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On modeling of the Ae_3 temperature of steel

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ABSTRACT

Ae_3 temperature of steel is required for many purposes for mechanical processing, thermal treatment and design of steels. However, the models available in the literature are not adequate. An attempt has been made to develop a relation for satisfactory prediction of the Ae_3 temperature of steel. Ae_3 temperature was expressed as a function of concentration of seven components of steels. The terms upto fourth order in concentration were retained. Total number of terms in the expression was 260. From a careful search of the literature 173 steels for which accurate values of the Ae_3 temperature were known were selected. Step wise multiple regression analysis was used to isolate the terms which made significant contribution to the Ae_3 temperature. Only nineteen of the 260 terms were found to be significant. These terms predicted the Ae_3 temperature with an accuracy which is much more than that offered by the other models. Although other investigators have tried to modify the model in various ways, the improvements have not been much. In all these treatments the exponents of the concentration parameters have been integral. It is possible to optimize allowing exponents as fractions with the help of genetic algorithm. However this technique also does not improve the over all quality of predictions appreciably.

INTRODUCTION

The austenite - ferrite transformation in pure iron occurs at a specific temperature but that in a multicomponent steel occurs over a range of temperatures. The austenite to ferrite transition temperature in hypoeutectoid steels has been described in the literature using a variety of symbols. The symbol, Ae_3, denotes the equilibrium transition temperature. It may be defined as the lowest temperature at which the

single phase austenitic structure is stable. It is often essential to know this critical temperature for designing steel for heat treatment. Ae_3 temperatures of only a limited number of steels are known. Therefore, attempts have been made to develop models for predicting Ae_3 temperatures of multicomponent steels.

The first formulation was proposed by Grange[1]. It is based on his experimental data on nineteen steels. His suggested analytical expression implies linear relationship between weight percentage of alloying elements, C, Mn, Si, Ni and Cr and the critical temperature and ignores interactions between the solutes. Andrews[2] modified Grange's model by incorporating interactions between carbon and nickel. However, other interactions were ignored. His model becomes inaccurate when Mn and Si increase beyond one percent. Baganis[3] considered equilibrium between ferrite and austenite and formulated equations to calculate Ae_3 temperature using free energies and activities of binary and ternary alloys. For dependable prediction of Ae_3 temperatures reliable thermodynamic data are required. However, such data are rarely available.

In this investigation a new model has been developed for estimating the Ae_3 temperatures of multicomponent low alloy steels. The parameters of the model have been evaluated using available data on the Ae_3 temperatures of steels. The predictions of this model are much more satisfactory than those of the previous models.

THE MODEL

Formulation

Let us consider the steel containing solutes, 1, ... i, ...n and the solvent 0 and let Te be the Ae_3 temperature of the steel. It may be expressed as a function of the composition of the steel Hence,

$$Te = F(x_1, \ldots\ldots x_i, \ldots\ldots y_n) \qquad \ldots 1$$

where xi is the weight fraction of solute i, Writing Eq. 1, as a polynomial,

$$Te = \Sigma_{m1}\ldots\ \Sigma_{mi}\ldots\Sigma_{mn}A_{m1\ldots mi\ldots mn}X_1^{m1}\ldots X_i^{mi}\ldots X_i^{mi}\ldots X_n^{mn} \qquad \ldots 2$$

where A is the coefficient and m stands for all positive integers including zero. By Tyalor's series expansion around the composition where the weight fraction of iron, x_0, is one, the coefficients can be expressed

as derivatives. Thus,

$$A_{ml,\ldots\ m_i,\ldots m_n} = \frac{1}{\pi_1^m\ m_i\ !}\left[\frac{\partial^{\gamma} Te}{\partial X_1^{ml}\ldots\ldots\partial X_i^{mi}\ldots\ldots\partial X_n^{mn}}\right] X_0^{-1} \qquad \ldots\ 3$$

$$\text{where } \gamma = \sum_1^n m_i \qquad \ldots\ 4$$

Eq.3, shows that the coefficients are measures of interactions between alloying elements.

