

Calculation of Physical Properties for Use in Models of Continuous Casting Process-Part 2: Steels

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The objective of the present study was to calculate physical property values for steels from their chemical compositions for subsequent use in mathematical models of the fluid flow, heat transfer and shell solidification in the continuous casting mould. Values of the following properties of steels are calculated for temperatures between 298 K and 2 000 K; Heat Capacity (C_p) Density (ρ) Thermal conductivity (k) and diffusivity (a) Electrical resistivity (R) Viscosity (η) Surface (γ_m) and Interfacial tension (γ_{msl}). In addition temperatures of transitions (Liquidus T_{liq} , Solidus T_{sol}) and various solid state transitions were also calculated. Ferritic and austenitic phases of Carbon - and stainless steels are both covered. The associated software is available on the following websites (i) <http://www.mxif.manchester.ac.uk/resources/software> (ii) <https://sites.google.com/site/shyamkaragadde/software/thermophysical-properties>.

KEY WORDS: low-alloy and stainless steels; thermophysical properties; continuous casting; mould slags.

1. Introduction

Recent mathematical models, coupling fluid flow, heat transfer and shell solidification in the continuous casting mould, have been shown to be capable of providing (i) reliable values for the horizontal heat flux and powder consumption and (ii) insight into the mechanisms responsible for defect formation.^{1,2)} However, these models require input data for the physical properties of both the steel and the mould powders used in the casting. Physical property determinations are both time-consuming and expensive. Thus it is unreasonable to use measured property data for all the steels being continuously cast. Consequently, in this study relations between property values for various types of steel and their chemical compositions are explored to provide property data for a wide range of steels since chemical composition data are routinely available. A similar study has been carried out for the mould powders in Part 1 of this communication.³⁾ The predicted physical property values can then be used as input data in the mathematical model to then calculate the fluid flow, microstructure, *etc.*

Thus the objectives of the study were:

- (i) To provide values of the physical properties of various steels calculated from their chemical compositions, and

- (ii) To continually improve the methods used for property estimations.

2. Calculation of Steel Properties

The physical properties of steels in the solid state are affected by the nature of the phase formed in the steel (*i.e.* ferrite or austenite). Thus differences in elemental concentrations (*e.g.* % C) tend to have a much larger effect on the property values when they result in a phase change from ferrite to austenite or *visa-versa* than when there is no phase change involved. Thus it important to determine whether a steel is ferritic or austenitic, or a mixture of the two phases. In order to demonstrate these property differences, calculations have been carried out for two steels (a peritectic, low alloy steel and an austenitic, stainless steel); the compositions are given in **Table 1**.

2.1. Calculation of Steel Composition

The chemical composition of the steel is first normalised to 100% and then mole fractions (X) are calculated. The mean molecular weight (M) of the steel is also calculated.

2.2. Classification of Steels

A directory has been developed to interrogate the composition to determine whether:

- (i) a steel was to be classified as a low alloy or a stainless steel, and

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Table 1. Chemical composition of two steels (mass%). LA=low-alloy and SS=stainless steel.

	Fe	C	Si	Mn	Cr	Ni	Mo	Ti	V	Al	S	P	N
LA	98.3	0.10	0.2	1.0	0.15	0.05	0.05	0.05	0.05	0.05	0.01	0.01	0.007
SS	50.5	0.17	2.24	1.74	24.4	20.6	0.24	0.05	0.05	0.05	0.005	0.015	0.023

(ii) it forms austenite or ferrite or a mixture of the two phases (*i.e.* peritectic).

In this study a steel was classified as a stainless steel if it contained >8% Cr.

The scheme used to differentiate between the steels is that devised by Wolf^{4,5)} and involves the calculation of the parameters, *ferrite potential* (FP) and *carbon potential* (CP) which are defined in Eqs. (1) and (2).

Wolf^{4,5)} introduced the term “*ferrite potential*” as a measure of the amount of peritectic reaction occurring in the steel. Although the ferrite potential is affected by the carbon content, it is also affected by other alloying elements; some of these elements stabilise the ferrite (*e.g.* Cr, W, Mo, Al and Si) whilst others stabilise the austenite phase (*e.g.* Ni, Mn, Co, N and Cu). For *low-alloy steels*, the ferrite potential (FP) can be calculated by Eq. (1) where CP is the carbon potential which is determined using Eq. (2).

$$\text{Low alloy: } FP = 2.5(0.5 - CP) \dots\dots\dots (1)$$

$$CP = (\text{wt}\%C) + 0.04(\%Mn) + 0.1(\%Ni) + 0.7(\%N) - 0.14(\%Si) - 0.04(\%Cr) - 0.1(\%Mo) - 0.24(\%Ti) \dots (2)$$

The phase is considered to be ferrite when $FP > 1.05$ and to be austenite when $FP = < 0.8$. The peritectic reaction is at a maximum at $FP = 1.0$ and the range, $FP = (0.8 \text{ to } 1.05)$, corresponds to the crack-sensitive range for steels. The peritectic range occurs between CP values of 0.06 and 0.17 and approximate values of fraction of ferrite (denoted f_α) formed are calculated by Eq. (3). For accurate values of fractions ferrite and austenite the reader is advised to consult thermodynamic software packages.

$$f_\alpha = 1 - f_\gamma = (0.17 - CP) / (0.17 - 0.06) \dots\dots\dots (3)$$

For *stainless steels* the FP is calculated from the (“Ni”/“Cr”) ratio using Eq. (4)^{4,5)} where “Ni” and “Cr” are defined in Eqs. (5) and (6), respectively.

$$\text{Stainless steel: } FP = 5.26(0.74 - \text{“Ni”} / \text{“Cr”}) \dots (4)$$

$$\text{“Ni”} = (\text{wt}\% \text{ Ni}) + 0.31(\%Mn) + 22(\%C) + 17.5(\%N) \dots (5)$$

$$\text{“Cr”} = (\text{wt}\% \text{ Cr}) + 1.5(\%Si) + 1.65(\%Mo) + 2(\%Nb) + 3(\%Ti) \dots\dots\dots (6)$$

