ON THE RELEVANCE OF MICROSEGREGATION MODELS FOR PROCESS CONTROL IN CONTINUOUS CASTING OF STEEL

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Abstract

Microsegregation in general is the consequence of the different solubility of alloying and residual elements in liquid and solid steel. The result is an enrichment of segregating elements between the dendrites due to incomplete diffusion equalization. This enrichment favours the precipitation of inclusions (e.g. MnS) during solidification as well as the formation of hot tear segregations (HTS) along primary grain boundaries. Hence, the modelling of microsegregation phenomena is an important task in order to predict the final product quality and to optimize the process parameters in continuous casting of steel.

A microsegregation model based on the analytical solution proposed by Ohnaka was implemented in an in-house 1D-FV solidification simulation software. Considering equilibrium partition coefficients from FactSage (FSStel2015) non-equilibrium solidus temperatures of various steel grades were calculated. These results show very good correspondence with values determined from an in-situ hot tensile on solidifying steel. Finally, the results were applied to calculate solidification in a continuous slab casting machine and to analyse the strain in the mushy zone subsequently. For selected steel grades the probability of HTS formation was predicted and the influence of operating parameters was quantified.

Keywords: solidification, microsegregation, continuous casting, hot tearing

1. INTRODUCTION

Elements generally show a different solubility in solid and liquid steel. In contrast to the thermodynamic equilibrium, the complete diffusion equalization of elements inside the solidifying microstructure is limited under continuous casting conditions. The consequence is an enrichment of alloying elements and tramp elements in the interdendritic melt. This phenomenon, known as microsegregation, has a decisive influence on the process quality and subsequently on the final product properties: The enrichment favours the formation of hot tear segregations (HTS) along primary grain boundaries as well as precipitation of inclusions during solidification. Further, the segregation on microscopic scale could lead to a macroscopic inhomogeneity in the center of the strand.

In the present work a microsegregation model based on Ohnaka's analytical solution [1] was implemented in an in-house 1D-FV solidification simulation software using input parameters from literature and FactSage (FSStel2015). Further, an evaluation of liquidus formulas by the comparison with results from Differential Scanning Calorimetry (DSC) measurements for a wide range of steel compositions was performed. A published formula could be slightly modified and improved. Calculated solidus temperatures are in good agreement with values determined from an in-situ hot tensile test on solidifying steel. Finally, the model was used for the solidification simulation and the prediction of hot tear formation in a continuous slab caster. Considering different steel compositions and secondary cooling strategies, the relevance of microsegregation modelling regarding quality control in the continuous casting process is shown.

2. MICROSEGREGATION MODELLING

2.1 Model description

Ohnaka [1] presented an analytical model of microsegregation during solidification based on the assumption of a quadratic solute distribution profile in the solid. The solution of the model is given in **equation 1**.

$$\frac{dc_l}{c_l} = \frac{(1-k)df_s}{1-\left(1-\frac{\beta k}{1+\beta}\right)fs} \tag{1}$$

c_l is the solute concentration in the liquid, f_s is the fraction of solid, dc_l ist the change of the solute concentration in the liquid corresponding to an increase of the solid fraction df_s and k is the equilibrium distribution coefficient. The backdiffusion parameter β depends on the dendrite geometry and the dimensionless Fourier-Number α (β=2α for the plate-like model and β=4α for the columnar model). In solidification processes α is generally defined by **equation 2**, where D_s is the diffusion coefficient of elements in the solid steel, t_f is the local solidification time and λ_2 is the secondary dendrite arme spacing (SDAS).

$$\alpha = \frac{4D_s t_f}{\lambda_2^2} \tag{2}$$

Setting Γ=1-βk/(1+βk) and assuming that the backdiffusion parameter is constant within an increase of solid fraction by Δf_s, integration of **equation 1** from f_s to $f_s+\Delta f_s$ results in the semi-integrated **equation 3** according to You et al. [2]. In the present work the semi-integrated form with a columnar dendrite structure (β=4α) is applied for the microsegregation calculation.

