USE OF THE THERMODYNAMIC DATABASE COMPUTHERM TO CONSTRUCT A REGRESSION EQUATION TO DETERMINE THE LIQUIDUS TEMPERATURE OF 41CR4 STEEL

[1]Lucie CHUDOBOVÁ, [1]Josef WALEK, [1]Michal SNIEGOŇ, [1]Jiří CUPEK, [1]Karel MICHALEK, [2]Mariola SATERNUS

[1]VSB - Technical University of Ostrava, Ostrava, Czech Republic, EU, lucie.chudobova@vsb.cz, josef.walek@vsb.cz, michal.sniegon@vsb.cz, jiri.cupek@vsb.cz, karel.michalek@vsb.cz

[2]Politechnika Śląska, Katowice, Poland, EU, Mariola.Saternus@polsl.pl

https://doi.org/10.37904/metal.2022.4449

Abstract

The subject of this paper is the analysis of phase transformation temperatures, specifically liquidus temperature (TL) for steel quality 41Cr4. To calculate the temperatures, 66 different variants of the chemical composition of a given steel grade were compiled. The calculations were performed in the CompuTherm thermodynamic database using the Lever microsegregation model. The resulting temperatures are further supplemented by multiple regression analysis, which considers the dependence on the chemical temperature. The results of the regression analysis are used to design a regression equation to calculate the liquidus temperature. It is clear from the obtained results that the chemical composition of the steel has a significant temperature effect on the change in the calculated values.

Keywords: Steel, phase, transformation, temperature, liquidus

1. INTRODUCTION

Steel changes its phase at different temperatures. The temperatures at which the state changes are referred to as the so-called phase transformation temperatures. The liquidus temperature (or melting point) is one of the most important phase transformation temperatures of steels. Its knowledge, in combination with the solidus temperature, enables the prediction of the tendency of the steel to internal defects, and enables the determination of the liquidus temperature of the steel by the correct setting of the steel casting temperature. These data are also used to set up numerical models that we model within the department. This knowledge allows us to optimize the setting of metallurgical processes and thus increase the quality of the steel produced, which is very important with the ever-increasing demands on steel quality [1-3].

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

Thermal analysis, dilatometry, or computational methods (using empirically determined equations or software) can be used to determine phase transformation temperatures. The results obtained after the computational determination of the phase transformation temperatures of the steel should also be verified by experimental methods [4]. The aim of this article will be to establish an empirical equation for calculating the liquidus temperature of 41Cr4 steel grade.

2. CHARACTERISTICS OF STEEL GRADE 41CR4

41Cr4 steel is a chrome manganese steel used in the manufacture of quenched and tempered bars. It is also suitable for induction hardening with a minimum hardness of 52HRC [5].

The cold-upsettable steel 41Cr4 can be cold-formed with suitable tools with a low to medium rate of forming according to the usual forming methods on single-stage and multi-stage presses. It is used for normed screws, driving elements as crankshafts, front vehicle axles, axle journals or steering components. Also used for high-strength parts manufactured according to drawings (eg. ball studs) [5,6]. The chemical composition of the steel used for the calculations is given in **Table 1**.

Table 1 Chemical composition of 41Cr4 steel used for calculations [5,6]

	Chemical composition of steel 41Cr4 (wt%)					
	C	**Si**	**Mn**	**P**	**S**	**Cr**
Range	0.380 – 0.450	≤ 0.40	0.60 – 0.90	≤ 0.025	≤ 0.035	0.90 – 1.20
Min.	0.380	0.00	0.60	0.000	0.000	0.90
Avg.	0.415	0.20	0.75	0.013	0.018	1.05
Max.	0.450	0.40	0.90	0.025	0.035	1.20

3. CALCULATION OF LIQUID TEMPERATURE USING EMPIRICAL EQUATIONS

Empirical equations are usually derived by regression analysis from laboratory measured data for a specific type of steel. Therefore, the equation determined in this way gives good results only for the studied steel. If the chemical composition of the steel changes, the regression equation may not provide a reliable calculation of the liquidus temperature in the required accuracy. Another problem may be the simple form of the equations, which are often linear composition functions, and thus applicable only to alloys with less diverse chemical compositions [7].

There are many empirical equations for calculating liquidus temperatures (from several different authors). The equations used for our calculations are given in [8] and **Table 2** shows the specified liquidus temperatures using these empirical equations.

