DETERMINATION OF PHASE TRANSFORMATION TEMPERATURES OF 20MNCR5 STEEL USING COMPUTHERM THERMODYNAMIC DATABASE AND DESIGN OF REGRESSION EQUATIONS

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Abstract

The paper presents analysis of phase transformation temperatures of 20MnCr5 steel. For calculations of required temperatures, i.e. liquidus temperature (TL) and solidus temperature (TS) was used CompuTherm thermodynamic database. The aim of this paper was the use calculated temperatures from CompuTherm thermodynamic database to design regression equations for calculation of the phase transformation temperatures. From the results it is obvious that in the calculation of individual temperatures, the chemical composition has a significant effect on changes of the values of given temperatures. The resulting temperatures also vary depending on the used calculation method (the Lever method proved to be the most suitable). The mean value of liquidus temperature is 1,508 °C and the solidus temperature is 1,462 °C (using CompuTherm and the Lever method). The range of the two-phase zone region for the average content of elements within the limits of 20MnCr5 steel grade is thus 46 °C. Furthermore, the resulting regression equations are given in the work, determined by regression analysis of 66 possible variants of chemical composition of steel 20MnCr5 phase transformation temperatures calculated for defined chemical compositions by thermodynamic database CompuTherm. These equations can be used in operational conditions for calculations of phase transformations in the limit values of the used chemical composition of a given steel grade. When using a different range of chemical composition, these equations can be used, but without guaranteed results.

Keywords: Steel, phases, transformation, liquidus temperature, solidus temperature

1. INTRODUCTION

Knowledge of the temperatures of the phase transformations of steel is very important either in its production or heat treatment. These temperatures allow us to understand the basic properties of steel, to determine the correct casting temperature or to optimize the settings of metallurgical processes [1-3].

Steel changes its phase at different temperatures. Temperatures at which the state of steel is changed are called phase transformation temperatures. The most important temperatures of phase transformations of steels include the liquidus temperature (melting temperature) and the solidus temperature (solidification temperature). The temperature range between the liquidus and solidus temperature determines the so-called two-phase zone, where the liquid phase changes to solid. Knowledge of the range allows prediction of steel tendency to internal defects, determination of steel liquidus temperature allows correct setting of steel casting temperature [2-6].

The temperature of phase transformations is affected by the chemical composition of the steel melt. Most elements reduce these temperatures [5].

Methods of thermal analysis, dilatometry or computational methods (using empirically determined equations or software) can be used to calculate phase transformation temperatures. The results obtained after the computational determination of temperatures should be also verified by experimental methods [7,8].

2. CHARACTERISTICS OF STEEL GRADE 20MNCR5

Steel grade 20MnCr5 is a case-hardening steel with the addition of manganese and chromium, sometimes it is additionally modified by a certain addition of boron. It is well hardenable and after case hardening it achieves good wear resistance due to high surface hardness. It is used for various applications in gears in rotary machines. Typical applications are valve bodies, pumps and fittings, screws, gears, machine tool components, shafts and other mechanical controls [9,10]. The chemical composition of the steel used for the calculations is given in **Table 1**.

Table 1 Chemical composition of 20MnCr5 steel used for calculations [11]

	Chemical composition of steel 20MnCr5 (wt%)						
	C	Si	Mn	P	S	Cr	Cu
Range	0.17 – 0.22	≤ 0.40	1.10 – 1.40	≤ 0.035	≤ 0.035	1.00 – 1.30	≤ 0.40
Min.	0.17	0.00	1.10	0.000	0.000	1.00	0.00
Avg.	0.20	0.20	1.25	0.018	0.018	1.15	0.20
Max.	0.22	0.22	1.40	0.035	0.035	1.30	0.40

3. CALCULATION OF LIQUID AND SOLID TEMPERATURES USING COMPUTHERM THERMODYNAMIC DATABASE

The CompuTherm thermodynamic database (version 13.5.5), which is part of the ProCAST software (version 2018.0) available at the Department of Metallurgy and Foundry, was used to calculate the required phase transformation temperatures of 20MnCr5 steel.

