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The Implementation Potential of the Hybrid Hot Metal Desulfurization Model – The Transformation of Research Results into Technological Recommendations

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Abstract

This study presents the development of a hybrid model for the desulfurization of hot metal using dual reagent injection of CaO and Mg, integrating thermodynamic equilibrium calculations with kinetic analysis based on Tank Theory. The objective is to provide practical technological recommendations that enable effective industrial application of the process. The model allows real-time simulation of sulfur concentration changes under varying parameters such as reagent dosage and mixing intensity, while an optimization module supports the selection of operating conditions by balancing desulfurization efficiency with material consumption and operational costs. The system adapts to changing technological conditions including feedstock composition and process temperature, ensuring flexibility in industrial practice. In addition to process control, the model incorporates economic evaluation by correlating reagent consumption with achieved technological outcomes, which enhances its practical value. The proposed solution represents a step toward intelligent desulfurization systems that combine the precision of physicochemical modeling with the adaptability of modern process control. Implementation of the hybrid model may lead to higher efficiency, reduced consumption of consumables, and stable achievement of target sulfur levels, thereby strengthening the economic competitiveness of iron production.

Keywords:

hot metal, desulfurization, hybrid, model, computer modeling

1. INTRODUCTION

Desulfurization remains a critical operation in iron and steelmaking, directly influencing the mechanical properties, weldability, and downstream process stability of final steel products. Sulfur, despite its low concentration, acts as a potent embrittling agent and must be removed efficiently at the earliest possible stage of production [1].

One promising approach is the desulfurization of hot metal using the dual reagent injection method of calcium oxide (CaO) and metallic magnesium (Mg), which leverages the simultaneous action of two complementary reagents with distinct thermodynamic properties. In this method, powdered CaO and Mg are introduced concurrently into the metal bath, typically using nitrogen as a carrier gas [2, 3]. A schematic diagram of the desulfurization station is presented in Figure 1. The reaction mechanism encompasses both heterogeneous reactions at the metal-slag interface and reactions within the bulk of the liquid metal, where gaseous Mg significantly enhances the diffusion of reactive species [4, 5].

A key advantage of the dual reagent injection method is the synergistic behavior of its components: magnesium initiates the process rapidly through an exothermic surface reaction ($Mg + S \rightarrow MgS$), while calcium oxide ensures deep desulfurization due to its high sulfur capacity under low oxygen activity [6, 4]. Both laboratory and industrial studies confirm that this synergy enables desulfurization degrees of up to 95%, while simultaneously reducing operational costs by 10–20% compared to single-agent desulfurizers [3].

To contextualize the proposed method, it is useful to contrast it with desulfurization techniques applied at later stages of steelmaking. In secondary metallurgy, calcium cored wire (CaSi) injection is commonly used to refine molten steel, improving cleanliness and mechanical performance. However, such techniques are not directly applicable to hot metal due to differences in temperature, slag composition, and oxygen activity [7]. CaSi wire is typically introduced under controlled ladle furnace conditions, whereas the CaO+Mg dual reagent injection method targets hot metal prior to converter processing.

The proposed technique is suitable for iron alloys intended for the production of low-sulfur carbon steels and low-alloy steels, where the sulfur content must be reduced below 0.005% to meet mechanical and weldability requirements. Early-stage desulfurization of hot metal not only improves downstream process stability but also reduces the burden on secondary refining operations.