Table 2 Calculated liquidus temperatures using empirical equations [own study]

Calculated liquidus temperatures for 41Cr4 steel (°C)				
Empirical equations	**T_L (min. wt%)**	**T_L (avg. wt%)**	**T_L (max. wt%)**	**ΔT_L (min. wt%) – (max. wt%)**
T. Myslivec	1,505	1,498	1,492	13
L. Šmrha	1,500	1,492	1,485	15
CLESIM	1,498	1,491	1,484	13
TECTIP	1,498	1,492	1,487	11
W. Dubovick	1,505	1,500	1,494	11
J. P. Aymard	1,501	1,493	1,486	15
W. Roeser	1,510	1,504	1,499	11
Vest Alpine	1,499	1,492	1,486	13
VSŽ Košice	1,498	1,492	1,485	13

From the results given in **Table 2**, the chemical composition of the steel has a significant effect on the liquidus temperature of the 41Cr4 steel. The difference between this temperature at the minimum and maximum content of the elements (see contents in Table 1) can in our case be up to 15 °C (in the case of calculation using the equation of J. P. Aymard).

There is also a difference between the calculated liquidus temperatures based on the empirical equation used, which can reach up to 14 °C (in the case of the maximum possible chemical composition). These differences are since each of the authors considers the influence of other elements in its equation and uses their various multiples. Therefore, for more accurate determination of liquidus temperatures for use in practice, it is recommended to verify these values using the available thermodynamic database and experimental measurements.

4. CALCULATION OF LIQUID TEMPERETURES USING COMPUTHERM THERMODYNAMIC DATABASE

The CompuTherm thermodynamic database (version 14.5), which is part of the ProCAST software (version 2019.0) available at the Department of Metallurgical Technologies, was used to calculate the required phase transformation temperatures of 41Cr4 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. For the calculation of steel, a calculation based on Fe is used, 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 [9].

CompuTherm calculations are performed by three different microsegregation models Scheil, Lever and Back Diffusion. The Scheil model does not consider solid state diffusion, while the Lever model assumes very good solid-state diffusion. Both models assume either complete mixing or infinite diffusion in the liquid. The Back Diffusion model is defined by the cooling rate. In the calculations using the Lever model, the change of the solid phase of austenite to ferrite is assumed [9]. Cooling rate 1 (K/sec) was used for the calculation using model Back Diffusion. The calculated temperatures with all models are given in **Table 3**.

Table 3 Calculated liquidus temperatures using the CompuTherm database [own study]

Calculated liquidus temperatures for 41Cr4 steel (°C)				
CompuTherm	**T_L (min. wt%)**	**T_L (avg. wt%)**	**T_L (max. wt%)**	**ΔT_L (min. wt%) – (max. wt%)**
Scheil	1,502	1,493	1,484	18
Lever	1,501	1,492	1,484	17
Back Diffusion (1K/sec)	1,501	1,492	1,484	17

From **Table 3** as can be seen, liquidus temperatures differ very little when using different models (maximum 1 °C), and all three microsegregation models are therefore suitable for its calculation. The liquidus temperature for the minimum content of elements within the given quality is about 1,501 °C, with the maximum proportion of elements for a given quality, the liquidus temperature drops to 1,484 °C.

5. DETERMINATION OF THE REGRESSION EQUATION FOR LIQUID TEMPERATURE CALCULATION

Calculations in the CompuTherm database were used to determine the regression equations. When 66 different variants of chemical composition were created for 41Cr4 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.

Regression analysis is one of the statistical methods. It consists in finding the dependencies of variables whose dependence expresses regression functions. To determine all regression equations, a multiple regression analysis was performed in an Excel spreadsheet, which considers the dependence of a given temperature on the chemical composition. The result of the regression analysis is a description of the dependence of the variables using a suitable mathematical model [10].

When calculating regression, we consider the standard significance level α = 0.05, ie. 5% unreliability of results (or 95% reliability). From the results obtained by the analysis, we then evaluate the statistical significance of the regression model. With the help of tests and the evaluation of parameters, it is possible to determine which aspects have the greatest influence on the change in temperature and which, on the contrary, do not substantially change its value.

Table 4 shows the results of regression statistics. **Table 5** shows the analysis of variance and in **Table 6** regression results are recorded (already arranged - according to the t Stat value).