This program allows you to calculate the thermophysical properties of steel after entering the chemical composition of steel and, if necessary, monitor changes in the required properties after adjusting the chemical composition. Calculable parameters include liquidus temperature, solidus, austenite decomposition temperatures, density, enthalpy, viscosity or thermal conductivity as a function of temperature. The calculation can be performed for metallic materials based on Al, Fe, Ni, Ti, Mg or Cu. For the calculation of steel is used the calculation based on Fe, where it is possible to further define the content of these elements: Al, B, C, Co, Cr, Cu, Mg, Mn, Mo, N, Nb, Ni, P, S, Si, Ti, V, W [12,13].

CompuTherm calculations are performed by three different microsegregation models Scheil, Lever and Back Diffusion. The Scheil model does not consider solid phase diffusion, while the Lever model assumes very good solid phase diffusion. Both of these models assume either complete mixing or infinite diffusion in the liquid. The Back Diffusion model is defined by the cooling rate. Using different calculation methods for the same alloy, we can get different thermophysical properties. The calculations using the Lever model assume a change in the solid phase of austenite to ferrite, the Scheil and Back Diffusion models do not predict this change, so they are not very suitable for calculating the liquidus and solidus temperatures of steel [12,13].

Figure 1 shows the interface of the software and solid phase distribution graph obtained after the calculation using the lever method.

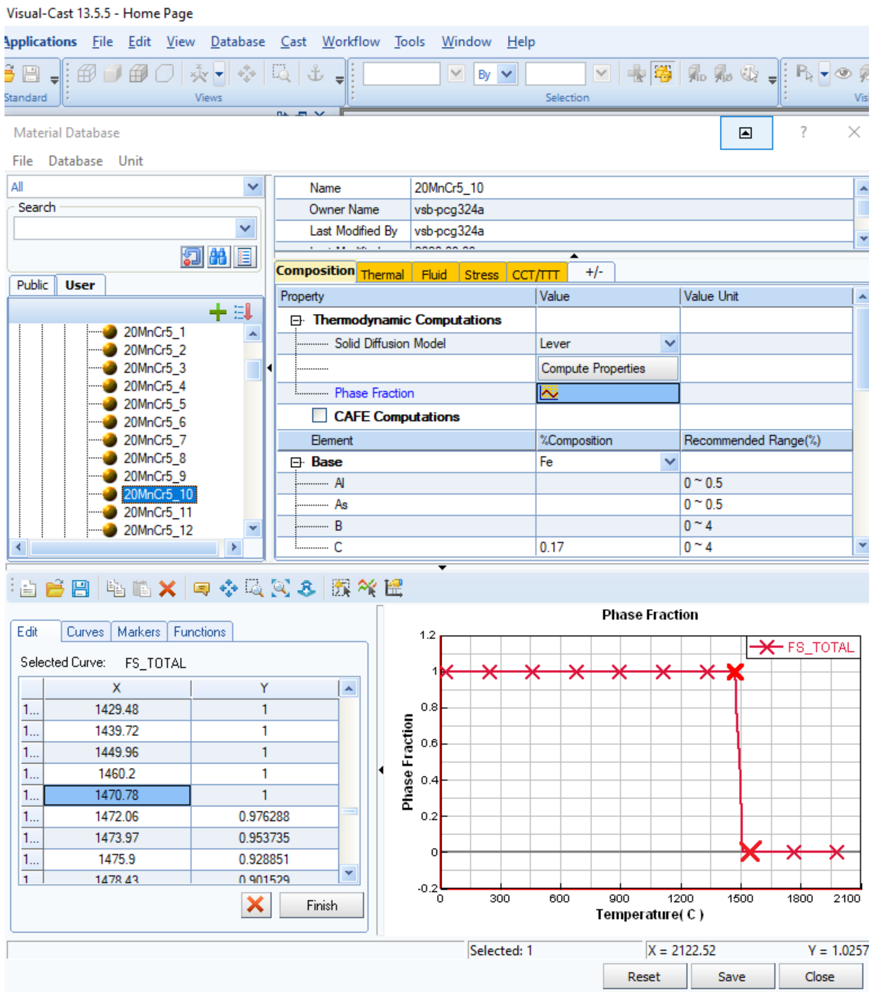

Figure 1 Interface of the CompuTherm and solid phase distribution graph [own study]