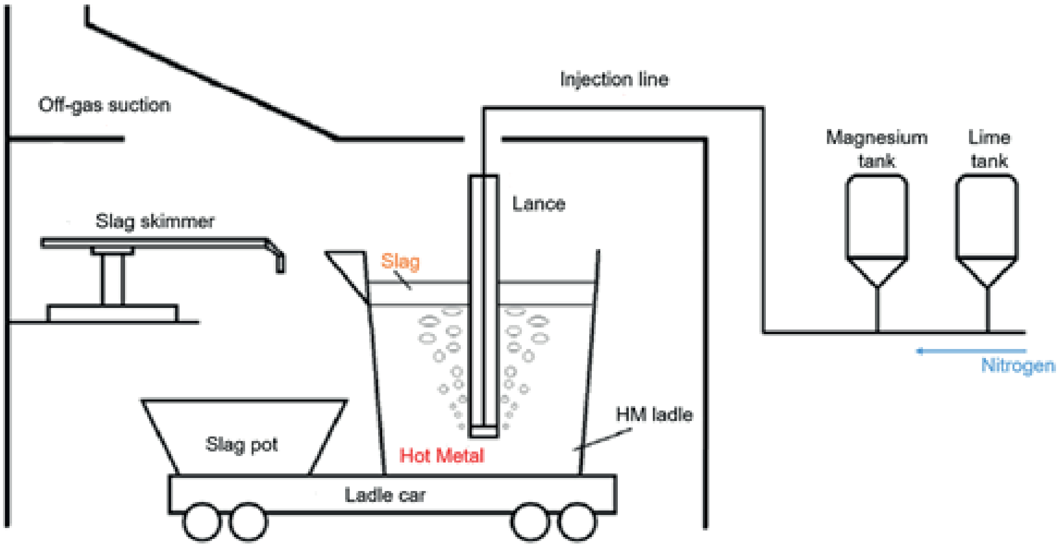

Fig. 1. Schematic diagram of the hot metal desulfurization station using the dual reagent injection method CaO+Mg [10]

The aim of this study is to evaluate the implementation potential of a hybrid model for hot metal desulfurization using CaO and Mg dual reagent injection, integrating thermodynamic equilibrium calculations and kinetic mixing analysis [8]. The model is designed to support technological decision-making under industrial conditions, enabling process optimization in terms of reagent consumption, sulfur removal efficiency, and economic performance [9].

2. RESEARCH METHODOLOGY

The initial task undertaken involved the identification of both control parameters and state parameters for the hot metal desulfurization process (Table 1). The objective of this step was to determine those factors for which modification would be feasible. It should be noted that both control and state parameters can be classified into two overarching categories: thermodynamics and kinetics parameters.

Table 1
Set of parameters for the hot metal desulfurization process: green colour represents control parameters, blue colour represents state parameters

Thermodynamics	Kinetics
Hot metal analysis (C, Si, Mn, P, S)	Average material flow during the process
Hot metal mass	Material injection time
Hot metal temperature	Pressure in material tanks
Final sulfur content (desulfurization level)	Transport gas pressure
Slag mass	Carrier gas flow
Injected material mass	
Initial material mass in the tanks	

The next stage of the research involved conducting simulations of the desulfurization process using historical data obtained from an actual metallurgical unit. The baseline (initial) values used in the simulation model reflect the process conditions of real industrial heat, which served as the reference case for all parameter variations. A complete set of these baseline parameters is presented in Table 2. To accurately assess the real impact of individual factors on the simulated sulfur content after the desulfurization process, a decision was made to change only one parameter at a time.

Table 2
Baseline process parameters used in the simulation model

Parameter	Value	Unit
Temperature	1391	°C
Hot metal mass	293	Mg
Sulfur initial	0.031	%
Mg mass injected	0.099	Mg
CaO mass injected	0.523	Mg
Slag mass	4	Mg

In the Tank Theory model, mass transfer streams between the elementary reactors were introduced to reflect the intensity of mixing and reagent dispersion within the ladle. These mass transfer values are directly linked to the nitrogen flow rate used in the industrial process, which governs the dynamic exchange of material between reactive zones. By adjusting these values, the simulation captures the influence of flow-induced mixing on desulfurization efficiency. A simplified schematic of the model operation is presented in Figure 2.

