Combining the power of computational thermochemistry with the convenience of Python within the digital Platforms of the SMS group

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ABSTRACT

For an optimal design and control of metallurgical processes, a deep understanding of the thermodynamics of the governing reactions is required. Modelling the thermochemical behavior of those reactions is complex, as it involves multi-component and multi-phase systems. For this purpose, thermodynamic computing systems such as FactSage™ (Bale et al., 2016), which combine Gibbs energy minimization routines with large databases of optimized thermodynamic data of solutions and compounds, have been used within the SMS group.

Recently, the successful integration of those thermodynamic computing systems into the digital platforms of SMS has been achieved through ChemApp, which made running complex thermochemical calculations in Python-integrated development environments possible. ChemApp is a programmer's package for thermochemistry and incorporates the Gibbs energy minimizer of FactSage™ as reported by Petersen and Hack (2007) as well as by Zietsman and Petersen (2018). The digital platforms link the fundamental and the industrial aspects together and can be applied as a process advisor, or for the evaluation of the environmental footprint and the economic implications of different process routes, as discussed by Reuter (2023). Two examples illustrating the progress of the developments in this regard will be introduced:

- The Tilting Refining Furnace (TRF) for copper scrap recycling and refining to anode copper (the BlueControlApp)
- Dephosphorization control for the Oxygen Steelmaking process (BOF)

INTRODUCTION

The future of metals is circular and carbon neutral. To achieve this, a thorough evaluation of the thermodynamic behavior of the systems involved is crucial. This evaluation is necessary for a comprehensive understanding of the system, allowing us to characterize its thermodynamic behavior to the full extent, quantify its limitations, and minimize the gap depicted in the top left of Figure 1.

Figure 1 illustrates the necessity of robust digital platforms for accurately quantifying the limitations of larger systems. These platforms facilitate scaling the physics of reaction interfaces in metallurgical reactors, which are instrumental in processing and recycling systems and guiding the product design. Consequently, it's crucial to thoroughly quantify the exergy efficiency of the entire system. Here, thermodynamics also plays an integral and important part in quantifying the performance relative to a rigorous baseline laying the groundwork for a comprehensive understanding of green premiums and their role in driving innovation within the system (Reuter (2023)).

FIG 1 – Integration of process understanding, digitalization, and innovation via the digital platforms of the SMS group.

Using ChemApp (Petersen and Hack, 2007; Zietsman and Petersen, 2018), it has become possible to run complex thermochemical calculations within the Python-based Integrated development environment (IDE). ChemApp is a programmer's package for thermochemistry and incorporates the Gibbs energy minimizer of FactSage™.

Later, two examples illustrating the progress of the developments in this regard will be introduced.

APPLICATION FOR THE TRF FURNACE: THE BLUECONTROL APP

In order to refine copper scrap, the SMS group uses a tilting refining furnace (TRF). By combining the tilting refining furnace with a casting wheel, high-quality anodes are produced. In other words, when combined with the casting wheel, TRF can execute the melting, refining, and casting of copper scrap in one flexible unit. However, as discussed by Reuter (2023), despite multiple advances in the process control of such furnaces, a certain degree of operator intervention is still required. Although there are modern process control methodologies available such as artificial intelligence techniques, the current process control input is primarily based on the operator's and/or metallurgist's expertise and intuition, rather than solely relying on these advanced techniques.

As shown in Figure 2, the tilting refining furnaces operate through a series of stages. Initially, the scrap is melted. Subsequent stages involve the removal of impurities such as Al, Fe, Ni, Pb, Sn, Zn, etc., which are transferred from the copper alloy into the slag by oxidation. This purification begins indirectly during the smelting of high-grade scrap, but due to limited slag uses, the final oxidation step(s) after charging and smelting are necessary.

