A Review of Mathematical Process Models for the Electric Arc Furnace Process

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The electric arc furnace is the main process unit in scrap-based steelmaking. Owing to its importance, numerous mathematical models for predicting the course of the electric arc furnace process have been developed. This article reviews mathematical process models proposed in the literature, identifying the most common modeling approaches, and uses mathematical descriptions for the main phenomena. Furthermore, the validation of such models is discussed in detail. Finally, the article identifies gaps in the existing knowledge and provides suggestions for the further development of mathematical process models.

1. Introduction

The electric arc furnace (EAF) constitutes the main process in scrap-based steelmaking.[1] Invented in 1889 by Paul Héroult, it was initially used mostly for production of special steels, but established itself as one of the main steelmaking processes in the later part of the 20th century.[1] In 2018, the EAF process supplied 523 918 000 t of steel worldwide, accounting for 28.9% of the total crude steel production.[2]

In comparison to the main route in iron ore–based steelmaking, the blast furnace and converter, the EAF route reduces the energy consumption by up to 61% and the carbon emissions by roughly 77%.[3] The process efficiency and productivity have improved dramatically through the introduction of technical improvements such as the increased use of oxygen, carbon and other sources of chemical energy, foaming slag, and post-combustion of CO.[4] Nevertheless, a significant potential for further optimization remains. This becomes apparent in the difference between the theoretical energy demand of roughly 400 kWh t−1 for the melting and heating of scrap and the actual average consumption of modern EAF that is around 375 kWh t−1 of electrical energy and a similar amount of chemical energy, resulting in a total efficiency of about 50%. [5–7]

The parameters necessary for analysis and optimization of the process, however, in many cases cannot be measured directly due to the harsh conditions inside the furnace. For example, the temperature and composition of the melt and slag can be determined only through spot measurements and potentially with some delay caused by the necessary analysis of the sample. While methods for the direct and continuous measurement of these parameters are being developed, they are not yet available for most furnaces.[8,9] Furthermore, plant trials that would be necessary to evaluate the impact of different optimization strategies may be impossible due to prohibitive cost or safety concerns. Mathematical models are thus a valuable source of information regarding otherwise unknown process parameters. Simulations can also be used as a less expensive, faster, and safer alternative for plant trials. For the EAF, a wide range of models has been developed with different purposes and modeling approaches. The aim of this work is to discuss fast and comprehensive process models. Unlike statistical equations for the prediction of endpoint conditions[6] or computational fluid dynamics (CFD) modeling,[10] these models have so far not been reviewed in detail.

2. The EAF Process

In the EAF, iron-bearing material is melted and refined to produce crude steel. The main feedstock is scrap, but other materials such as hot briquetted iron (HBI), direct reduced iron (DRI), or hot metal can be used as well. Energy is supplied through one or three electrode(s) as well as oxyfuel burners and chemical reactions facilitated by the injection of carbon and oxygen into the melt and slag. There are two different electrical concepts: alternating (AC) and direct (DC) current. In the AC furnaces, three electrodes and arcs are used, while DC furnaces have a single central electrode and arc in combination with a bottom electrode to close the electrical circuit. In both furnace types, the current is supplied through movable electrode arms that are adjusted to minimize the fluctuations in the electrical parameters induced...
by the movement of the scrap or melt surface. The furnace usually consists of a bottom vessel lined with refractory and containing an eccentric bottom tap (EBT) or tapping spout. Above that, there is a water-cooled furnace shell that may contain injectors and burners. A slag door allows the removal of slag and the insertion of lances for the injection of oxygen and carbon. The roof situated above the shell is water-cooled as well and contains openings for the electrode(s), the removal of off-gas, and potentially the charging of feedstock, slag-formers, or alloys. The furnace is mounted on a platform that is tilted for deslagging and tapping.[1,7,11] Figure 1 shows the main components of an EAF using an AC furnace as an example.

