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Computational Modelling of Sulfur Removal Mechanisms at the Steel–Slag Interface in Secondary Metallurgy

Výpočetní modelování mechanismů odsíření na rozhraní ocel–struska v sekundární metalurgii

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Abstract

Achieving the required steel purity and composition relies on effective secondary metallurgy processes, particularly during ladle refining. This study investigates sulfur removal mechanisms at the steel–slag interface using computational modelling. The research focuses on how slag composition and physical behaviour influence desulfurization during ladle treatment. A combination of CFD simulations and thermodynamic analysis was used to explore interfacial transport and reaction phenomena under realistic process conditions. Input data for the simulations were based on operational parameters and chemical compositions obtained from an industrial steelmaking plant. Statistical analysis and multi-parameter modelling were used to define the relationships between key slag properties—such as viscosity, basicity, and interfacial tension—and their influence on sulfur transfer efficiency. CFD simulations realized in Ansys Fluent captured the dynamics of multiphase flow and mass transfer, yielding results that closely reflect observed process trends. The study demonstrates that optimizing slag characteristics and refining parameters can significantly enhance sulfur removal during secondary steelmaking. The findings provide a computational basis for improving process control and refining strategies in industrial practice. By accurately modelling the steel–slag interface, this work supports the development of more effective and predictive tools for optimizing desulfurization in ladle metallurgy.

Keywords*: secondary metallurgy, CFD-simulation, steel-slag interface, steel desulfurization, ladle slag*

Abstrakt

Dosažení požadované čistoty a chemického složení oceli závisí na účinnosti procesů sekundární metalurgie, zejména během pánvové rafinace. Tato studie se zabývá mechanismy odstraňování síry na rozhraní ocel–struska s využitím numerického modelování. Výzkum je zaměřen na vliv složení strusky a jejích fyzikálních vlastností na průběh odsíření během pánvového zpracování. K analýze transportních a reakčních dějů na rozhraní za realistických procesních podmínek byla použita kombinace CFD simulací a termodynamického modelování. Vstupní data pro simulace vycházela z provozních parametrů a chemického složení získaných z průmyslového provozu. Pro stanovení vztahů mezi klíčovými vlastnostmi strusky – jako jsou viskozita, zásaditost a mezifázové napětí – a jejich vlivem na účinnost přenosu síry byla využita statistická analýza a víceparametrové modelování. CFD simulace realizované v prostředí Ansys Fluent zachycují dynamiku vícefázového proudění a přenosu hmoty a poskytují výsledky v dobré shodě s pozorovanými provozními trendy. Studie ukazuje, že optimalizace vlastností strusky a parametrů rafinace může významně zvýšit účinnost odsíření během sekundární metalurgie. Získané poznatky poskytují výpočetní základ pro zlepšení řízení procesu a návrhu rafinačních strategií v průmyslové praxi. Díky přesnému popisu rozhraní ocel–struska tato práce přispívá k vývoji pokročilých prediktivních nástrojů pro optimalizaci odsíření v pánvové metalurgii.

Klíčová slova: *sekundární metalurgie, CFD simulace, rozhraní ocel-struska, odsíření oceli, pánvová struska*

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1. Introduction

Secondary metallurgy plays a key role in producing high-quality steels by enabling precise control over chemical composition and non-metallic inclusions. Among the most important refining steps is sulfur removal, which is typically carried out in the ladle through reactions at the interface between molten steel and slag. The efficiency of desulfurization depends on several factors, including slag composition, basicity, viscosity, interfacial area, and stirring conditions [1-2].

While empirical approaches remain common in industry, computational modelling has become an increasingly valuable tool for analyzing and optimizing interfacial phenomena in steel refining. Modern CFD tools allow for the simulation of complex multiphase flows, interfacial mass transfer, and chemical reactions under conditions that reflect real ladle metallurgy operations [3-4].

This work presents a computational study of sulfur removal mechanisms occurring at the steel–slag interface using CFD simulations supported by thermodynamic analysis:

– The model incorporates realistic physical and chemical parameters derived from industrial data.
– The aim is to investigate how selected slag properties and operating conditions influence desulfurization efficiency, and to provide quantitative insights for improving ladle refining practice.
– The results contribute to a better understanding of interfacial behavior and support the development of more effective process control strategies in secondary steelmaking [5].

2. Materials and Methods

The computational model was developed to simulate sulfur removal at the steel–slag interface during ladle treatment using the CFD software Ansys Fluent 2023R1. A two-phase Eulerian multiphase model was applied to capture the interaction between the molten steel and slag layers, along with argon gas injection from the ladle bottom.

The geometry and mesh corresponded to the dimensions of an industrial ladle used for 170–180 tonnes of liquid steel. The mesh was refined in the interfacial zone to improve the resolution of gradients in velocity, concentration, and turbulence quantities. Turbulence was modeled using the realizable k–ε model with standard wall functions.

