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A Brief History of Metallurgical Modeling

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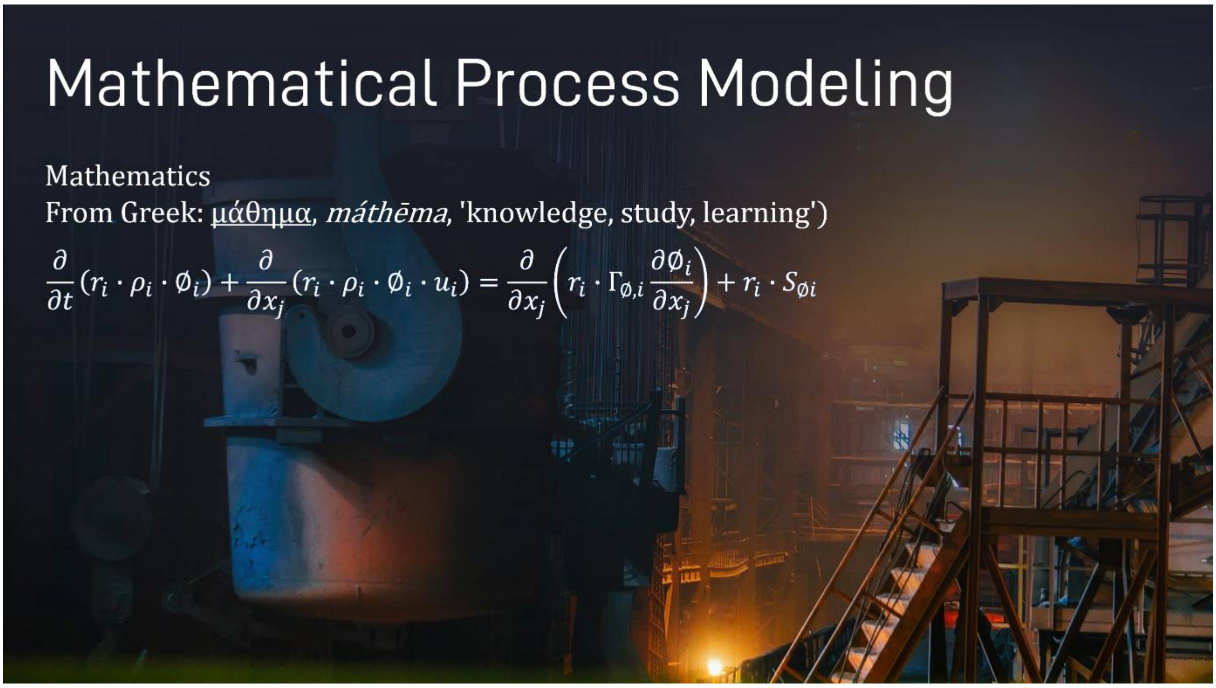
Modeling of steelmaking per se is not possible without a good grasp of steelmaking practice as well as the underlying scientific fundamentals [1].

In this article particular attention was paid to the state of holistic and fundamental models that can be applied to the various metallurgical refining processes. Generally, the present article tries to give the curious reader an overview of metallurgical process modeling by

- describing the most important fundamental-based disciplines to be considered,
- discussing the current state of the development of holistic process models and
- suggesting a methodical procedure to model development.



Mathematical Process Modeling

Mathematics
From Greek: μάθημα, *máthēma*, 'knowledge, study, learning')

$$\frac{\partial}{\partial t}(r_i \cdot \rho_i \cdot \emptyset_i) + \frac{\partial}{\partial x_j}(r_i \cdot \rho_i \cdot \emptyset_i \cdot u_i) = \frac{\partial}{\partial x_j}\left(r_i \cdot \Gamma_{\emptyset,i}\frac{\partial \emptyset_i}{\partial x_j}\right) + r_i \cdot S_{\emptyset i}$$

1 INTRODUCTION

The aim of this article is to give the interested reader a simple overview of the development of metallurgical process models. To put it more precisely, it is primarily about the mathematical modeling of the most important phenomena in the course of secondary metallurgy and how to build up a digital model, which depicts the fundamental metallurgical relationships holistically. Much of the work on metallurgical process modeling published in the relevant journals and conferences either concentrates only on individual phenomena of a process or was developed specifically for one of these processes (LF, VD, RH, VOD and AOD). Fundamental modeling of metallurgical processes is very complex, as the simultaneous multi-phase interactions, chemical reactions, heat transfer and turbulent flow patterns at high temperatures must be taken into account. It is therefore not surprising that only very few holistic models are described in the relevant literature which, based on fundamental theories, consistently take the occurring metallurgical phenomena into account.

