# KINETIC AND THERMODYNAMIC ASPECTS IN MATHEMATICAL MODELING OF HOT METAL DESULFURIZATION PROCESS

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**Abstract**

The aim of the research in the hot metal desulfurization process is to create a mathematical model that will include both kinetic and thermodynamic aspects of the process. This is intended to increase the accuracy of predicting and obtaining the level of sulfur content in the hot metal, as well as to optimize process costs. By physically modeling the phenomenon of mixing the metal bath, it was possible to determine the influence of the method of supplying the desulfurization agent on the time of complete mixing of the metal bath. This made it possible to determine how the reactants are distributed in metal bath, which influenced further stages of research. By applying the theory of elementary reactors and enriching it with thermodynamic equilibrium calculations using Thermodynamic Equilibrium Software (TES), it will be possible to model the change in sulfur content during the desulfurization process in individual elementary reactors. This approach to the problem will allow the use of a solution that will enable accurate tracking of the sulfur removal process from the metal bath in a given time step. Such use of knowledge in the field of process kinetics and thermodynamic aspects may lead to even better control of the hot metal desulfurization process.

**Keywords:** Hot metal, desulfurization, mathematical modeling, metallurgy

## 1. INTRODUCTION

The hot metal desulfurization process aim is to remove sulfur from the metal bath, which is crucial for the production of high-quality steel. Mathematical modeling of this process is a complex and multi-stage operation that allows for better understanding and, as a result, optimization of the industrial process. It involves creating abstract, mathematical representations of the process to analyze, simulate and optimize the desulfurization process. Due to the nature of the desulfurization process, both aspects like kinetics - mixing of the metal bath and thermodynamics - chemical reactions occurring should be taken into account [1-4]. The model constructed in this way, based on the above-mentioned aspects, will be able to model the processes occurring in a real metallurgical unit. Such action may allow for better control of the process and its optimization - shortening the duration, reducing the consumption of reagents and, consequently, reducing production costs. The aim of this research was to develop a mathematical model that takes into account kinetic and thermodynamic factors of the hot metal desulfurization process. The research also resulted in the development of a procedure for future software that includes the above-mentioned mathematical model, which will be implemented in a real metallurgical unit.

## 2. LITERATURE REVIEW

Mathematical models of the desulfurization process may have different structures and be based on various aspects. A good example of how different approaches to mathematical modeling can be is the diagram shown in **Figure 1** [5]. From models based on thermodynamics or process kinetics to data-driven models. From the

point of view of industrial implementation the choice of mathematical modeling method is related to the available data and tools. Due to the limited availability of time for real-time modeling, which is limited by the duration of the actual hot metal desulfurization process, and also due to the availability of data (**Figure 2**) [6], a mathematical model should be created that will meet the above limitations and at the same time its calculation results will be similar to real data.