3.1. Calculation of liquidus temperatures

From **Table 2** it can be seen that the liquidus temperatures differ very little when using different models (by a maximum of 1 °C), and all three microsegregation models are therefore suitable for its calculation.

The liquidus temperature for the minimum content of elements within the limits of a given quality is about 1,517 °C, with the maximum proportion of elements for a given quality, the liquidus temperature drops to 1,500 °C. The temperature difference is therefore 17 °C.

If a given steel grade were cast by continuous casting, then the melting chemical composition would play a crucial role in selecting the casting temperature. In addition, it is appropriate that the calculations should be supplemented by experimental studies of transformations [11].

Table 2 Calculated liquidus temperatures using the CompuTherm [11]

Calculated liquidus temperature (°C)				
	TL (min. wt%)	TL (avg. wt%)	TL (max. wt%)	ΔTL (min. – max.)
Scheil	1,517	1,508	1,500	17
Lever	1,516	1,508	1,499	17
Back Diffusion	1,517	1,508	1,500	17

3.2. Calculation of solid temperatures

From **Table 3** it can be seen that the results in calculating the solid vary greatly depending on the used model. It is clear that the Scheil model is not applicable for the calculation of solidus temperatures, as evidenced by significant differences in the resulting temperatures compared to the Lever and Back Diffusion models.

The Scheil model does not consider solid state diffusion, as mentioned above. In contrast, the Lever model represents equilibrium conditions and is the most suitable for determining solidus temperatures. The Back Diffusion model requires the correct setting of the cooling rate, which plays a role especially in continuous casting of steel. Since the cooling rate on the surface of the continuously cast billet is fundamentally different from the cooling rate in the center of the preform, is usually selected a mean value. The rate at which the center of a continuously cast billet is cooled can be determined approximately for example by using numerical modeling. However, when setting up the numerical simulation, it is necessary to redefine the thermophysical properties of the steel, which may distort the result to some extent. Therefore, the Lever calculation remains primarily the most appropriate choice [11].

Under equilibrium conditions, the solidus temperature calculated using the Lever method is 1,488 (for the minimum wt% of elements), resp. 1,448 °C (for maximum wt% of elements). If we add the liquidus temperatures, which amounted to 1,516, resp. 1,499 °C, then the range of the two-phase zone can vary in the range of 28 to 51 °C.

With a larger range of the two-phase zone, there is a risk of a larger range of macrosegration and central porosity in steel semi-finished products [11].

Table 3 Calculated solidus temperatures using the CompuTherm [11]

Calculated solidus temperature (°C)				
	TS (min. wt%)	TS (avg. wt%)	TS (max. wt%)	ΔTS (min. – max.)
Scheil	1,222	1,125	1,099	123
Lever	1,488	1,462	1,448	40
Back Diffusion	1,443	1,425	1,415	28

4. DETERMINATION OF REGRESSION EQUATIONS FOR CALCULATION OF TEMPERATURES OF PHASE TRANSFORMATIONS

Resulting temperatures calculated in the CompuTherm database were used to determine the regression equations. 66 different variants of chemical composition were created for 20MnCr5 steel. This is the minimum number of combinations to include all the possibilities of the minimum, average and maximum content of individual elements in the steel and for the subsequent correct regression analysis. The Lever microsegregation model was used for the calculation.