An approximate value for the fraction ferrite in stainless steels is calculated^{4,5)} from Eq. (7).

$$f_\alpha = 1 - f_\gamma = 5.28 \{ 0.74 - (\text{“Ni”} / \text{“Cr”}) \} \dots\dots\dots (7)$$

2.3. Calculation of Transition Temperatures

The thermodynamic temperature scale (K) is used throughout this paper except where certain authors have used Celsius in their equations; these were changed to K in the calculations. Routines for calculating approximate values of the transition temperatures are described below

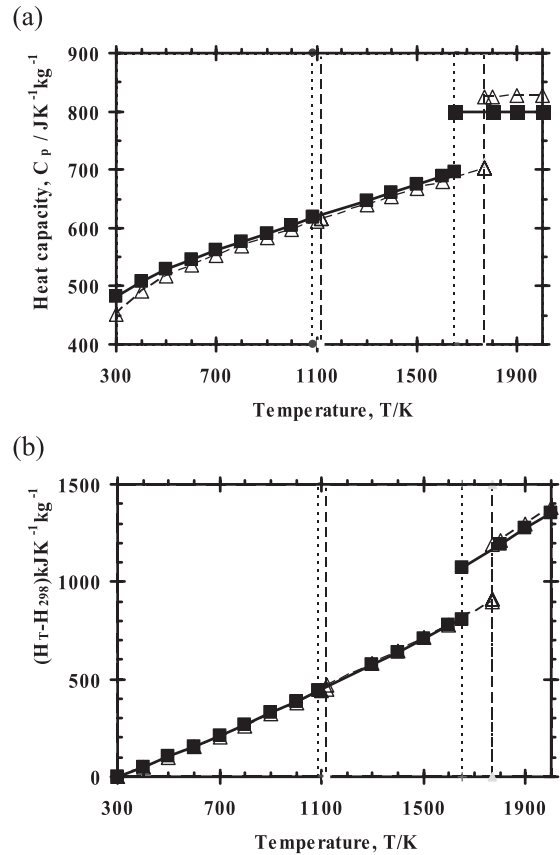


Fig. 1. Calculated values for (a) C_p and (b) Enthalpy ($H_T - H_{298}$) as functions of temperature for a peritectic low alloy steel (Δ) and an austenitic stainless steel (\blacksquare); Transition temperatures shown as vertical lines; dashed=low alloy; dotted=stainless steel.

since the properties are affected by the nature of the phase formed in the steel; for accurate values of these transition temperatures the reader should refer to thermodynamic software predictions.

2.3.1. Liquidus Temperature (T_{liq})

Several studies have reported equations relating liquidus temperatures as a function of the chemical composition of the steel.⁶⁻¹²⁾ In addition, Jablonka *et al.*¹²⁾ reported equations to calculate T_{liq} values for steels based on the Fe-C system for ferrite ($T_{liq}(K) = 1811 - 79\%C$) and austenite *i.e.* for steels with $C\% > 0.16$ ($56.02.\%C = (1811 \text{ K} - T_{liq}) - 1.13 \cdot 10^{-3} (1811 \text{ K} - T_{liq})^2$). The T_{liq} values for the steel calculated here for both low alloy and stainless steels were derived using Eqs. (8) to (11) due to Miettinen and Howe.¹¹⁾ The steels are classified according to the phase formed on solidification and interactions between elements are taken into account *e.g.* interaction between Cr and C on T_{liq} is covered in Eq. (8) by $\{0.033.\%Cr. (\%C)\}$. Miettinen and Howe cite an average uncertainty of $\pm 4 \text{ K}$ from a comparison of calculated with experimental T_{liq} values. The equations used to calculate T_{liq} values for the various categories of steel¹¹⁾

are given in Eqs. (8) to (11).

Low alloy Ferritic steels :

$$T_{liq,K} = 1811 - 76.2\%C - 10.35.(\%C)^2 - 11.66\%Si - 4.35\%Si.(\%C) - 5.62\%Mn - 0.223\%Mn.(\%C) - 1.95.\%Cr - 0.033.\%Cr.(\%C) - 2.2\%Mo - 0.845\%Mo.(\%C) - 3.58\%Ni - 0.836\%Ni.(\%C) - 24.78\%P - 12.94\%P.(\%C) - 32.8\%S - 17.72\%S.(\%C) \dots\dots\dots (8)$$

Austenitic

$$T_{liq,K} = 1801 - 60.1\%C - 6.14.(\%C)^2 - 11.49\%Si - 5.61\%Si.(\%C) - 4.26 * \%Mn + 0.453 * \%Mn.(\%C) - 2.47.\%Cr + 1.33.\%Cr.(\%C) - 4.36\%Mo + 0.07\%Mo.(\%C) - 1.97\%Ni - 0.589\%Ni.(\%C) - 30.92\%P - 5.35\%P.(\%C) - 33.2\%S - 10.09\%S.(\%C) \dots\dots\dots (9)$$

Stainless steels

Ferritic

$$T_{liq,K} = 1811 - 76.28\%C - 1.399\%Cr.\%C - 0.0837\%Ni\%C - 9.43\%Si - 0.2128\%Cr.\%Si + 0.2391\%Si.\%Ni - 7.55\%Mn + 0.1779\%Mn.\%Cr + 0.01\%Mn.\%Ni - 1.56\%Cr - 0.0236.(\%Cr)^2 - 2.87\%Mo + 0.044\%Cr\%Mo - 0.0205\%Ni\%Mo - 4.29\%Ni + 0.0095\%Cr\%Ni + 0.0428.(\%Ni)^2 + 12\%Nb + 0.0789\%Cr.\%Nb + 1.77.\%Ni.\%Nb - 18.55\%Ti + 0.0538\%Cr.\%Ti + 0.3514\%Ni.\%Ti - 42.64\%N - 1.2721\%Cr\%N - 1.0988\%Ni\%N + 0.002084.(\%Cr)^3 + 0.000695.(\%Ni)^3 + 238.96\%Ti\%N \dots\dots\dots (10)$$