The EAF process is a batch process that can usually be divided into four steps: charging with one or more scrap baskets, meltdown of the scrap, heating and refining, and finally tapping. At the beginning of the meltdown stage, the arcs bore down into the scrap pile with reduced power, to prevent electrode breakages. When the electrodes reach the melt surface, high power settings can be used with the scrap shielding the furnace walls and roof from the electric arcs. Oxyfuel burners using fuels such as natural gas or oil are often used to facilitate melting of the scrap around cold spots during meltdown and to increase productivity. Combustible contaminants and carbon partially burn in the furnace releasing flammable gases. Oxygen can be injected into the freeboard to allow the postcombustion of these gases inside the furnace, recovering some of the energy otherwise lost with the off-gas. The efficiency of burners and postcombustion depends on the amount and temperature of the solid scrap inside the furnace. Therefore, the use of burners and the injection of oxygen for postcombustion are discontinued when the meltdown has progressed far enough to make them inefficient. When the charge is mostly molten, the process enters the flat bath phase during which the steel melt is heated and refined. As the arc is no longer shielded by the scrap, more energy is lost to the water-cooled surfaces. By injecting oxygen and carbon into the melt and maintaining the correct slag properties, the slag can be foamed, partially shielding the arc and increasing energy efficiency. Oxygen is also necessary for the removal of impurities from the melt. Furthermore, the oxidation of carbon and trace elements releases additional chemical energy, increasing productivity. Different concepts for the preheating of scrap using burners or EAF off-gas are available and, in some cases, preheated scrap, hot metal, or other iron-bearing material is continuously charged into the furnace instead of using scrap baskets.[5,7,12]

2.1. Mass Balance

An exemplary mass balance for the EAF process is shown in Figure 2. The values given are the masses per ton of produced crude steel. While the values can vary in a wide range depending on the charge materials and specific operation strategy used for a specific EAF, it provides an overview of the mass flows relevant for modeling the EAF.

2.2. Energy Balance

Roughly half of the energy in the EAF is supplied by the electric arc(s),[11] and the other half being provided through chemical
reactions. The overall efficiency is around 50% with the main losses occurring through the water-cooling of furnace components and the off-gas.\textsuperscript{[5,7,13]} Figure 3 shows an exemplary energy balance for an EAF. Chemical energy is provided through the oxidation of injected or charged carbon sources, the carbon content of the scrap, and the consumption of the graphite electrode(s). Additional chemical energy is supplied by burners and the oxidation of iron and trace elements with the injected oxygen. The energy lost with the off-gas is mainly chemical energy in the form of unburned carbon monoxide and hydrogen, some of which can be recovered through postcombustion within the furnace.\textsuperscript{[13]} The share of chemical and electrical energy can
vary significantly depending on the operation strategy of a furnace, depending on the prices of energy sources and the desired product quality.\[3\]

Modeling and optimization of the EAF process constitutes a complex task due to the large number of variables such as the different charge materials, the share of different energy carriers, and the target composition and temperature. The different process phases, discontinuous changes during charging of material and many variations of the process with different furnace types, feedstocks, desired steel qualities, and operation strategies have led to the development of various modeling approaches.

3. Process Models

A process model is an “algorithm to predict the behavior of an open or closed system”[14] It allows predictive control and operator assistance, offline process optimization, improved understanding of the underlying physical phenomena, and the online estimation of parameters that cannot be determined directly through measurements.\[14\] Here, the term process model refers to deterministic models based on physical and thermodynamic relationships, and thus excludes purely statistical approaches.

3.1. Types of Process Models

Process models and other tools for simulation or prediction of industrial processes can be categorized based on their intended purpose and scope as well as the modeling approach used.

3.1.1. Categorization by Modeling Approach

Generally, models for industrial applications can be divided into those based on statistical evaluation of data, called statistical or empirical models, and those based on known physical or thermodynamic relationships, called mechanistic, analytic, or phenomenological models. Statistical models are applicable if the quality that is to be predicted can be measured and sufficient data are available, documenting both this quality and the process parameters influencing it. They are comparatively easy to develop, and the description of underlying physical relationships is not necessary. The accuracy of a statistical models is determined mainly by the accuracy and range of the data used to train the model. A general rule is that statistical models should not be applied outside the range of their training data as their capability for accurate extrapolation beyond this range is limited. This also means that the model is not transferable to a different process or plant without adjustment and it does not contribute to the understanding of underlying physical phenomena. In the case of complex processes such as the EAF process, analytical models are usually more difficult to develop than statistical models and may not reach the same degree of accuracy. They do, however, allow for extrapolation and are transferable because the physical and thermodynamic description is more universal.\[15,16\]

As stated earlier, only these analytical models fulfill the definition of a process model; however, statistical or mixed approaches are often used for similar applications.