$$c_l^{f_s+\Delta f_s} = c_l^{f_s}\left[\frac{1-\Gamma f_s}{1-\Gamma\left(f_s+\Delta f_s\right)}\right]^{\frac{1-k}{\Gamma}} \tag{3}$$

2.2 Input parameters

The temperature dependence of solute diffusion coefficients follows an Arrhenius approach (**equation 4**), where the gas constant R is 8.314 J / (mol·K) and T is the temperature in Kelvin. The used values for the activation energy Q and D_0 are listed in **Table 1**.

$$D_s = D_0 e^{-\frac{Q}{RT}} \tag{4}$$

Table 1: Diffusion coefficients of solutes in ferrite (δ) and austenite (γ) [3,4]

		C	Si	Mn	P	S	Al	Cr	Ni	Mo	Cu
δ	D_0 [cm^2/s]	0.0127	8.0	0.76	2.9	4.56	5.9	2.4	1.6	3.47	2.6
	Q [10^3 J/mol]	81.4	248.9	224.4	230.1	214.6	241.2	239.8	240	241.4	240
γ	D_0 [cm^2/s]	0.0761	0.30	0.055	0.01	2.4	5.1	0.0012	0.34	0.068	0.7
	Q [10^3 J/mol]	134.4	251.2	249.1	182.7	212.2	245.8	219	282.4	246.9	286

Equilibrium partition coefficients are taken from FactSage (FSStel2015). SDAS is computed as a function of local solidification time and carbon content as proposed by Pierer and Bernhard [5]. Further it was assumed, that if the enrichment of manganese and sulpher exceed the solubility product of manganese sulphid [6], precipitation takes place until the equilibrium concentrations are reached.

2.3 Evaluation of empirical equations for the estimation of liquidus temperatures

Numerous equations for the estimation of liquidus temperatures have been published in the past [7-11]. In general these empirical equations are based on regression analysis from thermal analysis measurements or thermodynamic calculations. With respect to microsegregation modelling, regression formulas are useful for a simple prediction of the current interdendritic temperature and the solidus temperature, respectively. Therefore, selected equations were evaluated with more than 300 Difference Scanning Calorimetry (DSC) measurements [12]. The results for a wide range of steel grades are shown in **Figure 1 (a) and (b)**. The formula according to Kawawa already differs at high temperatures from the experimental results and shows the highest deviation of 7.53 ± 9.20 °C, followed by Kagawa-Okamoto (K-O) equation with an average error of 5.77 ± 6.57 °C. The Howe and Schürmann-Stisovic (S-S) formulas show approximately the same accuracy. However, best correlation between experimental data and calculated temperatures was found for the Howe and Miettinen (H-M) regression polynoms with a deviation of 2.97 ± 3.48 °C. Based on the experimental data, an increase of the liquidus temperature by 2 °C / wt% was observed for aluminum contents up to 3 wt%. Considering this coefficient in the H-M equations, a further improvement could be achieved as the error decreases to 2.61 ± 2.32 °C. Since the optimized expression enables the precise determination of liquidus temperatures even at high amounts of alloying elements, it is particularly suitable for the application in the model.

