

DETERMINATION OF THE SOLIDUS AND LIQUIDUS TEMPERATURES OF THE REAL-STEEL GRADES WITH DYNAMIC THERMAL-ANALYSIS METHODS

DOLOČANJE SOLIDUSNIH IN LIKVIDUSNIH TEMPERATUR REALNIH JEKEL Z METODAMI DINAMIČNE ANALIZE

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Prejem rokopisa – received: 2012-10-10; sprejem za objavo – accepted for publication: 2013-02-22

The knowledge of the solidus and liquidus temperatures of the real-steel grades is one of the most important technological factors – especially when dealing with the processes of casting and solidification. These temperatures are critical parameters for proper settings of the models (physical or numerical) or in the final stage of an applied research of a real process. A correct setting of a production technology is significantly affecting the final quality of the as-cast steel (billets or ingots). Therefore, this paper is devoted to discussing the findings obtained during a utilization of dynamic thermal-analysis methods to identify the solidus and liquidus temperatures applicable to commercially produced steels. The results obtained with a differential thermal analysis (DTA) for three steel grades and with 3D differential scanning calorimetry (3D DSC) for two steel grades are compared with the results of the selected equations commonly used for liquidus and/or solidus temperature calculations. The calculations obtained with the CompuTherm SW for the discussed steels were also realized.

It can be stated that the equilibrium liquidus and solidus temperatures obtained with the above-mentioned methods for each steel grade differ. The differences between the calculated results, the thermodynamic calculations and thermal-analysis results are very unpredictable and vary individually for different steels. These differences are not marginal (tens of Celsius degrees). So, it is sometimes suitable to combine several methods for a proper determination of the liquidus and solidus temperatures for a correct setting of a steel-making process or its modelling. The best solution for a technological process is to obtain the liquidus and solidus temperatures for a concrete-steel grade from a given steelmaking practice – a thermal analysis of a concrete-steel grade is a possible way.

Keywords: steel, solidus temperature, liquidus temperature, thermal analysis, thermodynamic database, calculation

Poznavanje solidusnih in likvidusnih temperatur realnih jekel je med najpomembnejšimi tehnološkimi dejavniki – še posebno pri obravnavi procesov med ulivanjem in strjevanjem. Te temperature so kritični parametri za pravilno postavitev modela (fizikalnega ali numeričnega) ali pri končni stopnji raziskav realnega procesa. Pravilna postavitev proizvodne tehnologije pomembno vpliva na končno kvaliteto ulitega jekla (gredic in ingotov). Zato je ta članek namenjen razpravi o ugotovitvah, dobljenih med uporabo metod dinamične termične analize za ugotavljanje solidusne in likvidusne temperature pri komercialno proizvedenih jeklih. Rezultati, dobljeni z diferenčno termično analizo (DTA) za 3 jekla in s 3D diferenčno vrstično kalorimetrijo (3D DSC) za 2 vrsti jekel, so bili primerjani z rezultati iz izbranih enačb, ki se navadno uporabljajo za izračun temperature solidusa in likvidusa. Za obravnavana jekla so bili tudi izdelani izračuni s CompuTherm SW.

Ugotovljeno je bilo, da se ravnotežne likvidusne in solidusne temperature, dobljene z omenjenimi metodami, razlikujejo. Razlike med izračunanimi rezultati, termodinamičnimi izračuni in rezultati termične analize so nepredvidljivi in se različno spreminjajo pri različnih jeklih. Te razlike niso nepomembne (desetine stopinj Celzija). Zato je včasih pomembno kombinirati več metod za pravilno določitev likvidusne in solidusne temperature pri procesu proizvodnje jekla ali njegovem modeliranju. Najboljša rešitev za tehnološki proces je ugotavljanje likvidusne in solidusne temperature pri konkretnem jeklu iz dane jeklarske prakse – mogoča pot pa je tudi s termično analizo konkretnega jekla.

