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Mathematical modelling of thermal processes by the use of regression and neural models

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Abstract The paper presents a description of used methods and exemplary mathematical models which are classified into theoretical-empirical models of thermal processes. Such models encompass equations resulting from the laws of physics and additional empirical functions describing processes for which analytical models are complex and difficult to develop. The principle of developing, advantages and disadvantages of presented models as well as quality prediction assessment were presented. Mathematical models of a steam boiler, a steam turbine as well as a heat recovery steam generator were described. Exemplary calculation results were presented and compared with measurements.

Keywords: Mathematical model; Empirical functions; Neural modeling; Regression modeling

1 Introduction

Modelling is one of the fundamentals of science and engineering. The term mathematical model is understood as a set of relationships that create an image of a real process. Mathematical models used in engineering belong to a group of applied models, thus models representing only that part of knowledge of processes that are crucial for its purpose. The developed model enables the study of the effects of interactions on those quantities (which have physical equivalents in the process under investigation) for

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which such effects are observed. It should be characterized by sufficient prediction on the quantitative side of phenomena and a short computation time.

A mathematical model can be developed as an analytical model with the use of known physical laws, or, as an empirical model. The advantage of developing analytical models is that the process mechanism can be understood more accurately. Most often these processes are characterized by a high degree of complexity that makes model development difficult, or often impossible, based exclusively on a mathematical description of physical processes. Advances in measuring techniques and computer technology mean that empirical modelling techniques based on measurement data are more and more frequently used. Developing empirical models consists in converting a set of measurement data into a mathematical model that describes the most important process properties [1–3]. It is easier to develop empirical models than analytical ones, but the scope of its applicability is reduced to the parameters of the range of usability for which the model has been calibrated. Good results are obtained by building an analytical model with embedded empirical models. An analytical model is often built as a balanced model. These results from an easy introduction and the simple structure of balance equations. Additional empirical models describe processes that are difficult to express analytically, e.g., the combustion processes or the heat transfer. The regression and neuronal modelling belong to the most frequently used methods of empirical modelling.

2 Regression modelling

The foundations for linear regression in the form of the method of least squares were introduced by Gauss as a special case of the maximization of the error probability density function. The Gaussian rule was developed by Fisher in the form of the method of maximum likelihood. For a linear model, while assuming that random errors of the model are independent and have a normal distribution of the expected value of zero and constant direct variation, the estimates of the model coefficients obtained by using the method of maximum likelihood are identical to those derived from the method of least squares. When error distribution differs from the normal one, it is impossible to use the results obtained by the method of least squares. In general, the method of maximum likelihood that requires knowledge of the probability distributions is used and computations are much more complicated than those of the method of least squares. Normally, no analytical solution can be found and iterative methods are employed.

The conventional regression model contains the following components: response variable (a variable to be explained with model equations), explaining (explained) variables (used for description), structural parameters (parameters expressing a qualitative effect of a related variable on an response variable and a random component). The construction of a regression model requires the assumption of a model type and structure, a model parameter estimation of an established structure based on experimental results (measurements), the evaluation of the quality of the model's predictions and model verification. The model structure defines its construction with an accuracy to several unknown numeric constants. The model structure should reflect cause and effect relationships in phenomena which occur in the process. The model structure is established arbitrarily. Model parameters can be estimated when the model structure is known.

Model parameter estimation consists in determining the values of these parameters according to the adopted estimation criteria. The best known methods of model parameter estimation are the conventional method of least squares, maximum likelihood method, momentum method and Bayesian method. The simplest algorithm is obtained by adopting the minimization of the error sum of squares for a model as the estimation criterion [1–4]. This is the method of least squares. The concept of estimation by using the method of maximum likelihood estimation has already appeared in Gauss's papers. It consisted in such a selection of unknown parameters for which the highest probability of observations is made. If variables have continuous probability distribution, the estimation method comes down to searching of the highest value of the likelihood function that is defined as a product of the probability density function for individual variables. The method of maximum likelihood and proof of the properties of the obtained estimators were decisively formulated in Fischer's papers. The momentum method and Bayesian method are less often used. The application of the conventional method of least squares for model parameter estimation is presented in this paper.