Table 4 Results of regression statistics [own study]

Regression Statistics	
Multiple R	0.996952454
R Square	0.993914195
Adjusted R Square	0.993295299
Standard Error	0.33125827
Observations	66

Table 5 Analysis of variance [own study]

ANOVA					
	df	***SS***	***MS***	***F***	***Significance F***
Regression	6	1,057.343991	176.2239986	1,605.948421	2.05985E-63
Rezidual	59	6.474190439	0.109732041		
Total	65	1,063.818182			

Table 6 Ordered regression results [own study]

	Coefficients	***Std Error***	***t Stat***	***P-values***
Constant	1,537.194895	0.956712836	1,606.746389	1.2695E-138
Si	-16.99481253	0.254739804	-66.71439747	2.88339E-57
C	-84.13941014	1.622285348	-51.86474146	6.36701E-51
Mn	-4.95596681	0.398526528	-12.43572626	3.94672E-18
S	-40.59794834	3.300283394	-12.30135218	6.28621E-18
P	-34.77403218	4.342598192	-8.007655934	5.31109E-11
Cr	-1.593962672	0.402908924	-3.956136428	0.000206931

First, the statistical significance of the regression model will be evaluated. The achieved F-test significance level (Significance F) becomes 2.05985E-63, which is a much lower value than the selected significance level α. From this it can be said that the chemical composition has a significant overall effect on the liquidus temperature, which is characterized by the value R Square (0.994). According to this value, it can be said that the total influence of all elements on the liquidus temperature is 99.4%. The remaining less than one percent (0.6%) expresses the influence of other aspects, which are not the subject of this work.

Furthermore, the statistical significance of individual regression coefficients will be evaluated. The regression coefficients of all elements acquire lower values in the level of significance of the t test (P-values) than the selected level of significance α, therefore they have a statistically significant effect on the liquidus temperature.

The influence of statistically significant elements on the liquidus temperature decreases according to the t Stat column, ie. In this case, silicon has the highest effect on the liquidus temperature of the selected chemical composition of the steel and the method of determining the temperature using the CompuTherm thermodynamic database. The regression coefficients of the elements have negative signs, which means that the liquidus temperature decreases with increasing content of the given element.

The resulting regression equation for calculating the liquidus temperature of 41Cr4 steel has the following form:

$$TL = 1{,}537.2 - 17.0 \cdot (\%\ Si) - 84.1 \cdot (\%\ C) - 5.0 \cdot (\%\ Mn) - 40.6 \cdot (\%\ S) - 34.8 \cdot (\%\ P) - 1.6 \cdot (\%\ Cr) \qquad (1)$$

where:

TL – liquidus temperature (°C)

% X – content of element in steel (wt. %)

The calculated liquidus temperatures for the minimum, average and maximum representation of elements in the chemical composition of a given steel grade are given in **Table 7**.

Table 7 Calculated liquidus temperatures using equations, CompuTherm and equation (1) [own study]

Liquidus temperatures for 41Cr4 steel (°C)			
	T_L (min. wt%)	**T_L (avg. wt%)**	**T_L (max. wt%)**
Empirical equations (Avg.)	1,501	1,495	1,489
CompuTherm (Lever)	1,501	1,492	1,484
Regression equation (1)	1,501	1,492	1,484

6. CONCLUSIONS

The liquidus temperature, when calculated with the help of empirical equations, for the minimum content of elements within the given quality is about 1,501 °C, with the maximum representation of elements for a given quality, the liquidus temperature drops to about 1,489 °C. When using the CompuTherm thermodynamic database, the liquidus temperature is 1,501 °C, resp. 1,484 °C. When calculating the liquidus temperature with our regression equation (1), its values did not differ from the calculated temperatures, so this equation is suitable for the calculation of phase transformation temperatures for this steel grade.

If a given steel grade were to be cast in a continuous manner, then the melting chemical composition would play a crucial role in choosing the casting temperature. Furthermore, based on the results obtained, it should be noted that if we do not have a thermodynamic database and use empirical equations available in the literature to determine liquidus temperatures, then it is appropriate to have more equations and evaluate the results both in terms of elements in the equations and the grades of steel for which the empirical equations were compiled. In the case of calculation for this quality, the average value of liquidus temperatures is almost equal to the values obtained by thermodynamic calculation, but in the case of another quality, averaging may not be appropriate. Especially if we consider that in the calculation using empirical equations, the difference in liquidus temperature between the equations was up to 14 °C. For this reason, it is appropriate that the calculations be best supplemented by experimental studies of phase transformation temperatures.

Measurements on real steel samples can reveal material heterogeneity, and thus the effect of chemical composition or heating/cooling conditions on the actual liquidus temperature.

