

Representation of the Heat Specific Creep Rupture Behaviour of 9%Cr Steels Using Neural Networks

Olga Frolova^{1*}, Eberhard Roos¹, Karl Maile¹, and Wolfhart Müller²

¹ Material Testing Institut (MPA), University of Stuttgart, Pfaffenwaldring 32d, 70569 Stuttgart, Germany

² Technical University Mining Academy of Freiberg, Bern-von-Cotta-Straße 4, 09569 Freiberg, Germany

* corresponding author: olga.frolova@mpa.uni-stuttgart.de

Abstract. The present work aims to demonstrate an innovative way of application of modern data analysis tools for structural power plant materials, such as 9%Cr-steels. The purpose is the optimized prediction of the material behaviour considering the stress/time to rupture data and the determination of position of the specific melt in the scatter band for the given steel. This data is needed for an effective life time assessment of power plant components. The material behaviour is influenced by the multidimensional interdependencies between the individual elements of the chemical composition, the heat treatment parameters, product form, tensile properties and microstructure, which are difficult to describe using simple analytical methods. Modeling with neural network techniques therefore seems to be an interesting alternative. Moreover, the applied method takes away the requirement for long and expensive experiments. A large variety of data was used for training of a commercial neural network. By means of sensitivity studies the influence of specific data features was investigated with regard to an optimized correlation factor r . The interpretations of the neural network have been checked whether basic physical and metallurgical backgrounds are reflected. The results are compared with the real material behaviour gained by material tests. The applicability of the neural network tool for technical use in life time assessment was investigated.

Keywords: 9%Cr-Steels, data mining, creep-rupture behaviour, neural network.

1 Introduction

Modern non-destructive and destructive material testing experiments need novel data analysis methods that can automatically analyze data sets with a high number of attributes and data. In the past, data mining experiments have to be applied to a variety of different material testing applications [1], [2], [3].

For e.g., neural nets and decision trees have been developed for welding-seam inspection in order to judge if a component contains a crack or a hole [1], [2]. It has been shown that neural nets and decision trees have advantages and disadvantages that have to be taken into consideration before making the decision about what kind of data mining method should be used for the particular application [1].

Data from pump inspection were analyzed by genetic feature selection methods in order to figure out the relevant features among all the various features that were acquired during the experiment. The obtained highly-relevant features were used to build a classifier for in-situ pump inspection [3] in order to predict the life-time of a pump or a pump component.

We want to use data mining in order to judge the behaviour of the material before it is used for a particular component in a power plant or in another industrial plant with high-class claims.

In this paper we describe our work on using data mining for determining creep rupture behavior of the individual melt and extended to additional steels. The remainder of the paper has the following structure. The problem description is given in Section 2. The application is described in Section 3. We decided to use neural nets for data mining experiment since we expect our data highly correlated and neural nets can easily perform classification on non-linear decision surfaces. The objectives of our work are described in Section 4. The neural network model is described in Section 5. There we describe the data set and the application of neural networks. In Section 6 we present our results for modeling with creep rupture strength and time to rupture. We explain why we have to verify our neural network model and give an evaluation of physical and metallurgical backgrounds. Final we give conclusion in Section 7.

2 Problem Description

The experience has shown the fact that the old approaches for data mining and processing which were used in a past to evaluate power plant data, usually result in high data scatter or even deliver unrealistic or physically impossible results. In any case inaccurate outcome could cause high costs damages or unplanned idles.

Also modern non-destructive and destructive material testing experiments provide more and more data as well as new factors to be considered which make old methods outdated and ineffective.

Artificial neural networks have been proved as very effective tools for modeling of creep behaviour of weld metal based on knowledge of creep strength of wrought plates, which are available mostly for austenitic steels, Badeshia [4]. Even so these methods have some disadvantages, which have to be taken into consideration before application, as already mentioned above.

The main question of this research is: “How can an individual creep rupture curve of the melt be determined? “ There are several possibilities, which allow us to get the answer we are looking for. One way is creep tests, which requires minimum 4 years, so far as components made of given steel are expected to remain in service more than 100 000 hours. In addition, the technique is applicable just in case of availability of given steel grade, this is not the case for old power plants. The second way is a theoretical approach, so called Z-Factor, where the estimation of the dependencies between creep strength and the corresponding parameters is achieved using factor, according to Melzer [5], [6]. This approach is not empirically verified for modern steels.

The previous work on application of neural networks on assessment of long-term creep behaviour of heat-resisting steels was successfully done for the 11%Cr-steel X20CrMoV11-1, Balos [7].