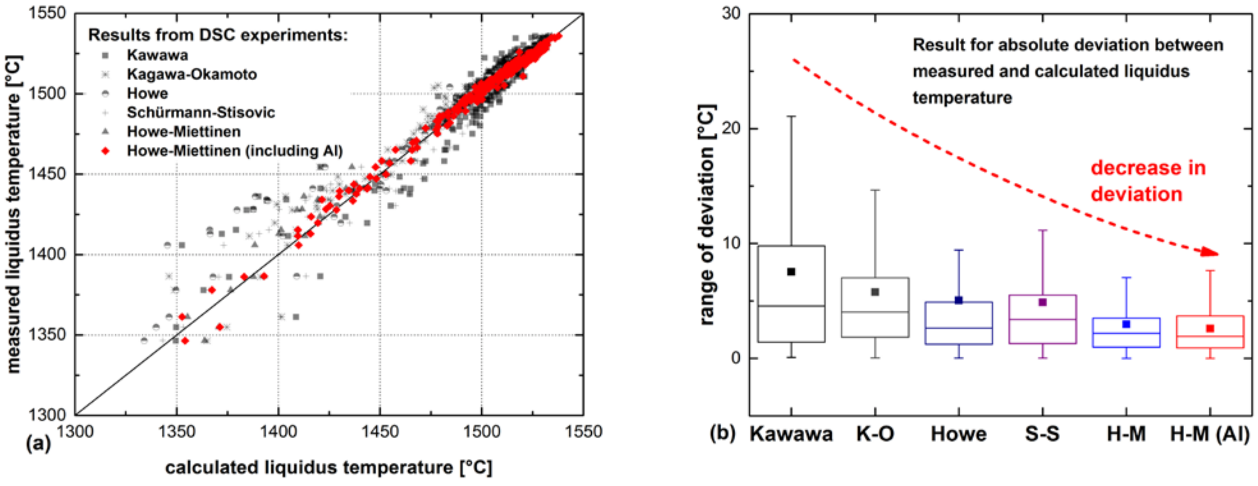

Figure 1: Comparison between measured liquidus temperatures by means of DSC measurements and using empirical equations (a) and resulting absolute deviation for selected equations (b)

3. VERIFICATION OF THE MICROSEGREGATION MODEL

At the Chair of Ferrous Metallurgy the hot tearing sensitivity of different steel grades can be investigated by the Submerged Split Chill Tensile (SSCT) -Test. The schematic representation of the SSCT-Test is shown in **Figure 2**. Within the experiment a cylindrical test body is submerged into a superheated melt. Simultaneously a thin shell solidifies on the surface of the test body and after a predefined holding time an in-situ tensile test starts during solidification. If the initiated strain exceeds a critical value, hot tears can be found in the following metallographic examination. The measured shell thickness and the detected position and number of hot tears can be used for the correlation with the numerical simulation. Finally, the evaluation of the calculated solidus temperature under non-equilibrium conditions and the prediction of critical strains for hot tear formation are possible. A detailed description of the experimental procedure and the numerical simulation of the SSCT test can be found elsewhere [13].

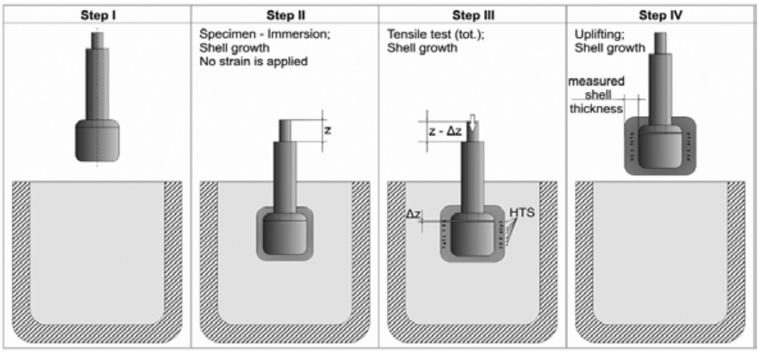

Figure 2: Schematic representation of the SSCT-Test at the Chair of Ferrous Metallurgy [14]

In a first step the present "stand-alone" microsegregation model was compared with an already evaluated model from You et al. [2] which is fully coupled with the thermodynamic database FSStel2015. On the example of medium carbon steel with an increased phosphorus content of 500ppm and assuming a cooling rate of 10 K/s, the calculated temperatures and concentrations in **Figure 3 (a)** show very good agreement. Since both models are based on Ohnaka's assumptions and use nearly the same input parameters, the high correspondence indicates, that the algorithm was properly implemented.

Subsequently, an in-house 1D-FV solidification software involving the microsegregation model was used to analyze more than 70 already available results from SSCT-Tests on Low Carbon (LC) und Medium Carbon (MC) steels. In **Figure 3 (b)** the experimental values are plotted against the calculated solidus temperatures. Although the deviation in case of MC steels (± 10 °C) is slightly higher than for LC steels (± 5 °C), the obtained results are highly satisfying and confirm the present method of microsegregation modelling.

