Use of machine learning methods for determinatuon of the boundary conditions coefficients in a FEM task for the case of accelerated cooling of hot-rolled sheet metal

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The article considers an approach to combine the FEM method with the machine learning method in modeling the process of sheet metal cooling in a laminar cooling unit. A model of rolled products cooling based on the FEM has been developed; it considers the variable properties of the material and phase transformations. The high importance of taking into account physical processes, which occur on the surface of rolled products during cooling, is shown, namely influence of the surface temperature of rolled surface on the heat transfer coefficient. In first iteration data from literature was used for this dependence, afterwards it was adapted for the concrete case using iteration method. Especial importance of this phenomenon for calculation of cooling processes for rolled heavy plates (with thickness more than 30 mm) is shown. Two ways to calculate heat dissipation from phase transformations based on the Avrami formula and using the curve of relationship between heat capacity and temperature are given; they are used in a model depending on availability of data for the examined steel grade. Heat transfer coefficient was determined using machine learning methods in order to increase accuracy of calculations. The training set was built on the basis of industrial data, cleared from serial production factor and errors in sensors data signals. Several machine learning models were examined, the model based on gradient boosting of the catboost library displayed the best results. The optimal model parameters were selected using the GridSearchCV method of the Sklearn library or other built-in methods. The most important factors (feature importance) were those that provide especial influence on the heat transfer coefficient - water flow, thickness of rolled products, temperature range of cooling, chemical composition of steel.

Keywords: rolled plates, cooling, machine learning, heat transfer coefficient, finite element method.
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Introduction

Modern rolling mills manufacture products via the controlled rolling technology, which is based on several structural mechanisms: grain refining, control of austenite-ferrite transformation and solid solution dispersion hardening.

Grain refining makes the maximal influence both on steel strength and cold resistance; at the same time the mist effect on ferrite grain size is provided by cooling of rolled products in accelerated cooling units. Such parameters as initial size of austenite grains before cooling, cooling rate and cooling termination temperature determine number of ferrite nuclei [1, 2].

Possibility of prediction of rolled product final properties and provision of the required above-mentioned cooling parameters allow to form different mathematical models, which can help to calculate both average temperature of rolled products after cooling and its distribution across width of these products [3, 4].

Many such cooling models for rolled products are based on the finite elements method (FEM) [5-7]. This method is characterized by high accuracy of obtained results; however, it needs a lot of time for calculation and accuracy of determination of boundary conditions. The first of these restrictions is decisive in the case of searching an optimal solution (e.g. choice of transportation speed or water flows in the cooling unit).

Neural networks are applied for modeling of cooling process of rolled products, e.g. as in the work [8], where the authors obtained optimal structures and parameters of radial-basic neural network and Takagi-Sugeno-Kanga neural network with demonstration of high accuracy of such approach.

A cluster of models on the FEM base and machine learning methods is used recently more and more often. For example, in the work [9] it is suggested to use neural networks for solving reverse Cauchy problem. Using multi-layer networks as approximation, discretization without a networks is presented for solving the problems. Numerical results for the cases from 2D to 3D show that the approach with neural networks is easily distributed for a multi-dimension case in comparison with finite elements method. The articles [10, 11] consider a neural networks on FEM base for solving the boundary problems. The neural networks consists of nodal units and sub-net elements, which synaptic weights are previously determined using FEM formulation procedure. Unknown networks entrances are renewed using the net inversion method in order to meet the requirements of the main law and the boundary conditions and, respectively, to solve the problem. Numerical modeling displays adequacy of this networks.

Thus, the combination of the most practical properties of each method allows to achieve accuracy and rapidity of calculations, so it is perspective to use such hybrid models on the second level of automation of rolling mills.

Goal setting

The average value of surface temperature after cooling is the aimed parameter for models which are used for control of cooling units. Determination of the average temperature of rolled metal depends mostly on heat transfer coefficient, which depends in its turn on water consumption and other factors such as water temperature, rolled metal surface temperature etc. In this paper, it is proposed to use machine learning methods to determine the heat transfer coefficient together with a FEM-based model to determine the average surface temperature of sheet metal after a cooling installation.

FEM model

To determine the temperature in each point of plate, it is necessary to solve non-stationary equation of heat conductivity with the boundary conditions of third type [12]:

$$\lambda \cdot \frac{\partial^2 T}{\partial x^2} + \lambda \cdot \frac{\partial^2 T}{\partial y^2} = \rho \cdot c \cdot \frac{\partial T}{\partial t} \text{ in the area } \Omega, \quad (1)$$

$$\lambda \cdot \frac{\partial T}{\partial n} = \alpha \cdot (T - T_{av}) \text{ along the boundary } \Gamma, \quad (2)$$

where λ – heat conductivity coefficient, ρ – density, c – metal heat capacity, t – time, T – temperature, T_{av} – medium temperature, α – heat transfer coefficient, Ω – area of the examined object, Γ – boundary of the examined object.