For convenience, Eq. 2, may be rewritten in the following manner

$$Te = A_0 + \Sigma A_i X_i + \Sigma A_{ii} X_i^2 + 1/2\ \Sigma_i \Sigma_k A_{ik} X_i X_k + \ldots. \text{ with } A_{ik} = A_{ki}, \ldots\ldots\ 5$$

where X is weight percent and i and k stand for the alloying elements and A_0 stands for $(Te)_{x0=100}$, which is the Ae_3 temperature of pure iron.

Eq. 5, suggests that Te becomes equal to the zeroth order term, A_0, when the solutes have no effect on the Ae_3 temperature. A_0 and the first order terms yield the value of Ae_3 temperature when the interactions between the alloying elements are zero. The higher order terms include contributions due to self interactions and those due to interactions between different solutes. All of these interactions may not be significant. Therefore, by making use of available data on the Ae_3 temperatures of low alloy steels, we wish to isolate those interactions which are significant.

Experimental Data

In order to evaluate the coefficients of Eq. 5, values of the equilibrium temperatures of a number of steels are required. Reliable values of the Ae_3 temperatures of low alloy steels and their compositions were taken from the literature. The steels selected include nineteen steels of Grange[1], eightyseven steels for which isothermal transformation diagrams have been determined[4,5], ten steels of Aaronson and Dominan[6], one steel of Hall, kinsman and Aaronson[7], three steels of Gilmour, Purdy and Kirkaldy[8], six steels of Kirchner and Uhrenius[9] and four steels of Swinden and Woodhead[10], Fifteen hypoeutectoid Fe-C alloys, five Fe-Mn alloys six Fe-Si alloys, Five Fe-Ni alloys, six Fe-Cr alloy and six Fe-Mo alloys were also selected from their phase diagrams[11].