Furthermore, models can be classed by the type of interaction that they describe. A model can either be based purely on cause and effect (deterministic) or include probabilistic elements (stochastic). The model can include linear or nonlinear behavior and continuous or discrete as well as lumped or distributed definition of variables. In practice, most models can be characterized as hybrids, as, for example, analytical expressions commonly include parameters that are determined empirically, or the parameters for an empirical model are selected based on known physical relationships.

3.1.2. Categorization by Scope and Application

A model can be developed to describe specific phenomena that characterize only certain phases or parts of a process or, often using several submodels and zones, a complete process such as the EAF from charging to tapping with the outside of the furnace forming the system boundary. Furthermore, the level of detail and the execution time must be balanced according to the intended purpose of the model. For online and optimization applications, the execution time must be kept low, while to understand complex physical phenomena on small scales a level of detail is required. This necessitates different models adjusted specifically for the respective application.

3.2. EAF Process Models

Due to the wide range of different applications of modeling the EAF and the complexity of the process, numerous approaches have been applied to derive models for the process. There are purely statistical or data-driven models, including neural networks, used, for example, to evaluate the power consumption[17] or the electrical system of an EAF.\[18,19\] Another class of models for the evaluation of EAF energy consumption uses a statistical approach based on parameters that are determined using physical relationships such as the expected power delivery from the use of oxygen or natural gas. Such energy consumption models, including some neural network approaches, have been reviewed recently by Carlsson at al.\[6\]

CFD is a branch of fluid mechanics concerned with modeling of fluid flows with high spatial resolution. CFD models are analytical models and, given a detailed and comprehensive model, can characterize all relevant phenomena, including fluid flow, electromagnetics, heat and mass transfer as well as chemical reactions. An up-to-date review on the application of CFD modeling to the EAF process has been presented by Odenthal,\[10\] who concluded that despite successes in developing CFD models that are computationally feasible for specific phenomena or components and promising developments toward a more comprehensive approach being made, there are still substantial limitations to CFD modeling of the complete EAF process. The main limitation is the wide range of different scales and phenomena involved, making comprehensive CFD models computationally expensive and unsuitable for online applications.

Process models can be seen as a middle ground between the energy consumption models and CFD modeling. Such models make use of some simplifications such as the introduction of
one or several lumped phases or zones and use some empirical parameters while maintaining a mainly analytical approach for the prediction of time-dependent qualities. This allows for the estimation of different time-dependent process parameters with a model that is simple and fast enough for online or optimization applications. Compared with process models, the energy consumption models represent a highly simplified and mainly statistical approach for the prediction of a single parameter, while CFD models offer a higher degree of detail and accuracy coupled with a significantly higher computational demand.

Process models have been developed not only for the complete process but also to describe specific phenomena within the EAF, for example, the heat transfer at the electric arc, the reaction of injected carbon with the slag, or the influence and potential of energy recovery within the off-gas system. In some cases these have then been incorporated into more comprehensive EAF process models. A brief overview of proposed EAF process models has previously been published by Logar et al. In this work, an in-depth review of the models is presented, encompassing both the models mentioned in Logar’s overview as well as several other models proposed before or since its publication. The aim of this work is to review the existing process models for the complete EAF, and the various solutions implemented for different phenomena such as phase changes, heat exchange, or thermochemistry. Table 1 shows the EAF process models found in the literature with the respective references and years of publication.

These process models are generally based on lumped zones with no spatial discretization except for the scrap charge that is discretized into multiple zones in some models. Heat and mass flows are exchanged between these zones and the surroundings and chemical reactions are usually considered within certain zones. Energy and mass balances are then used to track the temperature and composition of each zone. While most of these process models are dynamic, pseudodynamic approaches based on predefined process steps have also been proposed.