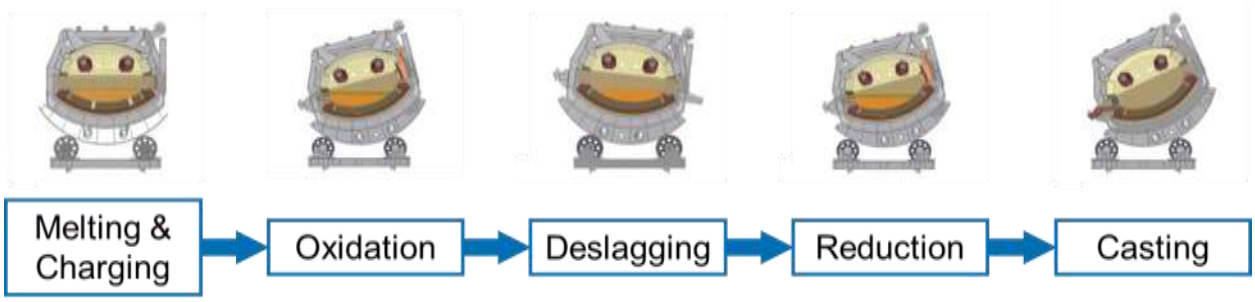

FIG 2 – Tilting Refining Furnace and its various steps, oxidation can happen in 1 to 3 steps depending on the scrap feed quality and required anode quality.

Non-linear solution chemistry of slag and copper affects the distribution of elements from copper to slag and off-gas. Obviously, the flow of gas through the system especially affects the distribution of elements and compounds with higher vapor pressure. Inefficiencies due to mass and heat transfer and fluid flow also have an effect.

Although a TRF is seemingly a simple system, various non-linear interconnected physical processes complicate the prediction of possible outcomes, i.e. metal quality. A full cycle of melting, oxidizing, refining, and casting typically takes approximately 24 hours. Optimizing the feed mix for a desired outcome requires substantial computational effort, as it involves repeatedly solving numerous 24-hour cycles using the Gibbs energy minimization method. Typical operational parameters to be optimized can include:

- correct quantity and mix of fluxes to achieve the desired flux type, fayalite/olivine (Figure 3), calcium- or calcium silicate-based;
- the processing steps and times;
- lambda of the burner, which denotes the ratio of actual air supply to the stoichiometric air requirement for complete fuel combustion;
- quantity and type of oxidizing and reducing gases;
- temperature;
- indirect parameters, such as viscosity;
- oxidation or reduction gas rate.

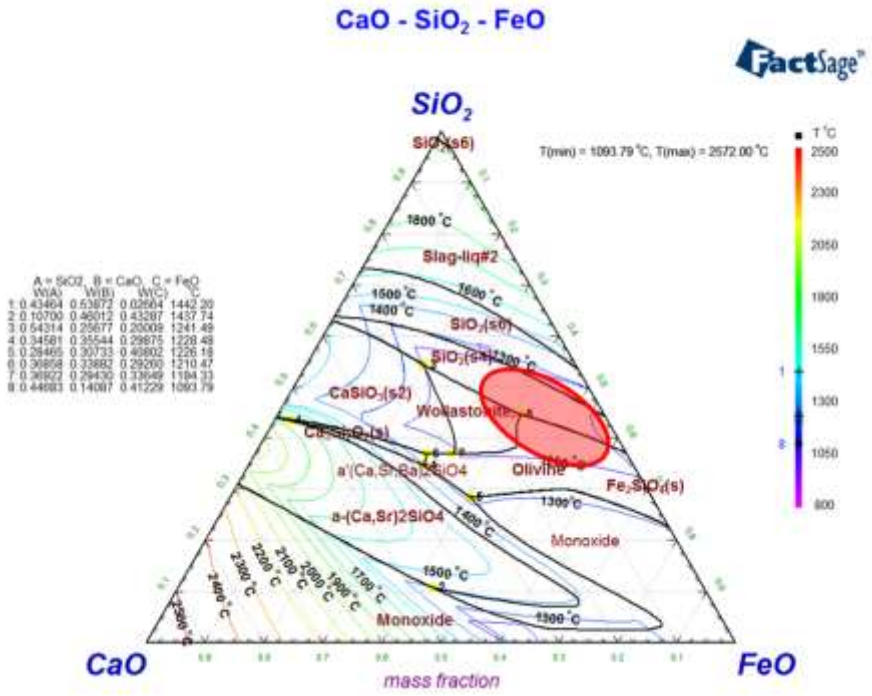

FIG 3 – Example target slag compositions for the copper refining for an operating point for an olivine.

The above said would suggest that the involvement of human intervention and decision-making in the production and refining processes of copper scrap may lead to various adverse outcomes. These might include inefficiencies in anode production mass, inconsistent anode quality, i.e. impurities outside of desired levels, unreliable parameters e.g. slag viscosity, significant deviations from customer yield targets, suboptimal refining processes i.e. not reaching the targets for an anode, lengthy decision-making periods, and heavy reliance on skilled operators and metallurgists with specialized knowledge of these processes. These downsides can lead to increased costs and reduced productivity.

