COMPUTER MODEL FOR PREDICTION OF MECHANICAL PROPERTIES OF LONG PRODUCTS AFTER HEAT TREATMENT[1]

Pavel Šimeček[2]
Rostislav Turoň[3]
Daniel Hajduk[4]

Abstract

The paper presents theoretical aspects and basic algorithms of the general metallurgical software tool (the static library MetaCool) developed for prediction of mechanical properties of steel after quenching and tempering. This model works independently of the concrete heat treatment technology and predicts final mechanical properties (hardness, ultimate tensile strength and yield stress) of steels cooled from austenitic state. The CCT-diagrams of steels are predicted from chemistry and conditions of austenitizing with taking into account the effects of transformation of deformed austenite. The MetaCool library can be linked to various off-line process simulation software or process monitoring systems created to design or control heat treatment or accelerated cooling technologies of concrete steel products. Examples of such technological software tools are presented together with some practical experience with the process simulation of heat treatment of tubes, bars and special profiles (QTSteel software).

Key words: computer model, mechanical properties prediction, steels, heat treatment, metallurgical monitoring

---

(1) *68th ABM Congress, 2013, Belo Horizonte, Brazil*

(2) *Ph.D. degree, technology & IT specialist, ITA Ltd., Ostrava, Czech Republic*

(3) *Technical university degree, technologist, Technology & Research, Trinecke zelezarny a.s., Trinec, Czech Republic*

(4) *Ph.D. degree, technology & IT specialist, ITA Ltd., Ostrava, Czech Republic*

1. Introduction

Increasing quality requirements of steel products market force steel producers to introduce more sophisticated technologies and process control systems into standard production. Various metallurgical software solutions became a part as process simulation as process control systems where provide processing of information about behavior of steels during deformation and subsequent cooling and predict mechanical properties of a final product.

Metallurgical software for computer simulation of heat treatment or accelerated cooling processes in steels can be divided to the following basic levels:

- Off-line Metallurgical Simulators – software that enables to study how changes of various technology parameters influent metallurgical quality of a final product.
- Metallurgical Monitoring Systems – software coupled with the process control system to provide metallurgical predictions based on real process data of already finished production.
- Metallurgical Cooling Control Systems – software providing the setup of cooling parameters necessary for achieving of required mechanical properties of final product before its production.

An essential part of each of those software tools is, if possible, simple and fast module, called Metallurgical Predictor, used for solving of direct heat treatment problem. It is required to calculate steel microstructure and mechanical properties after hardening and subsequent tempering for prescribed steel chemistry, properties of initial austenite and concrete temperature curve. Theoretical aspects of such concept of metallurgical predictor and some representatives of off-line simulation software based on it are presented.

2. MetaCool - basic concept of the metallurgical predictor

Although the steel processing technologies can differ, the physical background of ongoing metallurgical processes is similar. That was the reason why technology independent metallurgical predictor MetaCool was developed. The MetaCool is represented by the library of functions written in the C programming language with the data interface containing pure physical quantities as input (chemistry, temperatures, times, strains, cooling curve) and microstructure shares and final mechanical properties of steel (hardness, yield stress, ultimate tensile strength) as output. The MetaCool library is ready to be linked to various types of technology dependent process simulation or control software packages.

MetaCool is divided internally into 17 steel groups and covers carbon and structural steels with amount of carbon from 0.08% to 0.6% and with the total sum of alloying additions up to 10% and tool steels with amount of carbon from 0.6% to 1.8% with the total sum of alloying additions up to 5%. Assigning of the steel with specified chemical composition into particular groups is performed automatically and metallurgical algorithms differ from one steel group to another.

2.1 The CCT diagram model

The model of the CCT diagram consists of the set of lines (significant temperatures Ac3, Ac1, Ms) and curves (unsymmetrical parabolas) specified by time and

temperature coordinates if their significant points (nose, upper and lower branch). The position of lines and curves in the CCT diagram for specified chemistry was acquired from published diagrams processed separately for each steel group with the use of regression analysis. The following functions were used for approximation of time and temperature coordinates of definition points of the CCT Diagram:

$$T^0_{struct}(PT) = A_0 + \sum_i A_i \cdot c_i \quad (1)$$

$$S^0_{struct}(PT) = \exp(B_0 + \sum_i B_i \cdot c_i) \quad (2)$$

where

$S^0_{struct}(PT)$, $T^0_{struct}(PT)$	is time and temperature of the significant point,
struct	means particular start and finish lines and curves
A_0, B_0, Ai, Bi	are regression coefficients,
c_i	is percentage of alloying addition (i).