Ključne besede: jeklo, temperatura solidusa, temperatura likvidusa, termična analiza, termodinamični podatki, izračun

1 INTRODUCTION

A better control of the entire steel production cycle – from the selection of quality raw materials to a proper control of primary and secondary metallurgy processes and, finally, an optimum setting of the casting and solidification conditions, is necessary for a modern, competitive steel-making company. In the refining processes, optimizing the slag regimes,^{1,2} thermal and chemical

homogenization of the melt³ or filtration of the steel⁴ are very important stages. With respect to the casting and solidification of the examined steel, important steps toward optimizing the process of solidification of heavy forged ingots⁵ are currently being implemented.

It is not simple⁶⁻¹¹ to experimentally determine the phase transformation temperatures, especially the solidus and liquidus temperatures of the complex multicom-

ponent systems (steels), and at the level above 1000 °C. There are only a few methods that are suitable to provide these results. A comparison between them is shown in the literature.¹² Generally, these methods (briefly described below) are based on a detection of the temperature or a dimensional change induced due to a heat-treated process (an on-going phase transformation).

The direct thermal-analysis method^{13–15} is based on a direct measurement of the temperature of the sample during its continuous linear heating/cooling. The result is a heating/cooling curve. There is a deviation from the otherwise linear curve progression during the phase transformation in the samples. It is possible to obtain the temperatures of a phase transformation based on the curve deviations (e.g., liquidus and/or solidus temperatures).

The differential thermal analysis (DTA) and/or the differential scanning calorimetry (DSC)^{13–15} are the methods based on the same principle. The principle of these methods is a measurement of the temperature difference (heat-flow difference) between the measured sample and the reference. The reference can be an empty reference crucible or a reference crucible with a standard material. The sample and reference are subjected to the same setting of the temperature program of the continuous linear heating/cooling. The result is a DTA curve (a DSC curve) expressing the dependence of the temperature difference (the heat-flux difference) between the measured sample and the reference. If there is an on-going phase transformation in the sample, there is also a deflection from the baseline (a peak is formed). It is possible to obtain the temperatures of phase transformations by interpreting such peaks for given experimental conditions.

Dilatometry^{13–15} is a method based on monitoring the dimensional changes of a sample when it is exposed to a controlled temperature regime, most often to linear heating or cooling. The method is used mainly for the study of the phase transformation temperatures and dimensional changes of the samples in the solid phase. The measurement result is a curve, expressing the dimensional change of a sample in dependence on the

time or the temperature, respectively. The breaks on this curve (a significant deviation from the linear shape) indicate an on-going phase transformation. The temperatures detected with the phase transformations, under the conditions of the experiment, can be obtained by interpreting these deviations.

Apart from the above-mentioned dynamic methods of the thermal analysis, it is also possible to obtain the temperatures of the solidus and liquidus of steel using the broadly known and used equations (1–11).^{16–22} Different kinds of thermodynamic databases integrated into the software packages that are on the market, such as IDS or Computherm, can be used, too.

2 METHODS FOR DETERMINING THE LIQUIDUS AND SOLIDUS TEMPERATURES

Our study of the phase transformations in a high-temperature area was realized with the dynamic methods of the thermal analysis (TA), with the below-described equations and the thermodynamic software Computherm, in the new Laboratory for Modelling the Processes in the Liquid and Solid Phases. This laboratory was set up for the project establishing the Regional Materials Science and Technology Centre at the VŠB – Technical University of Ostrava, Faculty of Metallurgy and Materials Engineering in the Czech Republic. The liquidus and solidus temperatures were determined for the industrially produced steel grades taken from the production cycles in the companies represented by the above-mentioned coauthors.

2.1 High-temperature dynamic thermal analysis

It is possible to use three different laboratory devices for the thermal analysis in the conditions of the new laboratory: Netzsch STA 449 F3 Jupiter (STA-Simultaneous Thermal Analyser), Setaram SETSYS 18_{TM} and Setaram MHTC (Multi High Temperature Calorimeter) (Table 1).