Fig. 1 illustrates the ladle geometry and setup used in the simulation. Input parameters—such as slag composition, temperature, viscosity, basicity, and sulfur content—were based on representative values from actual industrial operations. The species transport model was used to simulate sulfur diffusion and its chemical consumption in the slag phase.

Thermodynamic equilibrium constraints for sulfur partitioning were incorporated through user-defined functions (UDFs), allowing the model to dynamically evaluate local desulfurization rates. Argon flow rates were varied in a parametric study to evaluate their influence on interfacial mass transfer and sulfur removal efficiency.

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Top diameter of the ladle	3330 mm
Bottom diameter of the ladle	3060 mm
Height of the ladle	3700 mm
Height of the steel phase	3150 mm
Thickness of the slag layer	110 mm
Nozzle diameter for gas injection	80 mm
Density of liquid steel	7020 kg/m^3
Density of slag	3500 kg/m^3
Density of argon	0.568 kg/m^3
Viscosity of liquid steel	0.0055 Pa.s
Viscosity of slag	0.124 Pa.s
Viscosity of argon	0.000085Pa.s
Surface tension between steel and slag	1.15 N.m
Surface tension between steel and argon	1.82 N.m
Surface tension between slag and argon	0.58 N.m

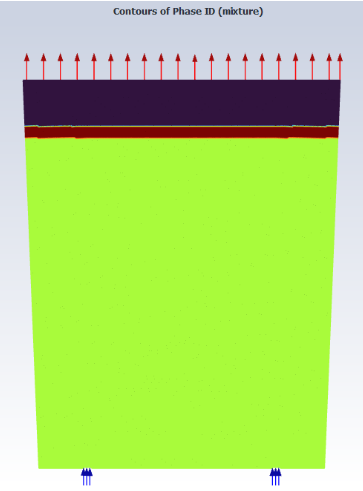

Fig. 1 Left: Dimensions of the ladle and simulation parameters; right: distribution of individual phases from the bottom view (steel, slag, atmosphere); argon gas inlets for inert media are shown at the bottom

Obr. 1 Vlevo: Rozměry pánve a parametry simulace; vpravo: rozložení jednotlivých fází při pohledu odspodu (ocel, struska, atmosféra); v dolní části jsou znázorněny přívody argonu pro inertní prostředí

3. Results and discussion

The CFD simulations provided detailed insight into the transport phenomena and sulfur removal behavior at the steel–slag interface. The desulfurization process was evaluated under varying argon flow rates (0 to 500 $l \cdot min^{-1}$), while keeping slag composition and steel temperature constant. **Tab. 1** and **Tab. 2** show the input chemical composition of the slag and steel phases.

Tab. 1 Input chemical composition of ladle slag
Tab. 1 Vstupní chemické složení pánvové strusky

CaO [%]	SiO_2 [%]	Al_2O_3 [%]	MgO [%]	S [%]
54.38	3.32	36.02	5.64	0.1550

Tab. 2 Input chemical composition of steel
Tab. 2 Vstupní chemické složení oceli

C [%]	Si [%]	Mn [%]	P [%]	S [%]	Al [%]
0.0520	0.003	0.138	0.0102	0.0077	0.338

Due to hardware and time constraints, the simulations were performed in a 2D format. The results were recorded in a vertical cross-section located on the left side of the ladle **Fig. 2**, assuming axisymmetric. Based on previously published research, symmetric flow behaviour is expected across both halves of the ladle volume, which justifies the use of a single representative section for analysis.

The computational results were consistent with known theoretical behavior and supported the assumption that both mixing intensity and slag properties strongly influence the desulfurization efficiency. The model provides a valuable basis for future optimization of ladle refining practices using simulation-based approaches.

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Fig. 2 illustrates the velocity vector field within the steel and slag phases. It can be observed that the injected argon bubbles drive circulation in the steel phase due to momentum exchange. In addition, high turbulent viscosity at the steel–slag interface enhances momentum, heat, and mass transport within the fluid, thereby increasing the turbulent diffusion of species. As a result, species near the steel–slag interface are transported at a higher rate compared to those near the bottom of the ladle.

In the simulation shown in **Fig. 3**, the intensity of steel desulfurization was analysed as a function of argon stirring applied from the bottom of the ladle. Argon flow rates ranged from 0 to 500 L/min. Bottom gas injection significantly accelerated the rate of desulfurization, as confirmed by the curve representing the simulation without gas injection.

The relationship between desulfurization rate and gas flow changes over time, as seen in **Fig. 3**, where the efficiency of sulfur removal decreases around 600 seconds. On the other hand, for argon flow rates ranging from 100 to 500 L/min, there is little to no improvement in desulfurization efficiency, indicating a saturation effect beyond a certain flow rate.