The model takes into account microstructure of initial austenite as well, especially its grain size and residual hardening if the transformation of deformed austenite is simulated. These quantities can shift curves of the diagram along time axe significantly. For example the time of noses is expressed in the model by the following equation:

$$\mathrm{Sx} = \mathrm{Sox} \cdot \mathrm{A_S} \cdot \exp((-\mathrm{B_S} + \mathrm{C_S} \cdot \mathrm{Ceq}) \cdot \varepsilon_R) \cdot \mathrm{d}_\alpha^{\mathrm{DS}} \cdot \exp(\mathrm{E_S} \cdot \mathrm{MICRO}) \cdot \varepsilon_R^{1/3})) \cdot \exp(\mathrm{F_S} \cdot \mathrm{B}) \quad (3)$$

where

Sx and Sox are times of shifted and original nose,

A_S, Bs, C_S, D_S, E_S, F_S are constants,

Ceq is the carbon equivalent,

d_α is the grain size of austenite expressed in microns,

ε_R is the residual strain of the deformed austenitic grain prior to its transformation,

B is an amount of boron in steel and MICRO = V+Nb+Ti.

2.2 Temperature curve and transformation kinetics

The MetaCool predictor supposes the cooling curve as a sequence of (time, temperature) couples that need not to be uniformly decreasing. Transformation kinetics of diffusion processes is described by the Avrami equation (4) that was modified for cases of cooling curves with non-uniform cooling rates

$$\mathrm{X(t,T)} = \mathrm{X}_\gamma \cdot (1 - \exp(-\mathrm{k(T)} \cdot \mathrm{t}^{\mathrm{n(T)}})) \quad (4)$$

where parameters k(T) and n(T) depend on the cooling rate, t is the time and Xγ is the rest of austenite. With the use of (4) the percentage of ferrite, pearlite and bainite is calculated in accordance with intersections of the cooling curve with particular CCT curves.

Process of martensitic transformation is not time dependent so the standard Koistinen-Marburger equation (5) is used

$$\mathrm{Xm(T)} = (1 - \exp(-\mathrm{b} \cdot (\mathrm{TMs} - \mathrm{T})^{\mathrm{n}}) \cdot \mathrm{X}_\gamma \quad (5)$$

where b, n are constants, TMs is the Martensite start temperature and Xγ is the rest of austenite.

2.3 Mechanical properties prediction

Basic step for prediction of final mechanical properties is calculation of HV hardness. The HV hardness after hardening has been determined by regression analysis for the shape function (6) with the percentage of alloying addition c_i, amount of particular structure shares X_{struc} and constants C_0, D_i, E_i, F_i and G_i :

$$HV = C_0 + X_F \cdot \sum_i D_i \cdot c_i + X_P \cdot \sum_i E_i \cdot c_i + X_B \cdot \sum_i F_i \cdot c_i + X_M \cdot \sum_i G_i \cdot c_i \qquad (6)$$

Relationship between HV and ultimate tensile strength is well known. The calculation of yield stress is more difficult. Except values from regression analyses the calculation of yield stress reflects the ferritic grain size effect in v Hall-Petch equation and influence of the cooling rate CR on the transformation of austenite and amount of fraction X_{struct}:

$$R_e = f\left(d_\alpha, CR, X_F, \sum (X_P + X_B + X_M)\right) \ [MPa] \qquad (6)$$

As tempered mechanical properties are calculated from the chemistry $c_{(i)}$ by the equation (7) based on the regression analysis of HV hardness of particular structure shares for various tempering temperatures T_{temp} but fixed tempering time 3hrs

$$HVx_3 = \left\{ \sum_i R_{(i)} \cdot c_{(i)} \right\}_{Ttemp,3hrs} \qquad (7)$$

The standard Hollomon-Jaffe parameter Hp is used for calculation of equivalent tempering regime with various tempering times and temperatures

$$H_P = (T_{temp} + 273.15) \cdot (C + \log t_{temp}) / 1000 \qquad (8)$$

where C is a constant varying between 15 and 21.

