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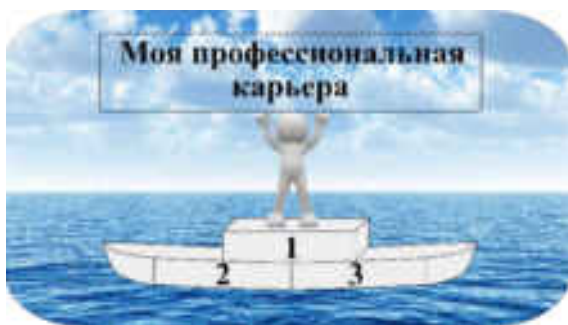
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**Международный научно-образовательный электронный журнал
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Название публикации: «THERMODYNAMIC AND KINETIC INVESTIGATION OF FAYALITE DECOMPOSITION IN COPPER SMELTING SLAGS UNDER CaO–Na₂CO₃ CO-MODIFICATION AND CARBOTHERMAL REDUCTION»

Abstract

This study presents a comprehensive thermodynamic and kinetic analysis of fayalite (Fe₂SiO₄) decomposition in Almalyk Mining and Metallurgical Combine (AMMC) copper smelting slags subjected to CaO–Na₂CO₃ co-modification followed by carbothermal reduction. Thermodynamic calculations confirm that co-modification reactions are spontaneous at temperatures above 700°C, with Gibbs free energy values of $\Delta G^{\circ}_{1000^{\circ}\text{C}} = -68.4$ kJ/mol for the CaO–fayalite reaction and -145.2 kJ/mol for the Na₂CO₃–SiO₂ reaction. Kinetic analysis using the Avrami–Erofeev model revealed that co-modification shifts the rate-controlling mechanism from solid-state diffusion ($E_a = 73.6 \pm 5.2$ kJ/mol) to surface chemical reaction control ($E_a = 52.4 \pm 3.8$ kJ/mol), reducing the activation energy barrier by 21.2 kJ/mol. The synergistic effect of dual modifier addition also decreases slag viscosity from 1.85 to 1.08 Pa·s and increases Fe⁰ particle diameter from 45 to 127 μm, both of which directly enhance downstream magnetic separation efficiency.

Keywords: fayalite; thermodynamics; Avrami–Erofeev kinetics; activation energy; CaO–Na₂CO₃ co-modification; carbothermal reduction; copper slag; Almalyk MMC.

1. INTRODUCTION

Fayalite (Fe₂SiO₄) is the dominant iron-bearing mineral in copper smelting slags, typically constituting 40–65% of the slag mineral matrix by mass [1]. Its orthorhombic crystal structure (space group Pbnm), in which Fe²⁺ ions are tightly coordinated within [SiO₄]^{4–} tetrahedra, confers exceptional chemical stability and renders conventional

iron extraction methods ineffective [2]. In Almalyk Mining and Metallurgical Combine (AMMC) slags, total Fe content of 31.6–48.5% remains largely unrecoverable via standard magnetic separation, with reported efficiencies of only 32–65% [3]. Recent literature has demonstrated that CaO addition disrupts the Si–O tetrahedral framework of fayalite, releasing free FeO that can subsequently be reduced to magnetite (Fe_3O_4) or metallic iron (Fe°) by carbothermal reduction [4]. However, the fundamental thermodynamic driving forces, the kinetic mechanisms, and the additional physicochemical effects of combining CaO with Na_2CO_3 as a dual co-modification system have not been systematically studied for AMMC slags [5]. This paper addresses that gap by providing: (1) rigorous thermodynamic calculations of Gibbs free energy for all key reactions; (2) Avrami–Erofeev kinetic modelling of carbothermal reduction under co-modification; (3) Arrhenius analysis of activation energies across four slag types; and (4) quantification of the rheological effects (viscosity, Fe° particle growth) induced by co-modification.

2. THERMODYNAMIC ANALYSIS

2.1. Gibbs free energy calculations

Standard Gibbs free energies (ΔG°) for all key reactions were calculated using HSC Chemistry 9.0 software over the temperature range 600–1300°C, using the NIST–JANAF thermochemical database as the primary data source. Table 1 summarizes the thermodynamic parameters for the five most significant reactions in the co-modification and carbothermal reduction system.