Table 1 shows the characteristic features of our experiment. It is possible to study thermophysical

Table 1: Experimental parameters of the used analytical systems

Tabela 1: Eksperimentalni parametri pri uporabljenih analitičnih sistemih

Parameter	Netzsch STA 449 F3 Jupiter	Setaram SETSYS 18 _{TM}	Setaram MHTC
Experimental method	c-DTA – "calculated curve"; TG/DTA; TG/DSC; TG	TG/DTA; TG/DSC; TG; TMA	HF DSC; DROP; DSC
Temperature range	20 °C to 2000 °C	20 °C to 1750 °C	20 °C to 1600 °C
Heating/cooling rate	0.01–50 K min ⁻¹	0.01–100 K min ⁻¹	0.001–50 K min ⁻¹
Temperature programme	Linear heating/cooling; isothermal holding; cycling		
Sample mass	Up to 30 g (35 g)	Up to 500 mg	HF DSC up to 2.5 g DROP up to 30 g
Atmosphere	Vacuum; inert; reactive		
Sensor type	Flat DSC sensor, S-type	DTA-tricouple sensor, S-type	HF 3D DSC sensor, B-type

Note: STA (Simultaneous Thermal Analysis), TG (Thermogravimetry), MHTC (Multi-High Temperature Calorimeter), DSC (Differential Scanning Calorimetry), HF (Heat Flux), TMA (Thermomechanical Analysis), DROP Calorimetry (a method based on throwing a sample to a pre-heated furnace at a defined temperature after measuring the heat absorbed, also known as the "throwing calorimetry" method)

properties, e.g., the liquidus and solidus temperatures of the steel grades under various experimental conditions: different sample masses, different heating/cooling rates, and different methods.

The measurements carried out in the laboratory are focused not only on determining the temperatures close to the equilibrium temperatures, or almost the equilibrium, but also on determining the phase-transformation temperatures depending on the cooling process and the subsequent thermomechanical treatment of the steels in the steel plants. The obtained temperatures can differ from the equilibrium, or close-to-equilibrium, temperatures, but can be also very important for an optimal setting of a real steelmaking technology. An example of such a solution was already presented²³.

To achieve the equilibrium state of a sample is, in some cases, very difficult. The equilibrium means that the structure and phases of the samples are at equilibrium. Moreover, an achievement of an equilibrium state during DTA (or DSC) is, due to the principle of these methods, not possible. For this reason the temperatures are set close to equilibrium, being almost equilibrium. Possible approximations to the equilibrium state, with respect to DTA or DSC, can be found, e.g., in^{9,24,25}.

Table 2: Studied steel grades, used devices, methods and sample mass
Tabela 2: Preučevane vrste jekel, uporabljene naprave, metode in masa vzorcev

Steel grade	Chemical composition, selected elements, w/%	Device, method	Sample mass, g
A	0.6 C; 5 Cr; 2 Ni + V	SETSUS; DTA	0.2
B	0.5 C; 8 Cr; 2 Ni + V		
C	0.04 C; 3 Si		
D	0.35 C; 0.08 Si; 1.3 Mn; 0.25 Cr; 0.2 Ni	MHTC; 3D DSC	2.6
E	0.25 C; 0.25 Si; 1.4 Mn; 0.1 Cr; 0.75 Ni		

Note: The publication of the chemical compositions of the steels was limited due to the requirements of the industrial partners

This paper is devoted to determining the liquidus and solidus temperatures for the selected real-steel grades (**Table 2**).

The content of carbon was determined with the combustion-infrared detection technique (LECO devices). The contents of the other selected elements were determined with the optical emission spectrometers. The steel samples were taken from different steel semi-products, depending on the used technologies in individual steelworks. For the sake of the heterogeneity of the steel samples, they were always obtained with the internal methods used to verify the crucial mechanical and other properties of the studied steel grades. In this way the possibility of the non-standard structural and chemical heterogeneity in the taken samples was minimized. The Setaram SETSYS 18_{TM} and Setaram MHTC devices were used.

The DTA method and the S-type measuring thermocouple (Pt/PtRh 10 %) was used to obtain the temperatures of the phase transformations with the SETSYS 18_{TM} equipment for the samples of the A, B and C steel grades. The samples were analysed in alumina (Al₂O₃) crucibles with a capacity of 0.10 mL. The weight of the analysed steel samples was approximately 200 mg. The experiments were performed at a linear heating rate of 10 °C min⁻¹ and 15 °C min⁻¹ using also a reference crucible – without the standard material. A constant dynamic atmosphere – inert argon with the purity of >99.9999 % – was maintained during the measurement. Such a high-purity gas is obtained by using a gas filtering device (a Getter gas purifier).