For this purpose, SMS has developed the BlueControl application, to support the metallurgists as well as the operators in designing, analyzing, controlling, and optimizing the copper refining process. The application can be further used for the training of operators and for calculating the process outcomes under different operating conditions (linked directly to the thermochemical software library ChemApp). As shown in Figure 4, the BlueControlApp has two main calculation features:

1. Simulation: The executed dynamic simulations use thermochemical equilibrium software FactSage™ (Bale et al., 2016), with a ChemApp interface, to perform Gibbs free energy minimization. Unfortunately, since the Gibbs free energy minimization algorithm uses the constrained and non-linear optimization method, the calculations can be time-consuming. For example, using FactSage™ with a ChemApp interface may take a single oxidation simulation (single refining cycle) up to 2 minutes and about 20 seconds to execute.

- Optimization: Based on the copper scrap weight and its composition, feed temperature, oxidation gas rate and reduction gas rate, the optimization application finds the ultimate fluxes combination. The resulting flux combination assures the highest possible copper amount and the lowest possible amount of impurities at the end of the refining process (purest copper anode). This will improve production efficiency, yield, quality, throughput and reduce production costs.

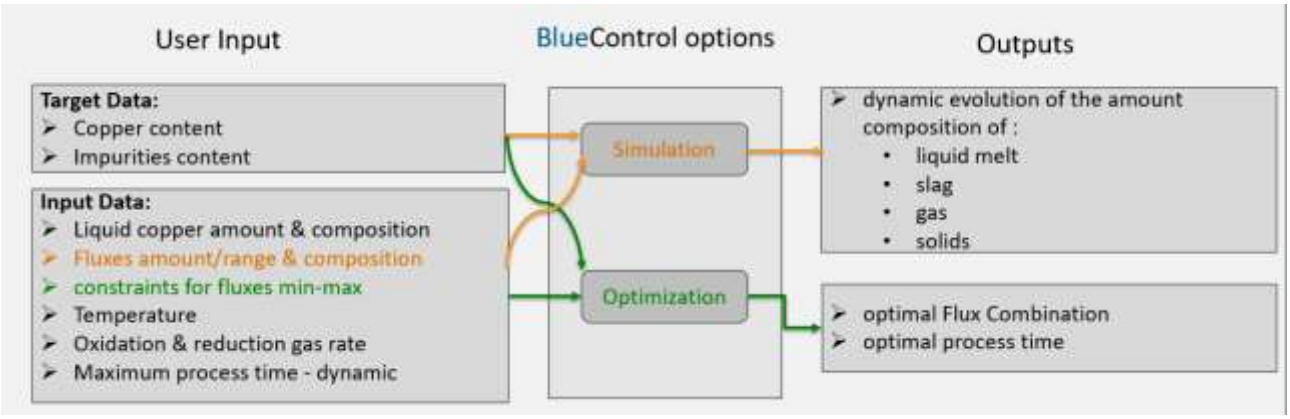

FIG 4. Schematics of BlueControlApp.

Moreover, the optimization process is based on the calculations done by the simulations, making it time-consuming. To illustrate more, using the BlueControlApp optimizer to find suitable fluxes combinations requires running a tremendous number of simulations, where each simulation resembles specific input values used during the copper refinement process. Recalling that such simulations are based on the time-consuming ChemApp interface, the optimization process itself will be also time-consuming. This can lead to tremendous production delays and an increase in production cost, thus making such analyses infeasible. To handle this issue, Akouch, Reuter, Kirmse et al. (2023) developed a surrogate model, which corresponds to a statistical model that accurately approximates the FactSage-based simulation outputs within seconds and not minutes.

The surrogate model is considered as a supervised machine learning model, where the model is trained to recognize patterns and physical relationships between the input-outputs of the copper refining process. Using the surrogate model as a core model to run BlueControl simulations/optimization, made it possible to accurately estimate in real-time the costly and time-consuming simulations/optimization.

APPLICATION FOR THE BOF PROCESS: DEPHOSPHORIZATION CONTROL

The next example illustrating the need to integrate computational thermochemistry into digital platforms is the control of phosphorous removal from steel during the oxygen steelmaking route, denoted as “steel dephosphorization”.