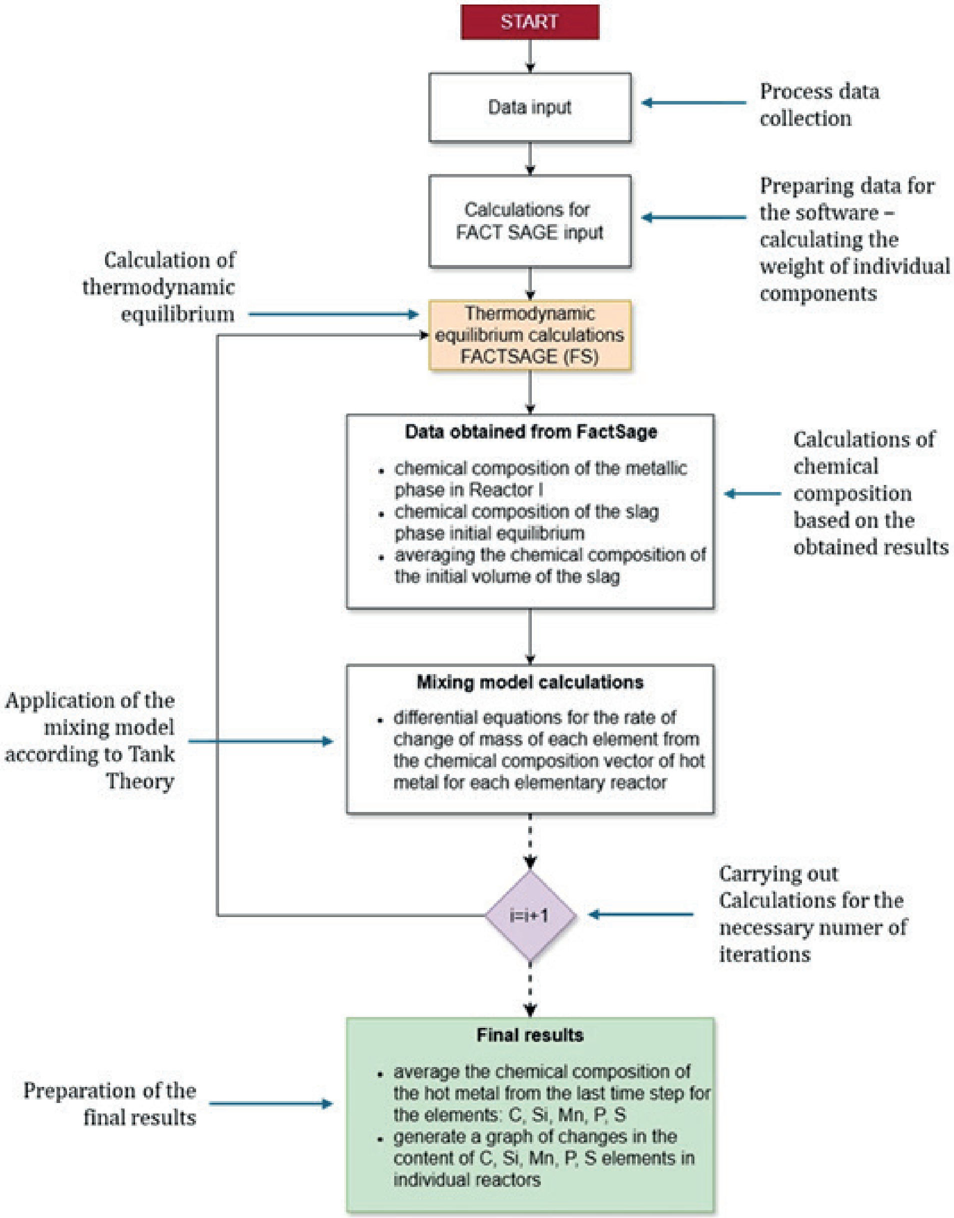

Fig. 2. Simplified block diagram of the hybrid hot metal desulfurization model

3. ANALYSIS AND DISCUSSION OF THE OBTAINED RESULTS

Simulations of the desulfurization model were conducted by varying the following parameters: the mass of blast furnace slag in the ladle, the amount of CaO introduced into the process, the amount of Mg introduced into the process, the temperature of the hot metal, the exchange of sizes between elementary reactors 1 and 3, as well as changes in the mass transfer rates between the elementary reactors. The sulfur content after the process, as a function of each investigated parameter, is presented in Figures 3–7.

To represent the mixing and reaction behavior within the hot metal bath, the system was conceptually divided into three elementary reactors arranged in series, following the Tank Theory model. Each reactor corresponds to a distinct zone of the ladle with different mixing intensities and reaction characteristics. Reactor 1 represents the surface region, where magnesium vapor reacts rapidly with sulfur at the metal-slag interface. Reactor 2 models the intermediate zone, characterized by partial mixing and reagent dispersion. Reactor 3 reflects the deeper region of the bath, where calcium oxide dissolves and reacts under low oxygen activity, enabling deep desulfurization. The exchange of sizes between reactors 1 and 3 simulates variations in the effective volume of reactive zones, while changes in mass transfer rates reflect differences in mixing efficiency and reagent penetration. This reactor-based approach allows the model to capture both thermodynamic equilibrium and kinetic limitations of the desulfurization process [2].