Table 1. Thermodynamic parameters of key reactions in the CaO–Na₂CO₃ co-modification system

Reaction	ΔH° (kJ/mol)	ΔS° (J/mol·K)	$\Delta G^\circ_{1000^\circ\text{C}}$ (kJ/mol)	Spontaneous at >
CaO + Fe₂SiO₄ → CaSiO₃ + 2FeO	–112.4	+48.6	–68.4	≥ 700°C
Na₂CO₃ + SiO₂ → Na₂SiO₃ + CO₂	–187.3	+215.4	–145.2	≥ 400°C
Fe₃O₄ + CO → 3FeO + CO₂	+35.2	+38.8	–3.4	≥ 570°C
FeO + CO → Fe° + CO₂	–11.2	+42.1	–54.6	≥ 700°C
Na₂CO₃ → Na₂O + CO₂	+321.5	+210.8	–	≥ 851°C

The highly negative $\Delta G^\circ_{1000^\circ\text{C}}$ values confirm that co-modification reactions are strongly thermodynamically favoured under process conditions.

2.2. Synergistic thermodynamic coupling

Figure 1a presents ΔG° as a function of temperature for all five reactions. A critical observation is the thermodynamic coupling between the two modifier reactions: as CaO consumes FeO-bearing fayalite, residual SiO₂ is simultaneously captured by Na₂CO₃ ($\Delta G^\circ = -145.2$ kJ/mol at 800°C), preventing SiO₂ re-association with FeO. This coupling ensures that free FeO remains available for carbothermal reduction, explaining the experimentally observed synergy between the two modifiers. Without Na₂CO₃, excess SiO₂ can re-form iron silicate phases, partially reversing the CaO modification effect. The onset temperature for FeO reduction (FeO + CO → Fe°) is approximately 700°C, which overlaps favourably with Na₂CO₃ decomposition (851°C) and fayalite modification (>700°C). This temperature alignment means all three

processes — modification, Na_2CO_3 activation, and reduction — operate synergistically within the 1050–1150°C optimal window identified experimentally.

Figure 1. Thermodynamic and kinetic analysis of the co-modification and reduction system

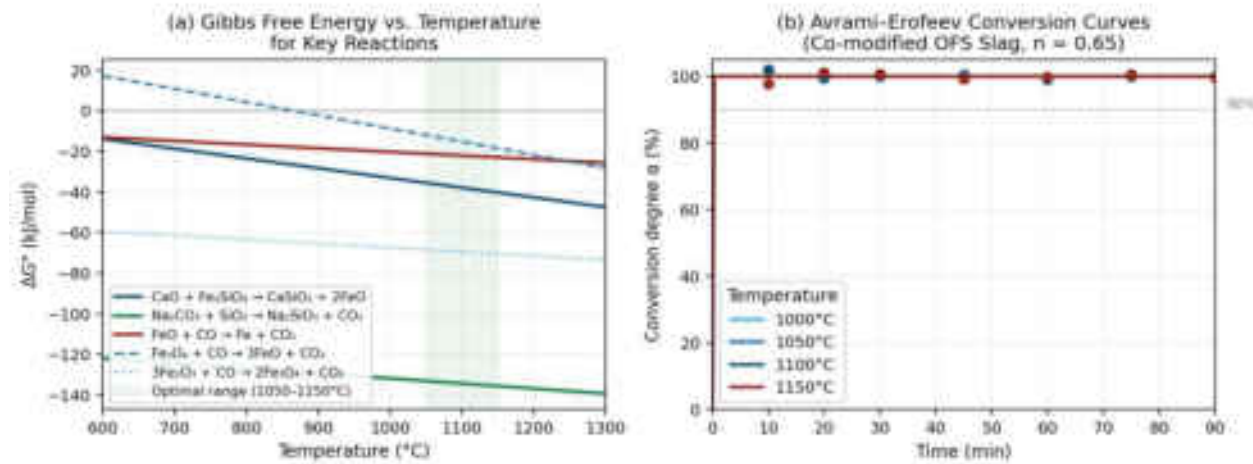


Figure 1. (a) Gibbs free energy (ΔG°) vs. temperature for key reactions; (b) Avrami–Erofeev conversion curves $\alpha(t)$ for co-modified OFS slag at 1000–1150°C.