Phosphorus is introduced to the blast furnace through the charged iron ore and ends up almost completely in the discharged liquid metal. The dissolved phosphorus must be removed from the liquid metal up to levels below 150 ppm due to its detrimental effect on the quality of steel. This occurs in the next aggregate, the BOF process (Basic Oxygen Furnace) through oxidation of phosphorus to P_2O_5, which is then bound into the slag phase. To ensure that the phosphorous oxide remains in the slag, the process should be operated in a way that sets favorable conditions for P_2O_5 stability in the slag. Otherwise, P_2O_5 is reduced, and the phosphorous returns to the liquid metal denoted as “steel rephosphorization”. It is well established that the dephosphorization potential of the slag increases with its CaO and FeO content while it decreases with temperature.

In previous works (Khadhraoui, Odenthal, Das et al., 2018, Khadhraoui, Hack, Jantzen et al. 2019, 2021; Khadhraoui, 2021), it has been reported that BOF slags are heterogeneous for a large part of the process containing a liquid phase and a variety of solid phases. The solid phase $2CaO.SiO_2$ (C2S) is particularly interesting for dephosphorization, as it is capable of dissolving phosphorous through the formation of the $2CaO.SiO_2$-$3CaO.P_2O_5$ (C2S_C3P) phase, which increases the dephosphorization potential of the heterogeneous slag. The formation of other solid phases, which do not dissolve phosphorous such as the $3CaO.SiO_2$ (C3S) phase, as well as the MgO- and CaO-based solid monoxide solutions, decreases the dephosphorization potential. Thus, the optimal slag zone for dephosphorization is suggested to lie within the single C2S saturation regions, indicated by the blue-marked area in Figure 5, which presents the phase diagram of the main oxide system for BOF slags, the CaO-FeO_x-SiO_2. However, the ratio of the C2S phase in the heterogenous slag has to be controlled carefully below a certain value, otherwise, its positive effect on dephosphorization can be counteracted by the negative effect on the kinetics of dephosphorization, as it decreases the

mass transfer coefficient of the slag. Thus, the target region for optimal dephosphorization has to be narrowed further, as indicated by circle A in Figure 5.

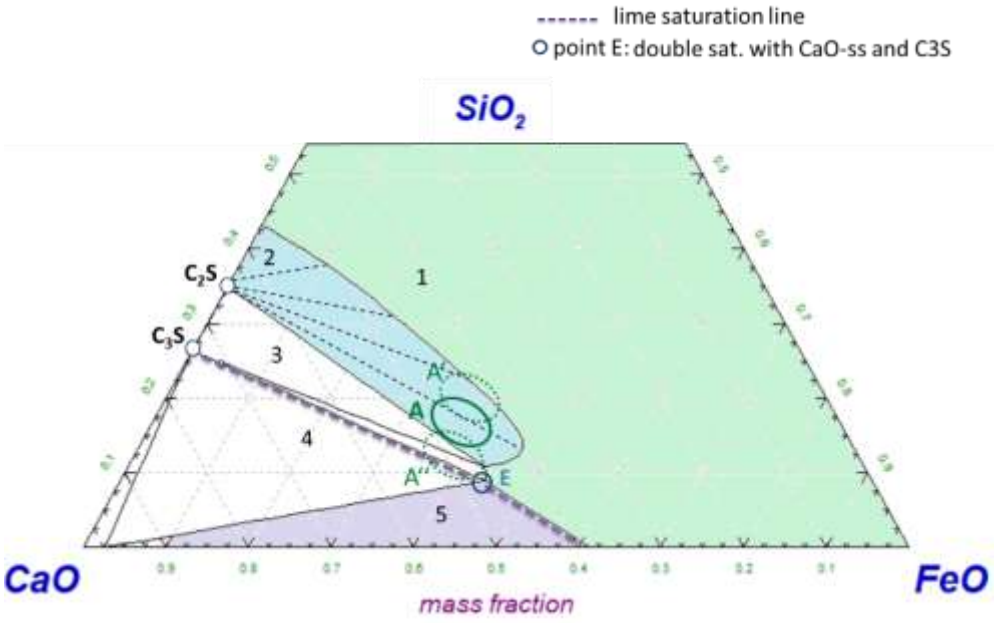

FIG 5 – Position of the alternative target slag regions A and B, suggested for optimal dephosphorization results in the $CaO\text{-}FeO_x\text{-}SiO_2$ system, at 1973 K (1700°C), and for a reduced $p(O_2)$ state.