Let us at first consider solution of the stationary task (i.e. the first part of the equation is equal to zero) via finite elements method, using rectangular elements. In this case the equation will be as follows:

$$\lambda \cdot \frac{\partial^2 T}{\partial x^2} + \lambda \cdot \frac{\partial^2 T}{\partial y^2} = 0 \quad (3)$$

Residual error of the solution is:

$$R_\Omega = \varphi - \overline{\varphi} \quad (4)$$

where φ – exact value of approximating function, $\overline{\varphi}$ – its approximation.

In order to decrease residual error, we need to equalize corresponding integrals within the whole area Ω to zero, while these integrals were taken with any weights W_i (these weights are accidental, but specially selected functions):

$$\int_\Omega W_i \cdot R_\Omega \cdot \partial\Omega = 0; i = 1, 2, 3... \quad (5)$$

In this case, execution of the boundary conditions can be provided in the same way via introduction of corresponding residual error, but along the object surface. If we summarize both residual errors and equalize them to zero, we shall get the following equation:

$$\int_\Omega W_i \cdot R_\Omega \cdot \partial\Omega \int_\Gamma W_i \cdot R_\Gamma \cdot \partial\Gamma = 0; i, l = 1, 2, 3... \quad (6)$$

The method of weighted residual errors for the heat conductivity equation (3) and the boundary conditions (5), as soon as these equations are considered as unknown functions, is expressed in the following way:

$$\int_\Omega W_i \cdot \left(\lambda \cdot \frac{\partial^2 T}{\partial x^2} + \lambda \cdot \frac{\partial^2 T}{\partial y^2}\right) \cdot d\Omega + \int_\Gamma \overline{W_i} \cdot \left(\lambda \frac{\partial T}{\partial n} - \alpha \cdot (T - T_{av})\right) \cdot d\Gamma = 0 \quad (7)$$

If we divide the examined object, which occupies the area Ω and has the boundary Γ, into a lot of areas Ω_i^e with boundaries Γ_i^e, then we can write down the equation for each of these sub-areas.

$$\int_{\Omega_e} \left(\frac{\partial W_i}{\partial x} \cdot \lambda \cdot \frac{\partial T}{\partial x} + \frac{\partial W_i}{\partial y} \cdot \lambda \cdot \frac{\partial T}{\partial y}\right) \cdot d\Omega_e + \int_{\Gamma_e} W_i \cdot (\alpha \cdot (T - T_{av})) \cdot d\Gamma_e = 0 \quad (8)$$

Let us agree, that approximation of the unknown temperature function T will be searched in the form:

$$\overline{T} = \sum_{m=1}^{M} T_m \cdot N_m, \quad (9)$$

where T_m – nodal function value, N_m – basic function, m – node number, M – number of nodes.

Now, if we consider the basic functions themselves as weighted functions (Galerkin method), we shall get from the equation (8)

$$\int_\Omega \left(\frac{\partial N_l}{\partial x} \cdot \lambda \cdot \frac{\partial \overline{T}}{\partial x} + \frac{\partial N_l}{\partial y} \cdot \lambda \cdot \frac{\partial \overline{T}}{\partial y}\right) \cdot dx \cdot dy + \alpha \cdot \int_\Gamma N_l \cdot \overline{T} \cdot d\Gamma = \alpha \cdot T_{av} \cdot \int_\Gamma N_l \cdot d\Gamma, \quad (10)$$

where l – element number.

Using here approximation (9), we obtain the following matrix equation:

$$K \cdot T = f, \quad (11)$$

When solving non-stationary problems, the partial discretization methods are widely used. In this case approximation of unknown function can be written down as:

$$\overline{T} = \psi + \sum_{m=1}^{M} a_m(t) \cdot N_m(x, y, z), \quad (12)$$

Where functions ψ and N_m are selected in such way, that the main boundary conditions will be executed. Then use of

the method of weighted residual errors allows to obtain the system of differential equations in vector form:

$$C \cdot \frac{dT}{dt} + K \cdot T = f. \quad (13)$$

Here C – so-called heat capacity matrix, its components can be expressed in the following way:

$$C_{lm} = \int_{\Gamma} \frac{c \cdot \rho}{\lambda} \cdot W_l \cdot N_m \cdot d\Omega, \quad (14)$$

where W_l – weighted function for the element l.

Other matrixes and their components can be found in the same way as for stationary case.