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2 METALLURGICAL PROCESS MODELLING

A good overview of metallurgical process modeling can be found in the publications by D. Mazumdar and J. W. Evans [1], B. G. Thomas and J. K. Brimacombe [2] and D. Sichen [3], to name just a few. The term modeling can be defined as a scientific representation of a process or phenomenon through a physical system or mathematical expressions. Physical modeling investigates a given phenomenon in a replica of the actual industrial unit. Mathematical modeling, compared to physical modeling, uses a series of equations and expressions to represent a particular phenomenon or process as closely as possible [1].

B. G. Thomas and J. K. Brimacombe [2] defined a process model as a system of mathematical equations and constants that are usually solved on a computer to make quantitative predictions about some aspect(s) of a real process. Similar to the “system of mathematical equations” definition, J. Wendelstorf [4] stated in his publication that a process model is defined as an implementation of an algorithm to predict the behavior of an open or closed system.

D. Sichen [3] stated in his work about modeling in secondary metallurgy that the rapid development of mathematical models can be traced back to the high demands placed on process optimization and process control. The control and optimization of metallurgical processes requires real-time models. Models that calculate the current state of the process and provide target values in the context of optimization. For such models the acceptable time to find a solution is key. Fully rigorous mathematical models based on physics and chemistry are often very complex and due to requirement of real-time calculations, numerous idealizations or at least some basic assumptions are often necessary in order to reduce the complexity.

Nowadays, or in the modern usage of buzzwords, the term digital twin is used in this context. In a a previous article we described in detail how to set up an intelligent digital twin for the processes of melting and refining of steel making. The approach includes all three levels of integration, i.e., the digital model, the digital shadow and the digital twin. Based on these levels of integration, we understand a metallurgical process model as illustrated in **Figure 1**.

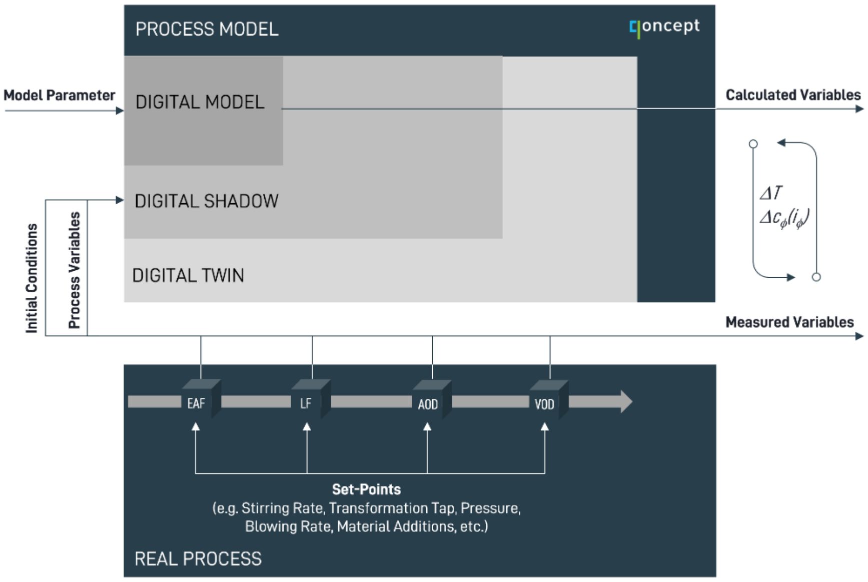

Figure 1: Interaction of the real process with a process model taking into account the different levels of integration

The picture below shows an example of the real process with melting in the EAF and a triplex route for the production of stainless steel (LF, AOD and VOD). The process control takes place via set-points, either manually by the experienced staff or by a software system for process control (Level 2). If the cyclical process variables (e.g. stirring/purging gas rate, oxygen blowing rate, etc.) and events (temperature measurements, material additions, etc.) that occur continuously during operation are used for the modeling in real time, one speaks of a digital shadow. Following this approach of the different levels of integration, a digital twin is realized if the process model also provides set-points and thus controls the process. However implemented, the digital model processes the process data and provides calculation results, which can then be compared with measurements from the real process.

To summarize this chapter, it can be stated that all the authors mentioned above agree on one thing:

> The simplification of complex processes while maintaining a strong hold on reality as well as the validation with realistic measurements is key in the entire development process.