The DSC method was used for analysing the D and E steel-grade samples. The HF 3D DSC sensor (B-type thermocouple: PtRh 6 %/PtRh 30 %) was used with the MHTC equipment. The samples were analysed in alumina crucibles (Al₂O₃) with a capacity of 0.7 mL. The weight of the analysed samples was approximately 2.6 g. A stable, dynamic atmosphere (helium, 6 N) and a linear

Table 3: Conditions and results of the thermoanalytical measurements; standard deviations and mean values of T_S and T_L

Tabela 3: Pogoji in rezultati termoanalitskih meritev, standardni odmik in glavne vrednosti T_S in T_L

Steel grade	Method	Sample mass/mg	Heating rate/ °C min ⁻¹	Determined temperature		Std. deviation		Mean value	
				T_S /°C	T_L^* /°C	T_S /°C	T_L /°C	T_S /°C	T_L /°C
A	DTA	210.1	10	1341.0	1464.4	0.6	0.6	1341	1465
		204.8	15	1340.1	1465.2				
B		190.1	10	1340.0	1458.5	2.8	1.0	1338	1458
		222.3	15	1336.0	1457.1				
C		198.3	10	1480.8	1495.5	0.3	1.3	1481	1497
		206.4		1481.1	1495.9				
	205.6	1481.0		1498.5					
	207.9	1480.5		1496.4					
D	DSC	2721.5	1	1437.7	1499.8	0.4	0.9	1437	1500
		2589.5	2	1437.2	1501.1				
E		2758.7	1	1454.2	1505.4	2.1	0.1	1456	1505
		2709.2		1457.2	1505.5				

Note: * T_L recalculated for the "zero" heating rate and "zero" mass of the sample