The method of estimating with the method of least squares incorporates the danger that it always enables an estimation of model parameters, even if the developed model accuracy is very low because of an improperly selected model structure or large measurement errors. The coefficient of determination is a parameter which enables the model to fit to the empirical data to be evaluated. It is equal to the square of the coefficient of correlation between the empirical and theoretical values of the response variable obtained from the regression model. The coefficient of determination takes values from $[0, 1]$. The square root of the coefficient of determination is referred to as the coefficient of multidimensional (multiple) correlation. The coefficient of determination indicates that there is a relationship between the output values derived from measurements and that obtained by model calculations. The coefficient of determination is a measure of model quality in terms of data variability. The closer to unity the value of determination coefficient, the higher model accuracy.

The determination of confidence intervals for estimated coefficients and model output data (response variable) requires assumptions for the probability distribution of model random errors to be made. In the conventional regression analysis, an independence – an expected value equal to zero and the constant variance of model random errors are assumed. A confidence interval for the model input variable is of special importance to the users. It is the narrowest in the middle of the measurement result area. The greater the distance from the mean of the measurement results, the higher the error in the expected value prediction. The best results of prediction should be found in the 'middle' of the measuring range.

Verification of the model consists in performing statistical tests to decide whether it can be accepted or not. A key issue in the verification of parametric models is the verification of model type and structure. The incorrect type and improper structure lead to a model of very poor predictive properties. To yield a usable equation for prediction purposes, as many functions as possible of input variables with different impacts on the output variable should be introduced into the model. An additional input variable introduced into the model equation may have a minute effect on the output variable because of its strong correlation with other variables present in the equation. In addition, a large number of estimated coefficients requires a large amount of available measurement data to assure the high accuracy of assessments; this can be cost consuming in industrial research. A compromise between these extremities is the selection of the best model equation. There is no general procedure for such a selection. The procedures based on statistical testing are most frequently used. They include elimination procedures. In the a posteriori elimination method, the procedure starts from the most complicated model equation containing all independent variables that are consecutively eliminated, until the suitability of the equation is decided. The a priori selection procedure is an attempt to achieve the same target in the reverse direction, i.e., by adding independent variables until a satisfactory model equation is obtained. The step regression procedure [4] is an improved version of this procedure. These improvements consist in examining the independent variables at each stage of statistical significance which have been introduced into the model in the previous stages. An independent variable that could have been the best single variable to be introduced in the previous stage, can be useless in a later stage due to its dependence on other independent variables which are present in the model equation. An F-Snedecor test is a decisive factor for introducing or removing variables from the model equation in the presented elimination methods. The advantages of the use of conventional regression analysis include known methods, algorithms and computer procedures of parameter estimation, prediction quality assessment and optimal model structure selection. However, this only applies to linear models with regard to estimated parameters. Regression models provide short computation time, computations that are not iterative, so not sensitive to the selected starting point. Disadvantages include the lack of effective estimation methods and statistical assessment procedures for models of nonlinear structure with regards to estimated coefficients and the necessity to inverse a matrix that for a large number of measuring points may have a significant size. The numerical inversion of matrices of such a considerable size causes computational difficulties, and rounding the errors affects the estimation result.

3 Neural modelling

Neural networks belong to the domain of artificial intelligence [5]. Fields of neural network technical applications include automation and robotics, as well as process identification and optimisation. In process identification and control, a neural network is a nonlinear model of the process which enables an appropriate control signal to be developed. Neural networks are used for modelling heat processes as numerical algorithms that can be employed for function approximation. A neural network is a set of interconnected neurons. In modelling heat processes a layered structure of the network without feedback is most commonly used. The best known representative of such networks is a multilayer perceptron. This network consists of a very large number of neurons connected in parallel and linked with weighted connections. Information is transmitted from the inputs of the first layer to the outputs of the last (output) layer. The output signals of consecutive layers are the inputs of the next layers. A neural network can have one or more outputs in the last layer.

The multilayer perceptron modelling includes several stages [6]: structure identification, neural-network connection weight identification and network testing. The network structure identification consists in determining the number of layers and the neuron type and number in each network layer. Nonlinear neurons with a sigmoid activation function are most often used. The network architecture contains an input layer, one or more hidden layers and an output layer. The output layer can have one or more neurons. Experience gained from neural network modelling shows that when modelling the heat processes of many outputs considerably better results are obtained by using individual models for each output than by building a model with many output neurons. There is no good quantitative approach in the literature – no quantitative criterion indicating the quality of the network structure. In practice, the network structure is selected through trial and error, i.e., if the learning process does not bring the desired results, the network structure is changed.