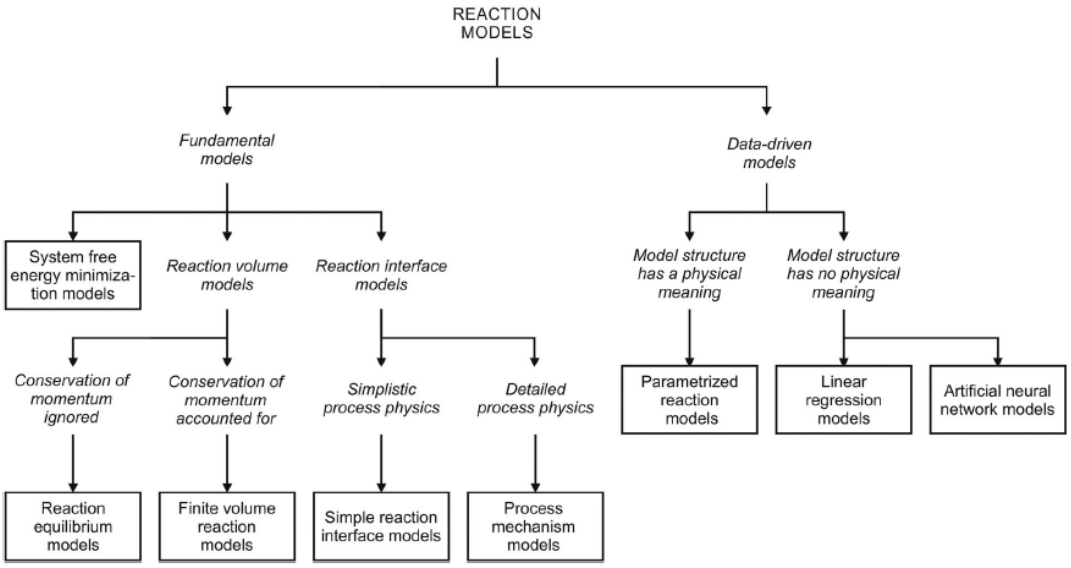


**Figure 1** Diagram of the proposed model categorization

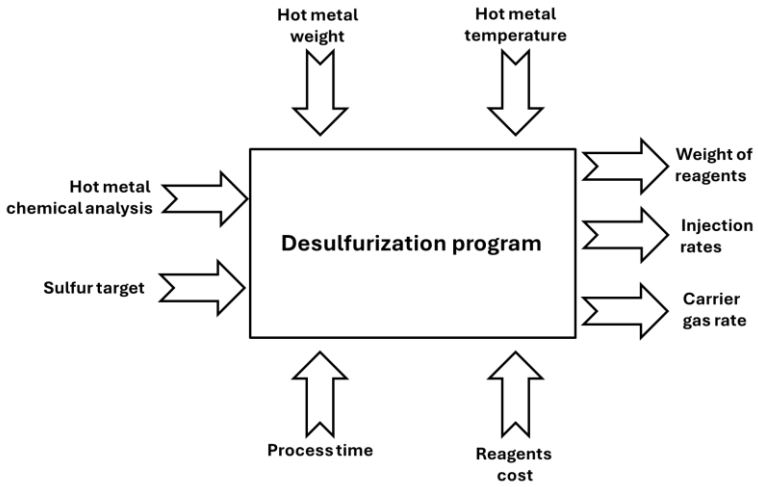


**Figure 2** Available inputs and outputs for the desulfurization program

## 3. KINETIC ASPECTS

In order to capture the kinetic aspects [7] of the hot metal desulfurization process, it was necessary to build a cold model based on a real metallurgical unit and then simulate the mixing of the metal bath [8]. Based on the experiments performed, experimental and simulation curves were determined the time for complete mixing. For this purpose the cold model of the hot metal desulfurization unit was designed (**Figure 3**) and built.

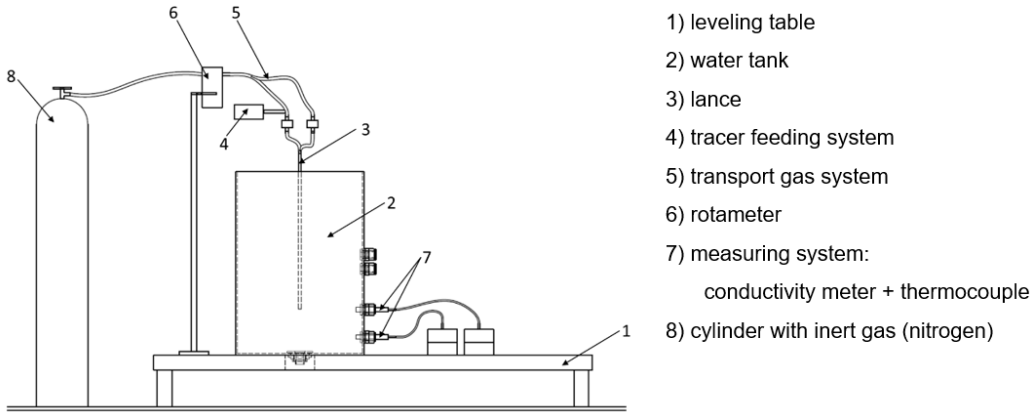


**Figure 3** Scheme of experimental setup

This model made it possible to simulate the actual mixing process of the metal bath during desulfurization in order to determine the time for its complete mixing (**Figure 4**).