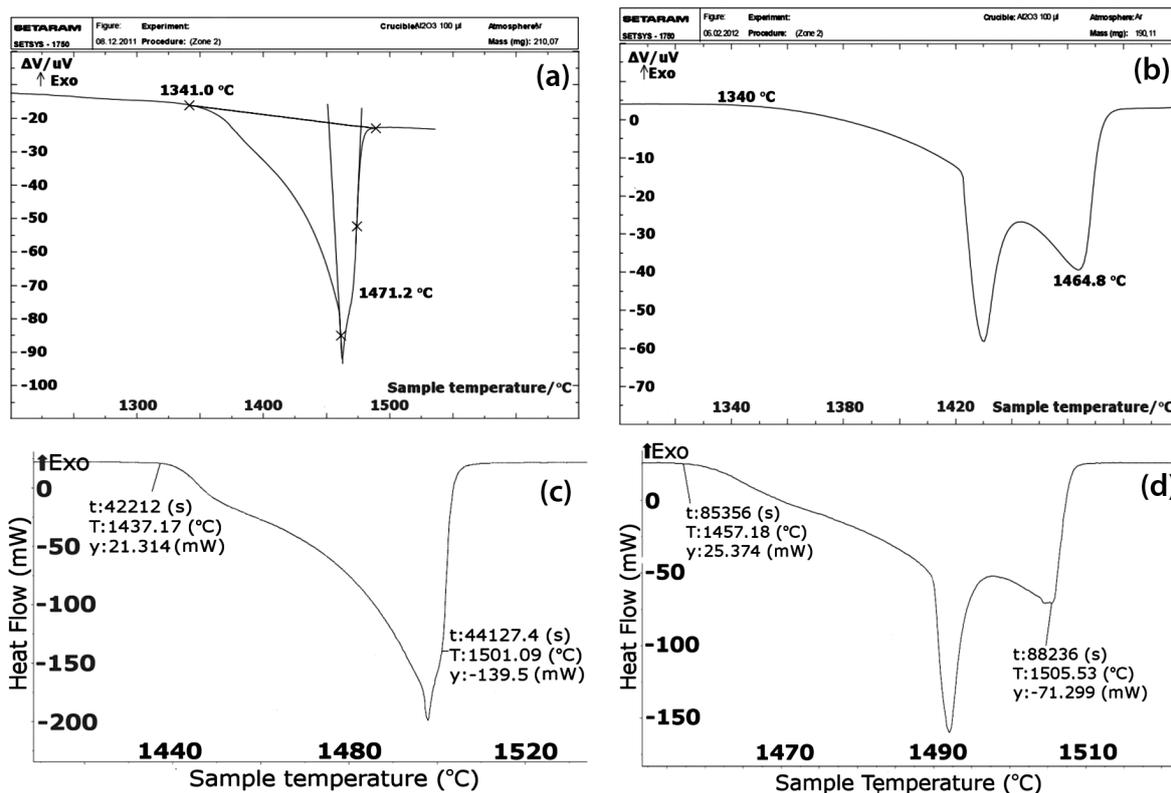


Figure 1: Examples of the selected DTA and DSC curves obtained with the measurements of the real-steel grades, liquidus and solidus temperatures: a) DTA curve, the heating rate of 10 °C min^{-1} , A steel grade, b) DTA curve, the heating rate of 10 °C min^{-1} , B steel grade, c) DSC curve, the heating rate of 2 °C min^{-1} , D steel grade, d) DSC curve, the heating rate of 1 °C min^{-1} , E steel grade

Slika 1: Primeri izbranih DTA in DSC krivulj, dobljenih med meritvami realnega jekla, likvidus in solidus temperature: a) DTA-krivulja, hitrost ogrevanja 10 °C min^{-1} , jeklo A, b) DTA-krivulja, hitrost ogrevanja 10 °C min^{-1} , jeklo B, c) DSC-krivulja, hitrost ogrevanja 2 °C min^{-1} , jeklo D, d) DSC-krivulja, hitrost ogrevanja 1 °C min^{-1} , jeklo E

heating rate of 1 °C min^{-1} and 2 °C min^{-1} were maintained during the analyses.

Each grade of steel was analysed two or four times at identical or almost identical conditions (the samples selected for DTA and the samples selected for DSC were treated separately). The final values of T_L and T_S were calculated as the mean values of the two or four experimentally obtained values (Table 3). The maximum standard deviation from the two or four measurements of the individual steel grades was 2.8 °C for T_S of the B steel grade.

The examples of the DTA and DSC curves for the studied steel grades are shown in Figure 1. The temperature of solidus was evaluated as the onset point of the first peak and the temperature of liquidus as the peak top (the last peak of the three observed peaks, e.g., 1501.09 °C for sample D – Figure 1c). Three thermal events (endothermic effects) were observed during the whole melting process, which demonstrated the melting of the steel (the melting region). The peak top, in comparison with the peak start (onset) temperature, is strongly dependent on the sample mass^{9,13–15,26} and heating rate.^{9,13–15,26} The correction with respect to the sample mass and heating rate (the experimental parameters) was undertaken.^{9,26} The temperature of liquidus was recalculated to the "zero"

heating rate and to the "zero" mass of the sample.^{13–15} The temperature calibration was also performed with the high-purity Ni and Pd (5N).

2.2 Calculation of the liquidus and solidus temperatures

The below-described equations and the Computherm software were used for calculating the liquidus (T_L) and solidus (T_S) temperatures of the above-mentioned steel grades.

The equations (1⁷, 2¹⁸, 3¹⁹, 4¹⁹, 5²⁰, 6²¹, 7²², 8¹⁹, 9¹⁹, 10²³, 11²³) are based on the effect of the contents of the selected elements (mass fraction (%)) of an element in the steel on the final liquidus/solidus temperatures. Only Computherm SW and equation (11) were used for the solidus-temperature calculations.

$$T_L = 1535 - 73(\%C) - 3(\%Mn) - 12(\%Si) - 28(\%P) - 30(\%S) - 7(\%Cu) - 1(\%Cr) - 3.5(\%Ni) - 3(\%Al) - 1(\%Sn) - 2(\%Mo) - 18(\%Ti) - 2(\%V) - 1.8(\%Co) \quad (1)$$

$$T_L = 1534 - [80(\%C) + 4(\%Mn) + 14(\%Si) + 35(\%P) + 1.4(\%Cr) + 2.6(\%Ni) - 1.2(\%Mo) + 3.4(\%Al)] \quad (2)$$

