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Optimizing Pig Iron Desulfurization Using Physics-Informed Neural Networks (PINNs) †

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Abstract: The aim of the presented research was to optimize a pig iron desulfurization process through data-driven machine learning methods. Utilizing historical data, chemical analysis of pig iron and slag, and the thermodynamics of the process including simulations of the chemical reactions between individual phases, a neural network was trained for the predictive modeling of desulfurization efficiency. The accuracy of the model was enhanced by integrating Physics-Informed Neural Networks (PINNs), which incorporate chemical reaction principles. The results show better performance of PINNs in comparison to the Feedforward Neural Network (FNN) in the generalization of the desulfurization process, bringing better reliability to the model.

Keywords: pig iron; steelmaking; desulfurization; neural networks; Physics-Informed Neural Networks (PINNs); data analytics; process optimization; chemical reactions; predictive modeling; cost savings; simulations

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1. Introduction

Steel production is a critical industry with wide-ranging applications in construction, automotive manufacturing, and various engineering sectors. One of the important challenges in the production of high-quality steel in closed loop is the effective removal of sulfur, known as the desulfurization process. An excessive sulfur content can adversely affect the mechanical properties of steel [1–3], making its optimization a priority for producers [3,4]. Traditional methods for desulfurization largely use physico-chemical fundamentals [1–9] and may not capture the complexities and nonlinearities of the chemical processes involved [10,11] that FNN can according to the universal approximation theorem [11]. Sulfur removal is possible in various stages of ironmaking and steelmaking.

In this presented paper, we discuss a novel approach aimed at optimizing the pig iron desulfurization process in a hot metal ladle using machine learning techniques. The methodology combines neural network models trained on historical production data with Physics-Informed Neural Networks (PINNs) [10,12,13] to improve the predictive accuracy. By integrating chemical principles into the machine learning model, a more efficient and accurate way to optimize the process is offered. Our work aims to show the significance of combining knowledge from data science with theory about processes. Figure 1 shows the scheme of the model training cost calculations.

In Physics-Informed Neural Networks (PINNs), there exists a pragmatic balance between theoretical precision and computational efficiency. The theoretical component of the PINN model used in this study adopts a simplified simulation approach to expedite the computer calculations. On the other hand, while the historical data inherently capture the influence of various parameters such as kinematics, temperature, and more, it is noteworthy that these specific variables were not actively monitored or explicitly recorded during

their entry into the database. This scenario underscores the interplay between empirical intricacies and theoretical generalities, laying the foundation for our investigation.

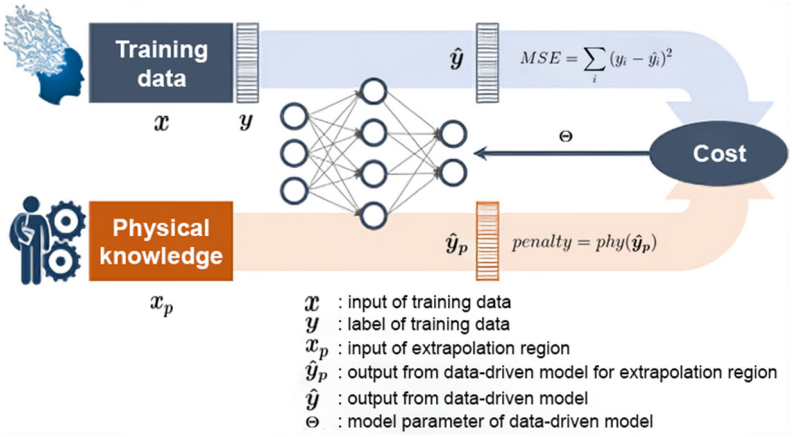


Figure 1. Scheme of PINNs model training.

2. Materials and Methods

2.1. Data Collection

The initial dataset consists of historical records of steel production from various plants, covering multiple years. Each entry includes metrics such as the temperature before desulfurization, the sulfur content, the sulfur activity, the chemical composition of pig iron, and the reagents used. The dataset underwent rigorous cleaning to handle missing values and outliers.

2.2. Neural Network Model

A neural network regression model for initial predictive modeling was utilized. The network was trained on 70% of the dataset, with 20% used for validation and the remaining 10% for testing. Both FNN and PINNs use the same regression structure: an input layer, 3 layers with 10 neurons, and an output layer.

2.3. Physics-Informed Neural Networks (PINNs)

To capture the underlying physics of the desulfurization process, Physics-Informed Neural Networks (PINNs) [10,12,13] were used. PINNs enable the integration of prior physical knowledge into the neural network model, allowing it to adhere to governing equations and physical laws.