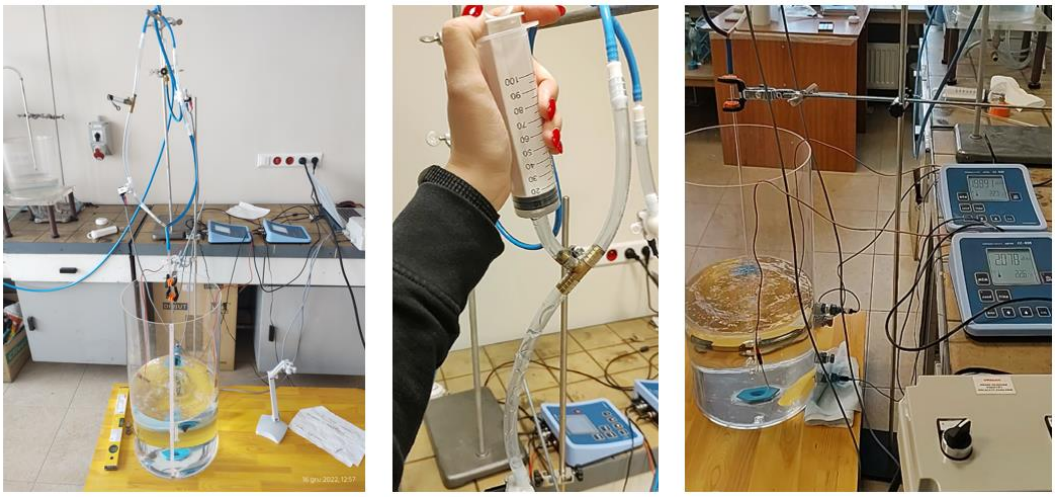

**Figure 4** Cold model of mixing metal bath

The next step was to create an experiment plan reflecting the actual conditions of the desulfurization process (variability of parameters: flow of transporting gas, tonnage of hot metal in the ladle, position of the working lance). Due to the need to compare the results of physical simulation for various configurations of the observed process parameters, standardization of the conductivity measurement results was required. It should be mentioned here that the concentration is linearly proportional to the specific conductivity of the tested system. The result of implementing the above-mentioned tasks was obtaining the results of the time of complete mixing of the metal bath. In the next stage, based on the data obtained, it was necessary to verify the mixing times of the metal bath. For this task, it was necessary to develop the structure of elementary reactors for the hot metal desulfurization process. It should be emphasized here that there is no information in the available literature on the use of Tank Model [9] in relation to the hot metal desulfurization process, and the development of the structure of elementary reactors was based on similarities to the steel argonization process in a steel ladle [10]. All the above activities are an introduction to the next stage of work - thermodynamic aspects.

## 4. THERMODYNAMIC ASPECTS

The concept of the desulfurization mathematical model will be based on a mixing model (cold model experiments) which was enriched with a thermodynamic model using Thermodynamic Equilibrium Software (TES). Thus it will be possible to simulate changes in sulfur content in individual elementary reactors using Tank Theory (**Figure 5**). It should be emphasized that Tank Theory is based on three main assumptions:

- at any instant of time t there is no concentration gradient of reactans within the each tank (ideal mixing)
- streams masses flowing in and out of the bath are defined
- reagents concentrations change in tank occurs in steps, with frequency resulting form the adopted calculation time step

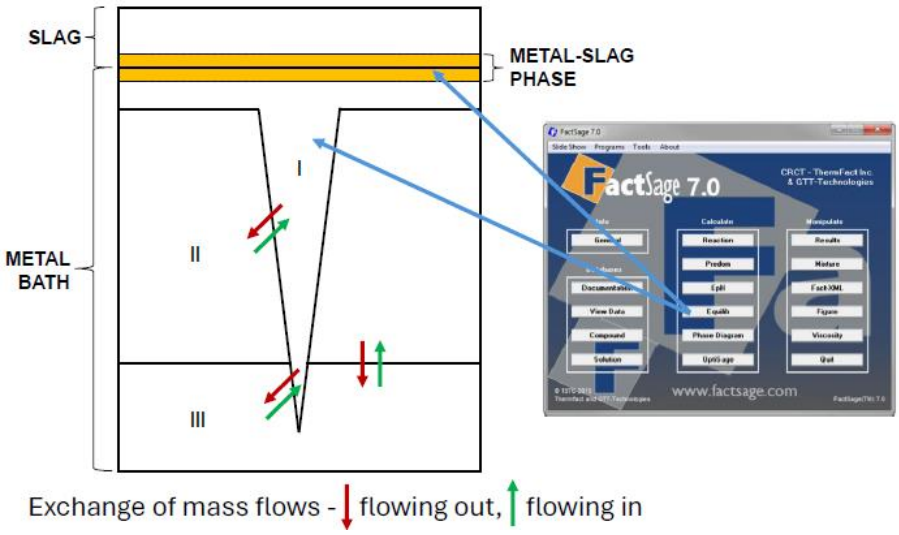


**Figure 5** Division of the metal bath in the ladle into reactors during the desulfurization process due to Tank Theory

Based on the experiments performed and the data obtained, mass flow streams between the reactors were defined, which made it possible to track changes in the chemical composition of the hot metal, and as a result, this solution will enable mathematical modeling of the desulfurization process.