$$T_L = 1537.7 - 100.3(\%C) + 22.1(\%C)^2 - 13.55(\%Si) + 0.64(\%Si)^2 - 5.82(\%Mn) - 0.3(\%Mn)^2 - 4.18(\%Ni) -$$

$$- 0.01(\%Ni)^2 - 4.1(\%Cu) - 1.59(\%Cr) + 0.07(\%Cr)^2 - 3(\%Mo) \quad (3)$$

$$T_L = 1535.6 - 88(\%C) - 8(\%Si) - 5(\%Cu) - 1.5(\%Cr) - 4(\%Ni) - 2(\%Mo) - 18(\%Ti) \quad (4)$$

$$T_L = 1535 - 66.73(\%C) - 7.8(\%Si) - 5(\%Mn) - 30(\%P) - 25(\%S) - 5(\%Cu) - 1.5(\%Cr) - 4(\%Ni) - 2(\%V) \quad (5)$$

$$T_L = 1535 - 80(\%C) - 14(\%Si) - 4(\%Mn) - 35(\%P) - 35(\%S) - 1.4(\%Cr) - 2.6(\%Ni) - 3.4(\%Al) \quad (6)$$

$$T_L = 1539 - K(\%C) - 8(\%Si) - 5(\%Mn) - 30(\%P) - 25(\%S) - 5(\%Cu) - 1.5(\%Cr) - 4(\%Ni) - 2(\%Mo) - 2(\%V) - 1(\%W) - 14(\%As) - 10(\%Sn) - 1300(\%H) - 90(\%N) - 80(\%O) \quad (7)$$

where the *K* coefficient varies with respect to different contents of carbon:

$$C \leq 1\%; \quad K = 65$$

$$C > 1\%; \quad K = 70$$

$$C > 2\%; \quad K = 75$$

$$C > 2.5\%; \quad K = 80$$

$$T_L = 1536.6 - K(\%C) - 8.1(\%Si) - 5.05(\%Mn) - 31(\%P) - 25.5(\%S) - 1.5(\%Cr) - 4(\%Ni) - 2(\%Mo) \quad (8)$$

where the *K* coefficient varies with respect to different contents of carbon:

$$T_L = 1536 - K(\%C) - 8(\%Si) - 5(\%Mn) - 30(\%P) - 25(\%S) - 1.7(\%Al) - 5(\%Cu) - 1.5(\%Cr) - 4(\%Ni) - 2(\%V) - 1(\%W) - 1.7(\%Co) - 12.8(\%Zr) - 7(\%Nb) - 3(\%Ta) - 14(\%Ti) \quad (9)$$

where the *K* coefficient varies with respect to different contents of carbon:

$$C \leq 2\%; \quad K = 65$$

$$C \in (0.2; 0.5)\%; \quad K = 88$$

$$T_L = 1536 - 8(\%C) - 7.6(\%Si) - 3.9(\%Mn) - 33.4(\%P) - 38(\%S) - 3.7(\%Cu) - 3.1(\%Ni) - 1.3(\%Cr) - 3.6(\%Al) \quad (10)$$

$$T_L = 1536 - 251(\%C) - 12.3(\%Si) - 6.8(\%Mn) - 123.4(\%P) - 183.9(\%S) - 3.3(\%Ni) - 1.4(\%Cr) - 3.1(\%Cu) - 3.6(\%Al) \quad (11)$$

It can be seen from the equations (1–10) that there are different elements and their multiples are taken into account in individual calculations. Some equations only include the effects of certain elements; on the other hand, other equations include a higher number of the elements. This fact can, in some cases, lead to substantially different calculated values of *T_S* and *T_L*. A discussion about the limitations of the mentioned and generally used equations is out of range of this paper.

Computherm SW is able to calculate both studied temperatures. It is possible to choose two microsegregation models (Scheil or Lever). In the case of Lever, the Lever rule has been applied, corresponding to a complete mixing of the solute in the solid (i.e., a very good diffusion in the solid). On the other hand, the Scheil model corresponds to a no-diffusion model for the solid phase (both models consider a complete mixing of an infinite diffusion in the liquid). The Back-Diffusion model allows for some diffusion in the solid and corresponds thus to the situation in between the Lever rule and Scheil. When the Back-Diffusion model is used, the average cooling rate (corresponding to the representative cooling rate of the casting to be modelled) should be specified in order to determine the amount of back diffusion. For iron and carbon steel, the Lever rule is still recommended.²⁷

The Computherm Fe-rich-alloy database has defined the limitations of the chemical composition and recommended composition limits for them.²⁸ The Lever rule was selected (without the Pb, Sn, As, Zr, Bi, Ca, Sb, B, N contents) for determining *T_L* and/or *T_S* in the frame of this paper.