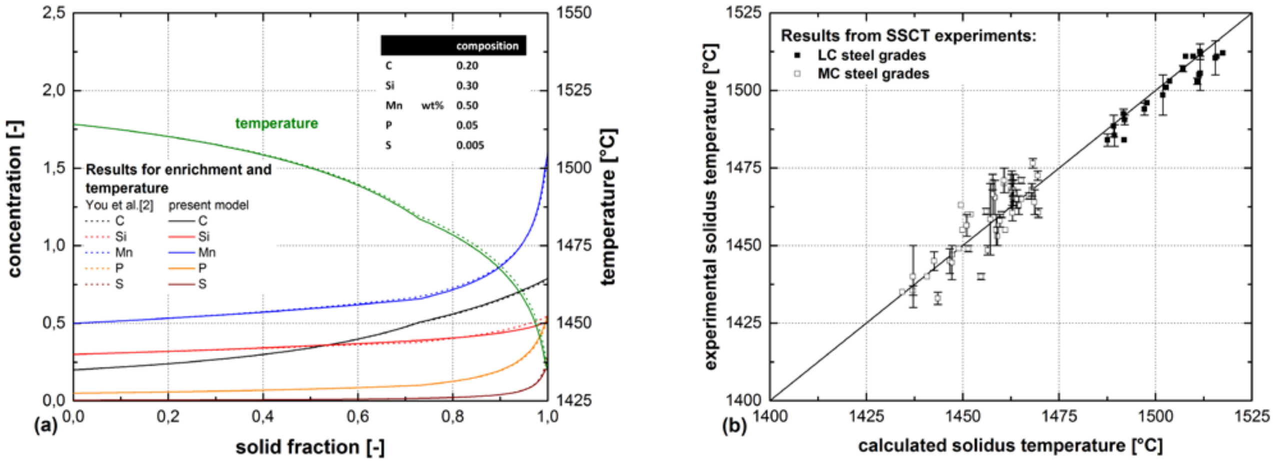

Figure 3: Comparison of the present „stand-alone" microsegregation model and a model which is fully coupled with the database FSStel2015 (a) and the correlation with results of SSCT-Tests (b)

4. SOLIDIFICATION SIMULATION OF A CONTINUOUS SLAB CASTER

The 1D-FV software was applied for the solidification simulation and strain analysis in a 250mm continuous slab caster considering a casting speed of 1.2 m/min. Thermal boundary conditions and casting machine configuration are taken from the previous work by Arth et al. [14].

In continuous casting of slabs the internal quality regarding macrosegregation is mainly improved by the installation of a softreduction close to end of the solidification. Practically, the final solidification point is determined by the numerical simulation of the process. The precision of the simulation may decide, if the softreduction is successful or not. In order to demonstrate the relevance of microsegregation modelling for the positioning of the softreduction, the calculated final solidification point is compared with the results obtained under assumption of equilibrium conditions (=Lever-rule). **Figure 4 (a)** shows the calculated metallurgical length for a Low Carbon (LC) and a Medium Carbon (MC) steel grade. Due to the low amount of alloying elements in the LC steel, the difference in the predicted final solidification point Δl_{MET} is negligible. Higher amounts of strongly segregating elements like carbon, phosphorus and sulphur raise Δl_{MET} significantly up to 0.2 m. Further, the influence of segregating elements on the difference in the metallurgical length is enhanced by the defined cooling program, as can been seen in **Figure 4 (b)**. Maximum values of Δl_{MET} are observed for slow cooling rates (= soft cooling strategy) and high carbon contents. The positioning of the softreduction according to the equilibrium conditions will miss the real final solidification point by 0.5 m. Deviation on this scale may lead to a downgrade of the slab, or in the worst case to a rejection.

