.

A statistical overview of the dataset is summarized in Table 2. The lifetime is the target value and all the other 30 features are considered as inputs. The data was initially split into training and test sets with a ratio of 85:15. The training set underwent a 5-fold Cross-Validation where 170 random combinations of the hyperparameters described in Table 3 were tested out. The activation function was set to ReLU and the learning rate was set to 0.001. The metric applied in this work was the Mean Squared Errors (MSE). After 2/3 of the random combinations were examined, a Bayesian optimizer was activated to focus the search on the space where most likely lives the best combination of hyperparameters. That is, the 5-fold Cross-Validation was wrapped on a Bayesian optimization algorithm. For this specific problem, not only the performance on average of each combination of hyperparameters was looked at, but also the error stability of each cross-validated fold. A ksample Anderson-Darwin test (ksample AD test) was performed on the cross-validation errors for all cases and the p-value annotated for a heuristic analysis. If the p-value is higher than a prespecified threshold, we retain the null hypothesis that the error distributions are the same. Not only the performance on average had to be satisfactory, but the error distributions should have a p-value higher than 0.01, the chosen threshold for the present work.

After selecting the model with the lowest MSE error that fulfills the condition of a ksample AD test p-value higher than 0.01, it was then tuned again with the whole training set (85% of the data) and its score obtained on the test set (15% of the data). An important remark is that all the inputs were rescaled into a comparable range by applying Eq. (1). This process is important to draw out the best performance of the ANN (Puheim et al., 2014). If the inputs are not rescaled, a feature of greater magnitude may have a larger impact on the ANN instead of others.

$$z = \frac{x-\mu}{\sigma} \quad (1)$$

Table 2. Dataset statistical characteristics

2223 Data Points	**Range**	**Mean (μ)**	**Standard Deviation (σ)**
Lifetime (h)	0.6 – 192,607	6,960.499	16,180.772
Stress (MPa)	18 – 544	163.933	96.493
Temperature (K)	723 – 977	867.782	62.102
[C] Carbon (wt%)	0.004 – 0.23	0.111	0.044
[Si] Silicon (wt%)	0 – 0.86	0.291	0.175
[Mn] Manganese (wt%)	0 – 0.92	0.500	0.126
[P] Phosphorus (wt%)	0 – 0.029	0.012	0.008
[S] Sulphur (wt%)	0 – 0.02	0.008	0.005
[Cr] Chromium (wt%)	2.165 – 12.9	8.476	3.263
[Mo] Molybdenum (wt%)	0 – 2.99	0.915	0.545
[W] Tungsten (wt%)	0 – 3.93	0.398	0.747
[Ni] Nickel (wt%)	0 – 2.9	0.277	0.387
[Cu] Copper (wt%)	0 – 0.87	0.072	0.109
[V] Vanadium (wt%)	0 – 0.28	0.119	0.099
[Nb] Niobium (wt%)	0 – 0.312	0.036	0.046
[N] Nitrogen (wt%)	0 – 0.165	0.030	0.027
[Al] Aluminium (wt%)	0 – 0.057	0.011	0.012
[B] Boron (wt%)	0 – 0.051	0.001	0.004
[Co] Cobalt (wt%)	0 – 3.9	0.161	0.558
[Ta] Tantalum (wt%)	0 – 0.18	0.001	0.009
[O] Oxygen (wt%)	0 – 0.035	0.010	0.004
[Re] Rhenium (wt%)	0 – 1.69	0.014	0.126
Normalizing Temperature (K)	293 – 1,453	1,279.235	79.069
Normalizing time (h)	0 – 33	1.996	3.749
Normalizing cooling method *0 – furnace cooling* *1 – air cooling* *2 – oil quench* *3 – water quench*	0 – 3	1.383	0.790
Tempering temperature (K)	823 – 1,133	978.191	70.394
Tempering time (h)	0.5 – 40	3.941	7.616
Tempering cooling method *0 – furnace cooling* *1 – air cooling* *2 – oil quench* *3 – water quench*	0 – 3	1.026	0.486
Annealing temperature (K)	293 – 1,069	437.122	272.851
Annealing time (h)	0 – 50	1.854	6.924
Annealing cooling method *0 – furnace cooling* *1 – air cooling*	0 – 1	0.949	0.221

Table 3. Examined Hyperparameter ranges

Hyperparameter	**Range**	**Step**
Hidden layers	(1,3)	1
Neurons per hidden layer	(32, 1500)	32
Epochs	(50,2000)	50
Batch size	(32, 128)	32

3. RESULTS AND DISCUSSION

The best combination of hyperparameters for this specific problem is described in Table 4. The 95% Confidence interval for the R^2 obtained through cross-validation is (82.24%, 89.13%) and the ksample AD test p-value obtained after comparing the error distributions is equal to 0.05, which is above the chosen threshold of 0.01.