3. Off-line metallurgical simulators

Some examples of the use of special off-line metallurgical simulators based on the MetaCool predictor are presented for technologies of heat treatment of standard bodies as bars and tubes and for technologies of on-line cooling of hot rolled special profiles from exit rolling temperature.

3.1 Heat Treatment of bars and tubes

The software QTSteel (Quenching and Tempering of Steels) is the off-line tool for calculation of mechanical properties of steels after hardening and subsequent tempering. QTSteel contains built-in 2D FEM temperature module that enables to calculate cooling curves for typical bodies as rectangular and rounded bars, cylinders, tubes and rings. There is possible to compile various time sequences of different cooling conditions to simulate requested strategies of cooling.

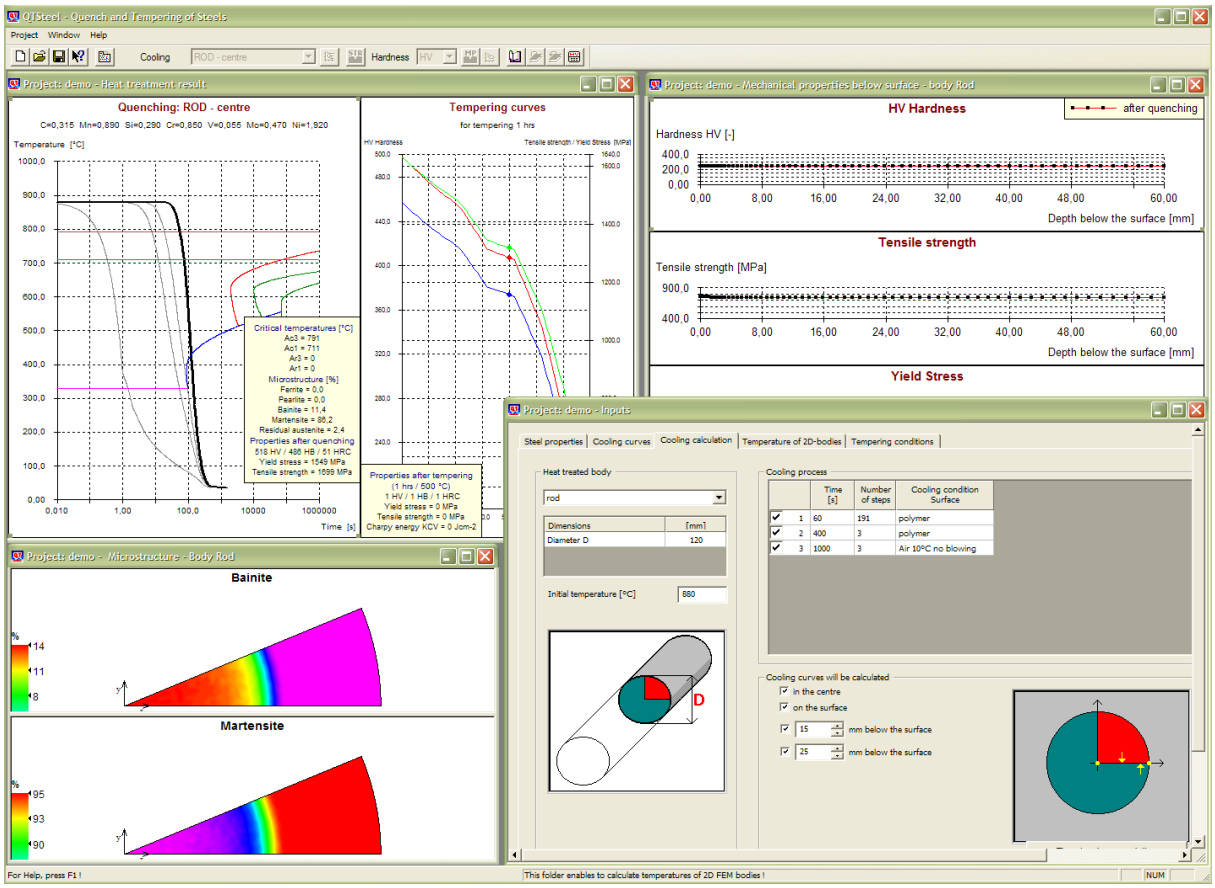


Figure 1. *Graphic User Interface of the software QTSteel*

To show abilities of the MetaCool predictor the simulation of the following 4 heat treated products were performed by the QTSteel software and resulting mechanical properties were compared with measured ones:

- 9 bars of diameters varying from 135 - 255mm, AISI 4330V, water quenched and tempered at 620 °C (hold time of 60 – 540 min)

C	MN	SI	CR	NI	MO	V
0,32	0,83	0,29	0,86	1,87	0,45	0,06

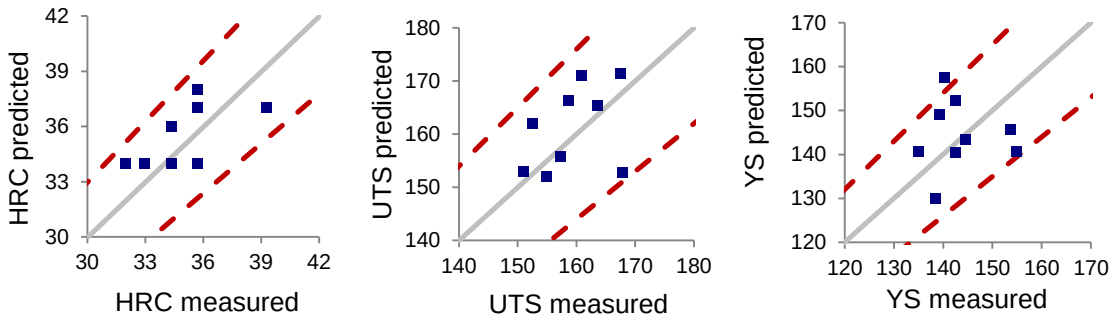


Figure 2. *Average chemistry and comparison of measured and predicted mechanical properties for bars AISI 4330V*

- 23 bars of diameters varying from 80 - 380mm, AISI 4130, water quenched and tempered at 650 – 700 °C (hold time of 60 – 680 min):

C	MN	SI	CR	NI	MO	CU
0,32	0,57	0,27	1,03	0,15	0,2	0,14

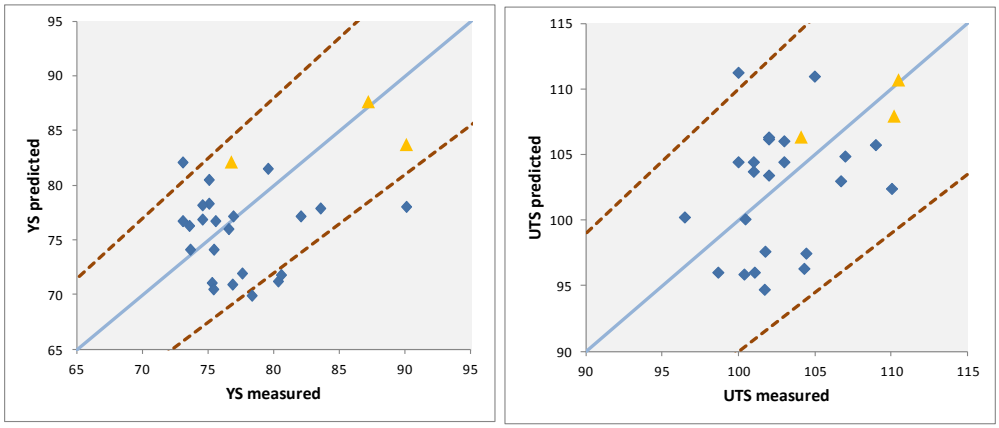


Figure 3. *Average chemistry and comparison of measured and predicted mechanical properties for bars AISI 4130*

- heat treated seamless tube of diameter 292mm and wall thickness 34mm, normalized and quenched by water spray, tempered 30min at 680°C:

C	MN	SI	V
0,4	1,4	0,2	0,17

	Ferrite %	**Bainite %**	**Martensite %**	**HV**	**UTS MPa**	**YS MPa**
Predicted outer surface	0	0	100	232	767	637
Predicted inner surface	5.2	81.1	13.7	224	690	524
Measured properties	-	-	-	-	**762**	**648**

Table 1. *The chemistry and comparison of measured and predicted mechanical properties for the tube 292/34mm*

- heat treated seamless tube of diameter 244.5mm and wall thickness 10mm, normalized and quenched by water spray, tempered 60min at 520°C:

C	MN	SI	CR	NI	AL	MO	TI	NB	B
0,25	1,3	0,2	0,14	0,4	0,037	0,2	0,04	0,002	0,0024

	Martensite %	**HV**	**UTS MPa**	**YS MPa**
Predicted outer surface	100	340	1058	1005
Predicted inner surface	100	339	1053	1001
Measured properties	-	-	**1050**	**996**

Table 2. *The chemistry and comparison of measured and predicted mechanical properties for the tube 244.5/10mm*

3.2 Cooling of hot rolled mining reinforcements

Hot rolled special TH profiles used for production of mining reinforcements lying on the cooling bed were cooled from the exit rolling temperature 1050°C by fans located at the bottom of the bed. Measurements of air flow on the cooling bed and temperatures of cooled profiles TH29 were performed and used for verification of boundary conditions for subsequent computer simulation to study how various conditions of air blowing influent mechanical properties of the final product. Computer simulations were performed by the software THCoool developed specially for these purposes.

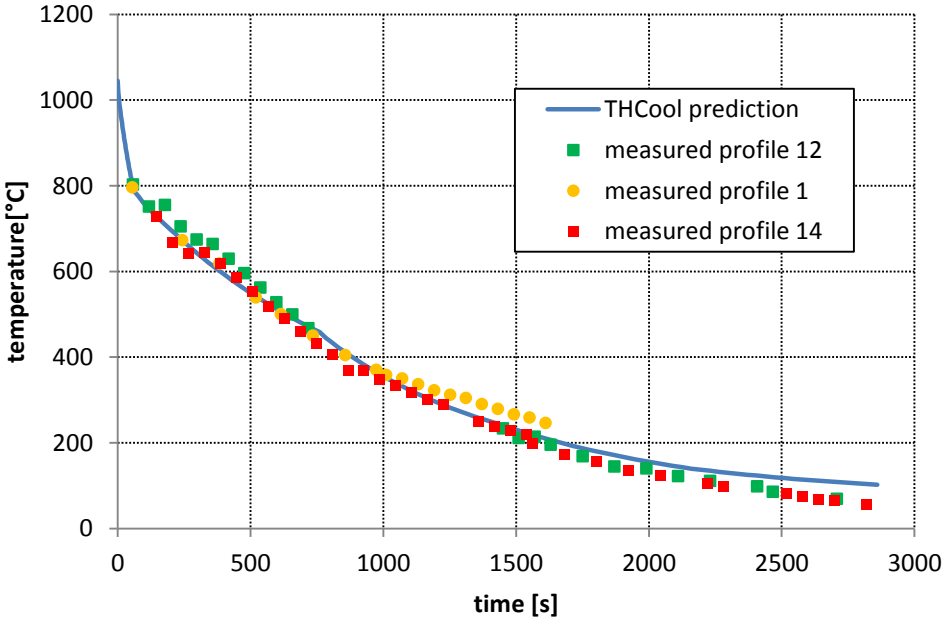


Figure 4. *Predicted and measured temperatures of the TH29 lying on the cooling bed*