The focus of the work described in this paper is an application of modern data analysis tools for structural power plant materials, such as 9%Cr martensitic steels. The purpose is the optimized prediction of the material behaviour considering the stress/time to rupture data and the determination of position of the specific melt in the scatter band for the given steel. In this paper we describe our work on using data mining for determining creep rupture behavior of the individual melt as a function of many parameters.

3 Application

Critical components in power plants are exposed to high temperatures and pressures. The material strength parameter, which is used for the design of the component, depends on time and temperature. This parameter normally will be determined by performing creep tests. That means, a specimen is exposed at a constant temperature to a constant load. During the experiment, the elongation of the specimen will be measured: a time-dependant creep elongation results in the deduction of the elastic strain and the strain at the time of load. The time to rupture of specimen represents the target of the investigation. The stress value calculated from the load test of the specimen is applied over the time until failure of the sample, so-called time to rupture. The result is the scatter band of the experimental data. With the help of various numerical methods, an estimation of the mean value can be determined. This mean value in turn provides the basis for the design of components. However, as it is shown in Figure 1, the experimental results represent a relatively large scatter band; the design value compared to the mean value will be lowered by 20%. This factor is to ensure that the use of an individual melt, whose strength value lies below the mean curve, won't lead the component to fail. Technically, it is accepted a scatter band of $\pm 20\%$ around the mean value. Since it is unknown what position has the built-in melt in the scatter band, for the determination of the consumed lifetime of component it will be forced to apply the lower scatter band limit. In that way, the conservative estimate of the calculated lifetime of component will be obtained. For example, the overestimation of the lifetime can be up to 300%, in case of melt at the upper scatter band situated.

The possibilities for the realistic calculation of the component lifetime arise as a result from:

- Determination of specific melt creep rupture curves
- The classification of individual melt in the scatter band via a correlation with melt-specific data.

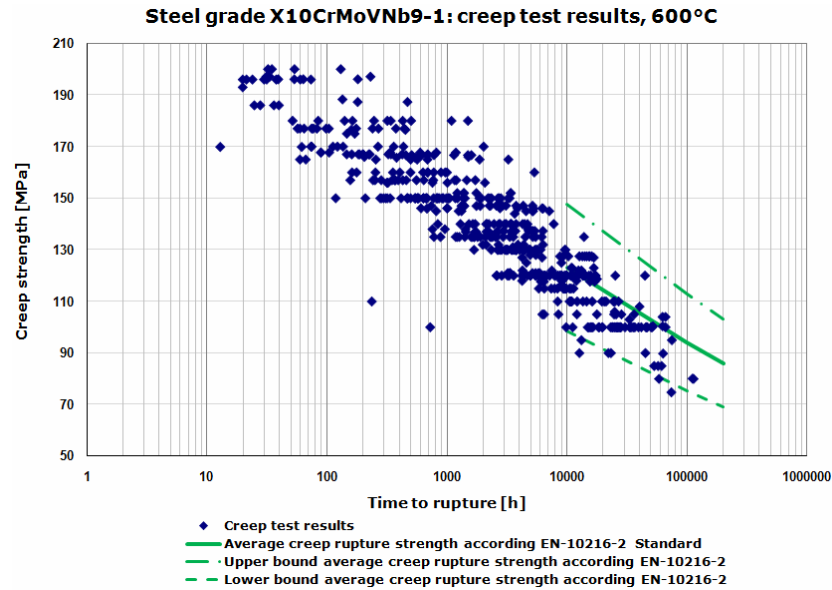


Fig. 1. Creep rupture strength at 600 ° C - scatter band of the material X10CrMoVNb9-1 and mean value according EN 10216-2 standard.

Other important properties, such as the creep rupture deformation, e.g. elongation, reduction of area or the short-term behaviour, e.g. yield stress, are often associated with individual characteristics, such as a particular value of an element that differs from the mean value or associated with parameters of the heat treatment parameters. However, from the metallurgical point of view, it's more unlikely that simple linear relationships exist for one feature only. It is rather to be expected that complex interactions between different features, i.e. characteristics lead to a different behaviour. These relationships can be studied, in principle, with the help of an artificial neural network (ANN). This helps to simulate the specific variation of the quantitative value of the feature, which has an influence on a target (creep elongation, creep stress, creep rupture deformations, short-term values) and compare the result with the actual behaviour.