Figure 3 illustrates the variation in the mass of blast furnace slag in the ladle. Simulations were conducted for the baseline heat as well as for two modified values: a reduction of 50% and an increase of 50% relative to the baseline slag mass. The simulation results indicate that changes in the mass of blast furnace slag affect the final outcome of the desulfurization process. Specifically, a lower slag mass leads to a reduced sulfur content after the process.

Figure 4 illustrates the variation in final sulfur content as a function of the amount of CaO added to the process. The simulation was performed for the baseline heat and four modified values of CaO consumption: −40% of the baseline CaO mass, −20% of the baseline CaO mass, +20% of the baseline CaO mass, and +40% of the baseline CaO mass. The simulation results indicate that increasing the addition of CaO to the desulfurization process leads to a lower final sulfur content, thereby enhancing the degree of desulfurization [11].

Figure 5 illustrates the variation in final sulfur content as a function of the amount of Mg added to the process. The simulation was conducted for the baseline heat and four modified values of Mg consumption: −40% of the baseline Mg mass, −20% of the baseline Mg mass, +20% of the baseline Mg mass, and +40% of the baseline Mg mass. The simulation results indicate that increasing the addition of Mg to the desulfurization process leads to a lower final sulfur content, thereby enhancing the degree of desulfurization.

Figure 6 illustrates the effect of varying the hot metal temperature on the sulfur content after the desulfurization process. The temperature range investigated was 1315°C to 1420°C. Based on the conducted simulations, it can be concluded that lower hot metal temperatures result in more efficient utilization of Mg, ultimately leading to a lower final sulfur content [12].

Figure 7 illustrates the impact of two key modifications applied to the simulation model: the exchange of sizes between elementary reactors 1 and 3, and a 100% increase in mass transfer rates between the reactors. These changes were analyzed in four distinct configurations, combining baseline and modified reactor geometries with baseline and modified stream parameters. A detailed representation of these simulation variants is provided in Table 3.