### 4. Heat Transfer

In modeling the heat transfer within the EAF, the distribution of the energy introduced through sources such as the arc(s) or chemical reactions (including burners and postcombustion) to

| Author          | Year       | References                  | Notes                                      |
|-----------------|------------|-----------------------------|--------------------------------------------|
| Boland/Billings| 1977, 1979 | [32,123]                    |                                            |
| Köhle           | 1982       | [30]                        |                                            |
| Hofer/Linninger et al. | 1995, 1997 | [37,113,167] |                                            |
| Hayman          | 1997       | [114]                       |                                            |
| Matson/Ramirez  | 1997, 1998, 1999 | [64,91,92] |                                            |
| Deneyes/Peaslee/Shah | 1997, 1998 | [31,63]                     |                                            |
| Cameron         | 1998, 1999 | [90,135]                    |                                            |
| Bekker et al./Oosthuizen | 1998, 1999, 2000, 2001 | [50–52,105,106,136] | Based on Bekker et al.[32,105,106,136] |
| Rathaba/Coetzee | 2005, 2006 | [38,125]                    |                                            |
| Modigell et al. | 1999, 2001 | [103,104]                   |                                            |
| Morales         | 2001, 2002 | [65,126]                    |                                            |
| Nyssen et al.   | 1999, 2002, 2004, 2007, 2011, 2015 | [28,145–148,161] |                                            |
| MacRosty/Swartz et al. | 2005, 2007, 2013 | [34,53,93,94,124] |                                            |
| Kleint et al.   | 2005, 2007, 2012, 2016 | [61,137–141] |                                            |
| Wendelstorf     | 2006, 2008 | [127,128]                   |                                            |
| Arnout          | 2006       | [62]                        |                                            |
| Clerici et al.  | 2008, 2011 | [115–118]                   |                                            |
| Natshläger      | 2007, 2008, 2009 | [119–122] |                                            |
| Matsuura/Forbes | 2008, 2010 | [176,177]                   |                                            |
| Frittella       | 2009, 2011 | [86,178]                    |                                            |
| Kho             | 2010       | [33]                        |                                            |
| Brooks          | 1997, 2012 | [129,130]                   |                                            |
| Logar et al.    | 2011, 2012, 2016 | [20,35,48,54,131,132] | Based on and in cooperation with Logar et al.[35,48,54,131,132] |
| Fathi/Saboohi   | 2017, 2018, 2019 | [39,42,43,133] | Based on and in cooperation with Logar et al.[35,48,54,131,132] |
| Meier, Hay      | 2016, 2017, 2018, 2019 | [13,36,49,87–89,107,142,143] | Based on and in cooperation with Logar et al.[35,48,54,131,132] |
| Opitz           | 2016, 2017, 2019 | [29,40,41,44,144] |                                            |
| Ringel          | 2020       | [47]                        |                                            |
| Steel University | –         | [111,112]                   | Website with browser-based model           |
the different phases inside the furnace must be described. The same is necessary for the energy removed, for example, by off-gas or cooling water. For a comprehensive characterization of the heat transfer and resulting energy content of the model zones, thermal radiation, conduction, and convection must be quantified. Models focused on the flat bath phase include very limited heat transfer or even assume isothermal phases,\textsuperscript{32,33} while models that include a description of the meltdown provide more detailed estimations of the heat flows inside the furnace and the impact of the changing geometry and temperature of the scrap charge.\textsuperscript{20,34–36} A highly simplified approach is the use of predefined heat flows, either as model input determined from measurements such as cooling water temperatures, or as fitting parameters. Similarly, empirical efficiency factors can be defined to determine the amount of heat delivered to certain phases or lost to off-gas and cooling. Alternatively, heat transfer between zones through conduction or convection can be described using heat transfer coefficients and specific surface areas. These are usually empirical model parameters and adjusted to fit measured data. To account for the varying surface area and conditions, heat transfer coefficients, specific surfaces areas, or efficiency factors can be adjusted using values such as the remaining scrap volume or the amount and condition of foaming slag.\textsuperscript{13,34,36–38} An even more exhaustive approach that has been implemented for EAF process models is the use of Nusselt number correlations to derive the heat transfer coefficients.\textsuperscript{20,39–41} Using the heat transfer coefficients, the heat flows between zones can be determined based on their temperature and the contact area, with additional information regarding physical properties and flow conditions needed if Nusselt correlations are to be used. The surface area is determined using empirical correlations and simplified geometries and often contained in a single empirical parameter together with the heat transfer coefficient. Different methods may be combined, for example, using efficiency factors or constant heat flows to account for energy losses through off-gas and cooling as well as heat transfer coefficients for the exchange between the scrap and melt.