Microstructure parameters such as precipitates, size and distribution are the direct response of the material to external conditions namely, heat treatment, temperature, stress and elongation, time to rupture in dependence of output features. Therefore, they are fundamentally appropriate as features for the description of dependencies between different parameters for application in neural networks. Indeed, these data are very limited, so that the following experience barely exists: in what form i.e. quantitative measure these parameters should be given in ANN to achieve an optimal

evaluation. Similarly, as with the other features it is necessary to determine to what extent namely, the number and quality of records, the raw data must be available for representation of reliable relationships.

In modern power plants for components e.g. headers, pipework exposed to temperatures up to 620°C martensitic 9%Cr-steels are used. Different steel grades with specific chemical composition and heat treatment are available, such as the X10CrMoVNb9-1 (P91), X10CrMoVNb9-2 (P92), and X11CrMoWVNb-1-1 (E911) grade.

4 Objectives

In the present work, the results of the previous project [7], [8] are summarized and the method of "artificial neural network" is established as a tool for determining creep rupture behaviour of the individual melt and extended to additional steels.

In particular, the following objectives will be pursued:

1. Application of the ANN-method to commonly used 9%Cr steels.
2. Conducting of sensitivity studies, i.e. estimation of what influence has a specific feature on an individual targets of the creep rupture properties.
3. With the addition of microstructure parameters to the feature values for 9%Cr steels, which have an influence on the creep rupture strength in the long-term range, and therefore to increase the sensitivity of the ANN, as well as to improve the accuracy of the expected outcome [9], [10].
4. It will be examined, whether the ANN is an appropriate method for the reproduction of the multi-dimensional relationships such as chemical analysis, heat treatment properties, etc., and what scope of work is necessary for this.
5. Reliability analysis of the ANN: which allows to estimate the creep rupture strength obtained with the help of ANN in comparison to practical results.

5 Neural Network Model for P91 Alloy

5.1 Dataset

The data shown in Table 1 were used for the analysis of the aforementioned 9%Cr steel grades.

Table 1. Data availability of the steels chosen for the analysis.

| Alloy Name | Number of data points/records |
|------------|-------------------------------|
| P91 | 1396 |
| P92 | 586 |
| E911 | 296 |

The investigation is very large and complex with extensive modeling with different chemical elements and other parameters of models. Therefore, just the scope is outlined with different types of models in 5.3. The presentation and results will be focused on the analysis of P91 steel as the most representative dataset within this paper.

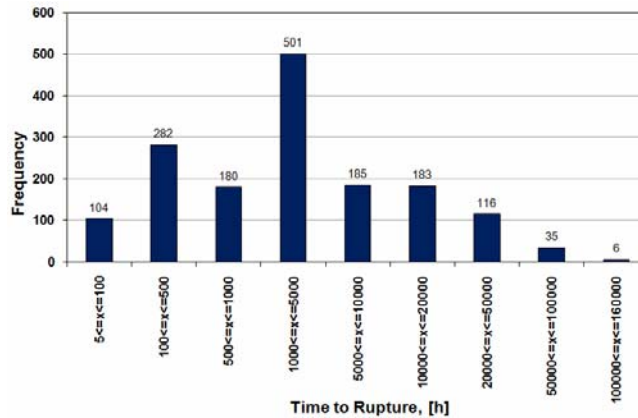


Fig. 2. Histogram of time to rupture values.

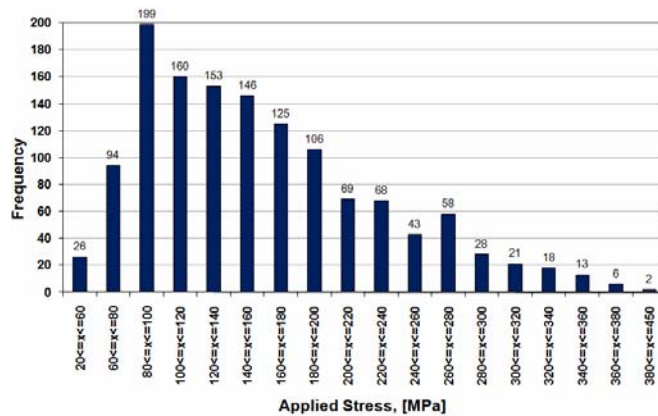


Fig. 3. Histogram of applied stress values.

A statistical analysis of the data frequency for P91 alloy, related to time to rupture and applied stress features, is represented in Figure 2, 3. The life time of the component, made of given steel, is designed for up to 20 years approximately. And the most interesting area in this study for target "time to rupture" after 100 000 hours is displayed in Figures 2 with a few data only. The prediction of long term creep rupture behaviour has been done here using ANN. It is known that the creep rupture test is temperature dependent. Most of the investigated data represent test temperature with four main temperatures: 500, 550, 600, 650°C.