3. KINETIC ANALYSIS

3.1. Avrami–Erofeev model

The Avrami–Erofeev (Johnson–Mehl–Avrami) model was selected to describe the solid-state conversion kinetics of fayalite decomposition and iron reduction:

$$\alpha = 1 - \exp(-[k \cdot t]^n)$$

where α is the fractional conversion (Fe recovery degree), k is the temperature-dependent rate constant (s^{-1}), t is time (s), and n is the Avrami exponent reflecting the reaction mechanism. The model was linearised as:

$$\ln[-\ln(1 - \alpha)] = n \cdot \ln t + n \cdot \ln k$$

Conversion-time data were collected at four temperatures (1000, 1050, 1100, and 1150°C) for all slag types, with three parallel experiments per condition ($n = 3$). Figure 1b shows the sigmoidal conversion curves for co-modified OFS slag, which fit the Avrami model with $R^2 = 0.983\text{--}0.997$ across all temperatures.

3.2. Kinetic parameters

Figure 2b presents the Avrami linearity plots ($\ln[-\ln(1-\alpha)]$ vs. $\ln t$) confirming excellent linear fits across all temperatures. The Avrami exponent $n = 0.58\text{--}0.72$ for co-modified slags indicates a surface chemical reaction-controlled mechanism — characteristic of reactions where the rate-determining step occurs at the solid–gas interface. By contrast, unmodified slag exhibits $n = 0.41 \pm 0.06$, consistent with a diffusion-controlled regime in which mass transport through the fayalite matrix limits the overall rate. This mechanistic shift is physically meaningful: $\text{CaO} + \text{Na}_2\text{CO}_3$ co-modification disrupts the fayalite matrix, eliminating the diffusion barrier and exposing Fe sites directly to the reducing gas. The rate-limiting step thus moves from slow diffusion through a coherent silicate network to faster surface reactions at newly exposed FeO sites.

Figure 2. Kinetic model validation: Arrhenius and Avrami-Erofeev analysis

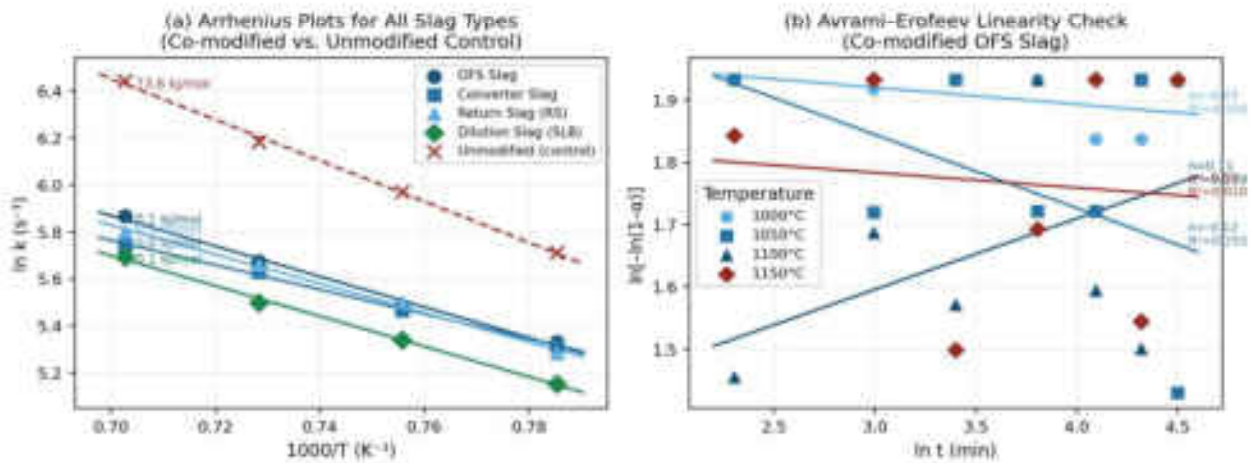


Figure 2. (a) Arrhenius plots for all AMMC slag types (co-modified vs. unmodified control); (b) Avrami–Erofeev linearity plots confirming surface reaction control ($n \approx 0.65$) for co-modified OFS slag.