Network weights are identified in the so-called network learning process [5,6]. The first step in the learning process is developing the training and validation sets. The training set is data set that should describe, as accurately as possible, the process within the range of variability under investigation. A single piece of data is called the teaching vector. It contains an input vector, i.e., input data entered into network inputs, and an output vector, i.e., data that should be generated in network outputs. After processing the input data vector its values are compared to the expected values and it is decided if the response is right and, if not, what the error is. This error is then propagated into the network but in the opposite direction to the input vector, i.e., from the output layer to the input layer. Based on this, weight correction is made in each neuron so that the reprocessing of the input vector causes a decrease in the response error. After processing the whole teaching course (this process is called an epoch) the error for the entire epoch is calculated and the whole cycle is repeated until the error is reduced below the permissible value.

After teaching, the network functionality should be verified. To do this, input vectors from a validation set are entered into network inputs to check whether the network can perform the learned task effectively. The validation set has the same properties as the training set, i.e., data accurately describing the process within the range of variability under investigation. However, it is important that the validation set data are not used for learning purposes. In the network verification process no error retrospection is performed, but only network responses are recorded and, on this basis, it is decided whether the network meets the assumed prediction requirements and can be used for process simulation. After teaching the network, it is worth repeating the whole procedure for another set of generated initial weights.

Empirical models built by using artificial neural networks can approximate any continuous or discontinuous functions. They have a high adaptability to modelling various phenomena (nonlinear, too) and efficiency, even in the presence of strong interferences. Modelling efficiency depends considerably on the method used and the selection of network learning parameters. In the learning process the following methods can be used: backward error propagation, backward error propagation and momentum, variable metric and Levenberg-Marquardt algorithm. The results obtained from modelling the heat processes indicate that the Levenberg-Marquardt algorithm is the most effective teaching method [3,7]. The choice of measuring points for training and validation sets has a significant effect on prediction results. Both the training and validation set should cover the whole range of the variability of the usability parameters for a process under investigation. Situations where some areas contain a lot of measuring points, while others contain only a few points should be avoided. In such situation, a neural model will feature high quality prediction within the areas of high concentration of measuring points. In industrial practice it is difficult to fulfill this condition. Most working points of power equipment are concentrated within the design parameter area. Only a few points are located on the boundary of the working parameter area. In such cases the best results are yielded by using the Levenberg-Marquardt algorithm.

The disadvantages of neural modelling include:

- a developed neural model is not unique; this means that there is a number of models of different structures and coefficients that can perform the same transformation; there are no unique methods for assessing the effect of structures and parameters on the quality of modelling;
- models based on artificial neural networks require much more compu-

tation time than parametric models, especially for linear models and when the Gauss's least square method is used for identification;

- structure of the models based on neural networks is often highly complicated and then the computational load may be a barrier limiting its application;
- the so-called over-training syndrome may occur, which means that the model properly reproduces training set standards, while being totally powerless for other standards not used in the learning process; a developed model may give unsatisfactory results of predictions when changing the working parameters of power equipment.

4 Simulation model of a steam boiler

Combustion flow of substance and heat exchange processes occur in a steam boiler. An analytical description of these processes is highly complicated, and numerical computation time is very long. Simpler models characterised by a short computation time are required for industrial purposes. Such models can be built by using empirical modelling methods. An empirical model of a steam boiler includes the relationship between efficiency and the energy losses of a boiler and working parameters, and can be formulated as a set of relationships between output variables and input variables without going into the physics of occurring phenomena. This is the so-called 'black box model'. Such a model developed by using neural modelling techniques is presented in the paper [7]. Empirical models of the 'black box' type have a limited range of applications. They can be used within the boiler operation range for which measuring data are available. Better prediction results are obtained by building an analytical model with embedded empirical models. An analytical model is most often built as a balance model. This is the result of the easy introduction and simple structure of balance equations. Empirical models that describe the complicated combustion and heat transfer processes can be built by using the regression and neural modelling techniques. They describe the relationship between the temperature of flue gas exhausted from a boiler and combustible fraction (in grams) in solid combustion products and the working parameters.