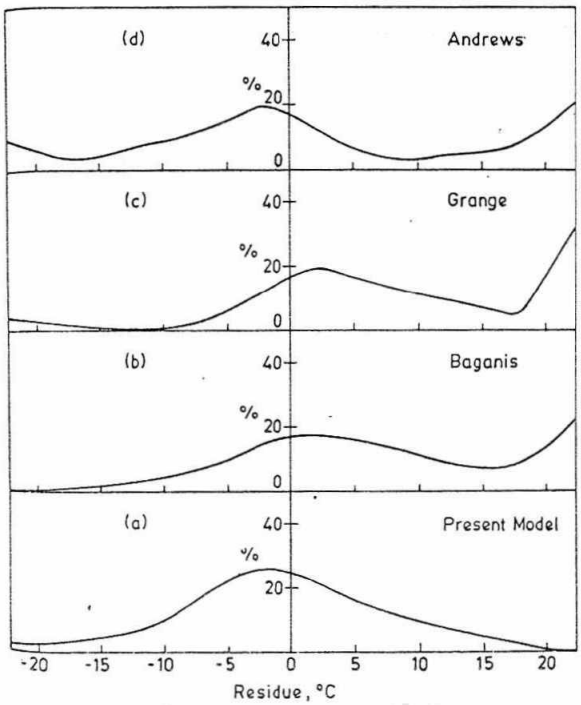

Fig.1 : Frequency distribution for residue from different models

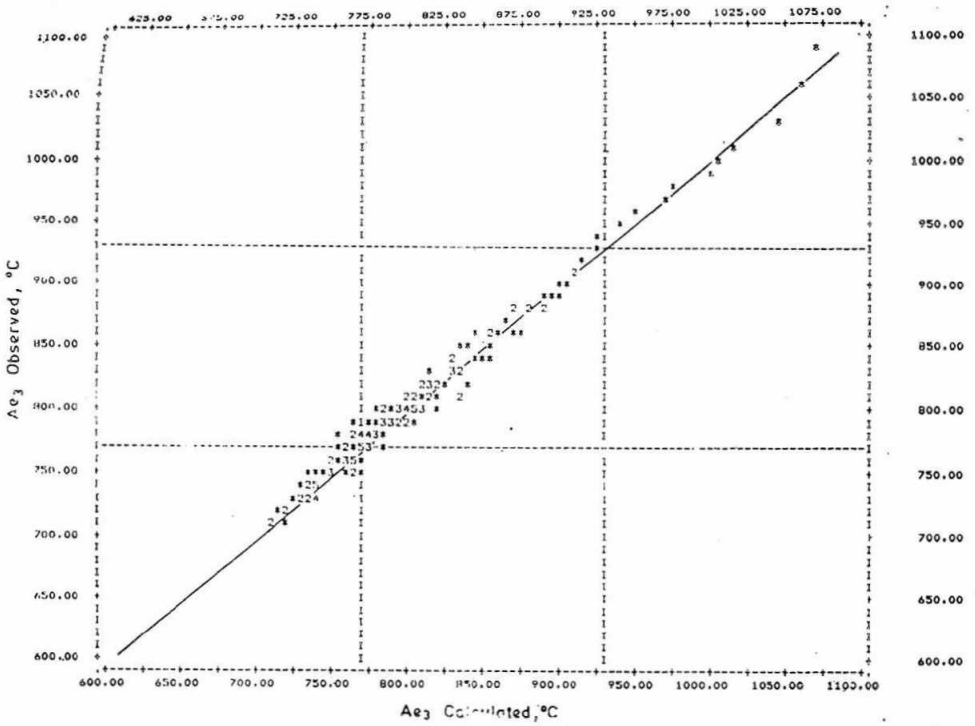

Fig. 2 : Scattergram for the present model

Thus, compositions of 173 alloys and their Ae_3 temperatures were compiled. The range of the weight percentages of alloying elements in these alloys were 0 to 0.758 for C, 0 to 5 for Mn, 0 to 1.83 for Si, 0 to 5.26 for Ni, 0 to 5.5 for Cr, 0 to 2.549 for Mo and 0 to 1.49 for Cu. The Ae_3 temperatures were in the range 710 to 1090°C.

Determination of Coefficients

The selected 173 alloys contain either all or some of the seven solutes, C, Ni, Mn, Si, Cr, Mo and Cu. For seven alloying elements, Eq. 5, would contain one zeroth order term, seven first order terms 28 second order terms, 84 third order terms, 140 fourth order terms and other higher order terms. If the equation is truncated after the fourth order terms, only 260 terms would remain. Copper is usually present in steels in small amounts. Therefore, the first order terms in copper has been retained while the seven second, tweentyeight third and 54 fourth order terms containing weight percentage of copper have been eliminated. The coefficients of the remaining 171 terms were determined using the Ae_3 temperatures of the 173 selected alloys.

Multiple regression analysis was used for the determination. This analysis takes into account the effect of all independent variables on the dependent variables. There are many computational methods available for multiple linear regression. However, the step wise regression is considered to be better than the rest[12,13]. The details about these techniques are available in the literature[12]. In this method the residue is defined as the difference between the functional value and the observed value of the dependent variable and the independent variable making the greatest reduction in the sum of the squares of residues is added at any step to the regression equation. The added variable is known as the entering variable.

A statistical parameter which gives the probability of variable not being a predictor variable is called significance level. The entering variable is required to have the minimum significance level amongst the variables not included in the regression equation. A variable is retained in the regression equation as long as its significance level is below a specified value. Thus, for a set of significance levels, $\alpha(1)$ and $\alpha(2)$ specified for entering and leaving variable respectively, the processes involving addition and removal of variables are continued, until variables are no more added to or removed from the regression equation. Thus, for a set of significance levels, the best set of coefficients

