Effects of Alloying Elements on the Ferrite Potential of Peritectic and Ultra-Low Carbon Steels

Rahul SARKAR,1)* Arunava SENGUPTA,1) Vimal KUMAR2) and Shiv Kumar CHOUDHARY1)

1) Research and Development, Tata Steel, Jamshedpur, 831001 India.
2) Metallurgical and Materials Engineering Department, NIT Trichy, Tiruchirappalli, Tamil Nadu, 620015 India.

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Solidification of steels involving the peritectic reaction are inherently prone to longitudinal facial cracking during casting, owing primarily to the large volume shrinkage associated with delta-ferrite to austenite transformation occurring at high temperatures. Therefore casting of those steels requires a lot of caution. Ferrite Potential (FP) is widely accepted as a measure of the tendency of steels to form delta-ferrite during solidification. However, the most commonly used definition of Ferrite Potential is strictly applicable only to plain carbon steels while commercial steels may contain several other alloying elements. Therefore, the existing definition may not express their actual Ferrite Potential. In view of this, a new correlation has been developed in the present work for evaluating the true Ferrite Potential for multi-component steels.

Influences of several common alloying/solute elements have been considered while developing the present model. Present model development involved rigorous thermodynamic calculations aimed at determining the interactions among various solute elements and their overall influence on the peritectic compositions and the peritectic transformation temperature. In addition, assumed quadratic dependence of peritectic compositions and temperature on the concentrations of alloying elements has been employed besides the application of non-linear multi-variate regression analysis. Finally, present correlations have been extensively validated against literature data as well as actual plant observations. In comparison to other models, reasonably better agreement between the current model predictions and plant data has been obtained. The present model has helped the plant operators in selecting the right parameters for casting operations.

KEY WORDS: steel; peritectic transformation; Ferrite Potential; longitudinal crack; continuous casting; alloying elements.

1. Introduction

Continuous casting of steel slabs having composition close to the peritectic point is often difficult as compared to other grades. These steels undergo the peritectic (L + δ → γ) transformation during solidification,1) which is accompanied by large volume shrinkage since the molar volume of γ(austenite) is considerably less than that of both liquid (L) and delta-ferrite (δ) phases. The temperature range in which this shrinkage occurs corresponds to the so-called zero-ductility-temperature range where the ductility of steels is very low and hence peritectic grades of steel are extremely prone to cracking. Thus, casting of such steels requires special precautionary measures like casting at a speed some 20% lower than that of ordinary carbon grades and using special type of mould fluxes.2)

As the propensity of cracking depends upon the extent of peritectic transformation, the tendency of steels to form delta-ferrite (δ) during solidification is an important parameter in continuous casting operations. This tendency is often measured in terms of its Ferrite Potential (FP) which is defined as3):

$$FP = 2.5 \times [0.5 - \frac{\%C}{25}]$$

where [%C] is the mass percent of carbon in steel and the constant terms (2.5, 0.5) are determined in such a way that FP satisfies the following criteria:

$$1 \text{ when } [%C] = C_A$$
$$FP = 0 \text{ when } [%C] = C_C$$
$$0.8 \text{ when } [%C] = C_B$$

where $C_A = 0.1$, $C_B = 0.18$ and $C_C = 0.5$ for simple Fe–C systems (Fig. 1).

Based on this definition of FP, plain carbon steels have been classified into two major categories:3)

- Depression Grades: 0.8 < FP < 1.0
- Sticker Grades: FP < 0 or FP > 1.0

It is the casting of depression grades that is more problematic, since they are more prone to longitudinal cracks as compared to the sticker grades. Therefore, in order to ensure smooth casting operation it is important to correctly classify peritectic steels into depression and sticker grades based on their chemical compositions.
The above expression of Ferrite Potential (Eq. (1)) is strictly valid only for plain carbon steels. Commonly, commercial steels are multi-component alloys of iron containing various alloying elements other than carbon. These elements may alter the peritectic transformation behaviour of steels by shifting the peritectic compositions \((C_A, C_B, C_C)\) either to the left or to the right and thereby affect their actual Ferrite Potential. Earlier efforts to determine the effects of alloying elements on Ferrite Potential consisted of simply replacing the \([\%C]\) in the definition of Ferrite Potential with carbon equivalent \([\%C_e]\) where \([\%C_e]\) may be obtained from one of the available correlations. But strictly speaking, in presence of other elements all the relevant peritectic compositions get shifted from their original values and replacing only \([\%C]\) with \([\%C_e]\) would not suffice. Rather, the definition of Ferrite Potential itself needs modification and a general expression based on composition dependent values of \(C_A, C_B, C_C\) needs to be developed.