Austenitic

$$T_{liq,K} = 1801 - 62.62\%C - 0.5175\%Cr.\%C - 0.20267\%Ni\%C - 8.29\%Si - 0.4646\%Cr.\%Si + 0.1755\%Si.\%Ni - 4.22\%Mn - 0.143\%Mn.\%Cr - 0.0377\%Mn.\%Ni - 2.59\%Cr - 0.034.(\%Cr)^2 - 0.26\%Mo + 0.0494\%Cr\%Mo - 0.0244\%Ni\%Mo - 1.69\%Ni + 0.0546\%Cr\%Ni - 0.0175.(\%Ni)^2 - 10.17\%Nb - 0.0225\%Cr.\%Nb + 0.0781.\%Ni.\%Nb - 16.91\%Ti - 0.0907\%Cr.\%Ti + 0.1422\%Ni.\%Ti - 21.6\%N + 0.1153\%Cr\%N - 0.2366\%Ni\%N + 0.000392.(\%Cr)^3 - 0.000356.(\%Ni)^3 + 154.98\%Ti\%N \dots\dots\dots (11)$$

2.3.2. Solidus Temperature (T_{sol})

Jablonka *et al.*¹²⁾ reported the following relations for the solidus temperature (T_{sol}) of ferritic ($T_{sol}(K) = 1811 - 460\%C$) and austenitic steels ($T_{sol}(K) = 1811 - 185\%C$) based on the Fe-C system. Since the alloying elements have a signifi-

cant effect on both T_{sol} and T_{liq} (see Eqs. (8) to (11)) it is not possible to use these relations to estimate T_{sol} for the wide compositional range covered in this study. Consequently, in the calculation of physical properties it has been assumed that fusion takes place abruptly at T_{liq} .

2.3.3. Solid State Transition Temperatures (T)

There are several solid state transitions in the Fe-C system. Jablonka *et al.*¹²⁾ reported the following relations to calculate transition temperatures for the Fe-C system; at the present time no corrections have been made for the effect of alloying elements on the various transition temperatures. Eqs. (12), (13) and (14) have been adopted to calculate the effects of C content on the transition temperatures for ($\gamma \rightarrow \delta$) and ($\alpha + \gamma \rightarrow \gamma$), respectively.

Transition ($\gamma \rightarrow \delta$) $T_{\gamma \rightarrow \delta} (K) = 1665 + 624.4\%C \dots (12)$

$C < 0.76\%$

$T_{\alpha + \gamma \rightarrow \gamma} (K) = A_3 = 1171 - 584\%C + 593\%C^2 - 190\%C^3 \dots\dots\dots (13)$

$C > 0.76\%$

$T_{\alpha + \gamma \rightarrow \gamma} (K) = A_{cm} = 865 + 24.1(\%C) + 159.2(\%C)^2 \dots\dots (14)$

Transition ($\alpha \rightarrow \gamma$) $T_{\alpha \rightarrow \gamma} (K) = A_1 = 990 K \dots (15)$

2.4. Heat Capacity (C_p) and Enthalpy ($H_T - H_{298}$)

The C_p and enthalpy are calculated using partial molar values (shown in Eq. (16) where P is the property being studied, X_i is the mole fraction of components of steel such as Fe, Cr, Mn, Ni *etc.*).

$$P_{steel} = \sum_{i=1}^N (X_i P_i) \dots\dots\dots (16)$$

The temperature dependence of heat capacity (C_p) for the solid phase is usually expressed in the form of Eq. (17) where a^* , b^* and c^* are constants and the enthalpy ($H_T - H_{298}$) is given by Eq. (18).

$$C_p = a^* T + b^* T - c^* / T^2 \dots\dots\dots (17)$$

$$(H_T - H_{298}) = \int_{298}^T C_p dT = a^*(T - 298) + 0.5b^*(T^2 - 298^2) + (c^* / T) - (c^* / 298) \dots\dots\dots (18)$$

However, C_p - T relations for Fe alloys contain a sharp peak in C_p around 1020 K due to the magnetic transition but the magnitude of the enthalpy associated with this transition tends to decrease with increasing alloy addition in steels. This makes it difficult to model. Consequently, the coefficients for a^* , b^* and c^* for Fe were obtained in the form of Eq. (18) from a best fit of enthalpy values for Fe. Thus the resultant C_p values do not show the enhanced peak in C_p associated with the magnetic transition but this has little effect on the enthalpy values.

The enthalpy of transition (ΔH^T) of ferritic steels for the various transitions are given below

$$\Delta H^{\text{tr}}_{\alpha \rightarrow \gamma} = 18.1 \text{ kJ kg}^{-1} \dots\dots\dots (19)$$

$$\Delta H^{\text{tr}}_{\gamma \rightarrow \delta} = 14.8 \text{ kJ kg}^{-1} \dots\dots\dots (20)$$

$$\Delta H^{\text{fus}} = T_{\text{liq}} \Delta S^{\text{fus}} \text{ kJ kg}^{-1} \dots\dots\dots (21)$$

The values of C_p and $(H_T - H_{298})$ are given in $\text{JK}^{-1}\text{kg}^{-1}$ and kJ kg^{-1} , respectively; values were converted from mol^{-1} to kg^{-1} by multiplying by $(1\,000/M)$ where M is the average molecular weight of the steel ($M = \sum X_i M_i$). The calculated values of C_p and $(H_T - H_{298})$ for low alloy and austenitic stainless steels are shown in Figs. 1(a) and 1(b), respectively. It can be seen that C_p and enthalpy are little affected by composition.