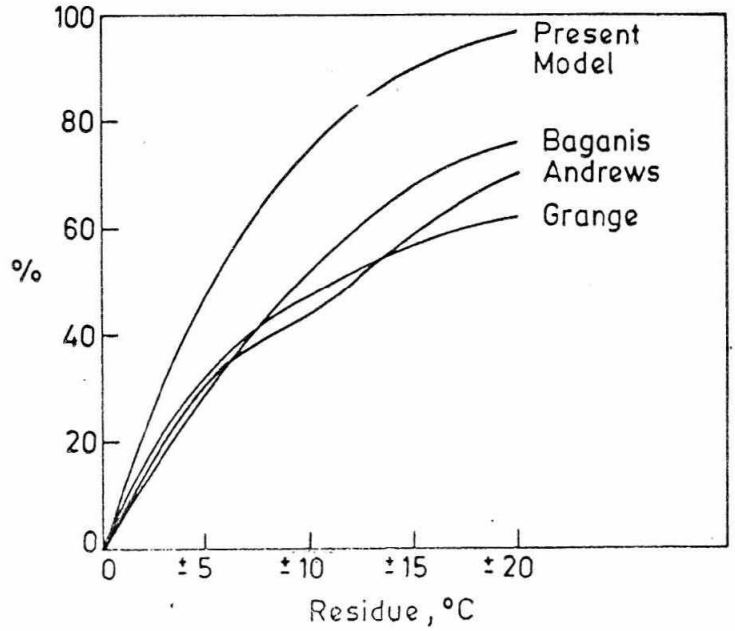

Fig. 3: Cumulative frequency distribution for residue from different models

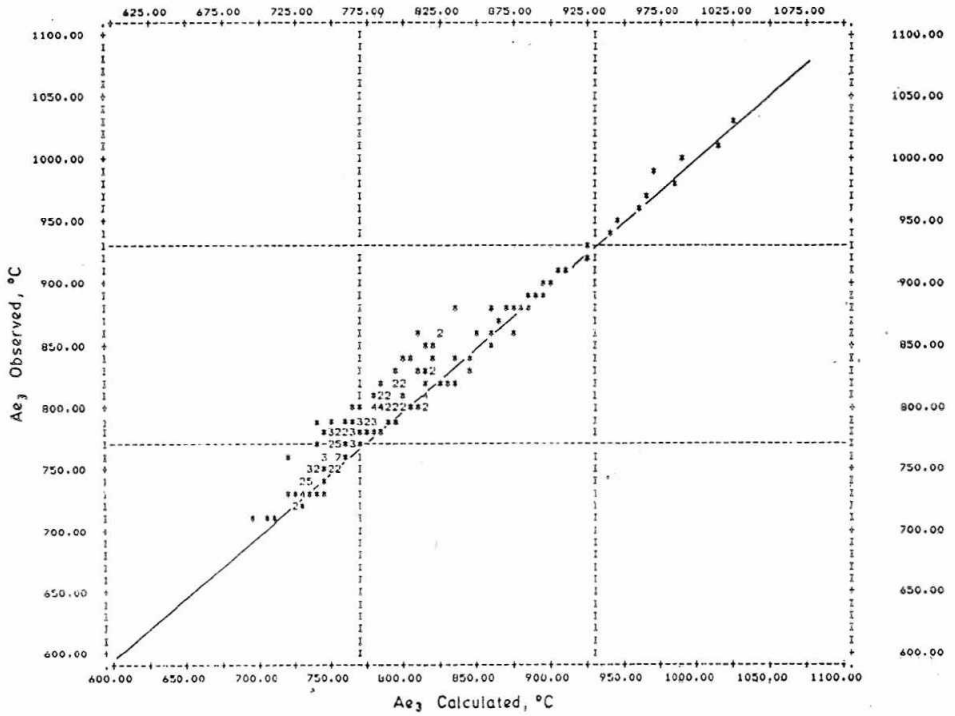

Fig. 4(a) : Scattergram for the Baganis' model

are calculated.