Preliminary attempts in determining the effects of alloying elements on the peritectic compositions and temperatures based on thermodynamics were made by Kagawa et al. More recently, efforts have been made to determine the effects of alloying elements on \(C_A\) and \(C_B\) through development of peritectic predictor equations using computational thermodynamic approaches. However, in none of the existing models/correlations effects of all types of alloying elements on the peritectic transformation have been considered. Also while such correlations seem to give good predictions in their respective composition ranges, the universality of these correlations is questionable since they are mostly regression based models. Insufficient information is available in literature on the effects of various alloying elements on the peritectic transformation behaviour of multicomponent steels, particularly those commercially produced at Tata Steel, India. In the new peritectic predictor model, equations for all the three relevant compositions marked in Fig. 2 (i.e. \(C_A, C_B\) and \(C_C\)) as well as the peritectic transformation temperature \(T_P\) (which also plays an important role in casting operations) have been developed. Finally, the predicted results were validated against plant data for checking their reliability.

2. Formulation

In general, the Ferrite Potential (FP) of an alloy-steel can be expressed by the following equation:

\[
FP = \left( \frac{C_C - [\%C]}{C_C - C_A} \right) \]

where, \(C_C\) is the carbon content of the steel.

The classification based on FP should be done as:

- **Depression Grades:** for \((C_C - C_B)/(C_C - C_A) < FP < 1\)
- **Sticker Grades:** for \(0 < FP < (C_C - C_B)/(C_C - C_A)\) or \(FP > 1\)

The compositions \(C_A\), \(C_B\) and \(C_C\) can be calculated from actual steel compositions.

2.1. Expressions for Composition Dependence of Peritectic Compositions and Temperature

In the present work, actual peritectic carbon compositions for multi-component steels (i.e. \(C_A\), \(C_B\) and \(C_C\)) have been assumed to have a quadratic dependence on the concentrations of the alloying elements and can be expressed by the following correlation:

\[
C = C_0 + \sum a_i [\%i] + \sum b_{ij} [\%i][\%j] + \sum c_i [\%i]^2 \]

where, \(C\) = actual peritectic carbon composition for multi-component steels

\(C_0\) = peritectic carbon composition for pure Fe–C binary system

\(a_i\) = coefficient of the first order concentration term for the alloying element \(i\)

\(b_{ij}\) = coefficient of the second-order concentration term containing the product of the concentration of alloying element \(i\) with that of \(j\)
\[ c_{ii} = \text{coefficient of the second order concentration term containing the square of the concentration of alloying element } i. \]

Besides composition, alloying elements also affect the peritectic transformation temperature \( (T_P) \). In fact, in the presence of certain alloys in higher proportion the peritectic transformation occurs over a range of temperatures rather than at a fixed temperature. Consequently, a three-phase \( L + \delta + \gamma \) appears in the phase diagram which is schematically shown in Fig. 2. The effects of alloying elements on the peritectic start temperature \( (T_{P, s}) \) have also been investigated in the present work. Following the same approach, \( T_{P, s} \) is expressed as a quadratic function of the concentration of elements:

\[ T_{P, s} = T_P + \sum d_i \% [i] + \sum \sum e_{ij} \% [i] \% [j] + \sum f_i \% [i]^2 \] ........................................ (4)

Where \( T_P = \) equilibrium peritectic transformation temperature for pure Fe–C system

\( d_i = \) coefficient of first order concentration term for an alloying element \( i \)

\( d_{ij} = \) coefficient of second-order concentration term containing the product of concentrations of alloying elements \( i \) with that of \( j \)

\( e_{ii} = \) coefficient of second order concentration term containing the square of the concentration of element \( i \).