2.5. Density (ρ)

Low alloy steels

The molar volume (V) of the steel at 298 K was calculated using partial molar volumes of the various steel components (Eq. (22)).

$$V_{298 \text{ steel}} = \sum_{i=1}^N (X_i V_i) \dots\dots\dots (22)$$

The density (ρ) can be calculated from the molar volume by using Eq. (23) where M is the molecular weight of the steel

$$\rho_{\text{steel}} = M / V_{\text{steel}} \dots\dots\dots (23)$$

Ferritic steels

The density of steel is also affected by the carbon content, Consequently, a correction was applied for the effect of carbon. The relations reported by Jablonka *et al.*,¹²⁾ shown in Eq. (24), were used where $g = 2.62 \times 10^{-2}$ for the α and δ phases and 1.46×10^{-2} for the γ phase.

$$\rho_{T, \text{ steel}} = \rho_{T, \text{ Fe}} (1 - g \cdot C\%) \dots\dots\dots (24)$$

Jablonka *et al.*¹²⁾ expressed the temperature dependence of $\rho_{T, \text{ Fe}}$ by Eq. (25) where $T^* = \{T - 273\}$. The temperature dependence of $\rho_{T, \text{ steel}}$ was obtained by substituting $\rho_{298, \text{ steel}}$ for 7 876 in Eq. (25).

$$\alpha \text{ and } -\delta \text{ - phases : } \rho_{T, \text{ Fe}} (\text{kgm}^{-3}) = 7\,876 - 0.297T^* - 5.62 \cdot 10^{-5} T^{*2} \dots\dots (25)$$

The transition ($\alpha \rightarrow \gamma$) is accompanied by an increase in density ($\Delta\rho_{\alpha \rightarrow \gamma} = +80 \text{ kgm}^{-3}$).¹²⁾

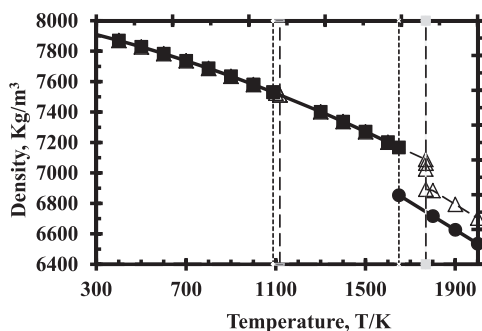


Fig. 2. Calculated values of the density of low-alloy steel (Δ) and austenitic, stainless steels (\blacksquare) as a function of temperature; Transition temperatures are shown as vertical lines; dotted = stainless and dashed = low-alloy steels.

Austenitic steels

Austenite has a higher density than ferrite. Jablonka *et al.*¹²⁾ reported the following relation for austenite, where $T^* = \{T(\text{in K}) - 273\}$. This equation was extrapolated to lower temperatures to calculate density values for the range, 298 K to $T_{\alpha \rightarrow \gamma}$. However, corrections were made for the effect of C content and the alloying content on $\rho_{298 \text{ Fe}}$.

$$\gamma \text{ - phase : } \rho_{T \gamma, \text{ Fe}} (\text{kgm}^{-3}) = 8\,100 - 0.506T^* \dots\dots (26)$$

The transition of austenite to δ -phase is accompanied by a decrease in density, $\Delta\rho = -42 \text{ kg m}^{-3}$.¹²⁾ The transition of δ -phase to liquid is also accompanied by a decrease in density, $\Delta\rho^{\text{fus}} = -250 \text{ kgm}^{-3}$.¹²⁾

Liquid steel

The density of the liquid at T_{liq} (denoted by the superscript m) was calculated using Eq. (27). Jablonka *et al.*¹²⁾ reported Eq. (28) for the effect of carbon on $\rho_{T, \text{ Fe}}$ for the liquid phase. Thus the density of the liquid was calculated by combining ρ^m_{liq} with the dependencies of density on the C content and temperature¹²⁾]; as shown in Eq. (28).

$$\rho^m_{\text{liq}} (\text{kgm}^{-3}) = \rho^m_{\text{sol}} - 250 \dots\dots\dots (27)$$

$$\rho_{T \text{ liq}} (\text{kgm}^{-3}) = \rho^m_{\text{liq}} - 0.835(T - T_{\text{liq}}) \dots\dots\dots (28)$$

It should also be noted that ρ^m_{liq} can be calculated from the relation ($V^m_{\text{steel}} = \sum (X_i \cdot V^m_{i, \text{ Fe}} + X_{\text{Cr}} \cdot V^m_{\text{Cr}} + (X_{\text{Ni}})^m + (X_{\text{Mn}})^m + (X_{\text{Si}})^m + \dots)$) and ($\rho^m_{\text{liq}} = M/V^m$) where the superscript, m indicates at T_{liq} . Values for (dV/dT) can be also calculated on a partial molar basis; this was used in the calculation of the temperature dependency of the liquid alloy. The effect of C content can be introduced by multiplying ρ^m_{liq} by $(1 - 0.01\%C)$.¹²⁾ These values were found to be in good agreement with the adopted values.

The calculated density values for low alloy and austenitic stainless steels are shown in Fig. 2.

Stainless steels

The densities of stainless steels were calculated using the empirical relation shown in Eq. (29).¹³⁾ It should be noted that although the ferrite to austenite transition is accompanied by an increase in density ($\Delta\rho$) the values of ρ_{298} for the two phases are similar because $\Delta\rho$ is largely offset by the higher thermal expansion coefficient for austenite.

$$\rho_{298 \text{ steel}} (\text{kgm}^{-3}) = 79.6(\% \text{Fe}) + 78.3(\% \text{Cr}) + 85.4(\% \text{Ni}) + 76.9(\% \text{Mn}) + 60.2(\% \text{Mo}) + 47.1(\% \text{Si}) \dots\dots\dots (29)$$

The linear thermal expansion coefficient (α) for austenitic stainless steels is given in Eq. (30).¹³⁾

$$10^6 \alpha (\text{K}^{-1}) = 15.8 + 0.6 \times 10^{-2} (T - 298) \dots\dots\dots (30)$$

The expansion coefficient for ferrite is significantly lower than that of austenite for temperatures between 298 and 1 000 K as can be seen from Eq. (31)¹³⁾ but increases abruptly for temperatures above 1 000 K with the formation of austenite (Eq. (32))

$$(298 - 1\,000 \text{ K}) \quad 10^6 \alpha (\text{K}^{-1}) = 10.2 + 0.6 \times 10^{-2} (T - 298) \dots\dots\dots (31)$$

$$10^6 \alpha (K^{-1}) = 14.2 + 2.4 \times 10^{-2} (T - 1000) \dots\dots (32)$$

Densities at various temperatures were calculated using Eq. (33) where T_{ref} is 298 K or 1 000 K in the case of ferrite at temperatures above 1 000 K.