Now it remains to apply the finite elements method or the finite difference method to the equation (13) in order to get the required temperatures of nodes. As a result, we shall obtain:

$$\int_0^1 \left[\left(\frac{C}{\Delta t_n} \cdot (-a^n + a^{n+1}) + K \cdot (a^n \cdot (1-\tau) + a^{n+1} \cdot \tau) - \right. \right. \\ \left. \left. - f \cdot (t_n + \Delta t_n \cdot \tau) \right) \right] \cdot W_n \cdot d\tau = 0. \quad (15)$$

Then, applying different routes of solution (with difference backward ($\tau = 1$), forward ($\tau = 0$) or central difference ($\tau = 0.5$)), it is possible to get standard matrix equations of the type (13).

Realization of the algorithm for solving matrix equations

As soon as Galerkin method was used for selection of weighted functions, all matrixes of elements inputs (and, respectively, global matrixes too) will be symmetric. Additionally, they will have weakly filled structure (sparse matrixes), what is typical for the finite elements method.

Iteration methods with preconditioning are the most efficient ways for solving such systems of linear algebraic equations (SLAE). There is also no need to store zero elements and provide actions with them in order to decrease the required time for calculations. Special methods of storage for sparse matrixes are used for this purpose; CSR route is chosen in this work [13].

To solve sparse SLAE, the conjugate gradients method with preconditioning in the form of Kholetsky dissolution is used in the model [14].

Taking the boundary conditions into account

Plate cooling in the accelerated cooling unit should be considered as a complex process, because the following processes take place during cooling [15]:

- forced convection;
- water heating up to the boiling temperature;
- evaporation;
- heat transfer through vapor (Leidenfrost effect).

As soon as physical nature of these processes is complicated [16], calculating of heat flows on the boundary of media separation is difficult in this case. Thereby use of the boundary conditions of third type will be optimal, because heat transfer coefficient will be considered as a complex parameter, taking into account all processes, i.e.:

$$\alpha = f(Q, T_{water}, ...), \quad (16)$$

where Q – water flow in the unit, T_{water} – water temperature.

Material properties and taking phase transformations into account

Material properties were preset on the base of literature sources for low alloy steels [17], while heat conductivity, heat capacity, density depend on temperature in the concrete networks node.

As soon as essential amount of heat is extracted in the process of austenite – ferrite (bainite) transformation, this phenomenon should be taken into account in plate temperature calculation.

We can take heat extraction into account, if we shall consider it as an internal heat source, according to the following formula [18-20]:

$$q = \Delta H_i \cdot \frac{dX_i}{dt}. \quad (17)$$

where ΔH_i – heat amount from transformation at the given temperature T_i, X_i – part of volume which was subjected to transformation, expressed in time function.

After air cooling, austenite decomposition is described as isothermal transformation. The Avrami formula can be used here:

$$\frac{X}{X^e} = 1 - \exp(-k \cdot t_n), \quad (18)$$

where X^e – thermodynamic equilibrium part, which can be determined from phase diagram for the given temperature and cooling rate, k and n – material coefficient.

It is necessary to consider non-isothermal character of transformation process in the case of water cooling. In its turn, transformation can be considered as a sum of discrete isothermal steps:

$$\frac{X}{X^e} = 1 - \exp(-k_i \cdot (t_i' + \Delta t_i)^n), \quad (19)$$

$$t_i' = \left[-\frac{1}{k_i} \cdot \ln\left(\frac{1 - X_{i-1}}{X_i^e} \right) \right]^{\frac{1}{n}}, \quad (20)$$

where t_i' - time required for transformation to the part X_{i-1} at the temperature at i-step, Δt – step in time.

There is an alternative approach to modeling of phase transformations – accounting of only heat capacity variation [21]. This approach is not so precise,

because it does not take into account kinetics of phase transformation and does not allow to calculate metal structure in time. However, the value of phase transformation heat can be obtained from the graph with dependence between heat capacity and temperature. It is equal to the figure (triangle) area, which reflects phase transformations in steel. It should be noted that this graph will differ for different cooling rates. Both methods were used in this work, and their use is determined by presence of data about the examined steel grade.

Interface of the FEM-based program

The above-described relationships and approaches are put in the basis of the developed Java software program, which allows to calculate cooling process of rolled metal in accelerated cooling unit at a plate rolling mill. The following parameters are used as the initial data:

- number of elements in plate length and thickness (non-uniform networks with a smaller element near the surface was used);