C	MN	SI	V
0,32	0,93	0,4	0,1

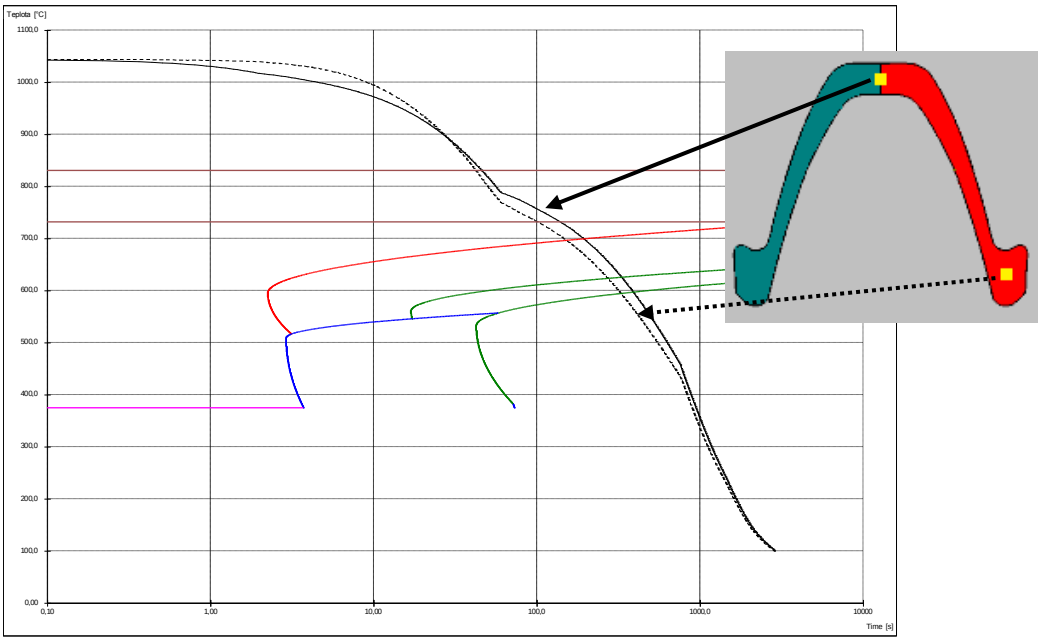
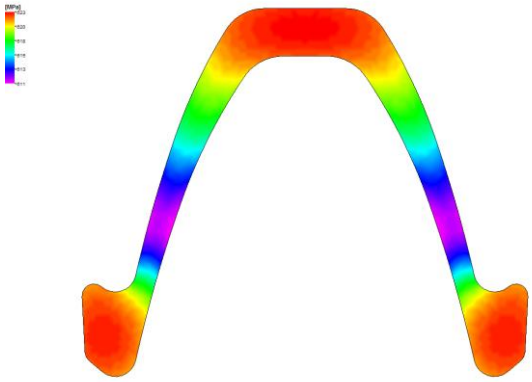


Figure 5. *The chemistry and predicted CCT-diagram with cooling curves*



predicted / measured Yield Stress [MPa]	396 / **370-380**
predicted / measured Tensile Strength [MPa]	642 / **640-650**

Figure 6. *Predicted Tensile Strength distribution and comparison of measured and predicted mechanical properties on the head of the TH29 profile*

5. Conclusions

Various implementations of the MetaCool Predictor was presented. Off-line applications as for example QTSteel and THCool can answer questions how microstructure and final mechanical properties of heat treated product are sensitive to changes of technology parameters. Mechanical properties of tubes, bars and special profiles predicted off-line by presented software tools were compared with measured ones to estimate possible precise.

This paper was supported from the budget of the Technology Agency of the Czech Republic within the ALFA - project TA01010838.

6. Literature

[1] ŠIMEČEK, P.; HAJDUK, D.: Prediction of metallurgical quality of strips as a component of the hot strip mill process control system. In: Steel Strip 2011 conference proceedings. Vysoké Tatry - Stará Lesná, Slovak Republic. 2011. pp. 65 – 73.

[2] ŠIMEČEK, P.; HAJDUK, D.: Metallurgical Monitoring – Prediction of quality of hot rolled production as a component of the process control system. In: SARUC 2011 conference proceedings, Vanderbijlpark, Gauteng, South Africa. 2011. pp. 88-91.

[3] ŠIMEČEK, P.; HAJDUK, D.: HRMM - software tool for prediction of metallurgical quality of hot rolled production as a component of the process control system. Metec InSteelCon 2011, Düsseldorf, Germany. 2011.

[4] ŠIMEČEK, P.; ELFMARK, J.; PROŠEK, M.: Computer simulation of heat treatment of high alloyed Cr-steel. SteelSim 2009 conference proceedings. Leoben, Austria. 2009.

[5] ŠIMEČEK, P.; HAJDUK, D.: Models for Level 2 control of cooling processes during hot rolling. 2nd International conference AITSIM´09: Automation and Information Technology in Iron and Steel Making Processes. Ranchi, India. 2009.

[6] http://www.ita-tech.cz/en/products-services/heat-treatment/software-qtsteel

[7] TOSCHI, F.; ŠIMEČEK, P.; CIMOLINO, M.: New process simulation tool for long product rolling. AISTech 2009. St. Louis, USA. 2009.
[8] ŠIMEČEK, P.; ČMIEL, K.; ELFMARK, J.; HAJDUK, D.: Computer simulation of metallurgical processes during hot rolling of bars. In: SteelSim 2007 conference proceedings. Graz, Austria, 2007. pp. 318 - 323.
[9] Computer simulation of metallurgical processes during hot rolling. Engineering Manual for MetaRoll and MetaCool Libraries. ITA Ltd. Ostrava, Czech Republic. 2012.