Equations (3) and (4) constitute the theoretical expressions for the actual peritectic predictor equations considered in the present work for steels containing various solute elements besides carbon.

3. Results and Discussion

3.1. Selection of Alloying Elements and their Composition Ranges

In the present calculations, the effects of 12 elements relevant to grades manufactured in Tata Steel, India have been investigated using ThermoCalc Version S (TCCS®) and TCFE7 database. The combined effects of these elements have been evaluated through several thermodynamic and regression based calculations. The composition ranges of solute elements are shown Table 1. Also, an index number has been assigned to each element in order to facilitate its reference later in the text, as shown in Table 1.

Out of these 12 elements, elements 1–7 are commonly present in almost all steels in varying quantities (Table 1). These elements are expected to affect the peritectic compositions and temperature not only because of their individual effects but also due to the interactions amongst them. We refer to these elements as primary alloying elements. Elements 8–12 on the other hand, are present only in some of the grades. Commonly, they are present in relatively much smaller proportions as compared to the primary alloying elements. Thus, although each one of them may have some effect on the peritectic compositions and temperature, the interaction amongst them as well as with the primary alloying elements can be neglected due to their small concentrations in steel. Those elements have been referred to as secondary alloying elements in the present case.

<table>
<thead>
<tr>
<th>Index</th>
<th>Element</th>
<th>Min. Comp. (wt.%)</th>
<th>Max. Comp. (wt.%)</th>
<th>Avg. Comp. (wt.%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Mn</td>
<td>0.13</td>
<td>1.4</td>
<td>0.765</td>
</tr>
<tr>
<td>2</td>
<td>Si</td>
<td>0.001</td>
<td>0.4</td>
<td>0.2005</td>
</tr>
<tr>
<td>3</td>
<td>Cr</td>
<td>0.001</td>
<td>0.46</td>
<td>0.2305</td>
</tr>
<tr>
<td>4</td>
<td>Ni</td>
<td>0.001</td>
<td>0.25</td>
<td>0.1255</td>
</tr>
<tr>
<td>5</td>
<td>Al</td>
<td>0.01</td>
<td>0.09</td>
<td>0.05</td>
</tr>
<tr>
<td>6</td>
<td>S</td>
<td>0.002</td>
<td>0.025</td>
<td>0.0135</td>
</tr>
<tr>
<td>7</td>
<td>P</td>
<td>0.01</td>
<td>0.09</td>
<td>0.05</td>
</tr>
<tr>
<td>8</td>
<td>Mo</td>
<td>0.001</td>
<td>0.011</td>
<td>0.0055</td>
</tr>
<tr>
<td>9</td>
<td>N</td>
<td>0.004</td>
<td>0.01</td>
<td>0.007</td>
</tr>
<tr>
<td>10</td>
<td>V</td>
<td>0.001</td>
<td>0.06</td>
<td>0.0305</td>
</tr>
<tr>
<td>11</td>
<td>Ti</td>
<td>0.001</td>
<td>0.02</td>
<td>0.0105</td>
</tr>
<tr>
<td>12</td>
<td>Nb</td>
<td>0.001</td>
<td>0.05</td>
<td>0.0255</td>
</tr>
</tbody>
</table>

3.2. Effect of Individual Elements on Peritectic Compositions and Temperature

In order to determine the influence of each element on the peritectic compositions and temperature, a large number of pseudo binary Fe-C-\( i \) phase diagrams were generated using ThermoCalc Version S (TCCS®) and TCFE7 database for each element \( (i.e. \ i) \) for their respective composition ranges as shown in Table 1. The corresponding relative deviation with respect to pure Fe–C binary was determined for each case.

3.2.1. Effect of Mn, Si, Cr and Ni

The effects of these four elements on peritectic compositions and temperature are shown in Figs. 3(a)–3(d). Mn and Ni being austenite stabilizers, shift all the three relevant peritectic compositions \( (i.e. \ C_A, C_B \) and \( C_C \) ) to the left. Si being a ferrite stabilizer, its effect is just opposite to that of Mn and Ni. Thus it shifts all the above three compositions towards the right in the pseudo-binary phase diagrams. The effect of Cr on the peritectic compositions is somewhat incongruous. Cr being ferrite-stabilizer shifts \( C_B \) to the right as expected. However, Cr shifts both \( C_A \) and \( C_C \) to the left, as can be seen in Figs. 3(a)–3(c).