The chemical reactions considered for the physics-informed part of the model are as follows:

$$(\mathrm{CaO}) + [\mathrm{S}] \rightarrow (\mathrm{CaS}) + [\mathrm{O}] \tag{1}$$

$$[\mathrm{S}] + [\mathrm{Mg}] + (\mathrm{CaO}) \rightarrow (\mathrm{CaS}) + (\mathrm{MgO}) \tag{2}$$

The corresponding time-dependent equations that describe the chemical kinetics for these reactions are incorporated into the PINNs loss function:

$$\frac{dc_{CaO}}{dt} = -k_1 c_{CaO} c_S^{2.5} - k_2 c_{Mg} c_S^{2.5} c_{CaO} + R_{CaO} \tag{3}$$

$$\frac{dc_S}{dt} = -k_1 c_{CaO} c_S^{2.5} - k_2 c_{Mg} c_S^{2.5} c_{CaO} \tag{4}$$

$$\frac{dc_{MgO}}{dt} = k_2 c_{Mg} c_S^{2.5} c_{CaO} \tag{5}$$

$$\frac{dc_O}{dt} = k_1 c_{CaO} c_S^{2.5} \tag{6}$$

$$\frac{dc_{Mg}}{dt} = -k_2 c_{Mg} c_S^{2.5} c_{CaO} + R_{Mg} \quad (7)$$

$$\frac{dc_{CaS}}{dt} = k_1 c_{CaO} c_S^{2.5} + k_2 c_{Mg} c_S^{2.5} c_{CaO} \quad (8)$$

Here, k_1 and k_2 are the reaction speed, and R_{Mg} and R_{CaO} are the agent gain constants. These equations provide constraints during the training of the neural network, ensuring that the model predictions are not only data-driven but also physically plausible.

All simulations and model training were conducted using Python 3.10. Figure 2 shows the results of the simulations for the differential Equations (3)–(8).

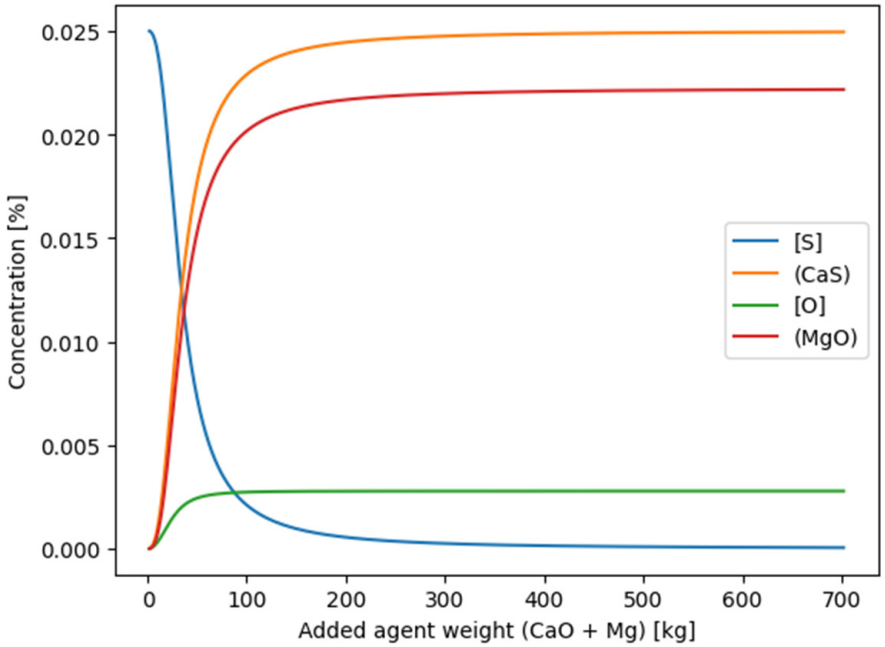


Figure 2. Simulation of chemical kinetics for Reactions (1) and (2).

2.4. Model Training

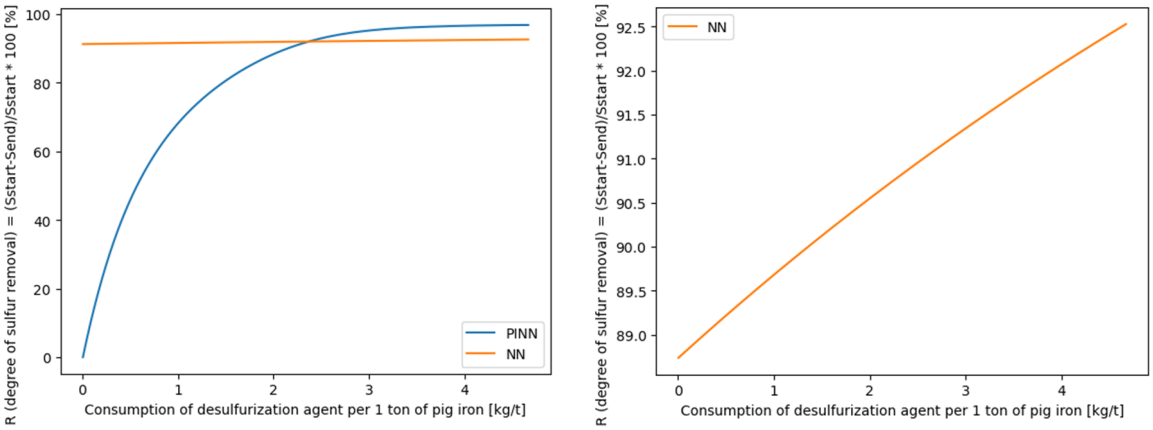
Both the FNN and PINNs models were trained using backpropagation with the Adam optimizer and the mean square error (MSE) loss function. The PINNs' loss was modified by the output of the physics simulation.