In the second part, the microsegregation model was used for strain analysis in the casting machine with respect to the formation of hot tear segregations (HTS). In **Figure 4 (c)**, the occurring strain ε due to bending, straightening, bulging and reheating (= accumulated strain) is compared with the critical strain measured by the SSCT-Test. Intensive cooling results in low values of the predicted strain whereas the soft cooling favours the strain accumulation during the process. However, under the assumption of 100 % maintenance of the casting plant, the calculated strain in this case never exceeds the critical value. In **Figure 4 (d)** it can be seen, that microsegregation has decisive influence on the accumulated strain: Even at low carbon contents (0.1 wt%) the calculated strain is nearly doubled compared to equilibrium conditions. Hence, the microsegregation phenomenon has to be considered to adjust the casting parameters and to prevent hot tear formation.

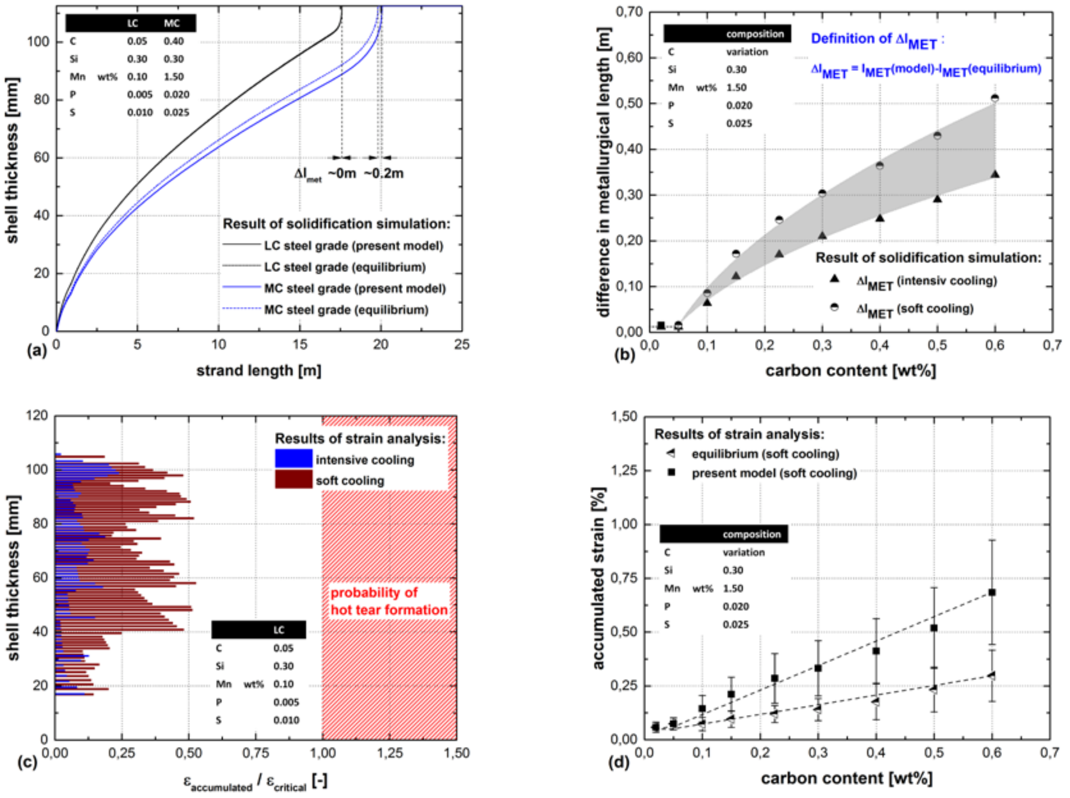

Figure 4: Difference in the metallurgical length compared to equilibrium conditions: (a) in presence of segregating elements and (b) in dependence of carbon content and cooling strategy; Calculation of accumulated strain during casting and comparison with critical values from the SSCT-Test (c); Influence of microsegregation modelling on strain accumulation compared to equilibrium conditions (d)