It is evident from Fig. 3(d) that Si has the most significant effect on \( T_{P,s} \). It considerably decreases the \( T_{P, s} \) temperature which is congruent with its tendency to stabilize ferrite. Ni being an austenite stabilizer increases \( T_{P, s} \) but its effect on \( T_{P, s} \) was found to be less pronounced. In the composition ranges presently considered, Cr hardly had an impact on \( T_{P, s} \). Manganese being an austenite stabilizer is expected to increase \( T_{P, s} \). However, in the chosen composition range Mn was found to slightly decrease the peritectic transformation temperature \( (T_{P, s}) \).

3.2.2. Effect of Al, S and P

Figures 4(a), 4(b) and 4(c) show the effects of Al, S and P on the peritectic compositions. Al being a ferrite-stabilizer shifts all the three compositions to the right. The individual effect of P on the peritectic compositions was found to relatively insignificant. However as will be discussed later, in presence of other elements especially Mn, P was found to
have a noticeable effect on the peritectic compositions and temperature. Sulfur seemed to have quite a significant effect on the peritectic compositions. Presence of S even in concentrations low (<0.025%) was found to influence the peritectic compositions $C_A$ and $C_B$ significantly by shifting them towards the left in the phase diagram. The effect of S on $C_C$ was found to be relatively less pronounced but nonetheless it also shifts $C_C$ to the left.

In the composition range considered, Al did not seem to have an effect on $T_{P_S}$. The effect of S on $T_{P_S}$ is not significant but the presence of S, even in very small quantities promotes the formation of $L + \delta + \gamma$ region. Congruent with its tendency to stabilise ferrite, P was found to decrease $T_{P_S}$ as shown in Fig. 4(d).
3.2.3. Effect of Mo, N, V, Ti and Nb

As evident from Table 2, Mo was found to have practically no effect on $C_A$, $C_B$ or $C_C$. Influence of elements N, V, Ti and Nb on $C_A$, $C_B$, $C_C$ and $T_{PS}$ are shown in Figs. 5(a)–5(d). Nitrogen being a strong austenite stabiliser shifts $C_A$, $C_B$ and $C_C$ towards the left. On the other hand, V, Ti, and Nb are all carbide formers and hence tend to stabilize the ferrite phase. But in the small composition ranges considered here, these elements could combine with only a very small amount of carbon and most of the carbon still remained in the solid solution. Thus, their ability to stabilize ferrite was found to be limited. V shifted $C_A$, $C_B$ and $C_C$ to the right and its effect on $C_C$ was more significant as compared to those on $C_A$ and $C_B$. Ti was observed to have very little effect on $C_A$, $C_B$ and $C_C$. Nb shifted both $C_A$ and $C_B$ towards left while its effect on $C_C$ was found to be less significant and can be neglected for all practical purposes. The effects of V, Ti and Nb on $T_{PS}$ were comparable and all of them tended to decrease $T_{PS}$.

3.3. Evaluation of Constants of Peritectic Predictor Equations

The effects of individual elements on the peritectic compositions and temperature have been discussed in Section 3.2. To determine the combined effects of these elements, a total of 298 pseudo-binary phase diagrams containing all the 12 pertinent elements have been constructed using ThermoCalc Version S (TCCS®) and TCFE7 database. Subsequently, coefficients of peritectic predictor equations were calculated using multi-variate non-linear regression analyses.