## 5. PROCEDURES FOR THE MATHEMATICAL MODEL

Based on the research conducted on the kinetic and thermodynamic aspects of the desulfurization process the procedure scheme for a mathematical model was formulated. Its simplified version is shown in **Figure 6**. The scheme of operation is as follows:

- First stage of modeling is the preparation of data that will be unchanged for each calculation performed, these are: volume fraction of elementary reactors, flow exchange matrix between reactors, hot metal density, slag mass entering equilibrium in one time step, time step length and chemical composition of the reactants.
- Second step is to enter data for a specific melt: mass of hot metal, its chemical composition, mass of slag in the ladle, slag chemical composition, mass of reagents, time of introducing reagents, nitrogen flow rate and number of iterations (time steps).

- Third step is to calculate the thermodynamic equilibrium in the Thermodynamic Equilibrium Software for reactor I. Obtained data: chemical composition of pig iron in reactor I, chemical composition of slag entering equilibrium.
- Based on the previous step, mass exchange between the reactors should be performed in a time step and their chemical composition should be averaged.
- The process should be carried out for a predetermined number of iterations (time steps).
- After performing an appropriate number of iterations, the chemical composition should be averaged over the entire volume of the ladle, the chemical composition of the slag should be averaged and the graphical representation of the change in the chemical composition of the hot metal during the process should be generated.

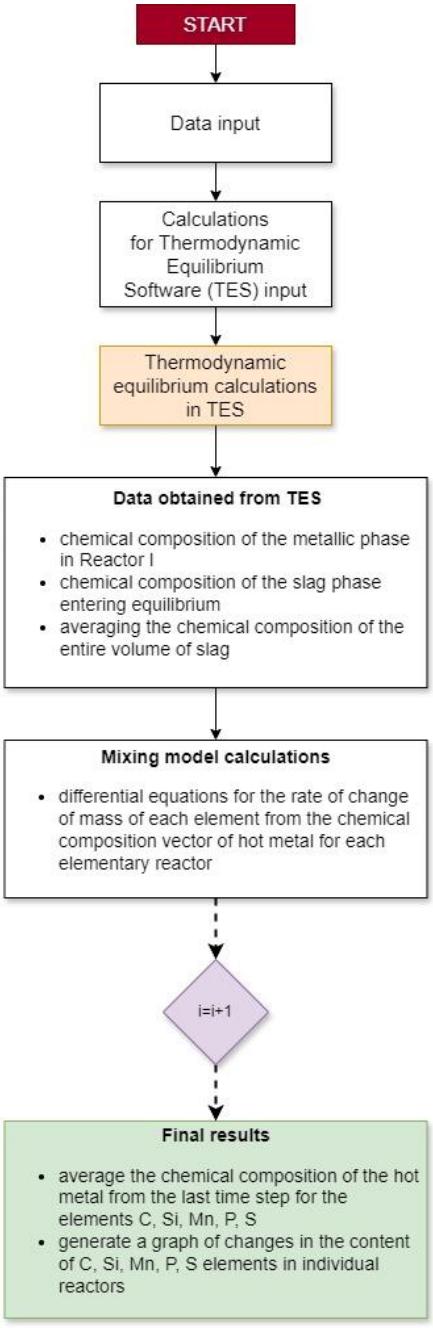


**Figure 6** Simplified procedure scheme for a desulfurization mathematical model

This procedure allows tracking the chemical composition of both hot metal and slag during the desulfurization process and also allows determining the actual weight of the slag that was created in the process. In case of any change in the desulfurization process - its time, the amount of reagents or the logistics of the entire steel production process, we are able to quickly determine the sulfur content in the hot metal without having to wait for chemical analysis, which may be crucial in extreme cases of failure of measuring devices.

## 6. CONCLUSIONS

Mathematical modeling of the hot metal desulfurization process allows for more detailed understanding and control of this process. Thanks to modeling, you can optimize process conditions, minimize costs and improve the quality of the final product. Modern computer techniques and numerical algorithms play a key role in the creation and validation of these models.

Based on the considerations and experiment, kinetic and thermodynamic aspects were used, thanks to which it was possible to construct the principles and procedure of a mathematical model that performs calculations in real time based on real data. The result of model calculations is the actual S content at a given moment in time. Thanks to this approach, from the point of view of the actual metallurgical aggregate, it will be possible to optimize the process in terms of costs and duration.

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