The 171 coefficients of Eq. 5 were calculated using the DEC 1090 computing system. For various sets of values of $\alpha(1)$ and $\alpha(2)$, the best results yielded nineteen non-zero coefficients for $\alpha(1) = 0.01$ and $\alpha(2) = 0.03$. Other sets of values of $\alpha(1)$ and $\alpha(2)$ increased the number of non-zero coefficients, without any significant reduction in the range of the residue.

The Ae_3 temperature, Te, can now be expressed in terms of the nineteen non-zero coefficients. However, the zeroth order term of the nineteen non-zero coefficients turns out to be 904.9°C while Ae_3 temperature of pure iron[14] is 911°C. In order to force Eq. 5, to yield 910°C for the zeroth order coefficient, the zeroth order coefficient was fixed as 910°C and the remaining eighteen coefficients were revaluated by the simple multiple linear regression method. The resulting coefficients were only slightly modified. Thus Eq. 5, reduced to:

$$
\begin{aligned}
Te = {} & 910.00 \\
& - 326.73X_C - 32.68X_{Mn} + 45.21X_{Si} - 36.26X_{Ni} \\
& - 6.82X_{Cr}^2 + 23.13X_{Mo}^2 + 69.74X_CX_{Ni} + 44.1X_CX_{Mn} \\
& + 95.69X_{Si}^3 - 9.46X_CX_{Ni}^2 - 74.83X_CX_{Si}^2 \\
& + 214.43X_C^4 - 46.05X_{Si}^4 + 0.17X_{Cr}^4 + 0.11X_{Ni}^4 \\
& + 8.48X_{Mo}X_{Cr}X_{Ni}^2 - 74.46X_CX_{Mo}^3 + 37.37X_C^2X_{Cr}^2
\end{aligned}
$$

Critical Appraisal of the Model

Several statistical parameters can be used to evaluate the reliability of a model and analyze the accuracy of any expression derived by regression. These parameters are standard error of estimate (SE), coefficient of multiple correlation (R), F-ratio and number of degrees of freedom[13].

The standard error of estimate, SE, is used to obtain a measure of how closely the calculated estimate of the dependent variable agrees with the experimental value [13]. The value of SE calculated from the errors of estimate is 9. The coefficient of multiple correlation, R, is the ratio of standard deviation of the estimated values to that of the experimental values. For perfect correlationship, the value of R would