A hybrid model of a boiler has been developed [6,8]. A balanced model was built based on standard PN-EN 12952-15 [9]. A neural model was developed to describe the relationship between the temperature of flue gases exhausted from a steam boiler and the working parameters. The neural network structure, including the number of layers and neurons in individual layers was experimentally chosen. A sigmoid activation function was adopted. The input quantities for this model are as follows: thermal power, heat flux transferred in the steam air preheaters, lower heat value (LHV) of fuel, oxygen content in flue gasses exhausted from the steam boiler, combustion air temperature and the boiler feedwater temperature. The step regression method was used for describing the effect of working parameters on the combustible fraction in solid combustion products. The set of variables analogical to that of a neural model for the temperature of flue gasses exhausted from a boiler was adopted. Figures 1 and 2 present sample simulation computations for the BP-1150 steam boiler.

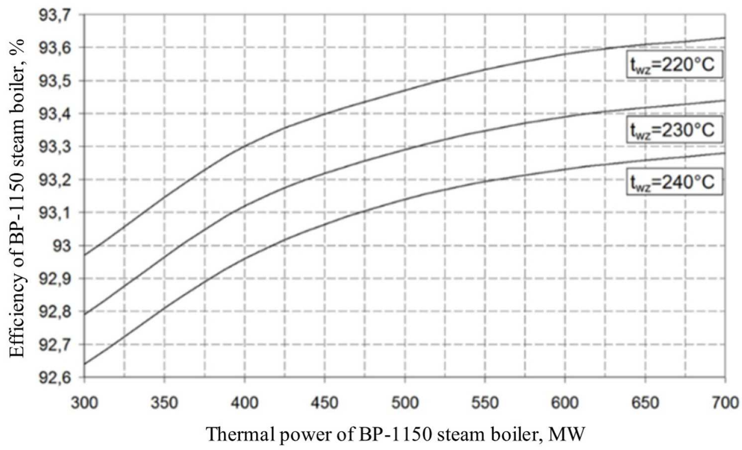

Figure 1: Dependence of boiler energy efficiency on thermal power and feedwater temperature.

An increase in boiler thermal power causes a rise in steam boiler efficiency. A decrease in feedwater temperature, while keeping other working parameters unchanged, also leads to an increase in boiler efficiency, but to a lesser extent. This results from better flue gas cooling, thus also reducing the relative energy losses of flue gasses. Regenerative feedwater preheating decreases boiler efficiency but increases the efficiency of the steam-water cycle operation. As a result, the efficiency of electricity production increases. Enhanced fuel quality increases steam boiler efficiency. This results from decreasing an unnecessary ballast in the fuel.

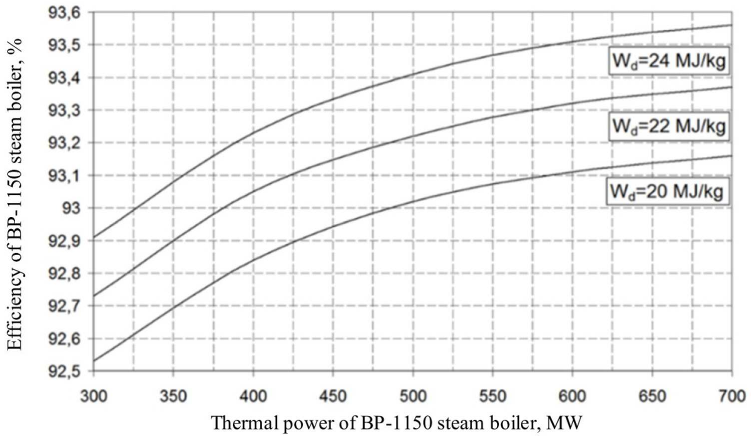

Figure 2: Dependence of boiler efficiency on thermal power and the LHV of fuel.