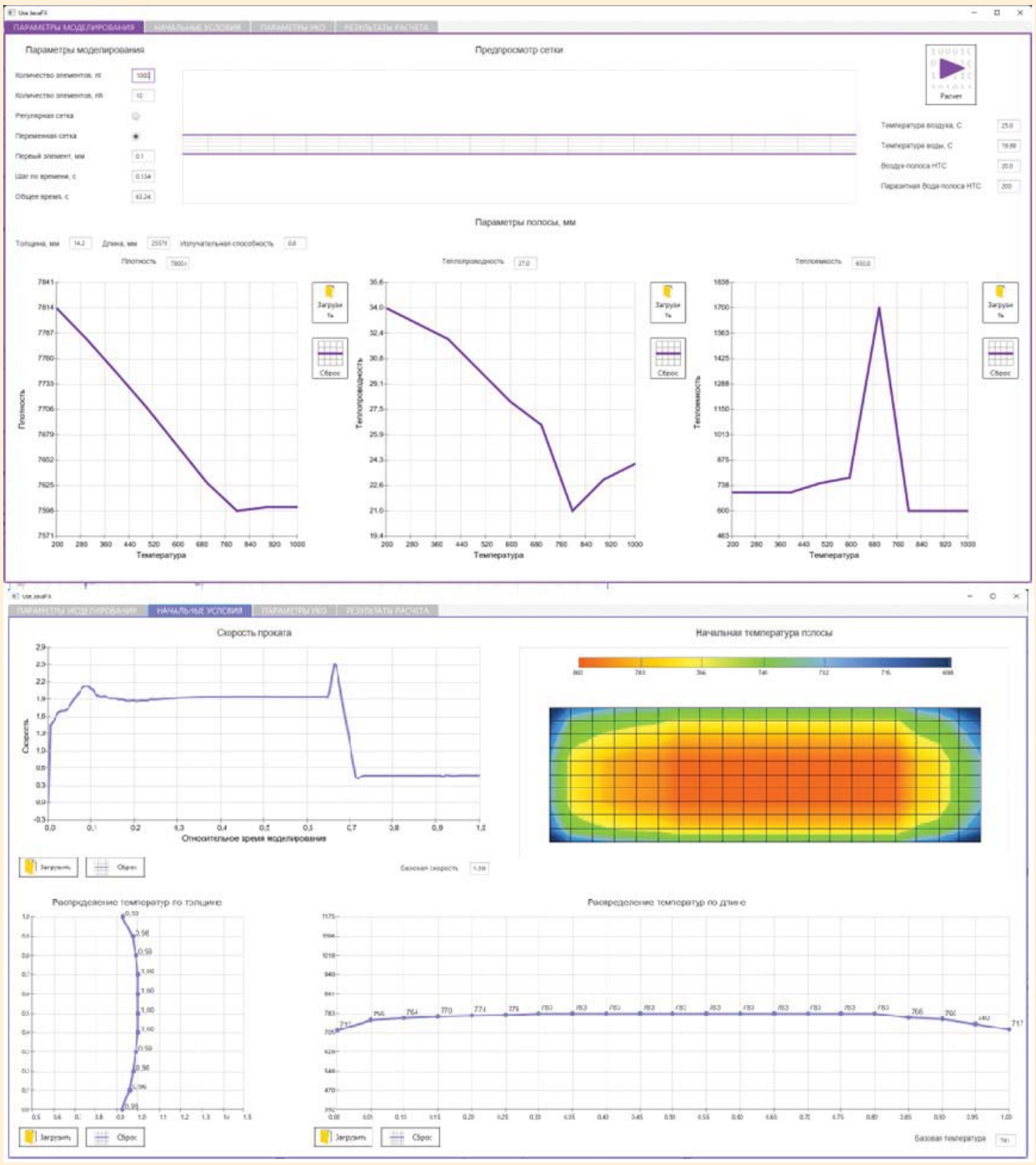

Fig. 1. General view of initial data in the model interface

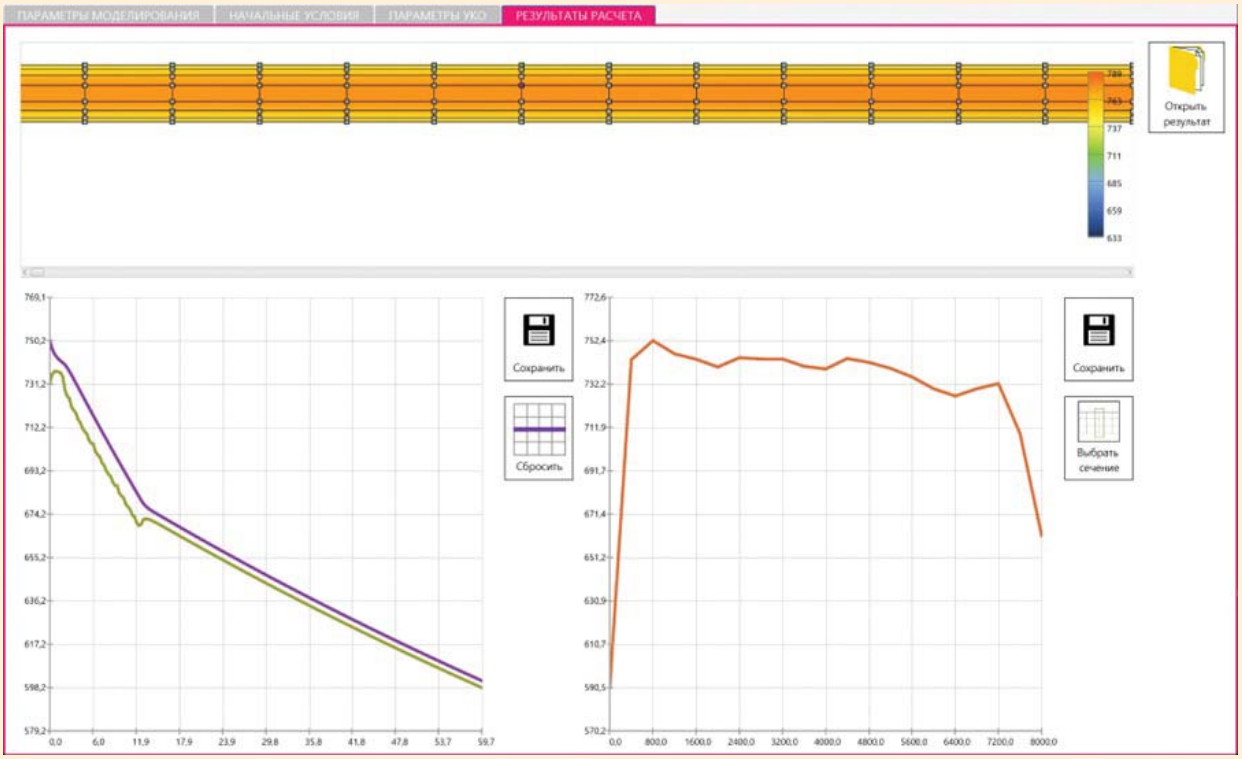

Fig. 2. Screen example with results of calculation

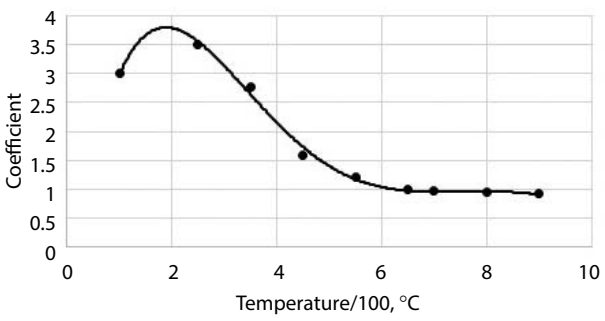

Fig. 3. Variation of the coefficient of heat transfer coefficient from the surface of rolled product depending on its temperature

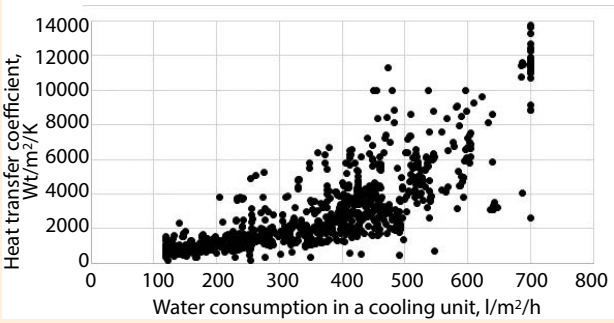

Fig. 4. Relationship between heat transfer coefficient and water consumption without accounting dependence from Fig. 3

- heat transfer coefficient from sheet to air (accepting 20 Wt/m²/C);
- heat transfer coefficient from sheet to extraneous water (accepting 200 Wt/m²/C);
- transportation speed in time;
- water consumption in time;
- water temperature;
- air temperature;
- sheet length and thickness;
- data on material properties (temperature conductivity, heat capacity, density, radiation capacity);
- temperature distribution along sheet length (a signal from pyrometer);
- temperature distribution across sheet thickness;
- time step.

General view of initial data in the model interface is presented on the **Fig. 1**.

The program calculation is resulted in temperature variation in each net node and also across its section (see the example on the **Fig. 2**).

General principle of heat transfer coefficient determination

It is known from the technical literature [22, 23] that heat transfer coefficient (HTC) during water cooling depends on many factors (such as surface temperature, transporta-

tion speed, scale structure etc.), but first of all on surface temperature. This dependence is characterized by permanent growth of this coefficient up to temperature 200-300 °C with its consequent lowering (Leidenfrost point). This circumstance was also taken in the developed model, however, a set of calculations within the above-described program was conducted for curve adaptation to industrial conditions and for provision of higher accuracy. The dependence was preset as HTC function from surface temperature and was approximated by a fifth degree polynom (see **Fig. 3**). This coefficient is multiplied during calculation on any basic HTC value.