$$\rho_{T \text{ steel}} (kgm^{-3}) = \rho_{T_{ref} \text{ steel}} (1 - \alpha_T (T - T_{ref}))^3 \dots\dots (33)$$

Liquid phase

The density of liquid stainless steel can be calculated using Eq. (34).

$$\rho^m_{liq} (kgm^{-3}) = 69.4(\%Fe) + 66.3(\%Cr) + 71.4(\%Ni) + 57.2(\%Mn) + 51.5(\%Mo) + 49.3(\%Si) \dots\dots (34)$$

However, it can also be calculated by using the calculated value of ρ^m_{sol} and the following relation, $\rho^m_{liq} = \rho^m_{sol} / 1.04$ (derived from Fe¹⁴). The calculated density values obtained with Eqs. (29) and (34) are subject to uncertainties of ca. ± 2%. Consequently, in order to avoid the situation where $\rho^m_{liq} > \rho^m_{sol}$, a mean of the ρ^m_{liq} values obtained by the two methods was used to avoid this anomaly.

2.6. Thermal Conductivity (k) and Diffusivity (a) and Electrical Resistivity (R)

2.6.1. Thermal Conductivity (k)

Experimental measurements of the thermal conductivity (k) of molten metals are prone to errors arising from con-

tributions from convection; these errors are accentuated by the low viscosities of metals. Values for the solid state are affected by the microstructure, which is, in turn, affected by the thermal and mechanical histories of the sample. Consequently, values cited here refer to annealed alloys *i.e.* with minimum resistivity. At high temperatures electronic conduction in metals is dominant¹⁵) Consequently, it has been proposed¹⁵) that the most reliable method of estimating thermal conductivities of liquid metals is *via* the Wiedemann-Franz-Lorenz (WFL) rule (Eq. (35) where R is the electrical resistivity).

$$k^{el}_T = 2.45 \cdot 10^{-8} (T / R) \dots\dots\dots (35)$$

Low alloy steels

The WFL rule does not apply to solids at lower temperatures where there are two contributions, namely,

- (i) *electronic conduction*, k^{el}_T (which can be calculated by combining Eqs. (36)¹⁶) and (35).
- (ii) *lattice thermal conductivity* k_T^{lat} which is calculated by an empirical relationship (Eq. (37))¹⁶

$$R_{298} (10^{-8} \Omega m^{-1}) = 100 \{ 0.11\%Fe + 1.92\%Cr + 3.53\%Mn + 0.97\%Nb + 2.1\%Ni + - 9.9\%Si + 3.34\%Ti + 7.9\%Al + 2\%Co + 8.28\%C + 2\%S + 1\%Ca + 0.11\%Nb + 0.6\%W + 4.5\%P \} \dots\dots\dots (36)$$

$$k_{298}^{lat} (Wm^{-1}K^{-1}) = 8.1\%Fe + 0.35\%Cr + 0.11\%Mn + 0.39\%Nb - 0.28\%Ni + -96.8\%Si - 1\%Ti + 100\%Al - 0.28\%Co + 246\%C + 1\%S + 1\%Ca + 0.81\%Nb + 4.6\%W + 1\%P \dots\dots\dots (37)$$

The effective conductivity (k_{eff}) at 298 K. can then be calculated using Eq. (38).

$$k_T^{eff} = k_T^{el} + k_T^{lat} \dots\dots\dots (38)$$

The thermal conductivity of ferrite (k_α) at 298 K is significantly higher than that of austenite (k_γ). However, α -ferrite transforms to γ austenite around 1 180 K in most low alloy steels and k_γ has a value of 25.4 $Wm^{-1}K^{-1}$ at this temperature.¹⁶) The k-T relations for temperatures between 298 K and $T_{\alpha \rightarrow \gamma}$ can be expressed in the form of Eq. (39) for both austenitic and ferritic steels. Note that values for the temperature coefficient (dk/dT) in this range will be negative for ferritic steels and positive for austenitic low-alloy steels

$$k_T (Wm^{-1}K^{-1}) = k_{298}^{eff} + \{ (k_{T_{\alpha \rightarrow \gamma}} - k_{298}) (T - 298) / (T_{\alpha \rightarrow \gamma} - 298) \} \dots\dots\dots (39)$$

The k^{eff} values for austenite in the temperature range ($T_{\alpha \rightarrow \gamma}^{tr}$ to $T_{\gamma \rightarrow \delta}^{tr}$) were calculated using the empirical relation shown in Eq. (40); the values for the δ -phase were derived by extrapolating the relation for the γ phase to T^{liq} . Note the calculated values are independent of the alloy composition in this range; any uncertainties due to composition were found to be within experimental uncertainties

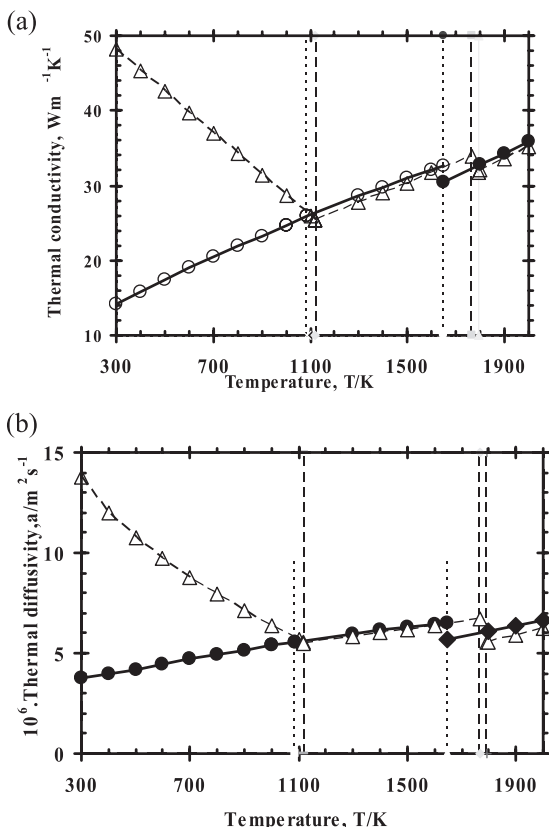


Fig. 3. Calculated values of (a) Thermal conductivity and (b) Thermal diffusivity as function of temperature for low alloy (Δ) and austenitic stainless (\blacksquare) steels.