4.1. Radiative Heat Transfer

Due to the high temperatures within the furnace and especially the electric arc, heat transfer through thermal radiation plays a significant role in the EAF. Some authors have therefore attempted to include comprehensive descriptions of the radiative heat transfer into their process models. MacRosty et al.\textsuperscript{34} introduced a geometry based on a cone-frustum-shaped void inside the scrap charge that increases in size as meltdown progresses. They assumed a rotationally symmetrical furnace with a single central electrode. Based on this geometry, the sizes and relative positions of surfaces necessary for the calculation of view factors can be determined based on the current volume of the scrap pile and the length of the arc. Figure 4 shows the different stages of the meltdown with an assumed cone frustum geometry.

Some simplifications were introduced to facilitate the computation of view factors. These include the omittance of the electrode and gas phase from the radiative heat transfer as well as deriving empirical functions for the estimation of view factors that cannot be determined using existing analytical expressions.\textsuperscript{34} Logar et al.\textsuperscript{35} based their work on a similar geometry and adjusted the calculation of view factors to reduce the number of empirical estimations used. In later works, Fathi et al.\textsuperscript{39,42} and Saboohi et al.\textsuperscript{43} included additional surfaces and a dynamic share of radiation of the energy emitted by the arc for more detailed studies of the radiative heat transfer. Meier et al.\textsuperscript{13,36} also based their work

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{cone-frustum-geometry.png}
\caption{Cone frustum geometry. Reproduced with permission.\textsuperscript{[13]} Copyright 2016, Mainz Verlag.}
\end{figure}
on Logar's model, adding the electrode and the gas phase including dust to the radiative heat transfer calculations. Opitz et al.\[44\] again adopted Logar's estimation of view factors and introduced several adjustments such as the impact of gas and dust on the radiative heat transfer and a more detailed representation of the scrap batch with several individual sections.

In the aforementioned models, all surfaces except the arc are assumed to be gray bodies with uniform surface temperatures. The shares of heat transferred through radiation, convection, and direct heating of melt and scrap at the arc are usually assumed to be constant\[13,34,36\]. A computationally efficient model for the estimation of this distribution has been developed and implemented within a process model by Fathi et al.\[19,42\]. Based on the calculated view factors and, if considered, the properties of the gas and dust, the radiative heat exchange can be quantified. The view factors for the simplified geometries are estimated using known analytical expressions for simple arrangements such as cylinder surfaces, view factor algebra, and some simplifying assumptions. Hernandez et al.\[45,46\] proposed a different approach for the estimation of view factors for EAF models based on a vertical cylinder, which can be interpreted as an extreme case of the cone frustum shape with a cone angle of 90°, using the Monte Carlo method to determine the resulting view factors. Hay et al.\[46\] adjusted the method proposed by Meier et al.\[13,36\] to this geometry and improved the estimation of view factors for several specific surface configurations. Ringel\[47\] developed another model based on that of Logar et al.\[35,48\] coupled with the geometry suggested by Hernandez et al.\[45\] and adjusted the view factors accordingly with similar results to those presented by Hay et al.\[49\].

Foaming slag can have a significant influence on the radiative heat transfer and the models can be adjusted accordingly. Oosthuizen et al.\[50,51\] introduced a calculation for the foaming slag height as an extension of the model proposed by Bekker et al.\[52\]. Based on this, Rathaba\[53\] added an adjustment of the arc efficiency parameter depending on the predicted slag height. MacRosty et al.\[53\] included a prediction of the foaming slag height in their model as well and adjusted the radiative heat flows into the wall and roof to account for the shielding of the arc. Logar et al.\[35,54\] used a similar approach but instead adjusted the view factors from the arc to the wall and roof, while Meier et al.\[13,36\] adjusted the distribution of the arc power by reducing the share of radiation and increasing the share of direct heating of the melt with increasing slag height instead.

Overall, even the more detailed models still require significant simplifications regarding the geometry and definition of the surfaces and temperatures involved. The error introduced by the assumptions and simplifications made is not usually quantified and local phenomena such as the formation of hotspots cannot be reproduced at all with such simplified approaches.