Table 4. Best combination of hyperparameters obtained through Cross-Validation

Hyperparameter	**Value**
Number of hidden layers	3
Neurons in the 1st hidden layer	128
Neurons in the 2nd hidden layer	1344
Neurons in the 3rd hidden layer	224
Batch size	64
Epochs	550

After tuning the ANN with the hyperparameters described in Table 4 with the whole training set and assessing its performance on the test set, a R^2 of 88.6% and the error histogram described in Figure 2 is obtained. The error is described as the expected value minus the predicted value. As can be noted in Figure 2, the prediction error is centered in zero, which indicates low bias. For few instances the error is massive, which signalizes that the algorithm should be used with caution and more data need to be fed into it to increase the overall performance. Since the error outliers are mostly negative, this means the model may overpredict the creep lifetime, which may lead to catastrophic failures if used without caution.

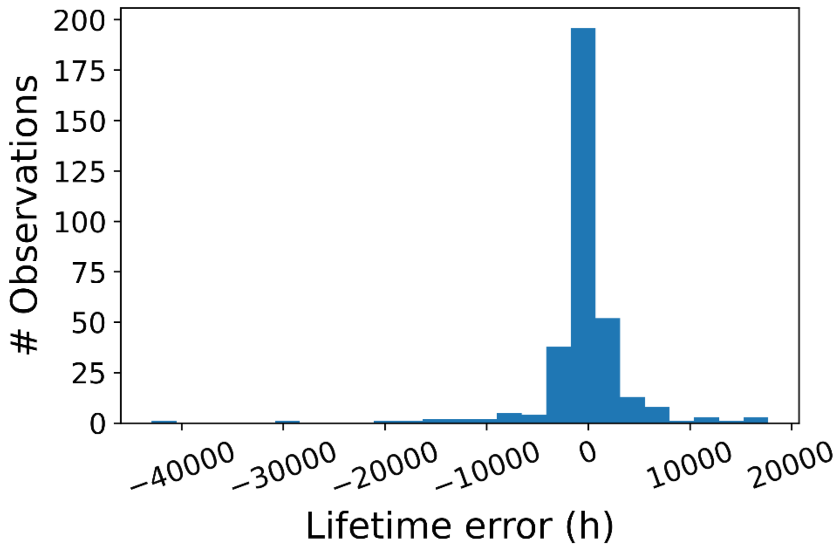

Figure 2. Error distribution obtained after checking the obtained ANN on unseen data

It should be remembered that two identical pieces of the same material under the same working conditions would not fail due to creep at the exactly same time. Although the ANN will always produce the same result if the inputs remain constant, it was tuned with values with an output that is probabilistic by nature, hence even if more data points are given to the algorithm, it will always have some considerable error attached to it.

To verify how the algorithm behaves when the temperature and pressure are changed but all the other parameters are set as constant, four materials with randomly generated chemical composition and randomly generated thermal treatment conditions were analysed. The characteristics of the four materials are described in Table 5. The log-log stress vs creep lifetime plots for these materials are displayed in Figure 3. It is interesting to see that when the lifetime is roughly below 10^5 h, there is almost a linear trend for all materials and conditions, but as the conditions are relaxed (lower stress and/or lower temperature) and lifetime increases past 10^5 h, the linear fit inclines downwards, which is in accordance to (Abdallah et al., 2018). The classical linear approach usually works well for short-term creep failures, but fails when dealing with long-term prediction. On the other hand, the ANN can capture the long-term behavior but struggles to output short-term creep lifetimes, as can be seen in Figure 3 where some trend lines are connected to the y-axis, indicating that a negative output was produced, therefore rounded to zero. For predicting the short-term creep lifetime, the author recommends plotting the stress vs creep lifetime curve in the log-log base, just as done in the present work, and create a linear plot with the ANN-generated outputs which are below the threshold of 10^5 h. This threshold was arbitrarily selected based on Figure 3 and may slightly vary depending on each case.