Table 4: Liquidus temperatures for the studied steel grades determined with the equations, Computherm and thermoanalytical methods

Tabela 4: Likvidusne temperature preučevanih jekel, določene z enačbami, s Computherm in termoanalitičnimi metodami

Method	Liquidus temperatures for steel grades, <i>T_L</i> /°C					Deviations of calculated <i>T_L</i> against <i>TA</i> results for steels/°C				
	A	B	C	D	E	A	B	C	D	E
(1)	1471	1471	1491	1499	1503	6	13	-6	-1	-2
(2)	1464	1465	1486	1495	1502	-1	7	-11	-5	-3
(3)	1461	1459	1495	1490	1495	-4	1	-2	-10	-10
(4)	1463	1465	1504	1492	1498	-2	7	7	-8	-7
(5)	1476	1476	1504	1499	1504	11	18	7	-1	-1
(6)	1465	1466	1487	1496	1502	0	8	-10	-4	-3
(7)	1479	1478	1508	1504	1508	14	20	11	4	3
(8)	1463	1465	1506	1493	1499	-2	7	9	-7	-6
(9)	1478	1477	1505	1501	1505	13	19	8	1	0
(10)	1473	1475	1509	1498	1504	8	17	12	-2	-1
SW	1467	1465	1492	1497	1503	2	7	-5	-3	-2
TA	1465*	1458*	1497*	1500**	1505**	0	0	0	0	0

Note: *DTA results; **DSC results

3 RESULTS AND DISCUSSION

Based on the above-described methods of the thermal analysis, the equations and calculations realized in Computherm SW, the liquidus temperatures for the selected, industrially produced steels were determined (**Table 4**).

It can be seen that certain variability between the obtained T_L values exists. Since the T_L values obtained with the thermal analysis (TA) – DTA/DSC measurement – were determined from the real-steel samples on the basis of the standardized methodology, it can be stated that the thermal-analysis results are the closest to the real T_L of the studied industrially produced steels. So, the thermal-analysis results are used as the core values for the next comparison.

The data based on the equations differs from the thermal-analysis results by 0 °C to 20 °C. It is not possible to identify the best equation for the T_L determination for all the analysed steel grades. The overall best agreement of the T_L calculated using equations (1–10) with the thermal-analysis results was achieved as the "zero" deviation for steel grade A if equation (6) was used. While calculating the T_L for steel grade A using equation (7), the calculated value is by 14 °C higher than the experimentally obtained T_L . However, the best agreement between the measured and the calculated results for steel grade B is reached using equation (3) – the calculated T_L is only 1 °C above the measured temperature. The overall poorest deviation for all the steels was obtained for steel grade B when comparing the value calculated with equation (7) with the TA measurements – this calculation is 20 °C above the thermal-analysis results. For the C steel grade, the T_L closest to the measurements (2 °C lower) was calculated with equation (3). The poorest value (12 °C above TA) was determined with equation (10). For the D steel, the TA measured T_L differs by 1 °C from the calculations made with the equations (1, 5 and 9). The poorest agreement between the equations and the TA results obtained with the DSC method was found for the D and E steels (this T_L is 10 °C lower than in the case of TA). The T_L value obtained with equation (9) fits the temperature found with the TA measurements.

Thus, the reason for this variability of the results can mainly be found in different contents of the alloying elements of individually studied steel grades. Moreover, the steel grades studied are such that they cannot be labelled as the common Fe-C systems.

If the Computherm calculation (SW line in **Table 4**) is compared with the thermal-analysis data, the difference in T_L is from 2 °C to 7 °C, and the mean difference value for all five steel grades is 3.8 °C. Focused on a comparison between the T_L computed with Computherm or calculated with equations (1–10) and the T_L measured with the DTA or 3D DSC methods, it can be postulated that the results achieved with Computherm are very close (unlike equations) to the thermal-analysis core measurements for the studied steel.