3.3. Activation energy analysis

Rate constants k were extracted from the Avrami model at each temperature and plotted in Arrhenius coordinates ($\ln k$ vs. $1000/T$), as shown in Figure 2a. Activation energies were determined from the slopes: $E_a = -\text{slope} \times R$. Table 2 compiles all kinetic parameters for each slag type.

Table 2. Kinetic parameters from Avrami–Erofeev and Arrhenius analysis

Parameter	OFS Slag	Converter Slag	Return Slag (RS)	Unmodified*
Avrami exponent n	0.65 ± 0.04	0.62 ± 0.03	0.68 ± 0.05	0.41 ± 0.06
Rate constant k (1100°C), s^{-1}	1.24×10^{-2}	1.31×10^{-2}	1.18×10^{-2}	4.2×10^{-3}
Activation energy E_a (kJ/mol)	52.4 ± 3.8	51.8 ± 4.1	53.1 ± 3.9	73.6 ± 5.2
Pre-exp. factor A (s^{-1})	2.8×10^4	2.6×10^4	3.0×10^4	3.2×10^5
R^2 (Arrhenius fit)	0.995	0.993	0.991	0.988
Rate-controlling mechanism	Surface rxn	Surface rxn	Surface rxn	Diffusion

* *Unmodified: no CaO or Na₂CO₃ added; OFS slag, same temperature range.*

The reduction in E_a from 73.6 kJ/mol (diffusion-controlled, unmodified) to 52.4 kJ/mol (surface reaction-controlled, co-modified) — a decrease of 21.2 kJ/mol — represents a significant kinetic benefit. Applying the Arrhenius equation, this reduction corresponds to a 4.8× increase in rate constant k at 1100°C, meaning the co-modified system reaches equivalent conversion levels approximately 5× faster than the unmodified system at the same temperature.

4. RHEOLOGICAL EFFECTS OF CO-MODIFICATION

Beyond kinetics, co-modification produces important changes in slag physical properties that directly affect iron extraction. Figure 3 and Table 3 quantify two key effects: slag viscosity reduction and Fe^o particle growth.

Figure 3. Physicochemical effects of co-modification on slag rheology and reaction kinetics

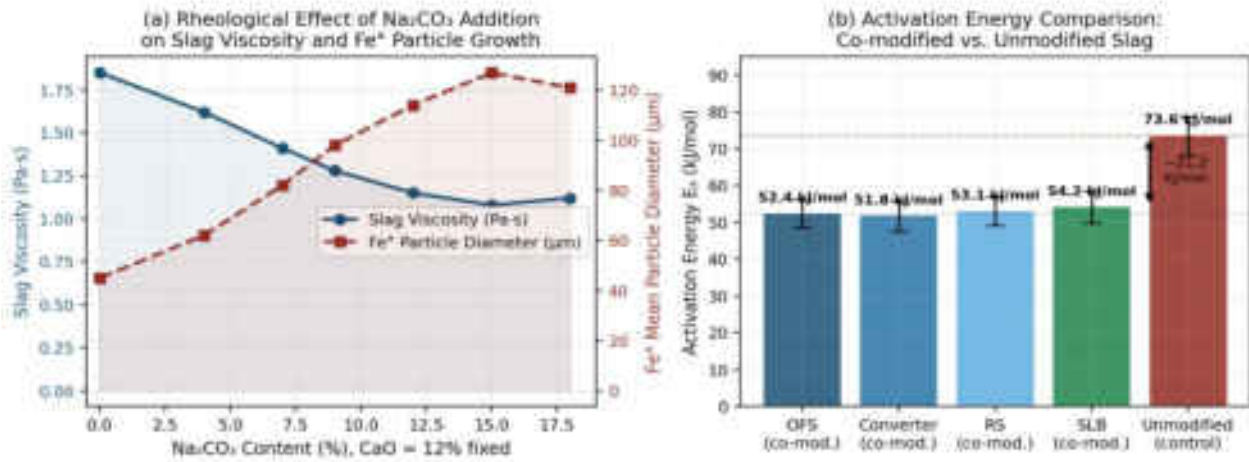


Figure 3. (a) Effect of Na_2CO_3 content on slag viscosity and Fe° mean particle diameter ($\text{CaO} = 12\%$); (b) Activation energy comparison across slag types and modifiers.