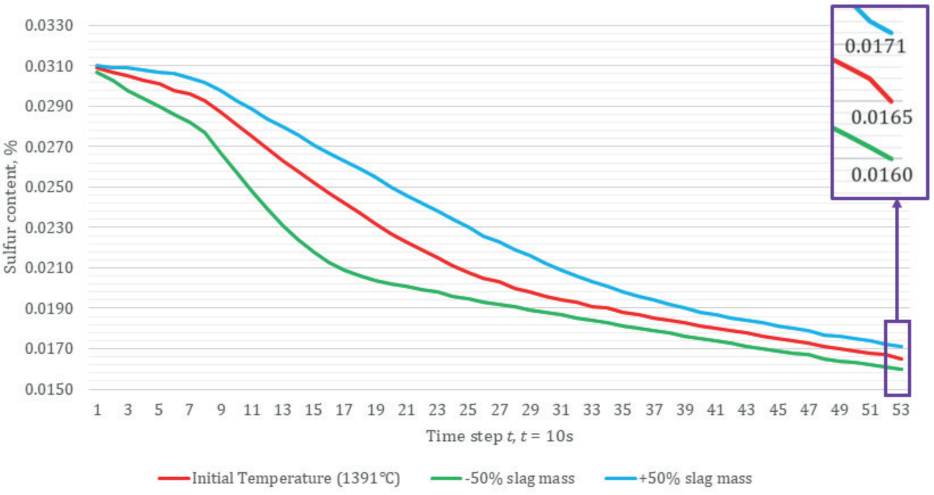

Fig. 3. Sulfur content depending on blast furnace slag mass

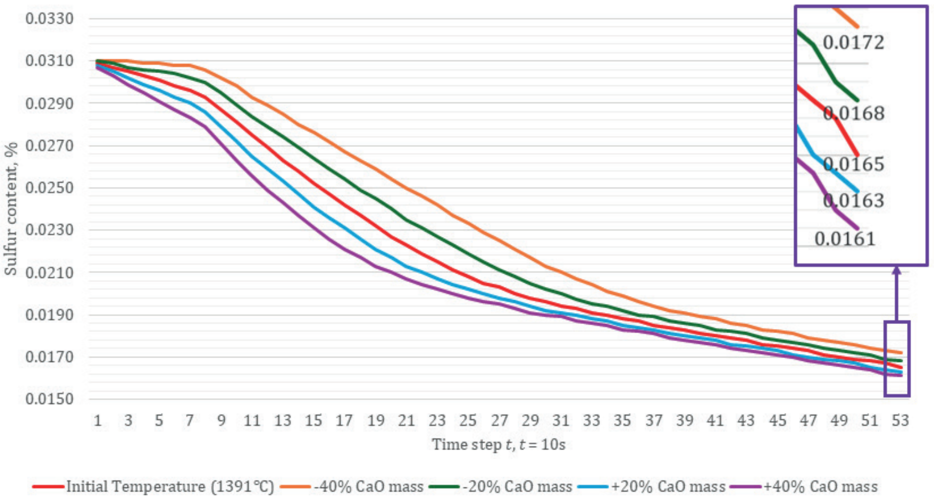

Fig. 4. Sulfur content depending on CaO addition

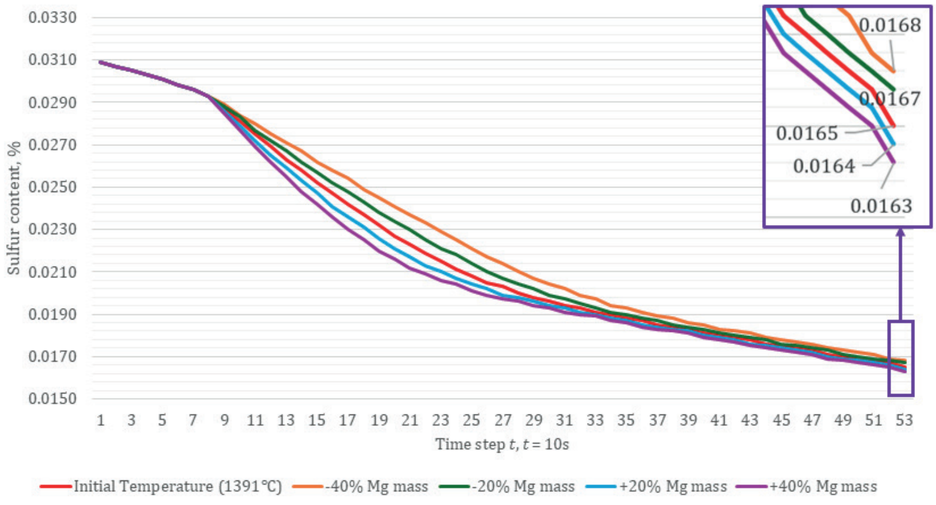

Fig. 5. Sulfur content depending on Mg addition

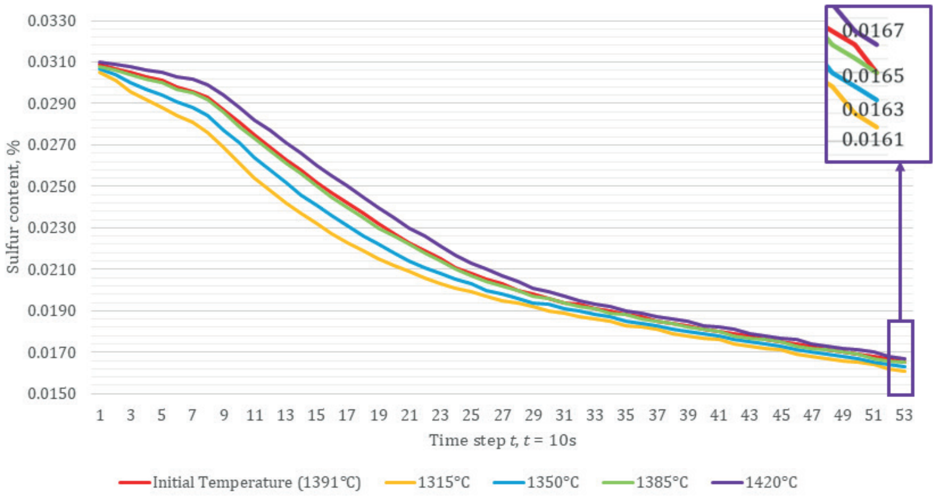

Fig. 6. Sulfur content depending on the HM temperature

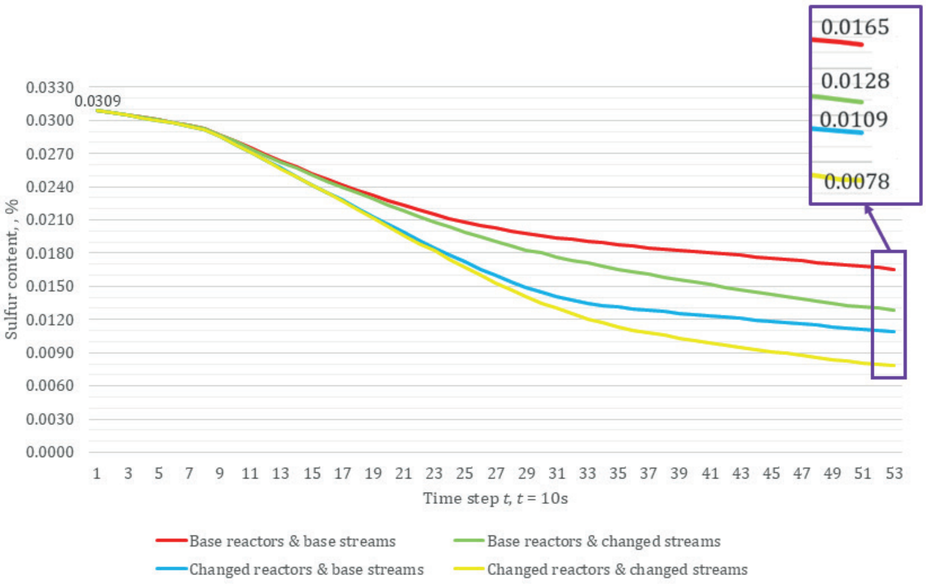

Fig. 7. Sulfur content depending on the parameter set

The results show that modifying the size of the elementary reactors leads to a lower degree of desulfurization for the same amount of reagents. This effect is attributed to the increased volume of reactor 1, which results in the delivery of a greater amount of sulfur to the chemical reaction zone. A similar trend is observed when the mass transfer rates between reactors are increased, indicating enhanced transport of sulfur to reactor 1. However, in this case, the effect also reflects intensified mixing within the ladle, which contributes to the overall reaction dynamics.

The configuration combining both modified reactor geometry and modified stream parameters yields the lowest final sulfur content (0.0078%), confirming that simultaneous optimization of spatial distribution and mass transfer enhances desulfurization efficiency.

Table 3
Simulation variants with reactor volumes and mass transfer stream values

Variant	Reactors volume	Mass transfer streams values
Based reactors & based streams	$V_1 = 30\%$ $V_2 = 50\%$ $V_3 = 20\%$	$V_{1-2} = 3\%$ $V_{1-3} = 2\%$ $V_{2-3} = 2.5\%$
Based reactors & changed streams	$V_1 = 30\%$ $V_2 = 50\%$ $V_3 = 20\%$	$V_{1-2} = 6\%$ $V_{1-3} = 4\%$ $V_{2-3} = 5\%$
Changed reactors & based streams	$V_1 = 50\%$ $V_2 = 30\%$ $V_3 = 20\%$	$V_{1-2} = 3\%$ $V_{1-3} = 2\%$ $V_{2-3} = 2.5\%$
Changed reactors & changed streams	$V_1 = 50\%$ $V_2 = 30\%$ $V_3 = 20\%$	$V_{1-2} = 6\%$ $V_{1-3} = 4\%$ $V_{2-3} = 5\%$