5 Simulation model of a heat recovery steam generator

Within a heat recovery steam generator (HRSG), a process of heat exchange between flue gas and working fluid is carried out. In order to develop a mathematical model of heat transfer process, often heat transfer correlations are used. However, they require knowledge about the dimensions and geometries of all heat exchangers in the HRSG. In addition, such models are relatively complex and often require iterative procedure. In many papers, instead of mathematical description of heat transfer process, constant values of pinch point and approach point are used [10,11]. At that time, the model of HRSG may be simplified to mass and energy balances and as a result, such model is characterized by shorter computing time, but it does not take into account the influence of technical HRSG condition on approach point and pinch point values.

Models, that are developed for thermal diagnostic systems, should be characterized by short computing time and take into account the technical condition of modelled machines. Therefore, in order to describe heat transfer process, empirical equations may be used, whose coefficients may be estimated on the basis of measured results. Such models contain mass and energy balance equations as well as empirical equations describing heat transfer process in all heat exchangers.

The heat flow, $\dot{Q}$, is described by Peclet's law [12]

$$\dot{Q}=U\,A\,\triangle t\ , \tag{1}$$

where: U – overall heat transfer coefficient, A – surface area, $\triangle t$ – logarithmic mean temperature difference.

The largest share in the total heat transfer coefficient is the resistance of the convection from the flue gas side. In the case of a superheater, the resistance of the convection from the superheated steam side is also essential. The product of overall heat transfer coefficient and surface area ($U\,A$) has been often approximated by the use of following empirical equations [11]:

- n economizer and evaporator:

$$\frac{(U\,A)}{(U\,A)_0}=\left(\frac{\dot{m}_{fg}}{\dot{m}_{fg\ 0}}\right)^{\beta_1}\left(\frac{c_p}{c_{p\ 0}}\right)^{\beta_2}\left(\frac{k}{k_0}\right)^{\beta_3}\left(\frac{\nu}{\nu_0}\right)^{\beta_4}, \tag{2}$$

- superheater

$$\frac{(U\,A)}{(U\,A)_0}=\left(\frac{\dot{m}_{fg}}{\dot{m}_{fg\ 0}}\right)^{\beta_1}\left(\frac{c_p}{c_{p\ 0}}\right)^{\beta_2}\left(\frac{k}{k_0}\right)^{\beta_3}\left(\frac{\nu}{\nu_0}\right)^{\beta_4}\left(\frac{\dot{m}_s}{\dot{m}_{s\ 0}}\right)^{\beta_5}, \tag{3}$$

where: β_1–β_5 – empirical coefficients, c_p – flue gas specific heat capacity, k – flue gas thermal conductivity coefficient, ν – flue gas kinematic viscosity coefficient, $\dot{m}_{fg}$ – flue gas mass flow rate, $\dot{m}_s$ – superheated steam mass flow rate, the subscript 0 refers to the design operational conditions; the symbols without subscript 0 represent the actual operational conditions.

On the basis of formulated mass and energy balance equations together with empirical equations describing heat transfer process, the model of double-pressure heat recovery steam generator was developed (Fig. 3).

The simulation model of the double-pressure heat recovery steam generator allows to calculate temperature, pressure as well as mass flow rates of working fluid at all characteristic points. In addition it also calculates among others the heat rate transferred in all heat exchangers and average value of overall heat transfer coefficient. Figures 4–7 present the comparison of the results of calculations with the results of measurements for mass flow rate and temperature of generated high-pressure (HP) and low-pressure (LP) steam.