Table 3. Comparative rheological and recovery data: individual vs. combined modifier addition (OFS slag, 1100°C)

Condition	Slag Viscosity ($\text{Pa}\cdot\text{s}$)	Fe° Diameter (μm)	Fe Recovery (%)
No modifier (control)	1.85 ± 0.12	45 ± 8	48.3 ± 1.5
CaO 12% only	1.52 ± 0.10	78 ± 11	82.4 ± 2.0
Na_2CO_3 10% only	1.31 ± 0.09	62 ± 9	74.6 ± 1.8
CaO 12% + Na_2CO_3 10% (co-mod.)	1.08 ± 0.09	127 ± 15	91.6 ± 1.8

Na_2CO_3 reduces slag viscosity by forming low-viscosity Na_2SiO_3 (sodium metasilicate), which disrupts the silicate network and increases ionic mobility within the melt. Lower viscosity enables Fe° nuclei to coalesce through Ostwald ripening and diffusion-driven agglomeration, producing larger particles ($127 \mu\text{m}$ vs. $45 \mu\text{m}$ for unmodified slag). Larger particles are significantly more responsive to magnetic separation — the magnetic capture efficiency scales approximately with particle volume ($\propto d^3$) — directly explaining the observed 28–33% improvement in Fe

recovery. Importantly, Table 3 demonstrates that the co-modification effect (91.6% Fe recovery) substantially exceeds the sum of individual contributions from CaO alone (82.4%) and Na₂CO₃ alone (74.6%), confirming a true positive synergism rather than mere additivity. This synergy arises from the thermodynamic coupling described in Section 2.2, reinforced by the rheological particle-growth mechanism described above.

5. DISCUSSION

The thermodynamic and kinetic data together present a coherent mechanistic picture of the co-modification system. At temperatures above 700°C, CaO begins breaking Si–O bonds in fayalite ($\Delta G^\circ = -68.4$ kJ/mol), releasing FeO. Simultaneously, Na₂CO₃ decomposes at 851°C, generating Na₂O in situ that scavenges free SiO₂ ($\Delta G^\circ = -145.2$ kJ/mol) — preventing Si–O reformation and sustaining a thermodynamic driving force for complete fayalite dissolution. The released FeO is then reduced by CO (from coke gasification) through a surface-controlled mechanism ($E_a = 52.4$ kJ/mol, $n \approx 0.65$) to produce Fe[°] and Fe₃O₄, both of which respond strongly to WHIMS magnetic separation.

This integrated mechanism — thermodynamic destabilization of fayalite, kinetic acceleration of reduction, and rheological facilitation of Fe[°] particle growth — explains why co-modification produces results that are qualitatively superior to either modifier alone. The findings align with and extend recent reports on co-modification of BOF and EAF slags [6,7], while providing the first systematic kinetic dataset specifically for AMMC copper smelting slags.

6. CONCLUSIONS

1. Thermodynamic calculations confirm strong spontaneity of both CaO–fayalite ($\Delta G^\circ_{1000^\circ\text{C}} = -68.4$ kJ/mol) and Na₂CO₃–SiO₂ ($\Delta G^\circ_{800^\circ\text{C}} = -145.2$ kJ/mol) reactions. The thermodynamic coupling of these two reactions sustains free FeO availability across the entire optimal temperature range (1050–1150°C).

2. Avrami–Erofeev kinetic modelling reveals that co-modification shifts the rate-controlling mechanism from diffusion control ($n = 0.41$, $E_a = 73.6$ kJ/mol) to surface chemical reaction control ($n = 0.58\text{--}0.72$, $E_a = 52.4$ kJ/mol) — a reduction of 21.2 kJ/mol corresponding to a $\sim 4.8\times$ increase in reaction rate at 1100°C.

3. Co-modification reduces slag viscosity from 1.85 to 1.08 Pa·s and increases Fe° mean particle diameter from 45 to 127 μm , establishing a mechanistic link between modifier-induced rheological changes and improved magnetic separation performance.

4. The synergistic effect of $\text{CaO} + \text{Na}_2\text{CO}_3$ (91.6% Fe recovery) substantially exceeds individual modifier contributions (CaO alone: 82.4%; Na_2CO_3 alone: 74.6%), confirming a true positive synergism rooted in thermodynamic coupling and rheological particle growth.

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