If radiative heat transfer is not considered directly in a model, it may be represented indirectly through adjusted heat transfer coefficients or other empirical model parameters such as globally defined efficiencies or heat flows. Table 2 shows an overview of the process models and the implemented descriptions for heat transfer. For several models, the published information does not allow a detailed evaluation of the exact implementation, and therefore only a qualitative summary of the respective approaches is listed.

### Table 2. Heat transfer in EAF process models.

| Study | Year | Implemented heat transfer | Notes |
|-------|------|--------------------------|-------|
| Boland/Billings\[32\] | 1977 | Constant EF and HF | Measured HF as model input |
| Köhle\[30\] | 1982 | Constant EF and HF | |
| Hofer et al.\[37\] | 1995 | Variable HTC | Radiative transfer mentioned, no details given |
| Hayman et al.\[314\] | 1997 | Variable HTC, RAD | Limited radiative transfer including gas |
| Deneyes/Peaslee/Shah\[51,53\] | 1997 | Constant HF | |
| Matson/Ramirez\[29\] | 1998 | Constant HF | Constant bath temperature during meltdown |
| Bekker et al.\[32\] | 1998 | Constant EF and HTC | |
| Nyssen et al.\[28\] | 2002 | Variable HTC | |
| Rathaba\[38\] | 2005 | Variable EF and HTC | |
| MacRosty/ Swartz et al.\[34\] | 2005 | Variable HTC, RAD | Gas/dust not considered, cone frustum |
| Kleint et al.\[61\] | 2005 | Constant EF | |
| Wendelstorf et al.\[127\] | 2006 | Constant HTC | |
| Arnoult et al.\[92\] | 2006 | Constant EF and HF | |
| Natschläger\[19\] | 2007 | Variable EF and HF | |
| Clerici et al.\[111\] | 2008 | Variable EF and HF | Based on measured data for gas phase |
| Kho et al.\[33\] | 2010 | None | Isothermal melt zone |
| Logar et al.\[33,48\] | 2011 | Variable HTC, RAD | Gas/dust not considered, cone frustum |
| Brooks et al.\[120\] | 2012 | Constant EF and HF | |
| Logar et al.\[20\] | 2016 | NHTC, RAD | Gas/dust not considered, cone frustum |
| Meier et al.\[13,36\] | 2016 | Variable HTC, RAD | Gas/dust considered, cone frustum |
| Opitz et al.\[40\] | 2016 | NHTC | |
| Fathi et al.\[49\] | 2017 | NHTC, RAD | Gas/dust not considered, cone frustum |
| Opitz et al.\[44\] | 2017 | NHTC, RAD | Gas/dust considered, cone frustum |
| Hay et al.\[39\] | 2019 | Variable HTC, RAD | Gas/dust considered, cone frustum |
| Hay et al.\[46\] | 2020 | Variable HTC, RAD | Gas/dust considered, vertical cylinder |
| Ringel et al.\[47\] | 2020 | Variable HTC, RAD | Gas/dust not considered, vertical cylinder |

\(^{4}\)EF, efficiency factors; HF, heat flows; HTC, heat transfer coefficients; NHTC, heat transfer coefficients based on Nusselt correlations; RAD, radiative heat transfer.
5. Scrap Melting

The heating and melting of scrap inside the steel bath and in the areas heated directly by the arc and burners needs to be accounted for to accurately model the meltdown of the scrap. While the heat fluxes into the scrap can be estimated using the heat transfer models described earlier, the resulting heating and melting rates cannot be determined based on the heat flows alone. The scrap is usually modeled as a single lumped zone, but the local melting of scrap can be accounted for by adjusting the melting and heating rates. Alternatively, the scrap charge can be discretized into several zones with different melting behavior based on their positions and composition.

