Non-linear Regression Model for Ac_3, Ac_1 Transformation Temperatures

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1 Ac_3 Introduction

This document presents a non-linear mathematical relationship between the chemical composition, heating rate, and the Ac_3 transformation temperature of various steel alloys. The model was developed using a second-order polynomial regression analysis based on a dataset of 824 experimental observations.

2 Methodology

The features used for the model include the weight percentages w_i of carbon, silicon, manganese, nickel, chromium, and molybdenum, alongside the heating rate ($\dot{T}$). To capture non-linearities and synergistic effects between elements, the model incorporates:

- Linear terms for primary alloying elements.
- Quadratic terms to account for diminishing or increasing returns of specific elements.
- Interaction terms to model how the presence of one element alters the influence of another.

2.1 Derived Equation

The resulting regression equation for Ac_3 (in °C) as a function of the wt% of solute and the heating rate in $\mathrm{K\,s^{-1}}$ is given by:

$$\begin{aligned} Ac_3 \approx\ & 918.88 - 529.00w_{\mathrm{C}} + 97.78w_{\mathrm{Si}} - 15.08w_{\mathrm{Mn}} - 30.95w_{\mathrm{Ni}} + 29.25w_{\mathrm{Mo}} \\ & + 430.98w_{\mathrm{C}}^2 + 0.99w_{\mathrm{Ni}}^2 + 6.99w_{\mathrm{Mo}}^2 - 84.13w_{\mathrm{C}} \times w_{\mathrm{Si}} \\ & + 50.44w_{\mathrm{C}} \times w_{\mathrm{Mn}} + 37.52w_{\mathrm{C}} \times w_{\mathrm{Ni}} + 7.95w_{\mathrm{C}} \times w_{\mathrm{Cr}} \\ & - 58.25w_{\mathrm{C}} \times w_{\mathrm{Mo}} - 29.28w_{\mathrm{Si}} \times w_{\mathrm{Mn}} + 18.13w_{\mathrm{Si}} \times w_{\mathrm{Mo}} \\ & + 2.53w_{\mathrm{C}} \times \dot{T} - 2.38w_{\mathrm{Si}} \times \dot{T} + 0.75w_{\mathrm{Ni}} \times \dot{T} \\ & - 0.14w_{\mathrm{Cr}} \times \dot{T} + 1.75w_{\mathrm{Mo}} \times \dot{T} \end{aligned} \tag{1}$$

2.2 Statistical Summary

The model demonstrates a strong fit to the experimental data, as summarised in the table below:

Metric	Value
Number of Observations	824
R-squared (R^2)	0.806
Adjusted R^2	0.801
F-statistic	166.7

Table 1: Model performance metrics.

2.3 Discussion

The high coefficient for w_C^2 indicates a strong curvature in the Ac_3 response to Carbon content. Furthermore, the significance of the interaction terms between alloying elements and the heating rate ($\dot{T}$) confirms that the kinetic response of the transformation is highly dependent on the specific chemical system of the steel.

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3 Ac_1 Introduction

This report provides a non-linear mathematical model relating the Ac_1 transformation temperature to the chemical composition and heating rate of various steel alloys. The model was derived from 824 experimental observations using polynomial regression.

3.1 Methodology

The regression model incorporates weight percentages w_i of alloying elements (C, Si, Mn, Ni, Cr, Mo) and the heating rate ($\dot{T}$). The model considers linear, quadratic, and interaction terms, with only statistically significant parameters ($p < 0.05$) retained to ensure predictive reliability.

3.2 Derived Equation

The equation for Ac_1 (in °C) is:

$$\begin{aligned} Ac_1 \approx\ & 836.00 - 225.36w_C - 135.23w_{Mn} - 27.44w_{Ni} + 11.06w_{Cr} + 2.16\dot{T} \\ & + 131.13w_C^2 + 33.65w_{Mn}^2 - 0.81w_{Cr}^2 - 0.0004\dot{T}^2 \\ & + 25.64w_C \times w_{Si} + 99.39w_C \times w_{Mn} + 23.61w_C \times w_{Ni} \\ & + 5.60w_{Si} \times w_{Cr} + 5.84w_{Mn} \times w_{Cr} - 1.15w_{Ni} \times w_{Cr} \\ & + 1.95w_{Cr} \times w_{Mo} - 3.61w_{Si} \times \dot{T} - 0.73w_{Mn} \times \dot{T} \\ & + 0.85w_{Ni} \times \dot{T} \end{aligned} \tag{2}$$

3.3 Statistical Summary

The performance of the Ac_1 model is summarized below:

Metric	**Value**
Number of Observations	824
R-squared (R^2)	0.812
Adjusted R^2	0.808
F-statistic	183.3

Table 2: Model performance for Ac_1.

3.4 Observations

- **Manganese**: Mn exhibits a strong depressive effect on Ac_1, but the positive w_{Mn}^2 term indicates this effect diminishes as concentration increases.
- **Interactions**: Significant interactions between chromium and molybdenum ($w_{\text{Cr}} \times w_{\text{Mo}}$) and nickel and chromium ($w_{\text{Ni}} \times w_{\text{Cr}}$) highlight the complex synergy of these elements in determining the onset of austenite formation.
- **Heating kinetics**: The Ac_1 temperature shows a non-linear sensitivity to the heating rate, influenced significantly by the presence of silicon and nickel.