3 THE FUNDAMENTAL DISCIPLINES TO BE MODELED

Since the metallurgical basics have already been dealt with in detail in a large number of technical books and publications, this chapter concentrates on the modeling of the different processes on the basis of a holistic approach. Essential content is based on the publication mentioned above [1-5] and are supplemented by relevant domain-specific articles and textbooks.

> Comprehensive understanding of steelmaking necessitates a sound knowledge of metallurgical thermodynamics and rate phenomena such as fluid flow as well as heat and mass transfer [1].

Nowadays the modeling technique is well established and shows its capabilities in a wide range of applications. Mathematical models can range from empirical to fundamental models. B. G. Thomas and J. K. Brimacombe [2] stated that all process models can be classified according to their empirical versus mechanistic basis. They understand a fully-empirical model in terms of a curve-fitting procedure on the results of a statistical study with no attempt to understand the reasons for the relationships. In contrast to such empirical models, fully-mechanistic (or phenomenological) models solve equations based solely on the fundamental laws. These laws include the conservation and transport of mass, momentum, mechanical force, electromagnetic force and energy, in addition to thermodynamics, phase equilibria, kinetics, and other relations. However, all models lie somewhere between these two extremes.

According to the relevant literature, the common modeling techniques can be classified into three groups, (1) computational thermodynamics, (2) computational fluid dynamics (CFD) and (3) computational kinetics, which will briefly described in the following:

(1) **Thermodynamic Models** enables the determination of the equilibrium distribution of species within the phases, the heat generated or consumed by these chemical reactions and the behavior of species in solution. The 2nd law of thermodynamics represents the fundamentals of these calculations. In order to thermo-dynamically describe a system, the phases and elements within the phases needs to be defined carefully. Moreover, each element defined in the model requires appropriate thermochemical data before any technique like the Gibbs free energy minimization can be applied [5].

(2) **CFD Models** are used to understand the fluid flow patterns and interaction between the phases and interaction between the phases [5]. The pioneer work was due to J. Szekely and S. Asai [6], who introduced the technique of fluid flow calculation from chemical engineering to metallurgical processes. In order to simulate fluid low, the equation of continuity and equation of motion must be considered, which leads to well know Navier–Stokes equation in case of incompressible liquid and Newtonian flow [3].

(3) **Computational Kinetics Models** calculate the changes in concentration within and between the phases over time. In general terms, the kinetic models gave answers in relation to the reaction rates and how they are influenced. The basis for predicting reaction rates is Fick's First Law. The law describes that the diffusion rate is proportional to the concentration gradient. By discretizing models over time t, the complexity can be reduced. In this context, time is often introduced into the equation as a differential variable [5].

The phenomena of thermodynamics, kinetics and fluid dynamics are closely related. The modeling methods also interact, for example, the results of CFD models provide important parameters for understanding convective mass transfer. Models of thermodynamics determine the limits of kinetic modeling. In the last few decades, the steadily increasing availability of powerful computers has reduced the calculation time of CFDs. Nevertheless, such models have so far only rarely been used for real-time modeling [5].

4 APPROACHES TO HOLISTIC PROCESS MODELING

A detailed literature search shows that basic models were developed that describe individual processes such as the removal of nitrogen or carbon or to predict the dissolution behavior after additions, the temperature, the sulfur and hydrogen removal, the reoxidation as well as the growth and removal of inclusions. The extent to which these fundamental model predictions have been verified with experimental data varies depending on the different metallurgical processes. The literature research also shows, however, that there are only very few holistic and fundamental-based models that consistently consider the ongoing processes.

D. Rohrberg [7] developed a holistic application for modeling of metallurgical processes. The developed tool was tested in two very specific use cases, (1) process modeling for the production of high-manganese steels and (2) investing the diffusion in the three-component system Fe-Al-Cr.

L. Jonsson et al. [8] published a concept based on so-called macro models. It describes some aspects of reality in an entire metallurgical plant or furnace. An integral part of these macro models are the reaction models, such as a model of desulfurization. The reaction models in turn consist of micro-models (e.g. the sulfide capacity). In order to gain a better understanding of how fundamental phenomena influence the process and make the process description more comprehensive, the authors recommend implementing these reaction models and micro-models as building blocks in the overall process model (see **Figure 2**).