5.2 Data Evaluation

The initial dataset of P91 alloy consisted from 3708 records, only creep tests were considered which ended in rupture, fourth part of the data have been removed including welded specimens.

After reduction, the data covers 186 distinct melts and 33 different chemical compositions.

Further, the selection of features was done for the data analysis. Based on the standard requirements and on the data availability, the basic set of parameters has been selected and the data were grouped into data levels. As a result of this evaluation step, the selected dataset with 1396 records meets the requirements according to the standards: VdTÜV material sheet 511 and DIN EN 10216-2 [11], [12], [13].

The data have been structured into three levels: from 16 up to 23 features for level 3 and for level 1 accordingly. Table 2 demonstrates that there are, indeed, many features available, but it is also apparent that some individual characteristics are weakly presented. The features are known as characteristics of tested specimens. A record, in this context, is composed of quantified variables, such as the alloying elements, the product form, heat treatment conditions i.e. temperature and duration of the austenitizing and tempering processes, the mechanical properties namely proof stress, tensile strength, elongation and the creep rupture data such as test temperature, time to rupture, creep rupture strength, elongation.

Overview of data availability and selection of the features, based on the original data levels, are completely filled in sub-matrices in Table 2.

5.3 Application of Neural Networks for the Modeling of Creep Rupture Behaviour

Artificial neural networks can be particularly beneficial for modeling, where a description of physical and mathematical models due to complex or unknown dependencies is not available. The model predictions are comparable to an accuracy of a classical-statistical modeling. The essence of artificial neural networks is to reproduce the operation and the structure of the human brain through mathematical models [14].

Badeshia [4] came to a conclusion that the regression analysis methods are applicable to the creep properties of materials, but with several limitations. He has pointed out that neural networks are seen as an appropriated tool for modeling of mechanical properties of materials, and, even more, for development and prediction of properties of new alloys. 2 ¼ Cr1Mo steel was investigated, based on chemical composition and heat treatment data, as those two groups of elements have greatest influence of the microstructure, and thus on creep properties of a material. According to [4], the neural network can find interactions between the inputs, which are nonlinear. ANN can be used to make predictions and to see how they depend on various combinations of inputs. There is strong fundamental evidence that a well designed neural network is the best way of extrapolating empirical data. The method should now be more widely exploited in the assessment of creep data [15].

Table 2. Overview of data availability and features according to the material P91.

| Alloy P91 | Number of Points | Availability, [%] | Matrix Number | | |
|--|------------------|-------------------|----------------|----------------|----------------|
| | | | 1 | 2 | 3 |
| Alloy Name | 1396 | 100% | | | |
| Melt Number | 1396 | 100% | | | |
| Product Form | 1396 | 100% | | | |
| Production Process | 723 | 52.79% | | | |
| Austenization Temperature | 1396 | 100% | 1 | 1 | 1 |
| Austenization Duration | 1031 | 73.85% | | | |
| Austenization Medium | 1346 | 96.41% | | | |
| Tempering Temperature | 1396 | 100% | 1 | 1 | 1 |
| Tempering Duration | 1105 | 79.16% | | | |
| Tempering Medium | 1346 | 96.42% | | | |
| C | 1396 | 100% | 1 | 1 | 1 |
| Si | 1396 | 100% | 1 | 1 | 1 |
| Mn | 1396 | 100% | 1 | 1 | 1 |
| P | 1396 | 100% | 1 | 1 | 1 |
| S | 1377 | 98.64% | 1 | 1 | |
| Cr | 1396 | 100% | 1 | 1 | 1 |
| Mo | 1396 | 100% | 1 | 1 | 1 |
| Ni | 1291 | 92.48% | 1 | 1 | |
| V | 1396 | 100% | 1 | 1 | 1 |
| Al | 1335 | 95.63% | 1 | 1 | |
| B | 253 | 18.12% | | | |
| Nb | 1384 | 99.14% | 1 | 1 | |
| N | 1344 | 96.27% | 1 | 1 | |
| As | 131 | 9.38% | | | |
| Co | 301 | 21.56% | | | |
| Cu | 584 | 41.83% | 1 | | |
| Pb | 137 | 9.81% | | | |
| Sn | 344 | 24.64% | | | |
| Ti | 328 | 23.50% | | | |
| W | 106 | 7.59% | | | |
| Proof Strength $R_{p0.2}$ (Room Temperature) | 1396 | 100% | 1 | 1 | 1 |
| Tensile Strength R_m (RT) | 1396 | 100% | 1 | 1 | 1 |
| Tensile Elongation A_5 (RT) | 1342 | 96.13% | 1 | 1 | 1 |
| Tensile Reduction Area Z (RT) | 555 | 39.76% | | | |
| Test Specimen Number | 792 | 56.73% | | | |
| Test Temperature | 1396 | 100% | 1 | 1 | 1 |
| Applied Stress | 1396 | 100% | 1 | 1 | 1 |
| Time to Rupture | 1396 | 100% | 1 | 1 | 1 |
| Creep Tensile Elongation | 1378 | 98.71% | 1 | 1 | 1 |
| Creep Tensile Reduction Area | 1314 | 94.13% | 1 | 1 | |
| Time to 1% Total Plastic Strain | 305 | 21.85% | | | |
| Testing Institution | 1396 | 100% | | | |
| Useful features for each data matrix / Data aggregation level | | | 23 | 22 | 16 |
| | | | Level 1 | Level 2 | Level 3 |