2.5. Evaluation Metrics

The models were evaluated based on the functions that were acquired after training. The graphs from the Neural Network and Physics-Informed Neural Network (PINN) were compared.

3. Results

After completing the training phase, Figure 3 shows the evaluation of both the neural network and the Physics-Informed Neural Networks (PINNs) models, based on their performance in predicting desulfurization effectiveness.



(**a**) Comparative Efficiency (**b**) NN Response

Figure 3. Comparative analysis of standard Neural Network and PINNs model predictions based on the desulfurization agent used.

One key observation, as shown in Figure 3a, is the disparity in the realism of the function graphs generated by the two models. While the standard neural network did exhibit a reasonable level of accuracy, its generated function graph appeared to lack information in extrapolation. This indicated that the model could generalize from the data to some extent; however, it might not fully capture the underlying physics of the desulfurization process, as is shown in Figure 3b, as the FNN is not able to extrapolate reliably.

In contrast, the PINNs model produced a function graph that not only aligned closely with the actual data but also adhered to the governing chemical equations. This resulted in a more realistic and physically plausible model.

These results demonstrate the efficacy of integrating physical principles into machine learning models for complex industrial applications like steel desulfurization. By offering a more accurate and reliable framework, the PINNs model stands as a significant advancement in the optimization of this crucial process.

4. Discussion

In this study, the benefits of integrating historical data and domain-specific knowledge are demonstrated to create a more reliable predictive model for steel desulfurization. The Physics-Informed Neural Network (PINN) model outperformed standard neural networks by incorporating both empirical data and real-world chemical equations. This multi-faceted approach not only improved the accuracy but added a layer of realism to the model. The key advantage of using domain knowledge to compensate for limited data is visually highlighted in Figure 4, underscoring its critical role in optimizing complex industrial processes like steel production.

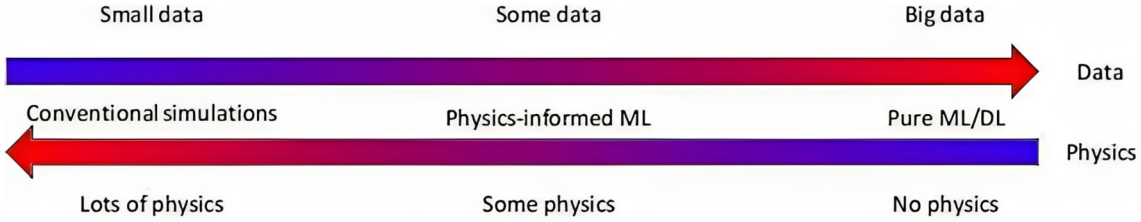


Figure 4. Trade-off between quantity of data and level of theoretical knowledge in model performance.

This study underscores the importance of merging data analytics with domain-specific knowledge for complex problem solving. It sets the stage for future research aimed at

refining the model for other variables and conditions that may be present in real-world steel production scenarios.

5. Conclusions

This study set out to explore the capabilities of machine learning models, specifically Physics-Informed Neural Networks (PINNs), in optimizing the steel desulfurization process. Our results indicate that the integration of domain-specific theoretical knowledge into neural networks can significantly enhance the model's performance and reliability. This is particularly valuable in scenarios where collecting a large volume of high-quality data is impractical or cost prohibitive.

The PINNs model generated graphs that were more physically plausible, highlighting the model's ability to grasp the underlying complexities of the desulfurization process. The synergy between historical data and domain-specific knowledge proved to be a compelling approach to problem-solving in complex industrial applications.

As industries increasingly turn to data analytics and machine learning for operational optimization, the findings of this study serve as a testament to the potential benefits of combining empirical data with theoretical understanding. Future research should focus on refining these models to account for more factors such as kinematics, thereby widening their applicability and efficiency in industrial settings.

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Conflicts of Interest: The authors declare no conflict of interest.

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