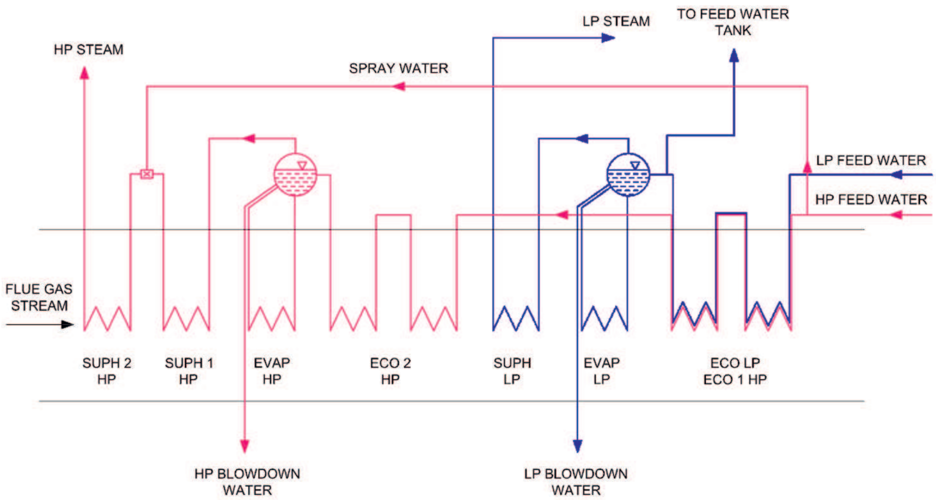

Figure 3: Schematic diagram of double-pressure heat recovery steam generator.

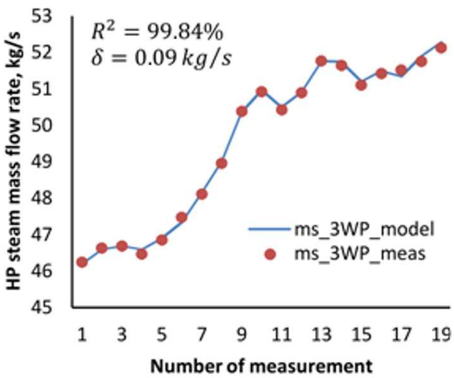

Figure 4: Comparison of the results of calculations with the results of measurements for HP steam mass flow rate.

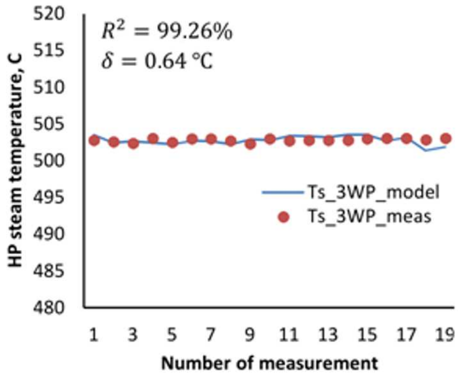

Figure 5: Comparison of the results of calculations with the results of measurements for HP steam temperature.

The presented comparison confirm the high prediction quality of the developed model. This is additionally confirmed with the high values of determination factors R^2 and the small values of model errors δ.

The high prediction quality of mass flow rates and thermal parameters of generated HP and LP steam is essential, because these values constitute input data to the simulation model of the steam-water cycle.

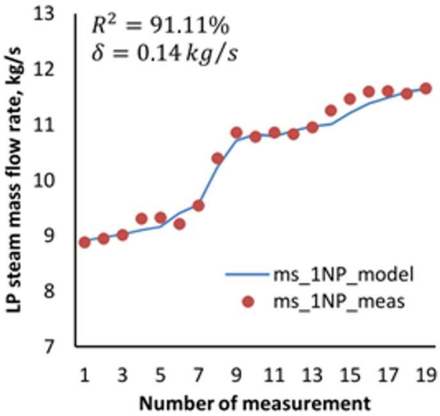

Figure 6: Comparison of the results of calculations with the results of measurements for LP steam mass flow rate.

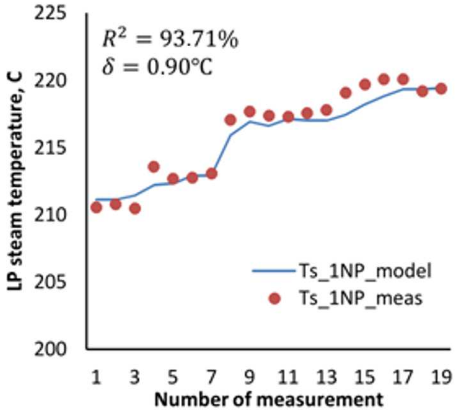

Figure 7: Comparison of the results of calculations with the results of measurements for LP steam temperature.