$$: (T^{\text{tr}}_{\alpha \rightarrow \gamma} - T^{\text{liq}}_{\gamma \rightarrow \delta})$$

$$k^{\text{eff}}_{\text{T}} (\text{Wm}^{-1}\text{K}^{-1}) = 25.4 + 0.013(T - T^{\text{tr}}_{\alpha \rightarrow \gamma}) \dots (40)$$

Values of k for the liquid phase were obtained by assuming that (i) $k^{\text{m}}(l)/k^{\text{m}}(s) = 1.07 = R^{\text{m}}(s)/R^{\text{m}}(l)$ (ii) the WFL Rule applied and (iii) the temperature coefficient $(dk/dT) = 0.015 \text{ Wm}^{-1}\text{K}^{-2}$.¹⁴⁾ The calculated values of $k^{\text{eff}}_{\text{T}}$ for low alloy and austenitic stainless steels are shown in Fig. 4(a) and the equivalent thermal diffusivity values are given in Fig. 4(b). It can be seen from Fig. 4(a) that (i) $k_{\alpha} > k_{\gamma}$ for temperatures between 298 K and 1 000 K (ii) the temperature coefficient (dk/dT) is negative in ferrite but is positive in both austenite and the liquid (iii) there is a small decrease in thermal conductivity and diffusivity on fusion.

Stainless steels

Values of k^{eff}_{298} can be calculated by deriving values for k^{el} using a combination of Eqs. (35)–(38). The values of k_{T} for austenitic steels are little affected by changes in chemical composition, so values of k_{T} above 1 100 K can be calculated using Eq. (37). Alternatively, k^{eff} can be calculated for austenitic stainless steels by using Eq. (41) for temperatures between 298 K and T_{liq} .¹³⁾

Austenitic :

$$k^{\text{eff}}_{\text{T}} (\text{Wm}^{-1}\text{K}^{-1}) = 9.2 + 0.0175 T - 2 \times 10^{-6} T^2 \dots (41)$$

Values of the thermal conductivities of ferritic stainless steels are also little affected by differences in concentrations of the alloying elements. However, ferritic stainless steels undergo a magnetic transition at *ca.* 1 000 K so two equations are needed to describe the temperature dependence of k . Thus Eqs. (42) and (43), respectively, describe k values in the temperature ranges (298–1 100 K) and (1 100– T_{liq} K). Uncertainties of $\pm 5\%$ and $\pm 10\%$ in the k values were reported for austenitic and ferritic stainless steels, respectively.

Ferritic (298–1 100 K) :

$$k^{\text{eff}}_{\text{T}} (\text{Wm}^{-1}\text{K}^{-1}) = 23.5 + 0.016(T - 298) \dots (42)$$

Ferritic (1 100– T_{liq}) :

$$k^{\text{eff}}_{\text{T}} (\text{Wm}^{-1}\text{K}^{-1}) = 25.4 + 0.013(T - 1 100) \dots (43)$$

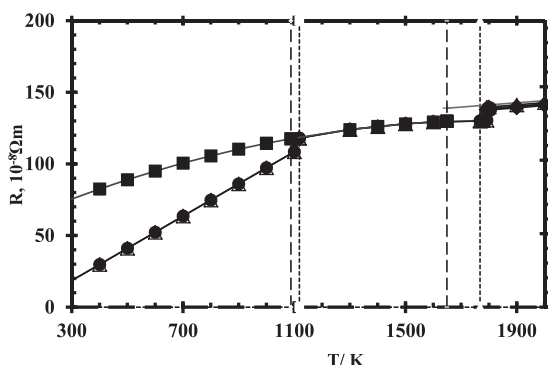


Fig. 4. The electrical resistivity (in $10^{-8} \Omega \text{ m}$) as a function of temperature for a low alloy steel (●) and an austenitic stainless steel (■).

2.6.2. Thermal Diffusivity (a)

The thermal diffusivity values (a^{eff}) are derived from the calculated values of C_p , ρ and k and the relation $a = (k/C_p \rho)$. The calculated values for the thermal diffusivity are given in Fig. 4(b). It should be noted that experimental values of thermal diffusivity show a sharp valley around 1 000 K due to the peak in C_p caused by the magnetic transition. The calculated C_p values do not contain this C_p peak; thus there is no pronounced valley in the calculated thermal diffusivity values.

Electrical resistivity (R) and conductivity (κ)

There is little demand for electrical resistivity values in the modelling of the continuous casting process. However, electrical resistivity values are calculated in the derivation of thermal conductivity values and electrical resistivity data for steels are needed for other steelmaking processes. Electrical resistivity values are cited in units of $10^{-8} \Omega \text{ m}$ (*i.e.* $70 \times 10^{-8} \Omega \text{ m} = 700 \text{ n}\Omega \text{ m}$).

Low alloy steels

The electrical resistivity of a steel at 298 K is calculated using Eqs. (36) to (38). Austenitic steels have a higher resistivity than ferritic steels. At high temperatures the values of electrical resistivity are little affected by chemical composition so constant values for specific temperatures can be adopted with little loss in accuracy. Values for the liquid can be calculated with an uncertainty of $\pm 10\%$ using Eq. (44) where R_i^{m} is the electrical resistivity at T_{liq} for the alloying constituents (*e.g.* Fe, Mn, Si *etc.*). However, $R^{\text{m}}(l)$ values can be calculated from the calculated $R^{\text{m}}(s)$ value and the relation $R^{\text{m}}(s)/R^{\text{m}}(l) = 1.07$ (*i.e.* equal to that for pure Fe¹⁴⁾); these latter values are considered to be more reliable and have been adopted.

$$R^{\text{m}}_{\text{steel}} (10^{-8} \Omega \text{ m}^{-1}) = \sum_{i=1}^N (X_i R_i^{\text{m}}) \dots (44)$$