### 3.3.1. Rationale Behind Selecting Terms in Peritectic Predictor Equations

From Eq. (3):

$$C = C_0 + \sum a_i \% i + \sum \sum b_{ij} \% i \% j + \sum c_{ii} \% i^2$$

Differentiating Eq. (3) with respect to $\% i$, for a particular $i$ we get:

$$\frac{\partial C}{\partial \% i} = a_i + \sum b_{ij} \% j + 2 c_{ii} \% i$$ \hspace{1cm} (5)

If $\% j = 0$, Eq. (5) reduces to:

$$\frac{\partial C}{\partial \% i} = a_i + 2 c_{ii} \% i$$ \hspace{1cm} (6)

From Eqs. (5) and (6) the following can be easily deduced:
- First, if $\% i = C$ curves at constant $\% j$ are straight lines, then $c_{ii}$s are all zeros.
- Second, if the slopes of $\% i = C$ curves at constant $\% j$ and at $\% j = 0$ are equal then $b_{ij}$s are all zeros.

In order to select the appropriate second order terms for peritectic predictor equations a large number of Fe-C-$i$(at constant $\% j$) and Fe-C-$i$-$j$(at constant $\% i$ and $\% j$) phase diagrams were constructed (where $i$ and $j$ represent different alloying elements considered in this study). All the different combinations of $i$ and $j$ have been considered. From different plots of $\% i = C$ at constant $\% j$ and $\% i = T_{PS}$ using the information from Eqs. (5) and (6), the necessary second-order concentration terms have been selected. It has been found that among all the different sec-

### Table 2. Effects of molybdenum on peritectic compositions and temperature.

<table>
<thead>
<tr>
<th>Mo (wt. %)</th>
<th>$C_A$</th>
<th>$C_B$</th>
<th>$C_C$</th>
<th>$T_{PS}$ (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.001</td>
<td>0.09274</td>
<td>0.17162</td>
<td>0.52729</td>
<td>1494.773</td>
</tr>
<tr>
<td>0.01</td>
<td>0.09279</td>
<td>0.17178</td>
<td>0.52785</td>
<td>1494.6933</td>
</tr>
</tbody>
</table>

Percent Shift

| 0.05885 | 0.09257 | 0.10691 | 0.00533 |

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**Fig. 5.** Effect of N, V, Ti and Nb on: (a) $C_A$; (b) $C_B$; (c) $C_C$ and (d) $T_{PS}$ (Online version in color.)
ond-order concentration terms, only four of them have significant effects on $C_A$, $C_B$ and $C_C$. Three out of these four terms involve the products of the concentration of Mn with Si, S and P while the fourth one is the square of the concentration of Mn. Thus only these four second order terms are retained in the equations for $C_A$, $C_B$ and $C_C$ and other terms are neglected. Similarly for $T_{P,s}$, it has been observed that only the second-order term involving the products of the concentration of Mn and P has a significant effect on $T_{P,s}$. As before, this term has been retained while the other second-order terms have been neglected in the equation for $T_{P,s}$.

The final predictor equations thus developed may be represented as follows:

$$C = C_0 + \sum a_i \times \left[ \% i \right] + b_{12} \times \left[ \% Mn \right] \times \left[ \% S \right] + b_{65} \times \left[ \% Mn \right] \times \left[ \% P \right] + c_{11} \times \left[ \% Mn \right]^2$$

$$T_{P,s} = T_F + \sum d_i \times \left[ \% i \right] + e_{17} \times \left[ \% Mn \right] \times \left[ \% P \right]$$

3.3.2. Final Predictor Equations

Total of 298 pseudo-binary Fe–C phase diagrams were generated using ThermoCalc Version S and TCFE7 database. Constant terms for the predictor equations have been estimated using non-linear multi-variate regression and the final peritectic predictor equations have been obtained as follows (Eqs. (9)–(12)). The ranges of application are shown in Table 1. High values of $R^2$ (Figs. 6(a)–6(d)) for all the correlations indicate excellent agreement between the calculated and the predicted values.