The network types which are most commonly employed in practice are multilayer perceptron with back-propagation learning for the supervised learning, and Kohonen's self-organizing feature maps for unsupervised learning [14]. Both models have a long history of successful application for various data behaviour modeling, starting from financial, medical sectors, traffic control and modeling of physical phenomena.

Multilayer Perceptron (MLP) neural networks [14] were applied as they are most efficient for the modeling of the dependency of creep rupture and time to rupture [4], [16]. The software package DataEngine [17] was used for the construction of neural networks.

As a result, several models were constructed for the analysis with the following dependent variables:

P91 steel:

Model 1: Proof strength by room temperature, [MPa]

Model 2: Creep rupture strength, [MPa]; time to rupture, [h]

P92 steel:

Model 3: Creep elongation at rupture A5, [%]

Model 4: Creep rupture strength, [MPa]; time to rupture, [h]

E911 steel:

Model 5: Creep rupture strength, [MPa]; time to rupture, [h]

9-12%Cr steels, product form "Tube":

Model 6: Creep rupture strength, [MPa]; time to rupture, [h].

The results in MLP can be analyzed and represented graphically. The software provides tools that can be used for calculation, variation and sensitivity analysis of the models. With the tools mentioned above it is possible to analyze how much the variation in the input parameters changes the values of output parameters, in our case time to rupture and creep rupture stress. For example, Figure 5 shows the sum of derivations for creep rupture strength of material P91. In this type of chart for each feature the derivations are added up, occurring when the input is changed. The resulting totals are displayed in a bar chart. The sensitivity analysis has shown the big influence of the time to rupture and test temperature variables on the target: creep strength. Figure 4 demonstrate the important influences/features for the same target.

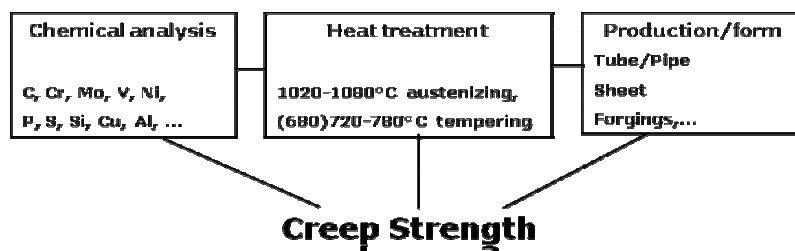


Fig. 4. Important influences/features on creep strength value.

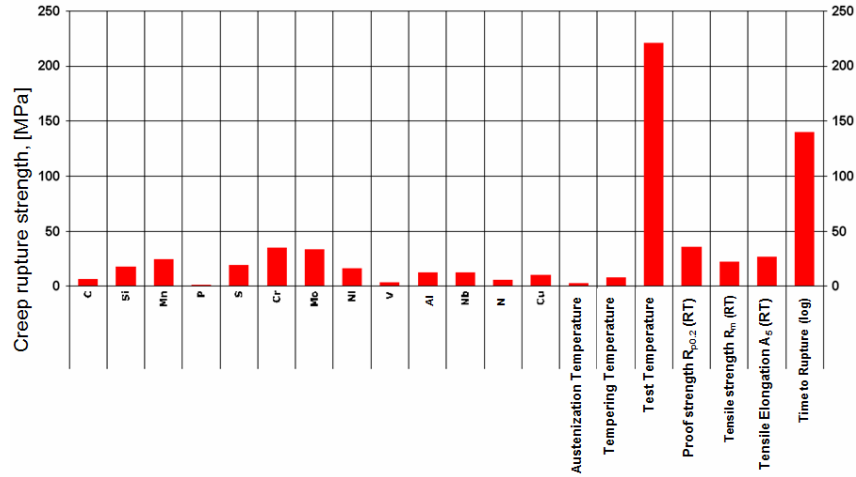


Fig. 5. Sum of the differentials graph for the P91 alloy.