Controlling the slag composition during the BOF process towards the target region, indicated by region A in Figure 5, is associated with the following challenges:

1. Identifying the actual composition of the slag: The CaO oxide is formed through the addition of CaO-containing fluxes such as lime and limestone. The further major components FeO and SiO_2 are formed through the oxidation of Fe and Si from the metal phase, respectively. Due to its high oxygen affinity, Si oxidizes almost completely within the first minutes of the process and the mass of SiO_2 in the slag remains constant for the rest of the process. The FeO content of the slag is distinguished by a dynamic behavior and is largely affected by the process operation (oxygen lance height, oxygen flowing rate, etc) and the decarburization rate. The FeO in the slag further acts as a fluidizing agent for the slag and helps dissolve the lime charged into the furnace. Thus, in addition to temperature, the amount of CaO dissolved in the slag is a strong function of FeO evolution. For identifying the actual position of the slag in the phase diagram shown in Figure 5, functions or modules for the determination of the evolution of the main slag components as well as the temperature based on the actual process data are required.
2. Identifying the target composition of the slag: The phase boundaries of the $CaO\text{-}FeO_x\text{-}SiO_2$ oxide system are a strong function of the process temperature, the $p(O_2)$ levels as well as of the minor oxide contents such as MgO, MnO, Al_2O_3. This implies that the composition of the target slag region, indicated by circle A in Figure 5 should be adjusted accordingly. Examples of adjustment of the target composition in case of an increase in temperature, in the presence of 7% MgO and 4 $\%Al_2O_3$ are presented in Figure 6-b), Figure 6-c), and Figure 6-d) respectively. For this purpose, ChemApp can be applied for the accurate determination of the thermochemical behavior of the actual oxide system at the conditions prevailing in a furnace.

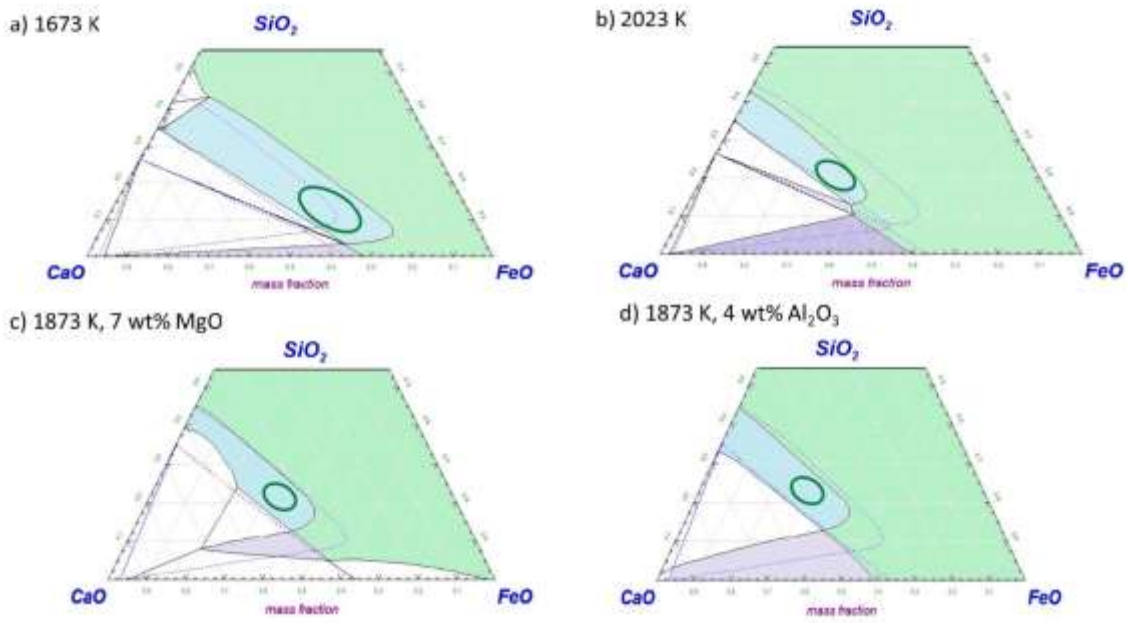

FIG 6 – Target slag compositions for optimal dephosphorization in the BOF furnace. Examples of the adjustment of the position of the optimal target slag region (green circle) in the CaO-FeO_x-SiO_2 oxide system at reduced p(O_2) state as a function of temperature: a) 1673 K (1400°C), b) 2023 K (1750°C), and depending on the minor oxide content of the system: c) 7 wt% MgO at 1873 K (1600°C), d) 4 wt% Al_2O_3 at 1873 K (1600°C). The dashed lines represent the phase boundaries of the ternary system at 1873 K.