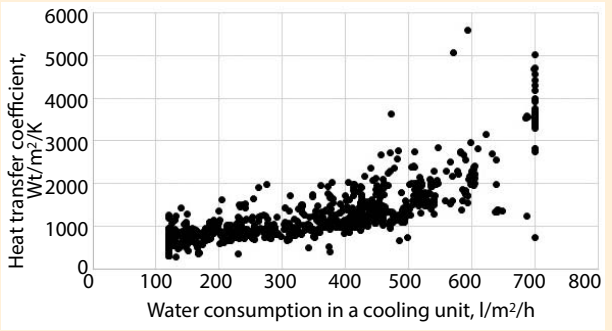

Fig. 5. Relationship between heat transfer coefficient and water consumption with accounting dependence from Fig. 3

The following algorithm was applied for adaptation process: the required parameters of cooled rolled plate and cooling unit were selected, then the average temperature value was calculated and compared with the really obtained data. Afterwards the curve profile was varied (peak displacement and coefficient distribution), and calculation was repeated until maximal accuracy of the experiments will be achieved.

It is especially important to take into account the heat removal efficiency factor when calculating the cooling of thick rolled products (>30 mm) and when cooling down to low temperatures (below 300 °C). The surface of rolled products with large thickness is cooled to the temperatures lower than 200-300 °C (with more hot core), that leads to high values of heat transfer coefficient. The surface of more thin rolled product, while being cooled to the typical temperatures about 500 °C, does not acceed temperatures close to the beginning of Leidentrost effect, thereby it is less sensitive to the examined coefficient. That's why, if we compare **Fig. 4**, where the coefficient is considered equal to 1, and **Fig. 5**, we can see principally larger HTC determination with the same water consumption for different strip thickness values and different cooling temperature ranges.

The value of heat transfer coefficient agrees with literature data and is within the range 500-14,000 Wt/m²/K (taking into account the coefficient value on the Fig. 5).

Table 1. **List of indicators for heat transfer determination**

Act_thk	Sheet thickness
Act_wdt	Sheet width
Act_len	Sheet length
Water_flow_lam_inner_bot	Average consumption in the upper collector
Water_flow_lam_inner_top	Average consumption in the lower collector
Plt_cool_spd_avg	Average transportation speed in f controlled cooling unit
Water_temp_laminar_cooling	Water temperature
Head_masking_top_length	Masking parameters
Head_masking_top_flow	
Head_masking_bottom_length	
Head_masking_bottom_flow	
Tail_masking_top_length	
Tail_masking_top_flow	
Tail_masking_bottom_length	
Tail_masking_bottom_flow	
Perc_C, Perc_MN, Perc_SI, Perc_NI, Perc_CR, Perc_TI, Perc_NB	Chemical composition
Collectors_number	Number of collectors
Pyr6	Average value at the entrance of a cooling unit
Flatness	Average value by flatness measuring device
Alfa	Calculated heat transfer coefficient

Creation of the model for prediction of heat transfer coefficient depending on water consumption and other parameters, on the base of machine learning methods

It was mentioned above that heat transfer coefficient depends on surface temperature, and it is especially observed during cooling of rolled product with large thickness (more than 30 mm). Thereby two models were developed on the base of machine learning methods: one for thicknesses less than 30 mm, another for thicknesses more than 30 mm. This circumstance was additionally substantiated by rather larger amount of manufactured rolled product with thickness < 30 mm.

The following indicators were presented as initial data (**Table 1**).

Initial data set consists of more than 10,000 sheets of pipe, micro-alloyed, high-strength and medium carbon steel grades; however, as soon as rolled products were manufactured in batches with 10-20 sheets in each of them, with equal cooling parameters within one batch, 5 sheets were selected from every batch for data balancing. These data were cleaned from error cases in pyrometer measurements (e.g. cooling lower that sensitivity threshold)m from errors in databases etc. The final data set included totally 1,849 sheets (1,315 sheets with thicknesses less than 30 mm and 534 sheets with thicknesses more than 30 mm). The main parameters of cooled rolled products within this data set are presented on the **Fig. 6**.

It is known that use of neural nets is inexpedient for such data set [24], what was checked within the framework of this