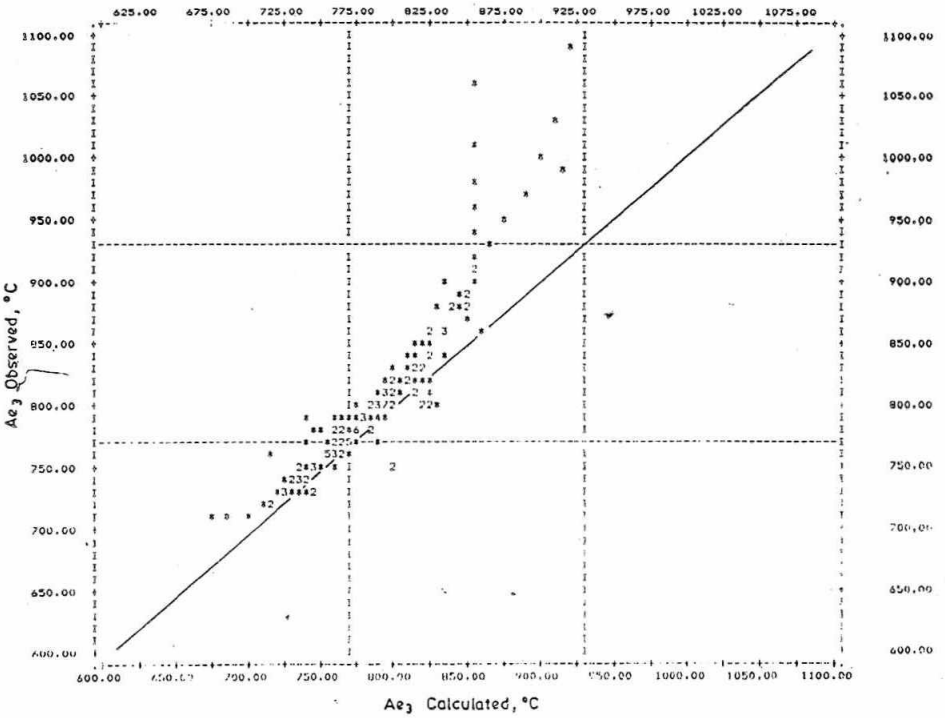

Fig. 4(b) : Scattergram for the Grange's model

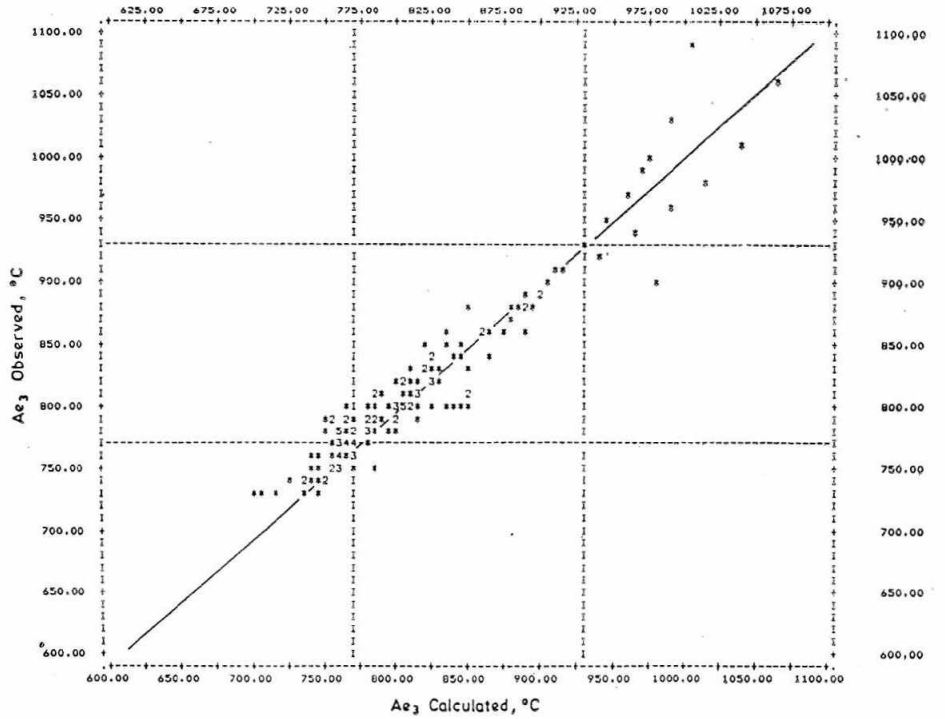

Fig. 4(c) : Scattergram for the Andrews' model

be 1.0 and it would be 0.0 for no correlation [13]. The value of R for the present model is almost 1. The F-ratio is a reliability parameter attributing a level of significance to the equation. It is equal to $(1-\alpha)$. If the F-ratio is more than 95%, the results are generally acceptable to a statistician[13]. The significance level of entering variable specified for developing the new model is 0.01 and that for the leaving variable is 0.03. Therefore, the model thus obtained has F value of more than 97%. The number of degrees of freedom is the difference between the total number of data points used to develop the model and the number of variables included in the model[13]. It illustrates the excess amount of data points available to be used in the regression equation. The accuracy of the model increases with increase in the degrees of freedom. There is, however, an economical limit above which a further increase in the degrees of freedom yields a lesser increase in accuracy. One hundred degrees of freedom and over is considered a respectable number for a regression system[13]. The number of degrees of freedom for the present regression analysis is 154 which is satisfactory.

The frequency distribution of the residue for the present model is shown in figure 1a. The distribution is symmetric. The mean error also turns out to be –0.6°C. The minimum and maximum values of error are –22.5°C and 20.5°C. In more than 97% of steels, the absolute value of residue is less than 20°C.

