Coupled Simulation of Heat Transfer and Phase Transformation in Continuous Casting of Steel

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A computer software package has been developed to simulate temperature, shell growth and phase transformations in continuous casting of steel. The package includes two earlier developed models, a heat transfer model and a thermodynamic-kinetic phase transformation model. The phase transformation model takes into account the effect of alloying and cooling on the phase transformation temperatures and on this basis, on important, solidification related thermophysical properties, enthalpy and thermal conductivity, generated by the model. Hence, while affecting these properties, the phase transformations have a special influence on the heat transfer in the strand. The output of these coupled calculations are temperature distribution, phase distribution (liquid, delta ferrite and austenite, and approximately, proeutectoid ferrite, pearlite, bainite and martensite) and volume distribution through the strand, and also, hardness distribution on the cross-section of the strand at room temperature. Characteristics of the coupled model and some results of calculations are presented.

KEY WORDS: simulation; heat transfer; phase transformation; continuous casting; steel.

1. Introduction

Applications of heat transfer analysis to continuous casting are numerous in the literature and give directly pertinent data like surface temperature and shell thickness. The heat transfer models are currently enhanced in several directions; one of these not very far developed includes the prediction of microstructure in continuous casting modeling. The heat transfer and microstructural models should be coupled, because the kinetics of phase transformations depends on cooling rate, and the thermophysical material properties needed in heat transfer calculations are related to the phases formed.

This paper presents a computer software package for the prediction of temperature distribution and some microstructural features such as phase fractions throughout a strand in continuous casting. The package includes two earlier developed models, a heat transfer model¹⁾ and a thermodynamic-kinetic phase transformation model.^{2,3)} The latter model also calculates the thermophysical material properties of steels,^{4,5)} taking into account the temperature, the cooling rate and the steel composition. Characteristics of the models and some results are presented.

2. Mathematical Models and Algorithms

2.1. Heat Transfer Model

The temperature field in the strand is described by the heat conduction equation with phase change. The model¹⁾ calculates the temperature field in the two-dimensional cross-section of the strand on its way through the casting machine as a function of casting parameters and steel grade. The heat conduction in the withdrawal direction is comparatively small and is

neglected. The equation takes the form:

$$\rho \frac{\partial H}{\partial t} = \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k \frac{\partial T}{\partial y} \right) \dots\dots\dots(1)$$

The necessary material data are the density, ρ , the enthalpy, H , and the thermal conductivity, k . Now, the enthalpy also includes the phase change heats. The numerical solution is obtained using the finite element method in space and the implicit finite difference method in time.

2.2. Phase Transformation Model

The solidification simulation of the phase transformation model²⁾ is made in one volume element set on the side of a dendrite arm; as a result of these calculations, one gets the fractions and the compositions of liquid (L), ferrite (δ) and austenite (γ) as a function of the decreasing temperature. The model solves the thermodynamic equilibrium at the interface of two solution phases, δ and L, γ and L, and γ and δ , using the chemical-potential-equality equations:

$$\mu_i^{\phi 1}(T, x_1^{\phi 1}, \dots, x_n^{\phi 1}) = \mu_i^{\phi 2}(T, x_1^{\phi 2}, \dots, x_n^{\phi 2}) \quad (i=1, \dots, n) \dots\dots\dots(2)$$

and the phase interface movement is simulated by means of modified interfacial material balance equations of solutes:

$$\Delta f^{\phi 1/\phi 2}(x_i^{\phi 2} - x_i^{\phi 1}) = S_i^{\phi 2}(T, x_i^{\phi 2}, D_i^{\phi 2}) - S_i^{\phi 1}(T, x_i^{\phi 1}, D_i^{\phi 1}) \quad (i=2, \dots, n) \dots\dots\dots(3)$$

In these equations, μ_i^{ϕ} is the chemical potential of component i in phase ϕ , x_i^{ϕ} is the mole fraction of the component in phase ϕ , T is temperature, n is the number of components in the alloy, $\Delta f^{\phi 1/\phi 2}$ is the fractional

movement of the ϕ_1/ϕ_2 interface, S_i^ϕ is a parameter describing the amount of solute i entering or leaving the interface, and D_i^ϕ is the diffusion coefficient of solute i in phase ϕ . Parameters μ_i^ϕ based on the use of the substitutional solution model and parameters S_i^ϕ involving Fick's first law of diffusion have been defined in references⁶⁾ and²⁾ respectively. The calculations are made stepwise and in each step, Eqs. (2) and (3) are solved simultaneously for each interface present. After solving these equations at a certain step, the solute diffusion in solid is simulated with a special finite difference application of Fick's second law.²⁾