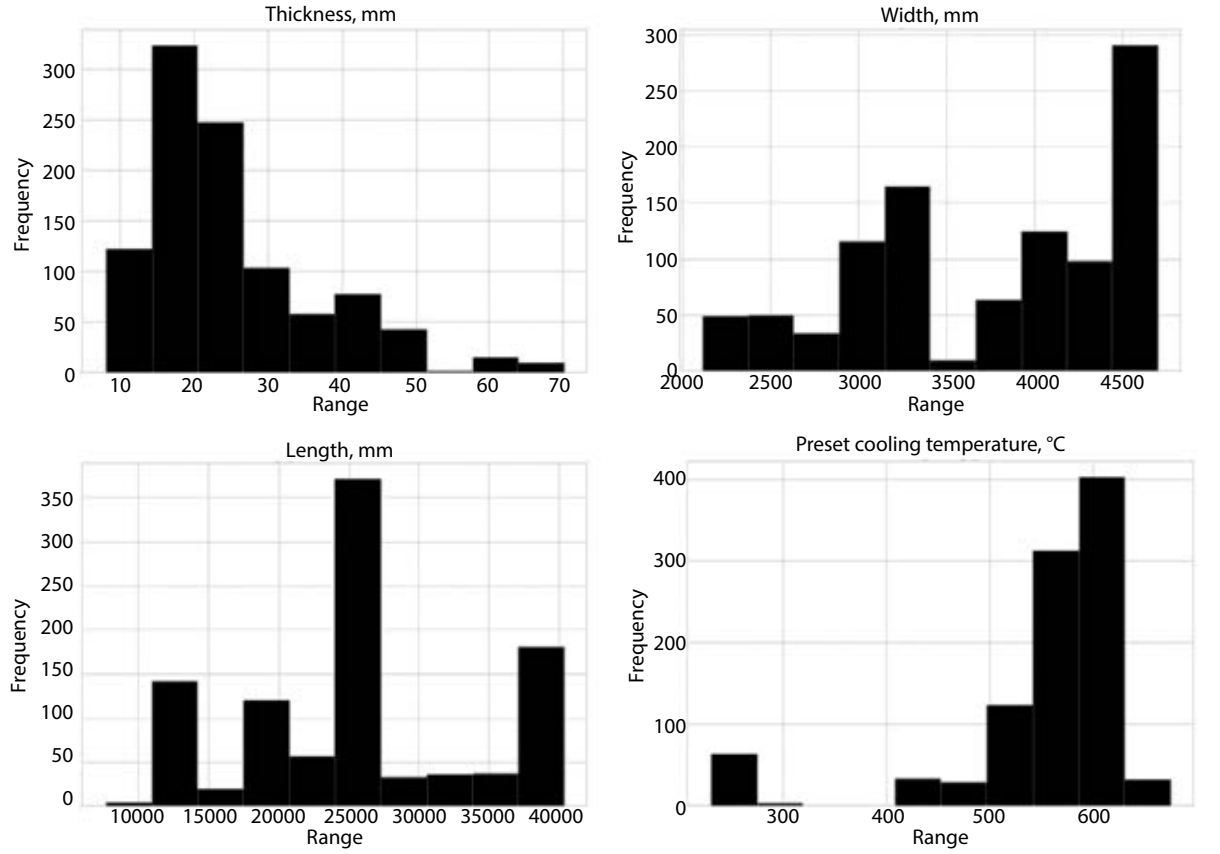

Fig. 6. The main parameters of cooled rolled products in the examined data collection

Table 2. **The results of models operation for thicknesses less than 30 mm**

Model	Determination coefficient R2 for training (testing) collections	Mean square deviation RMSE for training (testing) collections
Solving trees	0.89 (0.82)	98.5 (151.5)
Random forest	0.89 (0.80)	98.7 (159.9)
Catboost	0.98 (0.89)	39.4 (100.1)
LightGBM	0.91 (0.88)	102.6 (113.7)
XGBoost	0.93 (0.89)	81.4 (102.1)

research: neural nets provided essentially worse results in comparison with classic methods and with gradient boosting method.

To search the most exact model, the results of the following methods were analyzed:

- Solving trees
- Random forest
- Gradient boosting
  - Catboost library
  - LightGBM library
  - XGBoost library

The models were learnt with separation in testing and training sets with their relation 20 % to 80 %. To search the optimal parameters, the method GridSearchCV of Sklearn library (or other methods which are built in the libraries) was used.

The results of models operation for thicknesses less than 30 mm are presented in the **Table 2**.

The best results were noted for the model on the base of Cardboost library. The best parameters of this model are as follows: {'loss_function': 'RMSE', 'l2_leaf_reg': 10, 'depth': 6, 'learning_rate': 0.1 , 'max_leaves': 64, 'min_fold_size': 100}. Importance of features is presented on the **Fig. 7**.

The most important model features are thickness of rolled products, finishing cooling temperature (it was noted previously), water consumption, length of rolled products and speed of their transportation. Influence of alloying elements (variation of thermal physical properties of rolled products with different chemical composition) can be also seen.

The model on the base of Catboost library also displayed the best results for thicknesses more than 30 mm. Total accuracy of the models by RMSE is 87.3, calculation results are presented on the **Fig. 8**.

Calculation of the average sheet surface temperature value within the testing collection displayed satisfactory results (95.89 % of cases were located within the range ±30 °C from the aimed value) (**Fig. 9**). In this case all sheets from a batch and all thicknesses were taken into account.