4. CONCLUSIONS AND SUMMARY

The experimental verification of the hybrid hot metal desulfurization model demonstrated significant implementation potential. Considering the catalytic effect of sulfur on the degradation of steel's mechanical properties, as well as its limited reactivity in subsequent stages of steelmaking (converter process, secondary metallurgy), the optimization of desulfurization parameters at the hot metal preparation stage remains a critical metallurgical challenge [13]. Industrial data confirm that early removal of sulfur enables its content to be reduced to below 0.005% by mass while maintaining process profitability. Based on the conducted simulations, the following conclusions were formulated:

- Both magnesium and calcium oxide play a thermodynamic role in the desulfurization process. The effectiveness of magnesium, in particular, is influenced by the mass and basicity of the blast furnace slag, which affect the stability of the MgS phase and the extent of sulfur removal.
- The most effective configuration combined modified reactor geometry with increased nitrogen flow, yielding the lowest final sulfur content (0.0078%). This confirms that the simultaneous optimization of spatial distribution and kinetic mixing parameters significantly improves desulfurization performance.
- Simulation results indicate that increasing CaO addition leads to a greater reduction in final sulfur content than increasing Mg addition under the tested conditions, highlighting the strong thermodynamic driving force associated with CaO-based desulfurization. Hot metal temperature affects the desulfurization process — lower temperatures enhance the efficiency of sulfur removal by promoting favorable thermodynamic conditions and increasing the stability of sulfide phases. The kinetic factor contributing to the increased efficiency of the desulfurization process is the nitrogen flow rate, which governs the intensity of mass transfer between the elementary reactors. Higher nitrogen flow enhances mixing and accelerates the transport of sulfur to the reaction zone, thereby improving the overall desulfurization performance. Figures 3–7 reveal that desulfurization kinetics are significantly influenced by both thermodynamic and kinetic parameters. Variations in slag mass, reagent dosing (CaO and Mg), initial temperature, and reactor-stream configurations modify the rate and extent of sulfur removal over time. These changes are reflected in the slope and curvature of the sulfur reduction curves, confirming that process dynamics must be considered alongside equilibrium conditions.

Not all of the process parameters influencing desulfurization efficiency can be directly translated into technological control algorithms. A notable example is the temperature of the metal bath, which exhibits a contradictory impact on process indicators. Lowering the temperature to the range of 1350–1400°C increases the efficiency of desulfurizing agents by improving the thermodynamic affinity of the reactions. However, this adjustment simultaneously necessitates an increase in the specific consumption of hot metal in the oxygen converter to compensate for energy losses.

Figure 8 presents a structured set of recommendations for the implementation of process improvements based on the simulation results. The proposed actions are categorized into two groups: those requiring no financial investment and those that involve additional costs.

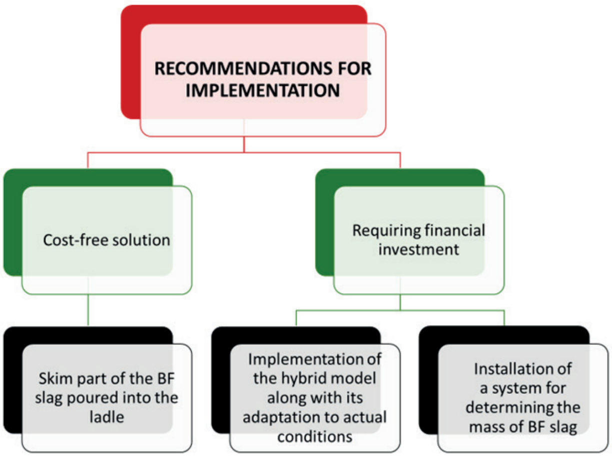

Fig. 8. Proposed recommendations

The cost-free recommendation involves partial skimming of the blast furnace slag poured into the ladle. This action aims to reduce the slag mass, which, as demonstrated in the simulations, can improve desulfurization efficiency by minimizing the dilution and buffering effects of the slag phase.

Recommendations requiring financial investment include the implementation of the hybrid simulation model adapted to actual operating conditions, and the installation of a system for determining the mass of blast furnace slag introduced into the ladle. These measures are intended to enhance process control and enable more precise reagent dosing, thereby improving the overall effectiveness of desulfurization [14].

The categorization of these recommendations reflects both the technical feasibility and economic consideration associated with their implementation.

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