6 Simulation model of a steam turbine

The turbine simulation model contains mass and energy balance equations for high-, medium, and low-pressure parts of the turbine taking into account leaks in the valves spindles seals and from the external glands, steam mass flow in the balance piston and inter-cylinder steam mass flow and the model of the steam expansion line for the individual groups of stages. To determine the steam expansion line in the turbine, analytical modelling or methods based on the steam capacity equation and internal efficiency equation are used [2,6,13,14]. Flow computations that require knowledge of flow system geometry are complicated and time-consuming. Computations based on the steam capacity equation and internal efficiency equation require an estimation of the empirical parameters of these functions based on the results of measurement [6,13]. For each turbine operating at a constant rotational speed, there is a strict relationship between the inlet parameters p_{in}, T_{in} and the outlet pressure p_{out} at the turbine stage group. This equation is called the steam-flow capacity equation. Approximate versions of this equation are most commonly used. The calculations which were carried out indicated that the exact identification of outlet pressure at the stage group is achieved for Flügel formula. In literature, there are many empirical forms of Flügel formula, among others [6,10,11,13,14]:

$$\dot{G}_{in}^2 \frac{v_{in}}{p_{in}} = A_1 \sqrt{1 - \left(\frac{p_{out}}{p_{in}}\right)^2} + B_1 \ , \tag{4}$$

$$\dot{G}_{in} = A_2 p_{out} \ , \tag{5}$$

where $\dot{G}_{in}$ – steam flow mass flow rate at the inlet of group of stages, v_{in} – steam volume at the inlet of group of stages, p_{in} – steam pressure at the inlet of group of stages, p_{out} – steam pressure at the outlet of group of stages, $A_1,\ A_2,\ B_1$ – empirical coefficients.

The unknown values of empirical coefficients $A,\ B$ are often estimated on the basis of measured results with the least-squares method. They result from the adjustment to measurement data and have no physical interpretation, unlike physical models.

The adiabatic internal efficiency of a steam turbine is expressed by the ratio of actual external work to theoretical work during adiabatic reversible expansion. In literature there are various empirical functions describing the internal efficiency of turbine stages. Most of them depend on outlet pressure at the stage group or the ratio of outlet pressure at the stage group to inlet pressure to the stage group [6,13–16]. Most commonly used relationships describing the internal efficiency include:

$$\eta_i = C_1 + D_1 \left(\frac{p_{out}}{p_{in}}\right) \ , \tag{6}$$

$$\eta_i = C_2 + D_2 \left(\frac{p_{out}}{p_{in}}\right)^{-1} + E_2 \left(\frac{p_{out}}{p_{in}}\right)^4 \ , \tag{7}$$

where: η_i – the internal efficiency of group of stages, p_{in} – steam pressure at the inlet of group of stages, p_{out} – steam pressure at the outlet of group of stages, C_1, D_1, C_2, D_2, E_2 – empirical coefficients.

Unknown values of empirical coefficients A, B, C, D, E are calculated by using estimation methods, e.g., regression method.

By using the substance and energy balance equation and the empirical model for steam expansion at individual turbine stages, the 18K370 turbine simulation model has been developed [14]. A computational scheme for this turbine is presented in Fig. 8. Figure 9 shows the steam expansion line based on this model (solid line) with marked measuring points for selected unit loads.