A plot-back can be used to show visually the difference between the calculated values of the Ae_3 temperature and their corresponding experimental values. A plot-back is a plot of the experimental Ae_3 temperature against the calculated ones. The dispersion of the plotted points about the 45° line is an indication of the deviation of the calculated values. The plot-back for the present model is given in Fig. 2. The digits plotted in these figures represent the number of coinciding data points whereas stars indicate single points. It is to be noted that the points lie close to the 45° line.

Out of the 19 coefficients in Eq. 5, a few are rather small in magnitude. However, if these coefficients are ignored, the range of the error of estimate appreciably increases. Also, the terms for which the coefficients are smaller, become appreciable in case of steels containing higher percentage of alloying elements. It is, therefore, not worthwhile to remove the terms where the coefficients are small.

The experimental uncertainties in the measured Ae_3 temperature have been reported to be 3°C to 10°C[1,6]. The steels for which the error

of estimate is more than 10°C were examined carefully. These differences are likely to arise because of several reasons. The interactions between the alloying elements may not have been fully taken into account. Also, the steels considered here are likely to contain impurities, some of which may contribute to the error. For example, Andrews[2] reported that phosphorous increases the Ae_3 temperature at the rate of 700°C per weight percent.

COMPARISON WITH EXISTING MODELS

Table 1 contains values of the mean of residue, standard error of estimates, minimum and maximum values of the residue and the coefficient of multiple correlation for all the models [1,2,3]. The 173 alloys examined in the study were used for evaluating the parameters for the present model and for Grange's[1] model. For determination of parameters for Baganis's[3] model only 171 steels could be used, as the computers program suggested by him did not yield values for the remaining two steels, 13 steels could not be used in the Andrews[2] model as his table does not have provision for steels with [C6 + (Ni/10)] greater than 0.7%. The number of alloys considered for each model is also listed in the table.

Table 1 shows that the standard error of estimate and the range of residue are minimum for the present model. Also the coefficient of correlation is about 0.99 and is the highest. The mean value of the residue of –0.6°C is very small. Andrews[2] model also gives a very small value of 0.2°C for mean value. However, the SE value for Andrew's model indicates that the spread in the residue is very large.

Tabel 1: Summary of the analysis of Ae_3 temperatures calculated using different models

Sl. No.	Description	Present model	Baganis model (3)	Andrews model (2)	Grange's model (1)
1.	Number of steel considered	173	171	160	173
2.	Mean of Residue	–0.6	9.6	0.2	17.2
3.	SE	9.0	13.8	19.2	33.3
4.	Residue (Min)	–22.5	–16.8	–78.8	–52.4
5.	Coefficient of correlation	0.992	0.977	0.961	0.909

The frequency distributions of the residue from all the models, shown in Fig. 1, suggested that the distributions for the models available in the literature are relatively asymmetric and the spreads are large. The cumulative frequency curves for the errors of estimate from all the models are shown in Fig. 3. It shows that for 30% of the steels the absolute value of the (or the magnitude of the) residue is more than 20°C for the three models of the literature whereas for the present model, only 3% of the steels have it greater than 20°C.

The plot backs for the three existing models are shown in Fig. 4. A comparison of these plot backs with that of the present model (Fig. 2) shows that the dispersion of the points about the 45° line is minimum for the present model. The present model thus, appears to be much more satisfactory than all the three existing models. Kumar[15] and Gupta[16] have tried to modify the present model using various techniques such as genetic algorithm. However, there is not much of overall improvement.

CONCLUSION

A model has been developed to predict the Ae_3 temperatures of multicomponent steels containing carbon, manganese, silicon, chromium, nickel, copper and molybdenum. The model is based on Ae_3 temperature of 173 alloys. The analytical expression for the Ae_3 temperature contains nineteen terms, many of which represent interactions between elements. The developed expression represents data much more accurately than the other relations in the literature.

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