In summary, the determination of the dynamic evolution of the slag composition and temperature, as well as the adjustment of the corresponding target zone are required for deciding on the necessary measures to be taken to achieve dephosphorization targets. Figure 7 provides an example of how computational thermochemistry can be integrated into the dynamic dephosphorization model through ChemApp. Actual process data, such as the oxygen blowing rate, the lance height profile, the input time, and the input amounts of fluxes define the input for dynamic process modules which are mainly based on mass and energy balance equations. The calculation output of other modules, such as the amount of dissolved lime is also required. The dynamic process modules deliver information on the evolution of the process temperature as well as on the evolution of the main slag components, such as CaO, FeO, SiO_2, MnO, and MgO. The results are fed into the ChemApp module, which, in turn, calculates the actual and the target slag compositions. The necessary corrective measures to be undertaken to minimize the deviation between actual slag and target slag state are determined and controlled by further dynamic modules. For example, the CaO content and/or the FeO content of the slag can be adjusted toward the target values by charging lime and/or modifying the blowing profile. The options available for undertaking the corrective measures may differ depending on the processing stage.

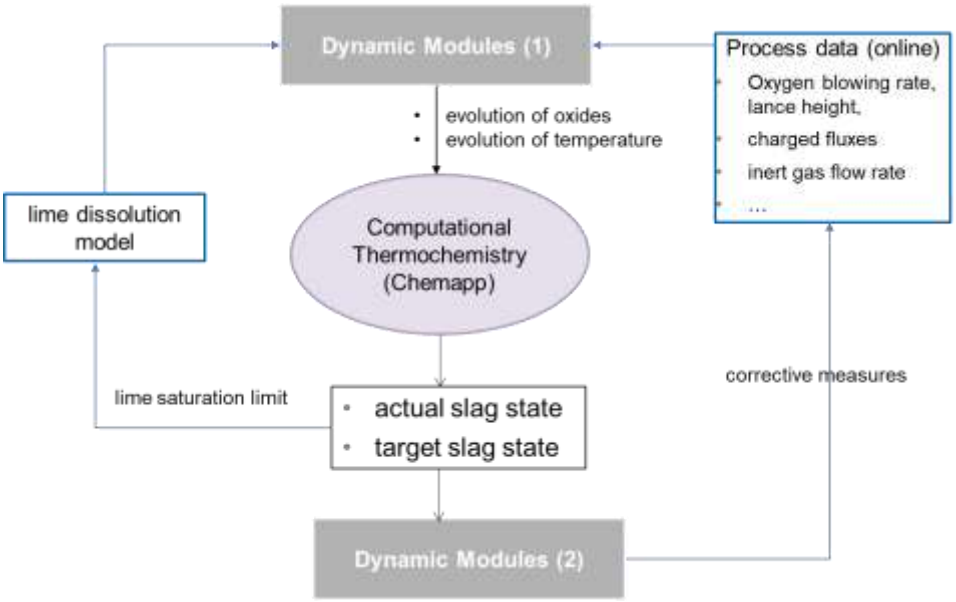

FIG 7 – Concept for the implementation of computational thermochemistry in the dynamic dephosphorization model.

To overcome the limitations associated with the high computational effort, the surrogate model approach, introduced in the previous section for the TRF furnace, can be applied.

CONCLUSION

The development of robust digital platforms serves as a basis for the integration of process understanding, digitalization and innovation into the industrial plants. The direct integration of computational thermochemistry into those digital platforms through ChemApp opens new possibilities for enhanced process control for the metallurgical industry. A surrogate-based modelling approach is adopted to overcome the limitations associated with the high computational efforts, thus making it suitable for online application. The examples discussed in this work illustrate the benefits for both the ferrous and non-ferrous metallurgical industry.

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