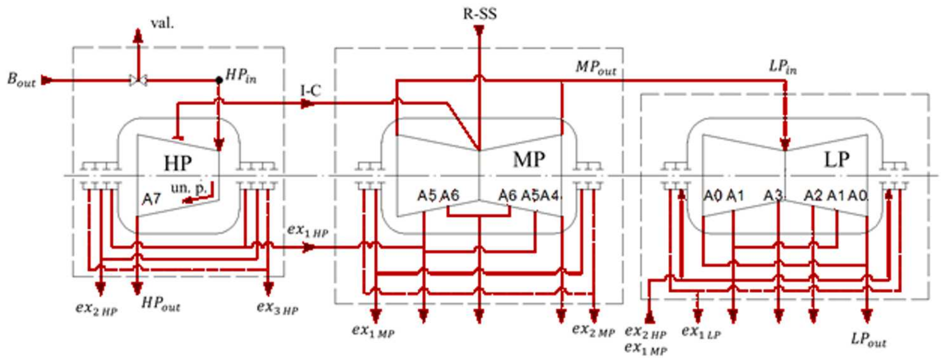

Figure 8: Schematic diagram of the steam turbine 18K370: B_{out} – the mass flow rate of fresh steam produced in the boiler, val. – the leaks in valves seals, HP_{in} – steam mass flow rate at the inlet of high-pressure (HP) part of the turbine, un. p. – mass flow rate on unload piston, I-C – mass flow rate of the inter-cylinder steam, HP_{out} – steam mass flow rate at the outlet of high-pressure part of the turbine, $ex_{i\ HP}$ – mass flow rate of the steam from the external HP glands, R-SS – mass flow rate of re-superheated steam from the boiler, MP_{out} – steam mass flow rate at the inlet of medium-pressure (MP) part of the turbine, $ex_{i\ MP}$ – mass flow rate of the steam from the external MP glands, LP_{in} – steam mass flow rate at the inlet of low-pressure (LP) part of the turbine, $ex_{1\ LP}$ – mass flow rate of the steam from the external LP glands, LP_{out} – steam mass flow rate at the outlet of low-pressure (LP) part of the turbine.

The presented model of the 18K370 steam turbine allows the calculation of non-measured operating parameters (particularly streams and thermal parameters of steam at the outlet of each group of stages) and energy assessment indicators, e.g. efficiency of each part of the steam turbine. An important benefit of the developed model is that it also features the capability of adapting to the changing technical conditions of the steam turbine. The model can be used in predictive control systems, in intelligent hierarchical control systems (OCL) and thermal diagnostics systems.

7 Summary

Theoretical fundamentals and the model construction rules which use the regression and neural modelling techniques are presented. The regression models ensure the availability of computer procedures for linear models and short computation time, but they require the inversion of the matrix which, for a large number of measuring points, may have a significant size. Models

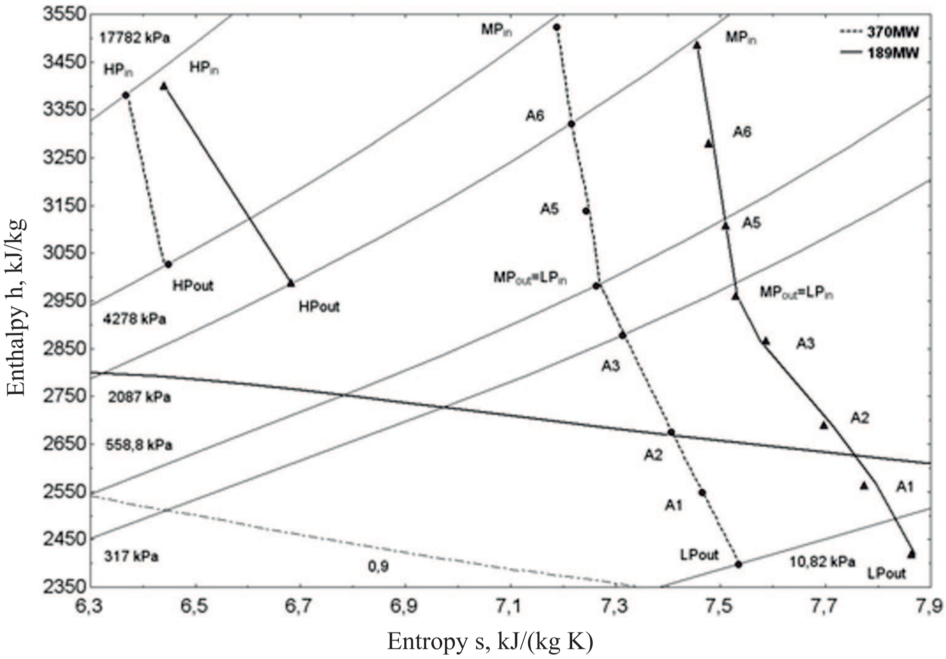

Figure 9: The exemplary steam expansion line for unit loads 370 MW and 189 MW.

developed by using artificial neural networks can approximate any continuous and discontinuous functions, but the model structure is often highly complicated and then the computational load may be a barrier limiting its application.

The mathematical models of the BP-1150 steam boiler, the 18K370 steam turbine as well as the double-pressure heat recovery steam generator have been presented. The values of prediction quality indices and the comparison of the calculation results with the results of the measurements indicate that a good modelling accuracy has been achieved, while maintaining a short computation time. The presented models were used in an operational control system at the Opole Power Plant and Zielona Góra comjbined heat and power plant to simulate unit operation and calculate working deviations.

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