Recently, the phase transformation model of solidification has been extended by another phase transformation model simulating the decomposition of austenite to various structures containing ferrite and cementite.³⁾ The austenite decomposition model applies the substitutional solution model using a para-equilibrium condition^{7,8)} during the cooling process, an analytical carbon diffusion model simulating the movement of the α/γ interface in spherical grains⁹⁾ and special regression formulas based on the German and the British CCT experiments,¹⁰⁻¹²⁾ taking into account the effect solutes C, Si, Mn, Cr, Mo, Ni, cooling rate and austenite grain size. The effect of stress on the transformation kinetics, however, has been ignored. The calculations of the new, extended phase transformation model have been compared with numerous solidification and CCT experiments showing a good correlation between the results.¹³⁾

Finally, special algorithms have been developed⁴⁾ for the calculation of important solidification-related thermophysical material properties, enthalpy, density and thermal conductivity needed in heat-transfer calculations taking into account the discontinuities caused by phase transformations. The data for these calculations are shown in references.^{5,6)}

2.3. Coupling of Phase Transformation and Thermal Calculations

The models of the work have been coupled as follows:

- 1) Assume a cooling rate for solidification and for austenite decomposition.
- 2) Calculate the material properties for the heat transfer model using the phase transformation model and the assumed cooling rates.
- 3) Calculate the temperature distribution and the cooling rates of each node using the heat transfer model.
- 4) If the calculated cooling rates on average match the assumed cooling rates, go to step 5). Otherwise, go back to step 1).
- 5) Calculate the microstructural evolutions through the strand with the phase transformation model. This is done separately for each node point in the finite element mesh using the nodal steel composition and the nodal cooling rates.

The calculation procedure is not yet fully coupled, because the material properties for the heat transfer model are calculated by mean solidification and cooling rates of the strand. Normally, the cooling rates vary at different points in the strand. To be precise, this should

be taken into account when solving the heat transfer equations.

2.4. Estimation of Microstructure Data

The phase transformation model applies special microstructure data as input data for the calculations. The secondary dendrite arm thickness of solidification is predicted as $d_2 = 150 \cdot \dot{T}^{-0.385}$ for low-alloyed steels¹⁵⁾ and as $d_2 = 68 \cdot \dot{T}^{-0.45}$ for stainless steels.¹⁶⁾ Here, d_2 is in μm and $\dot{T}$ is the cooling rate in $^\circ\text{C/s}$. The austenite grain size of an as-cast structure is roughly estimated as $d_{\text{GRAIN}} = 21 \cdot T^\gamma - 3152 \cdot [\exp \dot{T}/(1 + \exp \dot{T})] - 25088$ based on the work of Yasumoto *et al.*¹⁷⁾ T^γ is the highest temperature (in $^\circ\text{C}$) of a totally austenitic structure and $\dot{T}$ is the cooling rate of solidification in $^\circ\text{C/s}$. The validity of this equation, however, has not been checked beyond the cooling rate range 0.1 to 1.5 $^\circ\text{C}$ studied by Yasumoto *et al.*¹⁷⁾

2.5. Incorporating a Macroseggregation Profile

Normally, the austenite decomposition model applies the steel composition (either the nominal or the interdendritic composition) in the calculations. However, the macroseggregation profiles of solutes, if known, can also be used as input data. Depending on the degree of macroseggregation, one may then get different phases in different parts of the strand causing changes in volume and hardness through the strand.

2.6. Calculation of Volume Changes

Due to the different densities of ferrite and austenite, certain volume changes are expected to occur in the strand during the austenite decomposition process. The rate of these volume changes depends on the rate of the decomposition process influenced by the steel grade, the cooling conditions and the microstructure. Knowing the density function $\rho(T)$ obtained with the phase transformation model and the temperature distribution $T(x, z)$ obtained with the heat transfer model, the volume distribution of the strand can be expressed as $V(T(x, z)) = 1/\rho(T(x, z))$. Here V is given in cm^3/g , x is the distance from the strand surface and z is the distance from the meniscus.