Table 4. Randomly Generated Materials

	Material 1	Material 2	Material 3	Material 4
C (wt%)	0.064285	0.190235	0.184491	0.042429
Si (wt%)	0.706882	0.358567	0.235857	0.027008
Mn (wt%)	0.197058	0.83151	0.27359	0.620475
P (wt%)	0.000256	0.0219	8.34E-05	6.22E-05
S (wt%)	0.014697	0.013225	0.018775	0.016264
Cr (wt%)	10.11385	10.62377	3.400944	3.986633
Mo (wt%)	2.338712	1.41159	0.563426	1.665499
W (wt%)	0.332638	1.334667	1.500371	3.787182
Ni (wt%)	2.315403	2.868404	2.899432	1.335139
Cu (wt%)	0.140278	0.598417	0.347909	0.730964
V (wt%)	0.193304	0.029228	0.240519	0.032093
Nb (wt%)	0.225813	0.006796	0.231056	0.074489
N (wt%)	0.054714	0.079241	0.007827	0.161728
Al (wt%)	0.020274	0.037017	0.018406	0.047127
B (wt%)	0.01359	0.046209	0.0221	0.033932
Co (wt%)	0.091415	1.199478	1.332251	1.512165
Ta (wt%)	0.131605	0.056906	0.155265	0.091436
Re (wt%)	0.563935	1.152819	0.676063	0.932538
O (wt%)	0.005125	0.009689	0.021673	0.02826
Tempering temperature (K)	927.3916	1,128.108	843.7585	1,125.962
Tempering time (h)	37.10103	6.060461	10.70773	19.98397
Tempering cooling method (-)	1	0	3	3
Normalising temperature (K)	882.1041	1,437.568	1,228.493	1,441.611
Normalising time (h)	18.86701	25.33744	27.52958	16.79196
Normalising cooling method (-)	1	1	2	3
Annealing temperature (K)	1,022.647	1,088.764	1,086.915	977.6478
Annealing time (h)	14.31265	31.92376	32.22464	41.80881
Annealing cooling method (-)	0	1	1	0

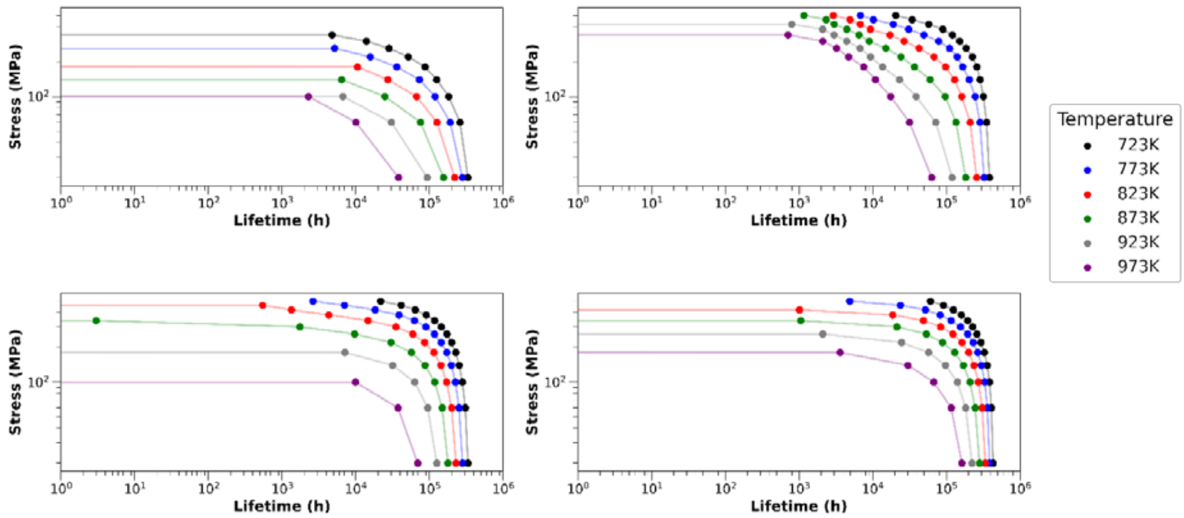

Figure 3. Typical stress vs creep lifetime plot for the four materials described in Table 5. a) material 1 represents the upper-left plot; b) material 2 the upper-right; c) material 3 the bottom-left and d) material 4 the bottom-right

Figure 4 is used to visualize a comparison between real-world data versus the ANN-generated data, where the top plot refers to data from Truck *et al.* (1991) and the bottom plot refers to data from Kaibyshev *et al.* (2016). The characteristics of each material and heat treatment is presented in Table 5. It is interesting to see that for both cases the creep lifetime was overpredicted by the ANN algorithm. It is important to emphasize that, although overpredicted, the ANN results were obtained without carrying out any experiments and can be used for an initial idea of the real creep lifetime of a material. As more data is fed into the ANN, it is expected to obtain better results that could lead to more accurate and more reliable predictions.