Stainless steels

The electrical resistivities are calculated for austenitic and ferritic steels using Eqs. (45) and (46), respectively.¹³⁾

Austenitic :

$$R(10^{-8} \Omega \text{ m}^{-1}) = 51.9 + 8.6 \times 10^{-2} T - 2.35 \times 10^{-5} T^2 \dots (45)$$

Ferritic :

$$R(10^{-8} \Omega \text{ m}^{-1}) = 23.8 + 12.9 \times 10^{-2} T - 4.17 \times 10^{-5} T^2 \dots (46)$$

2.7. Viscosity (η)

Low alloy steels

The experimental uncertainties for measurements on pure iron are about $\pm 0.5 \text{ m Pas}$ or about $\pm 10\%$. Steels are less pure and contain non-metallic inclusions which increase the viscosity; thus experimental uncertainties associated with viscosity measurements on steels are probably *ca.* $\pm 20\%$. With this level of experimental uncertainty it is difficult to determine the effect of alloy concentrations (*e.g.* Si%, C%) on the viscosity. For this reason, the viscosity of steel was taken to be that of pure iron (given by Eq. (47)).¹⁴⁾ However, this relation was amended (see Eq. (48)) to allow for the effects of (i) alloying elements and (ii) non-metallic inclusions on the viscosity. The calculated results are shown in Fig. 5.

$$\eta_{Fe} \text{ (mPas)} = 0.1896 \exp (6\ 206.5 / T) \dots\dots\dots (47)$$

$$\eta_{steel} = 1.1 \eta_{Fe} \dots\dots\dots (48)$$

Stainless steels

The following relation was derived from measurements of the viscosity of a stainless steel using oscillation viscometry.^{13,17)}

$$\ln \eta \text{ (mPas)} = -2.396 + (7\ 950 / T) \dots\dots\dots (49)$$

It can be seen from Fig. 5 that the viscosity values calculated for the two steels using the different methods lie within $\pm 10\%$ of one another.

2.8. Surface Tension (γ_m) and Interfacial Tension (γ_{ms})

Surface tension of steel (γ_m)

The surface tension of steel (γ) and its temperature dependence ($d\gamma/dT$) are both very sensitive to the concentrations (ppm levels) of *soluble* O and S contents of the steel. However, most steels contain Al contents of > 50 ppm, and these Al levels are sufficient to hold the *soluble* O content to *ca.* 5 ppm. Most alloying elements have little effect on the *soluble* S levels (the exceptions being Ca and the rare-earths). For this reason, the *soluble* S content approximates to the total S content. Thus, the surface tensions of steels are sensitive to the S content of the steel. Consequently, Eq. (50) due to Su¹⁸⁾ has been used to calculate the surface

tensions of liquid iron. The effects of alloying elements can be taken into account by (i) using density data for the elements and the method of Butler¹⁹⁾ or (ii) by using a partial molar approach for the alloy (excluding the S,O *i.e.* ($\gamma_{alloy} = \sum_{i=1}^N (X_i \gamma_i)$).²⁰⁾ However, the densities and surface tensions of the principal alloying elements tend to be similar to those of iron. Consequently, the simplified relation shown in Eq. (50) can be used for steels without much loss of accuracy.

$$\gamma \text{ (mNm}^{-1}\text{)} = 1\ 880 - 0.41(T - 1\ 803 \text{ (K)}) - 0.009T \ln \left(1 + e^{\frac{19\ 411}{T} - 4.6849} \times (\text{wt}\%S) \right) \dots\dots (50)$$

The calculated surface tension values for low alloy and stainless steels are shown in Fig. 6. It can be seen that:

- (i) The surface tension decreases with increasing S content.
- (ii) The temperature coefficient ($d\gamma/dT$) becomes increasingly positive with increasing c S content; ($d\gamma/dT$) is negative for 10 and 20 ppm S but is slightly positive for 50 ppm S but becomes progressively more positive with increasing S contents.

Stainless steels

A similar relation (Eq. (51)) has been reported which allows the surface tension of stainless steels to be calculated.^{13,21)} The temperature coefficient ($d\gamma/dT$) can be calculated using Eq. (52).

$$\gamma \text{ (mNm}^{-1}\text{)} = 1\ 840 - 0.4(T - 1\ 823 \text{ K}) - 0.056 \ln \{ 1 + e^{[(28\ 798/T) - 8.5647]} (0.68 \text{ wt}\%S) \} \dots\dots\dots (51)$$

$$(d\gamma / dT) = -0.4 - 0.056 \{ [28\ 798(1 - B) / BT] + \ln B \} \dots\dots (52)$$

Where $B = 1 + e^{[(28\ 798/T) - 8.5647]} (0.68 \text{ wt}\%S)$

Interfacial energy or surface tension (γ_{msl})

The interfacial *energy or interfacial tension* (γ_{msl}) is calculated from Eq. (53) where γ_{sl} = slag surface tension, γ_m can be derived from Eq. (34) and ϕ is an interaction coefficient, the magnitude of which was calculated in Part 1 (Eqs. (44)–(46)). The value of γ_{msl} is largely determined by γ_m since $\gamma_m \approx (4 \text{ to } 5) \gamma_{sl}$ and the value of γ_m , in turn, is largely determined

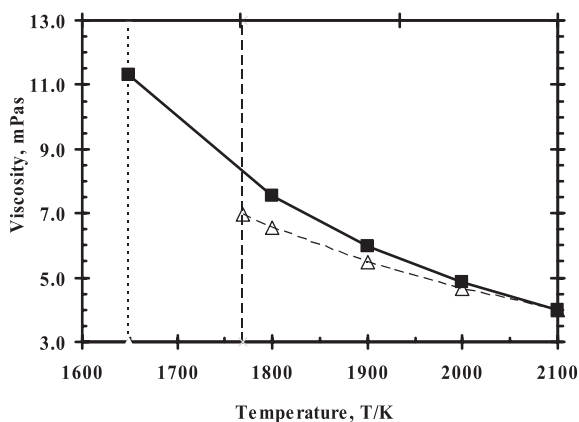


Fig. 5. Calculated values for the viscosities of a low alloy steel (Δ) and stainless steel (\blacksquare) as a function of temperature.