ACKNOWLEDGEMENTS

The work was supported by the project "Doctoral grant competition VŠB-TUO" number CZ.02.2.69/0.0/0.0/19_073/0016945 Ministry of Education, Youth and Sports of the Czech Republic entitled "Optimization of metallurgical processes using numerical simulations, laboratory melting and dilatometry" - DGS/TEAM/2021-002. The work was also created with the support of the project "Support for Science and Research in the Moravian-Silesian Region 2021 - RRC/10/2021" and with the financial support of projects "Student Grant Competitions" numbers SP2022/15 and SP2022/68. Furthermore, the work was created thanks to the project CZ.02.1.01/0.0/0.0/17_049/0008399 from EU and Czech financial funds provided by the Operational Program Research, Development and Education, Calls 02_17_049 Long-term cross-sectoral cooperation for ITI, managing authority: Czech Republic - Ministry of Education, Youth and Sports" and thanks to the project number CZ.02.2.69/0.0/0.0/16_018/0002706 - Strategic development of doctoral studying programmes at FMT VSB-TUO.

REFERENCES

[1] MANDAL, S. K. *Steel metallurgy: Properties, Specifications, and Applications*. USA, McGraw-Hill Education (India) Private Limited, 2015, 343 p. ISBN 978-0-07-184461-1.

[2] KAWULOKOVÁ, M., SMETANA, B., ZLÁ, M., KALUP, A., MAZANCOVÁ, E., VÁŇOVÁ, P., KAWULOK, P., DOBROVSKÁ, J., ROSYPALOVÁ, S. Study of equilibrium and nonequilibrium phase transformations temperatures of steel by thermal analysis methods. *Journal of Thermal Analysis and Calorimetry* [online]. 2017, vol. 127, no. 1. p. 423-429. [viewed: 2022-04-26]. Avalible from: http://doi.org/10.1007/s10973-016-5780-4. ISSN 1588-2926.

[3] TKADLEČKOVÁ, M., VÁLEK, L., SOCHA, L., SATERNUS, M., PIEPRZYCA, J., MERDER, T., MICHALEK, K., KOVÁČ, M. Study of solidification of continuously cast steel round billets using numerical modeling. *Archives of Metallurgy and Materials*. 2016, vol. 61, no. 1, p. 221-226. ISSN 1733-3490.

[4] BACHNIAK, D., RAUCH, L., PIETRZYK, M., KUSIAK, J. Selection of the optimization method for identification of phase transformation models for steels. *Materials & Manufacturing Processes* [online]. 2017, vol. 32, no. 11, p. 1248-1259. [viewed: 2022-04-26], Avalible from: http://dx.doi.org/10.1080/10426914.2017.1292035. ISSN 1042-6914.

[5] 41Cr4 Steel Grade. *Ambhe.com.* [online] [viewed: 2022-04-26]. Avalible from: https://ambhe.com/41cr4-steel/.

[6] 41Cr4 (1.7035). *European steel and alloy grades/numbers - SteelNumber*. [online] [viewed: 2022-04-26]. Avalible from: http://www.steelnumber.com/en/steel_composition_eu.php?name_id=331.

[7] MARTINÍK, O., SMETANA, B., DOBROVSKÁ, J., ZLÁ, S., KAWULOKOVÁ, M., GRYC, K., DROZDOVÁ, L., DOSTÁL, P., MARTINÍKOVÁ, P. Experimental and Theoretical Assessment of Liquidus, Peritectic Transformation, and Solidus Temperatures of Laboratory and Commercial Steel Grades. *Journal of Phase Equilibria and Diffusion.* [online]. 2019, vol. 40, no. 1, p. 93-103. [viewed: 2022-04-28]. Avalible from: https://doi.org/10.1007/s11669-019-00707-1. ISSN 1547-7037.

[8] CHUDOBOVÁ, Lucie. *Stanovení teplot fázových transformací oceli*. Ostrava, 2020. Diplomová práce (Ing.). VŠB-TU Ostrava, Fakulta materiálově-technologická, Katedra metalurgie a slévárenství, 2020-06-30.

[9] ProCAST 2019, User´s manual. ESI Group.

[10] Úvod do regresní analýzy. *StatSoft.cz* [online] [viewed: 2022-04-28]. Avalible from: http://www.statsoft.cz/file1/PDF/newsletter/2014_26_03_StatSoft_Uvod_do_regresni_analyzy.pdf.