2.7. Calculation of Hardness at Room Temperature

The British Steel Corporation¹²⁾ has given the following functions for the prediction of hardness (at room temperature) in various structures of low-alloyed steels: $HV^M = 127 + 949C + 27Si + 11Mn + 16Cr + 8Ni + 21 \cdot \log(\dot{T})$, $HV^B = -323 + 185C + 330Si + 153Mn + 144Cr + 191Mo + 65Ni + (89 + 53C - 55Si - 22Mn - 20Cr - 33Mo - 10Ni) \cdot \log(\dot{T})$ and $HV^{F+P} = 42 + 223C + 53Si + 30Mn + 7Cr + 19Mo + 12.6Ni + (10 - 19Si + 8Cr + 4Ni) \cdot \log(\dot{T})$, where $\dot{T}$ is the cooling rate in $^\circ\text{C/hr}$. Now, knowing the fractions of martensite (f^M), bainite (f^B), ferrite (f^F) and pearlite (f^P) through the strand, calculated with the austenite decomposition model, one can estimate the hardness profile of the final structure as $HV = f^M \cdot HV^M + f^B \cdot HV^B + (f^F + f^P) \cdot HV^{F+P}$.

3. Calculation Examples

This section shows two calculation examples for the

steels of Table 1.

3.1. Prediction of Phase Regions and Thermal Contraction during Solidification of Stainless Steel Slabs

Figures 1 and 2 show the calculated phase regions of solidification and the related thermal contraction for continuously cast AISI 304 and AISI 316 slabs. Assuming that solid fraction 0.80 can be related to the zero strength point of the steel, where dendrite arms have their first contact with each other and the liquid feeding becomes insufficient to totally compensate the shrinkage, one can approximate the mushy zone contraction as $\beta_{MUS}(\%) = 100(1 - \rho_{80\%}/\rho_{SOL})$. Here, $\rho_{80\%}$ and ρ_{SOL} are the densities corresponding to the temperature of 0.80 solid fraction and the solidus temperature. For AISI 304, this yielded $\beta_{MUS} = 1.35$ and for AISI 316, it yielded $\beta_{MUS} = 0.91$. The higher mushy zone contraction of AISI 304 can be explained by the greater amount of ferrite transformed away in the peritectic transformation region: in AISI 304, the ferrite fraction decreased from 0.80 to 0.45 (with a total fraction of 0.35) whereas in AISI 316, it decreased from 0.11 to 0.04 (with a total fraction of 0.07 only). Below the solidus temperature, one can apply the solid state contraction term $\beta_{SOL}(\%) = 100(1 - \rho_{SOL}/\rho_{S50})$ to estimate the contraction caused by the $\delta \rightarrow \gamma$ transformation, where ρ_{SOL} and ρ_{S50} are the densities at

Table 1. Nominal compositions (in weight %) of the studied steels.

Steel	C	Si	Mn	P	S	Cr	Mo	Ni	N
AISI 304	0.04	0.50	1.50	0.030	0.010	18.00	0.30	9.2	0.04
AISI 316	0.04	0.50	1.50	0.030	0.010	17.00	2.60	12.0	0.04
A320	0.43	0.24	0.88	0.008	0.027	1.01	0.23	0.2	0.05

Fig. 1. Calculated phase regions and contraction during solidification of continuously cast AISI 304 slab.

Fig. 2. Calculated phase regions and contraction during solidification of continuously cast AISI 316 slab.

the solidus temperature and at a temperature 50°C below the solidus. For AISI 304, this gave $\beta_{SOL} = 0.60$ (ferrite fraction reduced with 0.20), and for AISI 316, it gave $\beta_{SOL} = 0.35$ (ferrite fraction reduced with 0.02 only). Consequently, due to the higher shell contraction below the meniscus, AISI 304 may be more sensitive to hot spots and other surface defects than AISI 316.