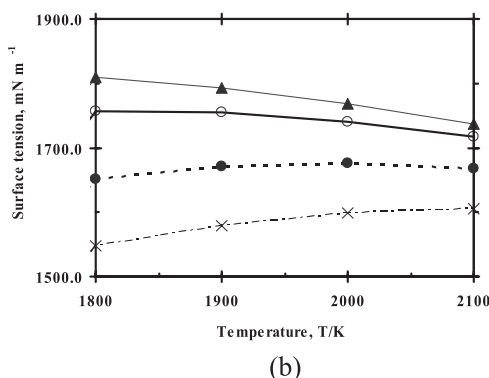
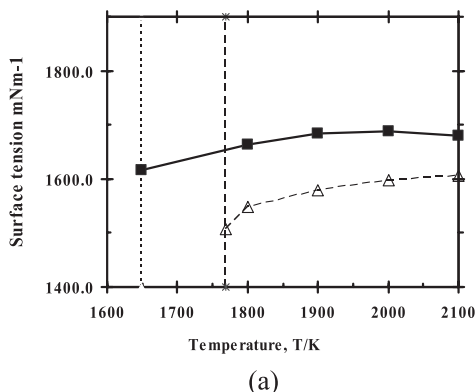


Fig. 6. Calculated values of surface tension as a function of temperature for (a) a low alloy containing 100 ppm S (Δ) and austenitic stainless steel containing 50 ppm S (\blacksquare) and (b) for steels with identical composition but containing different S contents: 10 ppm= \blacktriangle ; 20 ppm= \circ ; 50 ppm= \bullet ; and 100 ppm= \times .

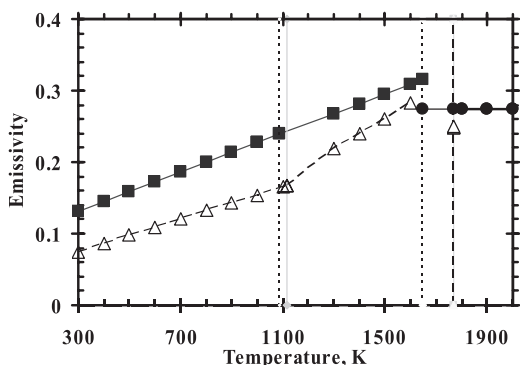


Fig. 7. Calculated values of the total normal emissivity as a function of temperature for a low alloy steel (Δ), an austenitic stainless steel (\blacksquare)^{22,23} and liquid steel (\bullet).

by the S content of the steel.

$$\gamma_{\text{msl}} = \gamma_m + \gamma_{\text{sl}} - 2\varphi(\gamma_m\gamma_{\text{sl}})^{0.5} \dots\dots\dots (53)$$

2.9. Emissivity (ϵ)
Low alloy steel

Emissivity is also a surface property. In practice, it is affected by the nature of the oxides formed in the surface layers with ϵ values varying from (0.1–0.3) for high vacuum conditions to 0.7 for oxidised conditions. Consequently, the emissivity values are affected by the partial pressure of oxygen (p_{O_2}). Since the atmosphere in the continuous casting mould is very reducing, the emissivity values reported here refer to low p_{O_2} values. The values of the total normal emissivity (ϵ_{TN}) of pure Fe¹⁴) were adopted for the steel; the following relations were used: The calculated values for a low alloy steel are shown in Fig. 7.

$$298 \text{ K} - T_{\alpha \rightarrow \gamma} : \alpha - \text{Fe} : \epsilon_{\text{TN}} = 0.075 + 0.000113(T - 298) \dots\dots\dots (54)$$

$$T_{\alpha \rightarrow \gamma} \rightarrow T_{\gamma \rightarrow \delta} : \gamma - \text{Fe (austenite)} : \epsilon_{\text{TN}} = 0.075 + 0.000208(T - T_{\alpha \rightarrow \gamma}) \dots\dots\dots (55)$$

$$T_{\gamma \rightarrow \delta} \rightarrow T_{\delta \rightarrow \text{liq}} : \delta - \text{Fe} : \epsilon_{\text{TN}} = 0.235 + 0.000136(T - T_{\gamma \rightarrow \delta}) \dots\dots\dots (56)$$

$$T > T_{\text{liq}} : \text{liquid} : \epsilon_{\text{TN}} = 0.275 \dots\dots\dots (57)$$

Stainless steel

Total normal emissivity values^{22,23}) reported for an austenitic, stainless steel are higher than those cited for low alloy steels; these data can be represented by Eq. (58). It can be seen that the values are in good agreement with the values for austenite in the low alloy steel.

$$\epsilon_{\text{TN}} = 0.122 + 0.0001(T - 298) \dots\dots\dots (58)$$

It can be seen from Fig. 7 that ϵ_{TN} values for the austenitic stainless steel are higher than those for the low alloy, peritectic steel.

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Symbols, Abbreviations, Units

- a= Thermal diffusivity (m^2s^{-1})
- C_p = Heat capacity ($\text{JK}^{-1}\text{kg}^{-1}$)
- H= Enthalpy (J kg^{-1})
- k= Thermal conductivity ($\text{Wm}^{-1}\text{K}^{-1}$)
- R= Electrical resistivity ($10^{-8}\Omega \text{ m}^{-1}$)
- T= Temperature (K)
- X= mole fraction
- α = Thermal expansion coefficient (K^{-1})
- γ = Surface tension (mNm^{-1})
- ϵ_{TN} = Total normal emissivity
- η = Viscosity (Pas)
- κ = Electrical conductivity ($10^{-8} \Omega\text{m} = 10\text{n}\Omega\text{m}$)
- ρ = Density (kgm^{-3})

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Appendix

User to Insert

a) Composition: %Fe; %Cr; %Ni; %Mo; %Ni; %Si; %Ti; %V; %Al; %Co; %C; %S; %O; %Ca; % Nb; %W. Note 5 ppm S=0.0005%.

b) T_{liq} and other T_{tr} values: Default values will be calculated (± 5 K) if no insert is made by the user.

Output

All calculated data as a function of temperature given on “Collected” Worksheet.