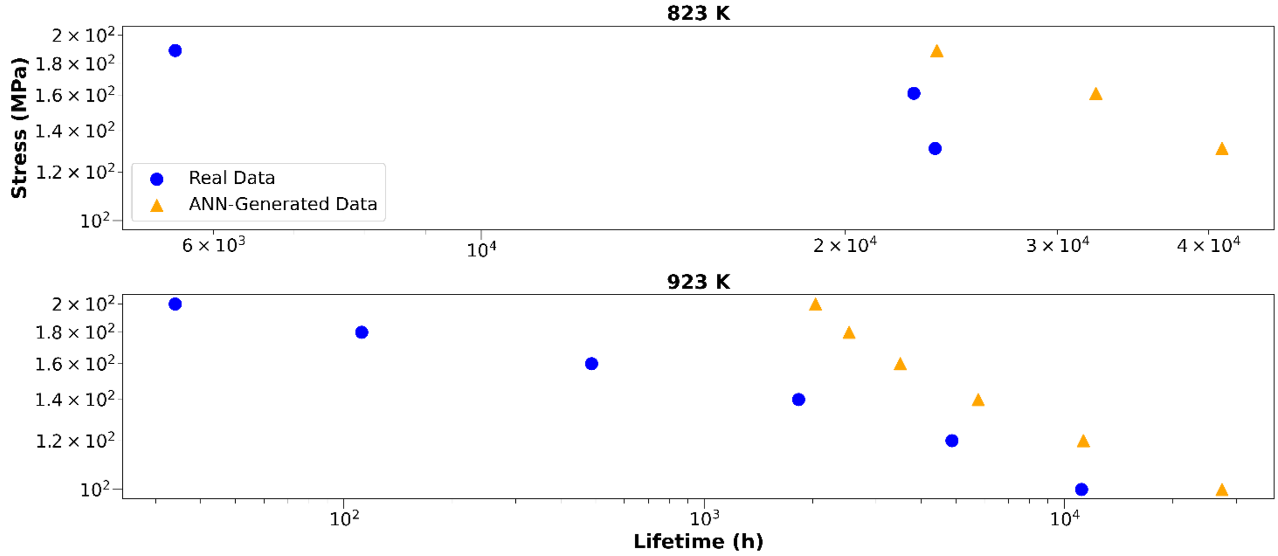

Figure 4. ANN outputs vs real data creep lifetime

Table 5. Chemical and heat treatment conditions for the materials illustrated in Figure 4. The star (*) indicates that the normalising time was not informed, so a value of 0.5 hours was assumed since the treatment was performed

	C	**Cr**	**Mo**	**Ni**	**Si**	**Mn**	**V**	**Nb**	**Normalising Temperature**	**Tempering Temperature**
823K	0.22	11.4	0.86	0.68	0.25	0.52	0.32	-	1323	1053
923K	0.12	9.5	0.44	0.04	0.08	0.2	0.2	0.06	1323	1023
	P	**S**	**Al**	**N**	**W**	**Co**	**B**	**Ti**	**Normalising Time**	**Tempering time**
823K	0.017	0.005	-	-	-	-	-	-	0.5	3
923K	-	-	0.01	0.05	2	3.1	0.005	0.002	0.5*	3

4. CONCLUSIONS

An Artificial Neural Network was created using as inputs the chemical composition, thermal treatment conditions and working conditions in order to predict the creep lifetime of low-carbon steels. The obtained model has a R^2 score equal to 88.6% on unseen data, which signalizes a great performance taking into account that no experiments are required to obtain the creep lifetime. Although the model has low bias, it has few overpredicted outliers, indicating that the result may be overestimated in some situations and it should not be blindly trusted. In addition, the model struggles to predict quick creep lifetimes, sometimes outputting a negative value – which is converted to zero – indicating that the prediction was unsuccessful. For those cases the author recommends to obtain some points from other working conditions with the ANN and fit a linear curve on a log-log stress vs lifetime plot, although this approach should be considered just as a rough estimate. The ANN utilized in the present work can be freely accessed and used for general purposes in the following repository: https://github.com/CorsettiS/COBEM2021---Creep-Lifetime-Prediction.

5. ACKNOWLEDGEMENTS

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