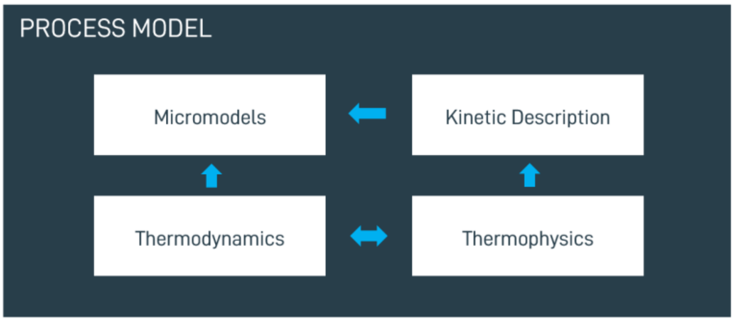

Figure 2: Structure of process models based upon micromodels according to L. Jonsson et al. [8]

The general basic model can be viewed as a system of equations in which each variable has its own line in the system and each equation is expressed in the form of a transport equation. To solve the resulting system of equations, thermodynamic and thermophysical properties, source terms, transport phenomena between different phases and boundary conditions for all variables must be provided. Used in this way, the result is a macro-model based on the combination of thermochemical and thermophysical relationships and macrokinetics. But assumptions also have to be made (for example for the thermal model, the fluid flow model, the transport equations and the incorporation of the slag phase into the model). The authors point out that there is a great advantage in using this process model structure: The integration of new models is possible without substantial reprogramming.

P. G. Jönsson and L. T. I. Jonsson [9] summarize it as follows: A well-founded and carefully tested model could be very useful as it is suitable for process optimization and the evaluation of new process flows as well as for improving treatment strategies. The reason is that basic models can be used for a multitude of different geometries, stirring conditions, metal and slag compositions, etc. For this purpose, the required reaction models must be coupled, desulfurization and reoxidation must be taken into account and the inclusion behavior must be modeled. Subsequently, these models could be integrated into a model for the vacuum treatment that is also coupled with a model of the degassing. This creates a complete model for vacuum treatment. In a similar way, coupled models of other metallurgical processes must be created. Ultimately, these could be incorporated into an overall model of the entire processes of secondary metallurgy.

5 POSSIBLE PROCEDURE TO MODEL DEVELOPMENT

According to Mazumdar and J. W. Evans [1] and B. G. Thomas and J. K. Brimacombe [2], the development of a mechanistic process model can be divided into several stages as illustrated in **Figure 3**.

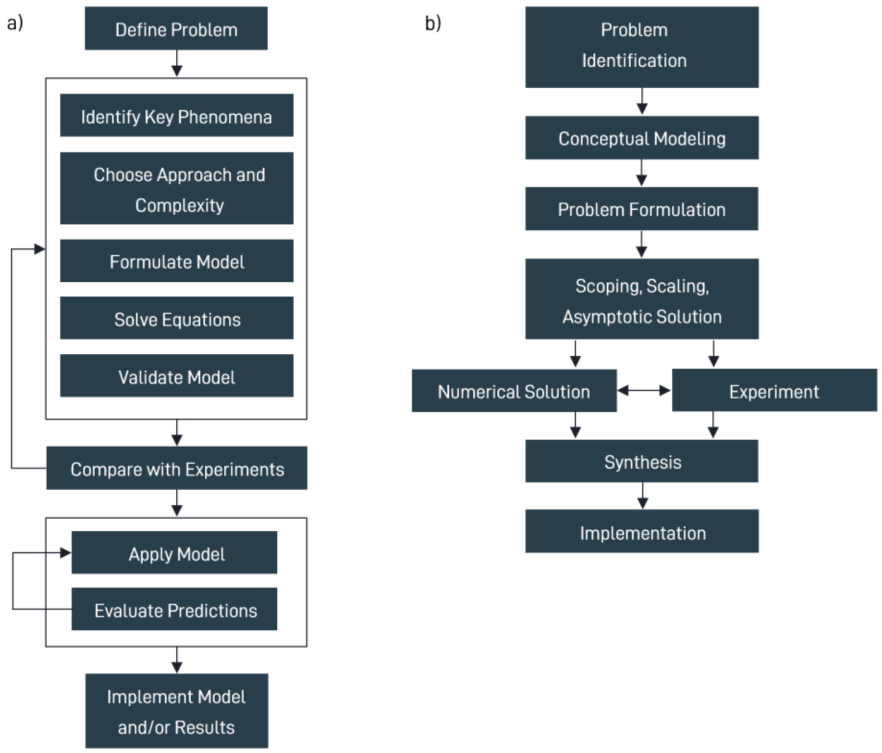

Figure 3: Steps in developing metallurgical models. a) according to B. G. Thomas and J. K. Brimacombe [2] and b) according to Mazumdar and J. W. Evans [1].