The solidus temperatures for the studied steel grades were obtained with only one equation (11), with the Computherm thermodynamic calculation (SW) and with the thermal-analysis methods (DTA or 3D DSC) – the results and their comparison are in **Table 5**.

Opposed to the liquidus temperatures, **Table 5** shows that there are big differences between the T_S values calculated with equation (11) or with Computherm SW, and the thermal-analysis results, ranging from 1 °C to 50 °C. The T_S determination for the B steel grade shows that the value calculated with equation (11) is 42 °C higher than the results of the TA experiments. This equation (11) was designed for the steels with low contents of alloying elements. On the other hand, the T_S obtained with this equation was only 1 °C higher for the C steel grade. The best fit of the SW prediction was obtained for the B steel grade (4 °C) and the poorest one for the C steel grade (50 °C). The reasons for such great differences can be connected with the limitations defined in the User Guide²⁶ in terms of a very specific (high) content of Si in this steel.

4 CONCLUSIONS

The aim of this paper was to present the current possibilities of determining the liquidus and solidus temperatures for the real-steel grades with a specific alloying-element content using the thermal-analysis methods, and their comparison with the calculated values obtained with the commonly used equations and the values obtained with the thermodynamic calculations performed with Computherm SW.

The thermal-analysis results were used as the core values for the comparison.

It is possible to conclude the following results:

1. The values of the liquidus (T_L) temperatures calculated with equations (1–10) differ from the experimentally obtained data by up to 20 °C.

Table 5: Solidus temperatures for the studied steel grades determined with the equations, Computherm and thermoanalytical methods

Tabela 5: Solidus temperature preučevanih jekel, določene z enačbami, s Computherm in termoanalitičnimi metodami

Method	Solidus temperatures for steel grades, $T_S/^\circ\text{C}$					Deviations of calculated T_S against TA results for steels/ $^\circ\text{C}$				
	A	B	C	D	E	A	B	C	D	E
(11)	1360	1380	1482	1425	1451	19	42	1	-12	-5
SW	1358	1342	1431	1429	1444	17	4	-50	-8	-12
TA	1341*	1338*	1481*	1437**	1456**	0	0	0	0	0

Note: *DTA results; **DSC results

2. A better conformity was observed between the experimentally obtained liquidus temperatures and the liquidus temperatures obtained with the Computherm calculations (differences between 2 to 7 °C).
3. Solidus temperatures (T_s) were also obtained on the basis of a DTA (DSC) curve evaluation. The experimental solidus temperatures differ significantly, in some cases, from the values obtained on the basis of the performed calculations; they differ by up to 50 °C from the Computherm SW results and by up to 42 °C from the calculated values, see equation (11).
4. Generally, it may be stated that the variability of the calculated values, in comparison with the thermal analysis of the real-steel samples, is due to the specific contents of the alloying elements in the studied specific steel grades.
5. The calculated values should be verified against the experimental results. The calculation equations and SWs have some limitations with respect to the composition, i.e., the composition ranges of the alloyed and admixed elements. We should not include the influence of the phases presented in the steel and the segregation of the elements. SW calculations also have limitations in the implemented calculation methods.

The best possible way of optimising the metallurgical process of steel casting is to obtain the theoretical values of the crucial parameters such as the liquidus and solidus temperatures and to verify them using experimental measurements, followed by simulations and an implementation into the real casting process.

Acknowledgements

This paper was created in the frame of the following projects:

- No. CZ.1.05/2.1.00/01.0040 "Regional Materials Science and Technology Centre" within the frame of the operation programme "Research and Development for Innovations" financed by the Structural Funds and by the state budget of the Czech Republic;
- FR-TI3/373 "Research and Development of New Subledeburitic Steels for Wood Working with Improved Performance";
- TIP programme, project No. FR-TI3/053 "Improvement of magnetic and quality properties of strips from grain oriented electrical steels";
- No. P107/11/1566 of the Czech Science Foundation;
- SGS (student's university project) project No. 2012/10.

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