5. CONCLUSION

By means of Difference Scanning Calorimetry measurements the published equation for the estimation of liquidus temperature by Miettinen and Howe [11] could be slightly modified. Based on the experimental data, an increase of the liquidus temperature by 2 °C / wt% was observed for aluminum contents up to 3 wt%. The consideration of the coefficient leads to a further improvement of the equation. The optimized expression enables the accurate calculation of liquidus temperature even at higher amount of alloying elements and is thus used for determination of the current temperature in the microsegregation model. The calculated solidus temperatures and concentrations performed with the present "stand-alone" model are in very good agreement with a model from literature which is fully coupled to the thermodynamic database FSStel2015 (FactSage). Further, the model has been evaluated with more than 70 hot tensile tests on Low Carbon and Medium Carbon steels. The solidification simulations of continuous slab caster and the subsequently strain analysis regarding hot tear show the relevance of microsegregation modelling for process control in continuous casting processes.

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REFERENCES

[1] OHNAKA, I. Mathematical analysis of solute redistribution during solidification with diffusion in the solid state, *Transactions ISIJ*, 1986, vol. 26, no. 12, pp. 1045-1051.

[2] YOU, D., BERNHARD, C., WIESER, G., MICHELIC, S. Microsegregation model with local equilibrium partition coefficients during solidification of steels, *steel research international*, 2016, vol. 87, no. 7, pp. 840-849.

[3] UESHIMA, Y., MIZOGUCHI, S., MATSUMIYA, T., KAJIOKA, H. Analysis of solute distribution in dendrites of carbon steels with δ/γ transformation during solidification, *Metallurgical Transactions B*, 1986, vol. 17B, no. 4 , 845-859.

[4] YAMADA, W., MATSUMIYA, T., ITO, A. Development of simulation model for composition change of nonmetallic inclusions during solidification of steels. In *6th International Iron and Steel Congress*, Tokyo, 1990, pp. 618-625.

[5] PIERER, R., BERNHARD, C. On the influence of carbon on secondary dendrite arm spacing in steel, *Journal of Material Science*, 2008, vol. 43, no. 21, pp. 6938-6943.

[6] XIA, G. Untersuchungen über das mechanische Verhalten von erstarrendem Stahl unter stranggußähnlichen Bedingungen, PhD Thesis, Chair of Ferrous Metallurgy, Montanuniversitaet Leoben, 1992.

[7] KAWAWA, T. Estimation of liquidus temperatures of steel, *Report of 6th Meeting on Solidification of Steel*, 1973, No. 6-III-9.

[8] KAGAWA, A., OKAMOTO, T. Influence of alloying elements on temperature and composition for peritectic reaction in plain carbon steels, *Materials Science and Technology*, 1986, vol. 2, no. 10, pp. 997-1008.

[9] HOWE, A. Estimation of liquidus temperatures for steels, *Ironmaking and Steelmaking*, 1988, vol. 15, no. 3, pp. 134–142.

[10] SCHÜRMANN, E., STISOVIC, T. Berechnung der Liquidustemperatur aus der chemischen Analyse legierter Stahlschmelzen, *Stahl und Eisen*, 1998, vol. 118, no. 11, pp. 97–102.

[11] MIETTINEN, J., HOWE, A. A. Estimation of liquidus temperatures for steels using thermodynamic approach, *Ironmaking and Steelmaking*, 2000, vol. 27, no. 3, pp. 212–227.

[12] PRESOLY, P., PIERER, R., BERNHARD, C. Identification of defect prone peritectic steel grades by analyzing high temperature phase transformations, *Metallurgical and Materials Transactions A*, 2013, vol. 44, no. 12, 5377-5388.

[13] PIERER, R. Formulation of a new hot tearing criterion for the continuous casting process, PhD Thesis, Chair of Ferrous Metallurgy, Montanuniversitaet Leoben, 2007.

[14] ARTH, G., BERNHARD, C., ILIE, S., SCHADEN, T., PIERER, R. Experimental und numerical investigations on hot tearing during continuous casting of steel, Berg- und Hüttenmännische Monatshefte, 2015, vol. 160, no. 3, pp. 103–108.