5.1. Melting of Scrap Submerged in Liquid Steel

The melting of scrap that is submerged within a liquid steel bath is not only relevant to the EAF but also to the basic oxygen furnace (BOF) and has been studied thoroughly both through experiments and numerical simulations.\[^{55-60}\] By submerging samples and observing the change in mass and composition, the relevant phenomena and numerical models can be derived for specific geometries under controlled conditions. The carbon content of the sample and metal bath, their temperatures, flow conditions within the bath, and the geometrical arrangement of the samples have a significant influence on the resulting rates of mass, temperature, and composition changes.\[^{55,56,59,60}\] Numerical models have been developed to reproduce both the behavior in experiments with specific sample types\[^{56,59,60}\] and the conditions within a BOF converter\[^{58}\] or EAF.\[^{57}\] For the EAF, additional phenomena such as the melting of scrap around the arcs and sources of chemical energy such as burners need to be considered.\[^{53}\] In addition to that, the EAF is usually charged with more than one scrap basket per heat, meaning that unlike the BOF, fresh scrap is charged onto the previous, partially melted charge. This requires complex models and discretization to account for local phenomena, making it difficult to incorporate such detailed models for the melting of scrap into EAF process models. Furthermore, many of the parameters such as the shape and composition of the scrap or the flow conditions within the bath would need to be estimated in most cases. Therefore, simplified approaches relying on empirical equations are used in EAF process modeling.

5.2. Modeling of the Meltdown in EAF Process Models

Some authors use a single parameter defined as the specific energy demand for each charged material and determine the progression of the meltdown according to the fraction of this energy that has been supplied up to the current point of time.\[^{10,61,62}\] Shah et al.\[^{63}\] use a similar approach by dividing their pseudodynamic process model into predefined process steps that account first for the heating of the scrap to a certain temperature, then the melting, and for the final steps assume liquid steel for the calculation of chemical equilibrium. This simple energy balance approach is mainly used to determine the end of the meltdown and not to characterize the actual phenomena such as the change in geometry due to scrap melting and the resulting impact on heat flows.

Another simple but slightly more accurate approach is the division of the total net heat flow into the scrap zone(s) into one that is used to heat the remaining scrap and one that is used for melting. The melting rate is then determined based on the second fraction and the temperature change based on the first. These fractions are usually calculated using an empirical equation based on the current temperature of the scrap zone and the bath temperature or the melting temperature of steel with the assumed average carbon content of the scrap. Additional factors such as the current power delivery of burners and arcs may be considered as well when determining the distribution into melting and heating. This approach has been used in the models proposed by Bekker et al.\[^{52}\] MacRosty et al.\[^{14}\] Logar et al.\[^{48}\] and the models based on them. Linninger et al.\[^{17}\] mention both heating and melting based on the heat supplied to the solid zones without giving further details on how the specific rates are determined.

A more detailed description of the melting and heating rates can be found in the model proposed by Matson et al.\[^{64}\] where the scrap is represented as spheres and differential equations are derived to calculate the temperature distribution and the resulting melting and heating rates. Nyssen et al.\[^{28}\] divide the scrap zone into several sectors with different heat transfer conditions depending on the location (submerged in melt or in the freeboard, position in relation to arc and burners, etc.) and composition (determined by the layers of different scrap types charged). A specific melting rate is then calculated for each sector. However, the exact method of determining the heating and melting in the different sectors is not described in detail. The structure of the scrap zones proposed by Nyssen et al.\[^{28}\] is shown in Figure 5.

Similarly, Opitz\[^{29}\] uses different sections within the scrap zone to calculate local heat flows. For each separate zone, an energy balance approach is implemented, initially heating all the scrap within the zone to melting temperature and then progressively melting it. Once a sector is fully liquid, the content is added to the liquid zone and eliminated from the scrap zone, resulting in a discretized melting profile with discontinuous mass changes. Morales et al.\[^{65}\] consider a charge consisting purely of DRI and derive an empirical melting rate for their model.

The different approaches implemented for the melting of scrap in EAF process models are shown in Table 3.

6. Thermochemistry

Up to half of the energy input for the EAF is provided by the energy released through chemical reactions.\[^{15,18}\] and for this reason thermochemical descriptions are an essential part of comprehensive process models for the EAF. In particular, thermochemical descriptions are required for determining the thermal effect of material additions as well as for solving metal–slag reaction equilibria and gas phase equilibria in the freeboard.

6.1. Thermal Effect of Scrap and Other Material Additions

The heating up and melting of the scrap charges constitute a main component of the energy requirement in the electric arc
furnace. Unfortunately, as mentioned in the previous section, the composition, shape, and density of the scrap vary from one batch to another, making scrap one of the most varying parameters in the process.\[66\] Consequently, managing the variation in the properties of the scrap is a key factor for technoeconomically viable EAF processing.