$$C_A = 0.0927 + 0.0471 \times \left[ \% Mn \right] - 0.0859 \times \left[ \% Si \right] - 0.0237 \times \left[ \% Ni \right] - 0.5429 \times \left[ \% S \right] - 0.3553 \times \left[ \% N \right] - 0.0361 \times \left[ \% Ti \right] - 0.0136 \times \left[ \% Nb \right] + 0.0106 \times \left[ \% V \right] + 0.1097 \times \left[ \% Mn \right] \times \left[ \% Si \right] - 5.6239 \times \left[ \% Mn \right] \times \left[ \% S \right] - 0.0165 \left[ \% Mn \right]^2$$

$$\left( R^2 = 0.996 \right)$$

$$C_B = 0.1716 - 0.0589 \times \left[ \% Mn \right] - 0.1776 \times \left[ \% Si \right] - 0.0053 \times \left[ \% Cr \right] - 0.0410 \times \left[ \% Ni \right] + 0.0473 \times \left[ \% Al \right] - 0.9453 \times \left[ \% S \right] - 0.0160 \times \left[ \% P \right] - 0.6884 \times \left[ \% N \right] - 0.0283 \times \left[ \% Ti \right] - 0.0147 \times \left[ \% Nb \right] + 0.0285 \times \left[ \% V \right] + 0.2342 \times \left[ \% Mn \right] \times \left[ \% Si \right]$$

$$\left( R^2 = 0.992 \right)$$

$$C_C = 0.5274 - 0.0124 \times \left[ \% Mn \right] - 0.1424 \times \left[ \% Si \right] - 0.0154 \times \left[ \% Cr \right] - 0.0981 \times \left[ \% Ni \right] + 0.0934 \times \left[ \% Al \right] - 0.3871 \times \left[ \% S \right] - 0.0553 \times \left[ \% P \right] - 2.0916 \times \left[ \% N \right] + 0.1226 \times \left[ \% V \right] + 0.2363 \times \left[ \% Mn \right] \times \left[ \% Si \right] + 0.0729 \times \left[ \% Mn \right] \times \left[ \% P \right] - 0.05 \times \left[ \% Mn \right]^2$$

$$\left( R^2 = 0.993 \right)$$

$$T_{P,s} = 1.494.643 - 18.846 \times \left[ \% Si \right] - 1.295 \times \left[ \% Cr \right] - 71.433 \times \left[ \% S \right] - 55.847 \times \left[ \% P \right] + 87.915 \times \left[ \% N \right] - 12.138 \times \left[ \% Ti \right] - 12.175 \times \left[ \% Nb \right] - 11.283 \times \left[ \% V \right] + 79.916 \times \left[ \% Mn \right] \times \left[ \% P \right]$$

$$\left( R^2 = 0.996 \right)$$

3.4. Validation of Regression Models

Correlations developed in the present work have been validated against the literature data as well as plant data.

![Fig. 6. Comparison between the calculated and predicted values of: (a) $C_A$, (b) $C_B$, (c) $C_C$ and (d) $T_{P,s}$.](image-url)
One-year data on longitudinal cracks observed in various slabs were collected and critically examined and used for the validation of the present work.

3.4.1. Validation with Literature Data

The predictor equation for \(C_B\) has been compared with other existing correlations between \(C_B\) and composition developed by Xu et al.\(^5\) and Blazek et al.\(^6\) Figures 7(a)–7(c) show the co-relation between the calculated values of \(C_B\) and those predicted by the different models.\(^5,6\) The present model represents a greater value of \(R^2\) and a smaller value of RMSD (Root Mean Square Deviation). It can thus be concluded that in the composition ranges considered here, the present correlation fits the calculated data much better than any of the pre-existing models.

The reliability of the present predictor equations was also tested by comparing the calculated and predicted values of Ferrite Potential (FP). A steel sample having each alloying element in the average composition (Table 1) has been selected. The calculated values of FP as a function of \([\%C]\) are then plotted against the values predicted by three of the existing models and the current model. These three pre-existing models include the one based on the equation for plain carbon steels (Eq. (1)), one based on carbon equivalent formulation by Wolf\(^3\) and another based on Blazek’s et al.’s correlation.\(^6\) It is once again evident from Fig. 8 that the current model fits the calculated values of FP much better than other models.\(^3,6\) Also, it is interesting to note that for the steel sample considered here, the presence of alloying elements has shifted the carbon range for depression grades from an initial value of 0.1–0.18% to 0.055–0.11% (as demonstrated in Fig. 8) thereby elucidating the need for the classification of peritectic steels based on actual compositions rather than based solely on carbon percentage.