4.1. Regression analysis

Regression analysis is one of the statistical methods. It consists in finding and examining the dependencies of variables (so-called regressors), the values of which are usually obtained during the implementation of experiments. It is used to describe and determine the dependence of the quantity Y on X, the dependence thus obtained is expressed by a regression function. To determine all regression equations, multiple regression analysis was used, which considers the dependence of a given temperature on the chemical composition. Regressors are usually multiplied by so-called regression coefficients [14,15].

The Excel spreadsheet processor, which is part of the Microsoft Office package, was used for data processing using the multiple regression analysis method.

In the regression calculations, was considered the standard significance level α = 0.05, ie. 5% unreliability of results (or 95% reliability). From the result provided by this program, was evaluated the statistical significance of the regression model as a whole, using Fisher's F-test (Significance F), there is also an important parameter Reliability value R. Furthermore, the statistical significance of individual regression coefficients is evaluated, namely using the results of the Student's t-test (t-Stat), an important parameter here is the level of significance of the t-test (P value).

With the help of the mentioned tests and when evaluating the mentioned parameters, it is possible to determine which aspects have the greatest influence on the change of temperatures and which, on the contrary, do not substantially change its value [14,15].

4.2. Liquid temperature regression equation

The chemical composition has a statistically significant effect on the liquidus temperature of 20MnCr5 steel from 99.3 % and from 0.97 % other influences affect the liquidus temperature. The regression coefficients of all elements acquire lower values in the level of significance of the t-test (P value) than the selected level of significance α, therefore they have a statistically significant effect on the liquidus temperature. In this case, silicon has the greatest influence on the liquidus temperature. The obtained equation (1) has the following form:

$$TL = 1537.4 - 16.4 \cdot (\%\ Si) - 82.8 \cdot (\%\ C) - 5.1 \cdot (\%\ Mn) - 3.7 \cdot (\%\ Cu) - 40.5 \cdot (\%\ S) - 31.5 \cdot (\%\ P) - 1.4 \cdot (\%\ Cr) \quad (1)$$

4.3. Solid temperature regression equation

The chemical composition has a statistically significant effect on the solidus temperature of 20MnCr5 steel from 89.7 % and from 10.3 % the solidus temperature is influenced by other influences. The higher percentage of influence of other aspects at the solidus temperature is due to the reactions taking place in the two-phase zone. The regression coefficients of the elements Si, S, C, P, and Cu acquire lower values in the significance level of the t-test (P value) than the selected significance level α, therefore they have a statistically significant influence on the solidus temperature. The coefficients of the elements Cr and Mn do not meet this condition, and therefore their effect on the solidus temperature will not be significant. The obtained equation (2) has the following form:

$$TS = 1515.9 - 29.3 \cdot (\%\ Si) - 316.2 \cdot (\%\ S) - 158 \cdot (\%\ C) - 193.3 \cdot (\%\ P) - 7.6 \cdot (\%\ Cu) - 1\ .7 \cdot (\%\ Cr) - 1.1 \cdot (\%\ Mn) \quad (2)$$

5. CONCLUSION

Paper was devoted to calculations of phase transformation temperatures of steel and the determination of regression equations for their calculation. Temperatures are determined using the CompuTherm thermodynamic database. From the above results it is clear that in the calculation of individual temperatures, the chemical composition has a significant effect on changes in the values of given temperatures. The resulting temperatures also vary depending on the calculation method used (the Lever method proved to be the most suitable).

The average liquidus temperature is 1,508 °C and the solidus temperature is 1,462 °C (using CompuTherm and the Lever method). The width of the two-phase zone for the average content of elements within the limits of quality 20MnCr5 is thus 46 °C.

Regression equations stated in the work (1 - 2) are determined by regression analysis of 66 possible variants of chemical composition of steel 20MnCr5 and phase transformation temperatures determined for defined chemical compositions by thermodynamic database CompuTherm. These equations can be used in operational practice for calculations of phase transformations for steel grades similar to 20MnCr5.

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