3.2. Prediction of Phase, Volume and Hardness Distribution in an As-cast Bloom

Table 2 shows composition profiles measured from an as-cast A320 bloom of Imatra Steel. As can be seen, the profiles are quite uniform except for the slight carbon peak in the center of the bloom. Table 2 also shows the cooling rates of different nodes between 700 and 500°C obtained by applying the coupled calculations to the continuous casting process of Imatra, and the grain sizes calculated with the equation of Sec. 2.4. Using the data of Table 2, a phase and a hardness distribution of Fig. 3 was obtained. The as-cast structure contained 13 to 25% ferrite, 63 to 75% bainite, 10 to 14% martensite, and 1 to 2% rest austenite, and the hardness varied between 300 and 360 HV correlating well with these measured hardness data points. The phase distribution

Table 2. Solute contents (in weight %), austenite grain size, and cooling rate at different distances from the surface of a continuously cast A320 bloom.

x (mm)	C	Si	Mn	Cr	Mo	Ni	d_{GRAIN} (μm)	$\dot{T}$ ($^{\circ}C/s$)
140	0.517	0.243	0.905	1.022	0.243	0.197	2454	0.048
135	0.466	0.240	0.894	1.013	0.239	0.197	2454	0.048
128	0.395	0.236	0.878	1.001	0.233	0.196	2453	0.049
119	0.404	0.240	0.882	1.002	0.232	0.196	2452	0.049
110	0.405	0.237	0.878	0.998	0.228	0.196	2451	0.050
100	0.406	0.234	0.873	0.993	0.223	0.196	2448	0.051
90	0.409	0.235	0.877	0.995	0.225	0.196	2444	0.052
80	0.412	0.237	0.881	0.998	0.228	0.196	2437	0.054
70	0.415	0.238	0.885	1.000	0.230	0.196	2426	0.055
60	0.415	0.238	0.884	1.001	0.232	0.196	2404	0.058
50	0.415	0.238	0.884	1.003	0.234	0.196	2361	0.060
40	0.415	0.238	0.883	1.004	0.236	0.196	2261	0.062
31	0.414	0.238	0.883	1.006	0.238	0.196	2034	0.065
23	0.414	0.238	0.882	1.007	0.240	0.196	1666	0.067
17	0.414	0.238	0.882	1.008	0.241	0.196	1288	0.069
12	0.414	0.238	0.881	1.008	0.242	0.196	1058	0.071
7	0.414	0.238	0.881	1.009	0.243	0.196	986	0.074
3	0.414	0.238	0.881	1.010	0.244	0.196	980	0.076
0	0.414	0.238	0.881	1.010	0.244	0.196	980	0.078

Fig. 3. Calculated phase and hardness distribution at room temperature in an as-cast A320 bloom.

Fig. 4. Calculated phase and hardness distribution at room temperature in an as-cast A320 bloom using reduced grain size or cooling rate (reduction of 20%).

Fig. 5. Calculated volume distribution in certain nodes of a continuously cast A320 bloom (points are 1=135 mm, 2=128 mm, 3=90 mm, 4=80 mm from the strand surface).

is quite uniform: no specific discontinuities were caused by new phases or remarkably changed phase fractions. However, by changing these input data slightly (by reducing the original grain size or cooling rate data by only 20%), two separate pearlite regions were formed (Fig. 4). This resulted in certain volume changes in the boundaries of the pearlite region as shown in Fig. 5: the region between points 2 and 3 expanded whereas points 1 and 4 around the region did not (at least, not before the bainite formation temperature at 520°C). Consequently, tensions are formed in regions 1 and 4 which may cause cracks during the cooling process. The present example clearly shows the sensitivity of the input parameters of Table 2 to the results: with slight changes of parameters, a certain transformation "nose" may scarcely be passed resulting in a totally different phase and volume distribution in the bloom.

4. Conclusions

Two earlier developed models, a heat transfer model and a thermodynamic-kinetic phase transformation model were coupled to predict the temperature, phase, volume and hardness distribution in a continuously cast strand. The calculation procedures were not fully coupled, because the material properties for the heat transfer model were calculated using mean cooling rates of the strand. A closer coupling of calculations will be made in the future. Some test calculations were presented for two stainless steel slabs showing that due to the higher shell contraction below the meniscus, AISI 304 could be more sensitive to surface defects than AISI 316. The model was also used for the prediction of phase, volume and hardness distribution in an as-cast bloom of Imatra Steel. The phase distribution was not measured experimentally but the calculated hardness data correlated well with the measured hardness values through the bloom. The work will be continued.

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