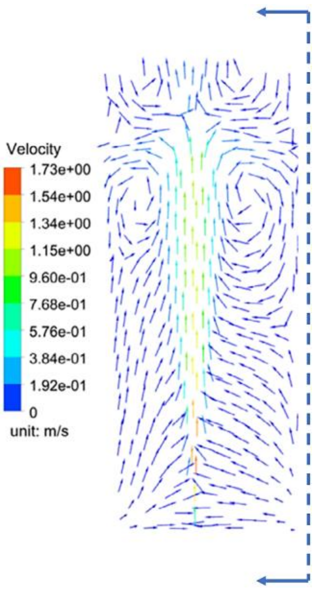

Fig. 2 Visualization of velocity vector directions within the ladle volume

Obr. 2 Vizualizace orientací vektorů rychlosti v objemu pánve

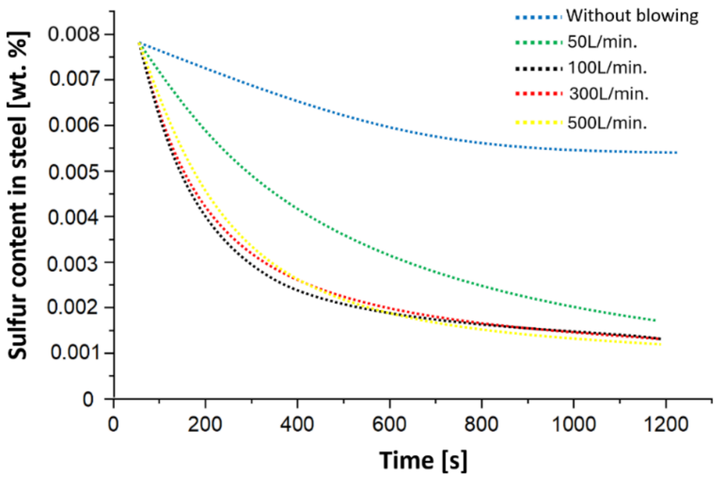

Fig. 3 Predicted sulfur content in steel at different argon flow rates over time

Obr. 3 Predikovaný obsah síry v oceli při různých průtocích argonu v průběhu experimentu

As shown in **Fig. 4**, the sulfur content in molten steel decreased over time, with the rate of desulfurization increasing significantly at higher argon flow rates (150 L/min. at this simulation). Enhanced stirring promoted better contact between the steel and slag phases, increasing the interfacial area and accelerating mass transfer.

The simulation results confirmed that argon injection is a key parameter for improving desulfurization kinetics.

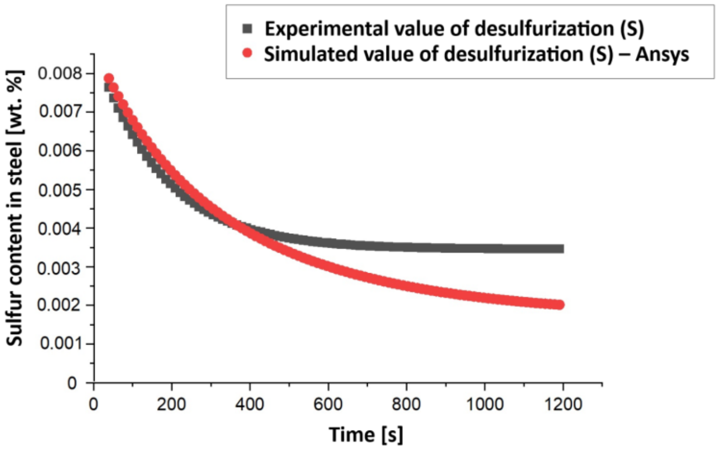

Fig. 4 Desulfurization progress of steel: computational model vs. predicted experimental values

Obr. 4 Průběh odsíření oceli: výpočetní model versus predikované experimentální hodnoty

4. Conclusion

This study demonstrated the applicability of CFD modelling for analysing sulfur removal mechanisms at the steel–slag interface during ladle refining. The simulations provided valuable insight into the effects of argon stirring and slag properties on the overall desulfurization efficiency. The results showed that bottom gas injection significantly enhances interfacial mass transfer by increasing mixing intensity and expanding the active reaction area. However, the effectiveness of desulfurization does not increase proportionally with gas flow beyond a certain threshold, indicating diminishing returns. High turbulent viscosity at the interface was found to be a key factor in promoting momentum and species transport.

The developed model, based on industrially relevant input data and validated physical assumptions, successfully captured the dominant transport and reaction phenomena in the ladle. It serves as a useful tool for evaluating process conditions and optimizing refining strategies in secondary metallurgy. Future work may include the transition to fully three-dimensional simulations and the integration of more complex thermodynamic and kinetic sub models to further improve the predictive accuracy of the computational approach.

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