Maximal error was observed for thicknesses about 10 mm, what can be explained by maximal sensitivity of thin

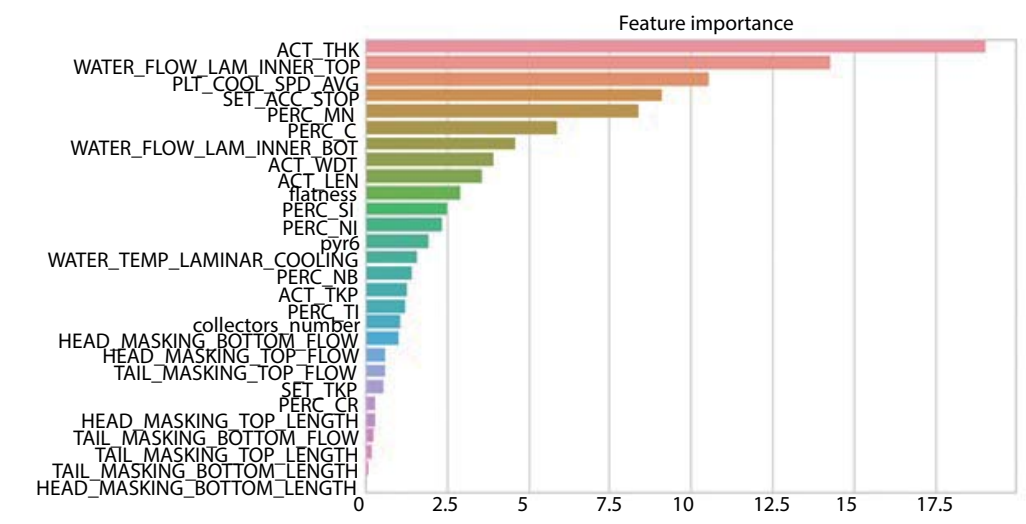

Fig. 7. Importance of model fetaures for determination of heat transfer coefficient

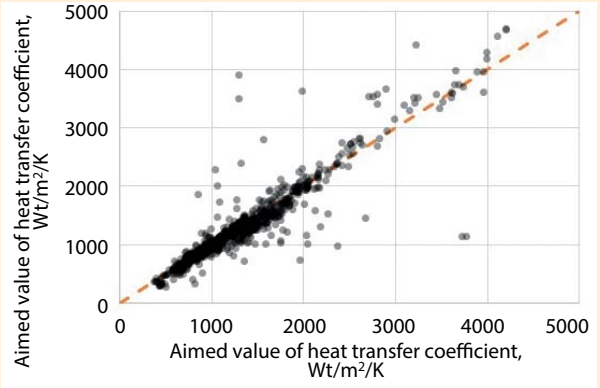

Fig. 8. Obtained accuracy of heat transfer coefficient determination

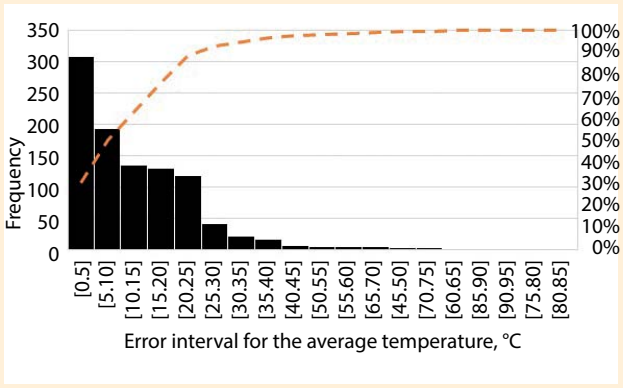

Fig. 9. The error in average temperature calculation for sheet surface after accelerated cooling unit

rolled products during cooling to errors in heat transfer coefficient determination. In general, such accuracy of average temperature determination on rolled products surface in a cooling unit of plate rolling mill meets the requirements to the models which are used at production sites.

Conclusions

1. The developed FEM-based cooling model for rolled products in accelerated cooling unit, which takes into account variable material properties, phase transformations and dependence of heat transfer coefficient from surface temperature, allows to determine average temperature of rolled product surface after accelerated cooling with satisfactory accuracy in production conditions.

2. Influence of relationship between surface temperature dependence on determination of heat transfer coefficient and high importance of accounting of this effect for calculation of cooling procedure of heavy plates (with thickness more than 30 mm) is shown.

3. The gradient boosting method on the base of Catboost library provided maximal accuracy of determination of heat transfer coefficient. The coefficient of determination for the model R2 = 0.98-0.89 (for training / testing collection), mean square deviation RMSE = 39.4-100.1.

4. The most important parameters for determination of heat transfer coefficients were defined: rolled product thickness and length, finishing cooling temperature, water consumption, transportation speed of rolled metal.

5. Of the considered sample of 10,000 plates, more than 95.89% of the calculated values were within the range of ±30 °C from the target value, which is acceptable in the production of rolled products using the controlled rolling technology.

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