6 Results

6.1 Modeling with Targets: Creep Rupture Strength and Time to Rupture

A prerequisite for modeling with ANN is a sufficiently large and representative dataset. Moreover, the influence of reliability and accuracy of the data is very essential for the prediction ability of a constructed model. First objective evidence on the quality of input data and ANN model provides the correlation coefficient. A graphical comparison between measured and model values is the better way, in this case, to represent the degree of agreement or discrepancy. Figure 6 and Figure 7 represent corresponding graphs for the targets: creep rupture strength and time to rupture for the data level 1.

It should be mentioned, that the correlation coefficient r between the model- and measured values for the target "time to rupture" is significantly worse in comparison with the "creep rupture strength" and has most values between 0.8 and 0.9. The model and target values for the "creep rupture strength" show significantly better correlations with r values > 0.94 .

Four additional models were trained for the data levels 2 and 3 with the same 2 targets for P91 alloy. The correlation coefficients for these models are represented in Table 3 and Table 4.

In summary, it can be concluded that an increasing number of records with fewer features does not automatically have to be beneficial. Because the level 3 has shown a high degree of spreading of values for the target "time to rupture". The deviation at low creep strengths or long-term duration will not become necessarily lower through increased number of feature's values. Therefore, the conversion of the data in the ANN will be considered advantageous with a data structure constructed in accordance with data level 2 or level 1 which is thus used for training in ANN.

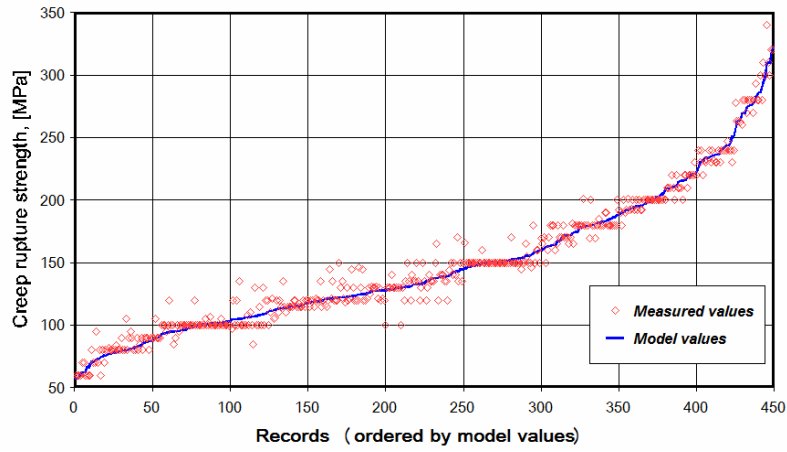


Fig. 6. Creep rupture strength: comparison between model- and measured values: data level 1, 20 features, 449 records, correlation coefficient=0.989.

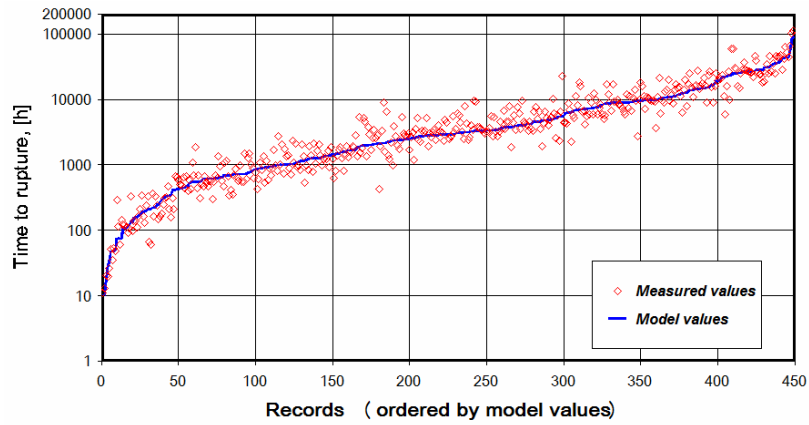


Fig. 7. Time to rupture: comparison between model- and measured values: data level 1, 20 features, 449 records, correlation coefficient=0.939.