Although these two flowcharts may seem different at first, they take a very similar approach. In a first step, you must ask yourself which questions should be answered or what purpose the model should serve. B. G. According to B. G. Thomas and J. K. Brimacombe [2] the different reasons to develop a process model are (1) increase fundamental understanding of a process, (2) assist in scale-up, (3) design of experiments, (5) evaluation of experimental results, (6) quantifying property measurement, (6) technology transfer and (7) online process control and optimization.

Identifying, defining and most importantly understanding the problem at the fundamental level is the next important step. A common feature of both drawings is the comparison of the model with measurements, which can be derived from physical models, pilot or full-scale steel processing units. Going a step further, this takes two forms: verification and validation. The verification ensures that the solution is created correctly. Validation ensures that the right product is being developed. The analysis of development risks is not explicitly shown in the figure above, but from our point of view it is of crucial importance.

The development of a holistic approach to modeling, i.e. the transformation of the individual process-specific models into a basic model for melting and refining, is an extraordinarily complex project. This risk can be countered with modern agile methods. **Figure 4** shows the methodical approach we developed for all of our projects, so that the risks are identified and minimized at an early stage.

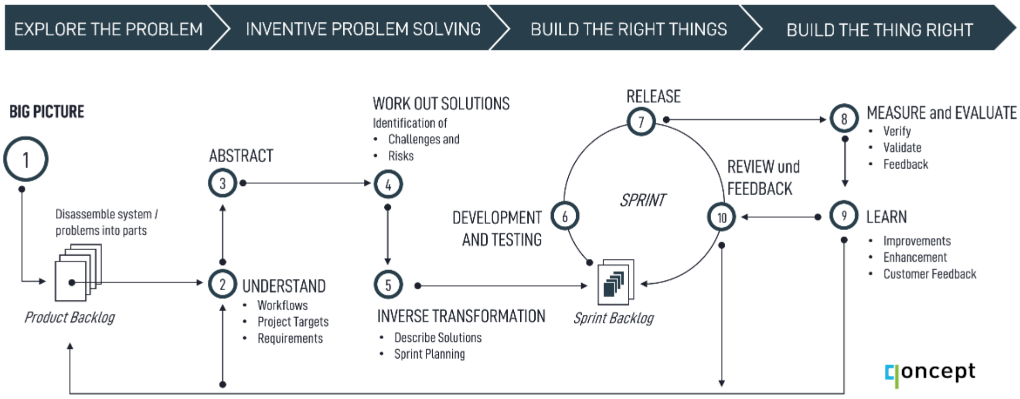

Figure 4: Methodical approach to develop a holistic process model

This methodical approach is based on methods of Design Thinking, Design Sprint, Lean Startup, Scrum and Business Model Canvas and their combination. The start of development begins with the creation of a big picture, i.e. which questions should be answered or what purpose the model should serve. Steps 1 to 5 follow the idea of Design Sprints and an inventive problem-solving approach. This is very much about analyzing and abstracting the task and the problems to be solved so that solution can be described and conceptually developed. The result of this phase is a sprint backlog for the actual prototype development. This phase follows the Scrum method, with the idea of Lean Startup already being integrated into the Scrum cycles. The Scrum method defines which work packages and which to-dos will be done by whom and when. We keep testing what works and what does not. This means that the development can be readjusted again and again. The latter is the starting point for the lean startup method with the central terms build, measure and learn. This allows improvements and extensions to be derived again and again. These flow back to the review of the development process (sprint) and, if necessary, are also fed back into the design sprint.

6 SUMMARY

The present article briefly describes the concept of metallurgical process models, not only from the point of view of the classical modeling literature but also in the context of the degree of integration. Particular attention was paid to the development status of comprehensive modeling approaches, i.e. holistic and fundamental-based model which can be applied for the different metallurgical processes of refining. Such a holistic approach is discussed conceptually in the relevant literature but reports on case studies or concrete applications are missing. In contrast, the relevant literature describes a large number of models of individual ennoblement phenomena. The motivated developer of holistic metallurgical models can access and build on these publications. Here the wheel no longer must be reinvented, but the challenge is much more the intelligent orchestration of these model approaches in the context of the holistic approach.

Finally, we illustrated our approach of model development which is based on different agile methods and follows the following steps: *Explore the Problem → Inventive Problem Solving → Build the Right Things → Build the Thing Right.*

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