Direct validation of the regression model for \(T_{PS}\) was not possible since there is no literature available on the effects of alloying elements on \(T_{PS}\). However, Wang et al.\(^8\) proposed an equation for calculating the liquidus temperature \(T_{LIQ}\) from the concentration of its alloying elements. Noting that for \([\%C] = C_C, T_{LIQ} = T_{PS}\), the predicted values of \(T_{LIQ}\) (for \([\%C] = C_C\)) are plotted with calculated values of \(T_{PS}\) in Fig. 9.

From Fig. 9, it is evident that the calculated values correlate very well with those predicted by Wang et al.\(^8\) (the maximum deviation is <10°C). This difference might be due to two reasons. First of all, Wang et al.’s\(^8\) correlation does not take into account the effects of N while the alloys selected for calculations contained N in the range 40–100 ppm (Table 1). Nitrogen is expected to decrease \(T_{LIQ}\) still further but its effect cannot be quantified since there is no literature available on the effects of N on \(T_{LIQ}\). Secondly, the equation by Wang et al.\(^8\) have been derived by considering simple Fe-\(i\) binary systems while the present calculations have been done for actual pseudo binary systems containing all the alloying elements. Thus, the equation predicted by Wang et al.\(^8\) neglects the effects of interaction between different ele-
ments. A correction factor has later been introduced into the proposed equation to account for the interactions but the use of a constant term seems unreasonable because the interaction terms are expected to be strong functions of compositions. Hence the equation overestimates the values of $T_{\text{liq}}$ thereby accounting for the small difference between the calculated and the predicted values.

Further, to test the accuracy of the calculated phase diagrams, some of the measured values of liquidus temperature ($T_{\text{liq}}$) from Wang et al.\(^8\) and austenite formation temperature ($T_{\gamma}$) from Xu et al.\(^5\) have been compared with the calculated values for the same steel compositions (Tables 3 and 4) and plotted in Fig. 10.

As evident from Tables 3 and 4, there is reasonably good agreement between the measured and the calculated values (the deviation in all the cases being <10°C) which indicates that the present calculations done using TCCS® are correct. Also, the present set of calculated values for $T_{\gamma}$ correlates excellently with those calculated by Xu et al.\(^5\) using FactSage and both of these values are slightly higher than the measured values. This is because the calculated values are for equilibrium conditions while the measured data are for actual industrial (non-equilibrium) conditions. Under cooling rates relevant to industrial processes, $L + \delta \rightarrow \gamma$ transformation takes place at temperatures lower than the equilibrium

![Comparison between the calculated values of $T_{\text{liq}}$ with the values predicted using Wang et al.\(^8\)](Online version in color.)

<table>
<thead>
<tr>
<th>Steel Components, %</th>
<th>Measured Temp. (°C)</th>
<th>Calculated by Wang (°C)</th>
<th>Present Calculation (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C  Si  Mn  P  S  Ni  Cu  Mo  Cr</td>
<td>1508 1510 1516.72</td>
<td>1490 1494 1499.88</td>
<td>1486 1490 1496.41</td>
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<table>
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<tr>
<th>Steel composition (Mass %)</th>
<th>Measured Temp. (°C)</th>
<th>Calculated by Xu (°C)</th>
<th>Present Calculation (°C)</th>
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<tr>
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</table>
transformation temperature (Fig. 11). For the same reason, the calculated values of \( T_{\text{liq}} \) are also slightly higher than the measured values as evident from Table 4.

3.4.2. Validation with Plant Data

The regression models developed to predict peritectic behaviour is also validated using industrial data for slabs cast in LD2&SC, Tata Steel Jamshedpur Works over the past one year. Typical dimension of slabs cast is 11 m * 1 250 mm * 215 mm. The casting speed varies in the range of 1.2–1.7 m/min and the average casting speed is 1.5 m/min. Figure 12(a) shows a typical longitudinal crack observed in one of the low carbon steel slabs. Slabs in which longitudinal cracks were observed all contained carbon in the range 0.035–0.185%. This range was divided into 10 classes in intervals of 0.015% and in Fig. 12(b) the relative frequency of longitudinal cracks \( \eta \) is plotted against the carbon range for each class. This quantity \( \eta \) is defined as:

\[
\eta = \frac{\text{Number of slabs with longitudinal cracks in the specified carbon range}}{\text{Total number of slabs with longitudinal cracks}} \times 100\%
\]

It is evident from Fig. 12(b) that \( \eta \) is maximum in the range 0.095–0.11% and it decreases both to the left and also to the right of this range. Thus it can be concluded that in the composition ranges of different elements presently considered (Table 1), the tendency of slabs to develop longitudinal cracks is maximum when carbon is in the range 0.095–0.11%.