Table 3. Correlation coefficients for target “creep rupture strength”, P91 steel

| Correlation coefficients | Data level 1 | Data level 2 | Data level 3 |
|--------------------------|--------------|--------------|--------------|
| | 0.989 | 0.994 | 0.989 |

Table 4. Correlation coefficients for target “time to rupture”, P91 steel

| Correlation coefficients | Data level 1 | Data level 2 | Data level 3 |
|--------------------------|--------------|--------------|--------------|
| | 0.939 | 0.809 | 0.894 |

6.2 Verification of Neural Network Models

The functionality on the basis of above described ANN is shown below on an examination of an individual melt. The verification procedure has been done as follows: the features of selected melt were given to the trained network i.e. model. Based on this, the ANN calculates stress values for the given times, which can be then connected to a creep rupture curve. In other words, the predicted values can be compared with the real measured values of the selected melt.

The evaluation of the data was carried out for the data levels 1 and 2 at temperatures 550, 600, 650°C. Figure 8 demonstrates a good agreement of the model values of data level 2 for the melt number 801141 at 650°C with target "creep rupture strength" and as well the mean curve according to EN-10216 standard of the given steel.

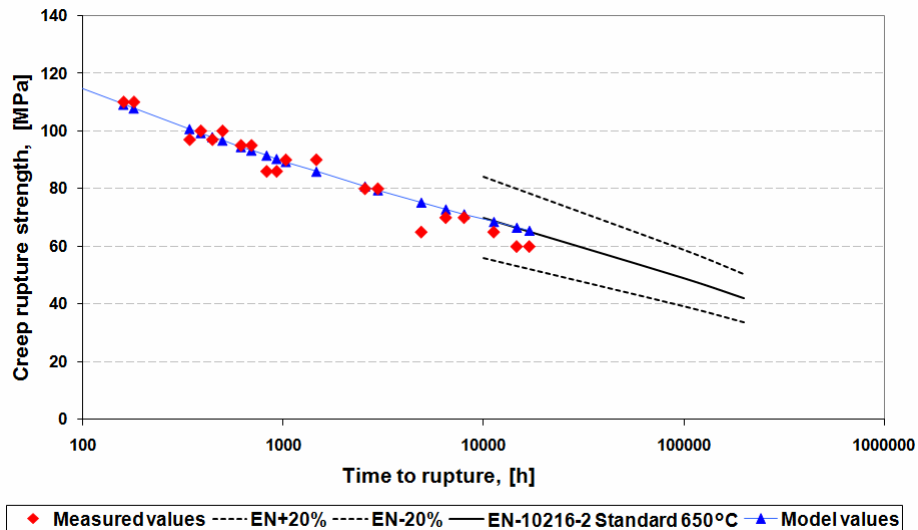


Fig. 8. Determination of the melt position with NN for the melt No. 801141, 650°C, Data level 2, with target: creep rupture strength, P91 alloy.

6.3 Evaluation of Physical and Metallurgical Backgrounds

The analysis of the influence of the individual chemical and other alloying elements on creep strength was done with the help of an artificial melt. The artificial melt represents the mean of all independent features of all available melts by the variation of time to rupture. Four test temperatures 500, 550, 600, 650°C were taken into consideration for the artificial melt.

As an example, here will be demonstrated the influence of chromium content on the creep rupture strength. Figure 9 shows the determination of the artificial melt position with ANN by chromium variation from 8.0% up to 9.5% according EN-Standard which specifies the range, for target "creep strength", data level 2 and

600°C. For this purpose, the separate model was calculated with ANN for each chromium value, not trained! As shown on Figure 9, with the increasing chromium content, the curve is shifted upwards significantly. And the difference between the curves of maximum and minimum chromium content becomes smaller with the temperature increase from 500 to 650°C. In the literature [18] it is described that an increase of chromium has a positive effect on the creep strength:" in almost all projects with the test temperature 650°C it was initially intended to use the experimental alloys with 11-12% chromium to achieve a sufficient oxidation resistance. Almost all results indicate that the highest creep rupture strength can be achieved only with a chrome-mass fraction below 11%, possibly even just from 9 to 10%."

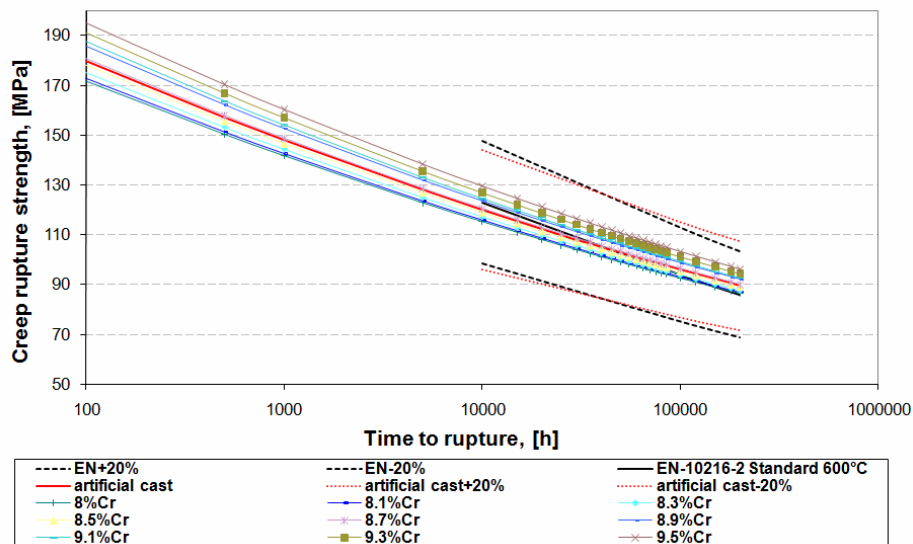


Fig. 9. Determination of artificial melt position with NN – chromium variation from 8% to 9.5% specified in EN-standard range, level 2, 600 °C, with target: creep strength, P91 steel.

6.4 Considerations to the Accuracy of Prediction of the Creep Rupture Behaviour

Within this section the residual analysis is demonstrated. It is known that ANN tries to minimize the squared distance between the predicted and measured values, in other words, the ANN is characterised by the residuals [14],[17], [19].

The training process is based on the minimization of the residuals, both on mean and max scale. Moreover, the learning rule uses additional techniques to prevent the "overfitting" or so called "learning by heart" effect. The learning algorithms SuperSAB and Resilient Propagation were applied within the training process. For P91 models the mean residual error has the margin $\pm (4.1-5.3)$ MPa for creep strength depending on applied data level, which is acceptable. This means, that each model

value is associated on average with an uncertainty of about ± 5 MPa. The distribution of the residuals is demonstrated on the Figure 10.

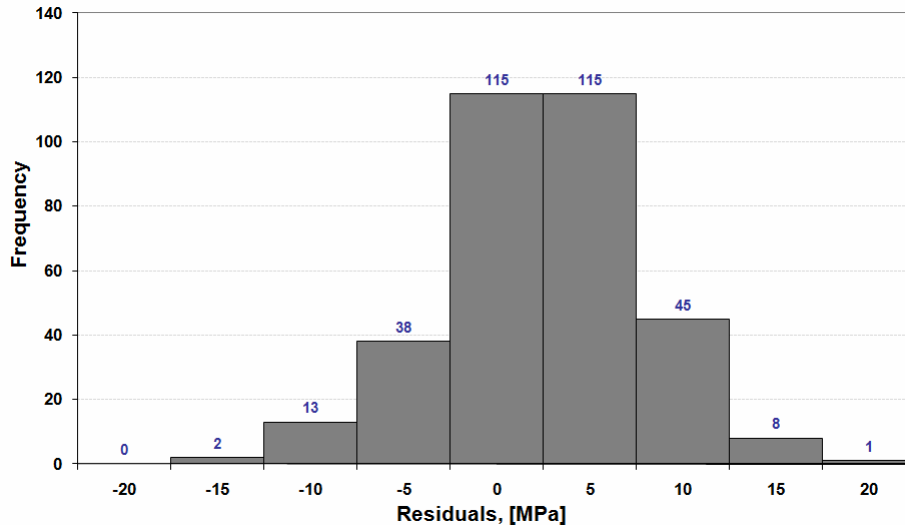


Fig. 10. Distribution of residuals, data level 1, learning algorithm: Resilient Propagation. P91 material, target "creep rupture strength"

7 Conclusion

The present work has demonstrated an innovative approach to the use of modern tools for data analysis. The goal is the optimized prediction of a material behaviour under consideration of the creep strength and duration i.e. time to rupture data and determination of the position of the specific melt in the scatter band for 9%Cr steels.

The material behaviour is influenced by the multidimensional interdependencies between the individual elements of the chemical composition, the heat treatment parameters, product form, tensile properties and microstructure, which are difficult to describe using simple analytical methods. Modeling with neural network techniques therefore seems to be an interesting alternative. Moreover, the applied method takes away the requirement for long and expensive experiments.

In summary, the results described in the present paper are:

- It was shown that the neural network models used in the current study process the assumed metallurgical connections
- The framework conditions for the successful training of the neural network have been determined
- The results of the forecasting have provided plausible estimations.

In summary it can be held, that it is very reasonable to continue the work by involvement of new steels which are already in use and therefore to expand the state of knowledge and to further enhance the existent models.

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