To correlate the industrial data on cracks with the peritectic behaviour, \( \eta \) is plotted against the deviation from peritectic composition (\( [\% C] - C_b \)) for different carbon ranges in Fig. 13 where \( C_b \) is calculated using Eq. (10). Also to compare the efficacy of the present model vis-à-vis other existing models, \( \eta \) is plotted against the values of this deviation (\( [\% C] - C_b \)) predicted by other available correlations in the same Fig. 13. Under non-equilibrium conditions the Fe–C phase diagram shifts down and \( C_b \) shifts to the left by \( \Delta C_b \) which has been shown schematically in Fig. 11. Hu et al.\(^9\) estimated the value of \( \Delta C_b \) for cooling rates relevant to thin slab casting. But in thick slab casting, the cooling rate of the solidifying shell is relatively lower and hence the \( \Delta C_b \) is smaller than that for thin slab casting. However, in the absence of any data on this shift \( \Delta C_b \) for thick slab casting, we start with the value of \( \Delta C_b \) reported by Hu et al.\(^9\) and then simulate it in our model to best-fit the industrial data for thick-slab casting. Presently, \( \Delta C_b = 0.02 \).

It is evident from Fig. 13 that if \( C_b \) is calculated using the
proposed correlation (Eq. (10)), \(\eta\) is maximum when the deviation from peritectic composition ([%C] - \(C_B\)) is zero. This is consistent with the industrial results because the tendency to develop longitudinal cracks is expected to be the greatest at the peritectic composition, that is when [%C] = \(C_B\).\(^{10}\) Xu et al.\(^{5}\) also reported that the propensity of longitudinal cracks is maximum when the value of this deviation ([%C] - \(C_B\)) is zero. However if \(C_B\) is calculated using any of the other existing correlations,\(^{5,6}\) \(\eta\) does not show a peak at [%C] = \(C_B\) which is not consistent with the industrial results. This happens because for the composition ranges considered here each of these correlations over-estimates \(C_B\) (Figs. 7(a), 7(b)) and hence the peak is obtained at some negative value of this deviation ([%C] - \(C_B\)). Thus, it is proved once again that the regression model developed in the present work is most appropriate for the chosen composition ranges and can thus be reliably used in the design and optimization of steel compositions for different applications. Furthermore, the results can be used as a reference for selecting the process parameters for continuous casting of low carbon as well as peritectic steels.

4. Conclusions

Salient features of the present work are as follows:

1) New correlation for evaluating the Ferrite Potential (FP) has been proposed taking into account the effects of various alloying elements on the peritectic transformation of multi-component steels.

2) Influence of various elements on the peritectic compositions (\(C_{A}\), \(C_B\) and \(C_C\)) and the peritectic start temperature (\(T_{PS}\)) has been investigated based on rigorous thermodynamic calculations.

3) While developing the current predictor equations (for \(C_{A}\), \(C_B\), \(C_C\) and \(T_{PS}\)), interactions amongst various alloying elements were also taken into account. Developed correlations exhibited reasonably good degrees of goodness of fit as indicated by the high values of \(R^2\) (>0.99) and low values of RMSD. In addition, the proposed models were found to provide relatively better description of peritectic transformation in comparison to other existing ones.

4) Adequacy of model prediction was rigorously evaluated against the literature as well as extensive plant data of longitudinal cracks. Good agreement between the predicted and the calculated values of liquidus and solidus temperatures indirectly proved that the thermodynamic calculations done in the present work were correct. Model predictions were also found to be consistent with the industrial data on longitudinal cracks thus further validating the calculations.

5) Finally, present model has been found to be useful for selecting the casting parameters for various grades of steel in the plant.

REFERENCES