For the EAF, the main phase transformation is the melting of scrap; the associated enthalpy change is also referred to as the latent heat of melting. In addition to scrap, a chilling effect is brought by other material additions and process gases. Their effect on the heat balance can be calculated similar to that of scrap. If the specific heat capacity of a given material addition is unknown, a rough estimate of the specific heat capacity can be obtained by using the Neumann–Kopp rule.\[67\] Furthermore, possible dissolution enthalpies should also be accounted for as a phase transformation. Specific heat capacity is typically described with temperature-dependent polynomials for different temperature intervals. In practice, it is common for EAF models to use a simplified description by treating the \( c_p \) values as constant over temperature, incorporated into the constant parameters described in the previous section. In this way, some computational expense is saved, while the structure of the model becomes somewhat simpler.

### 6.2. Metal–Slag Reaction Equilibria

During the flat bath phase, the molten metal starts to react with the slag phase. Owing to poor mixing in the EAF vessel, the kinetic conditions for these reactions are more of a limiting factor than in some other steelmaking processes, e.g., converters or ladles. In the literature, different methods have been applied for calculating metal–slag equilibria in the EAF process. The equilibrium constant method is used for relatively simple reaction systems, while more complex phase equilibria are solved typically using Gibbs energy minimization. Regardless of the method used, the calculation of metal–slag equilibria requires thermodynamic descriptions of species in metal and slag phases. As for the standard Gibbs energy of reaction, many authors have used values that are averaged over temperature, thus inducing a potential source of error. Furthermore, the treatment of the excess Gibbs energy requires descriptions for the non-ideality of the metal and slag phases. While there are numerous models which describe metal–slag equilibria, many of them do not account for the non-ideality of metal and slag species or use purely empirical approaches. A summary of the description of activities used in EAF modeling is shown in Table 4. A detailed discussion on the different approaches for activities of species in metal and slag phases is provided in the following.

#### 6.2.1. Activity Models for Liquid Steel

In the case of infinitely dilute solutions, the Henrian activity coefficient of species in the metal phase can be described using the Wagner–Lupis–Elliott (WLE) formalism, shown later for the Raoultian reference state using first- and second-order terms\[68\]

\[
\ln \gamma_i^R = \ln \gamma_i^0 + \sum_{j=2}^{N} e_{ij} X_j + \sum_{j=2}^{N} \rho_{ij} X_j^2 + \sum_{j=2}^{N} \sum_{k=2}^{N} \rho_{jk} X_j X_k
\]

\[1\]
where \( \gamma_i \) is the activity coefficient at infinite dilution, \( f_{ij} \) are the molar-based first-order interaction parameters, \( X \) denotes the mole-fraction, and \( \rho \) are the molar-based second-order interaction parameters. It should be noted that in the WLE formalism the solvent (iron) is represented by index 1.

Noting that the Wagner formalism does not fulfill the Gibbs–Duhem rule, Pelton and Bale [69] proposed a modified expression, named unified interaction parameter (UIP) formalism, which is applicable for both dilute and nondilute solutions. Using first- and second-order terms, the Raoultian activity coefficient for each solute \( (i = 1, \ldots, N) \) can be calculated using the following two equations

\[
\ln \gamma_i = \ln \gamma_i^\infty + \ln \gamma_{\text{solvent}} + \frac{1}{2} \sum_{j=1}^{N} \sum_{k=1}^{N} f_{ij} X_j X_k - \frac{2}{3} \sum_{j=1}^{N} \sum_{k=1}^{N} \sum_{l=1}^{N} f_{jkl} X_j X_k X_l
\]

where \( \gamma_{\text{solvent}} \) is the activity coefficient of the solvent and \( f_{ijkl} \) are the molar-based second-order interaction parameters. The UIP formalism has been used extensively in thermodynamic databases for dilute liquid iron solutions. Later, Ma et al. [72] derived an interaction parameter formalism, which provides a slightly more detailed description for both the solvent and the interaction of the solutes.

As second- or higher-order terms are not always available for all systems of interest, they are usually neglected in mathematical modeling of unit processes. Compilations of interaction parameters relevant for EAF steelmaking are readily available in the literature.

As shown in Table 4, the most used approaches are the WLE and UIP formalisms. Owing to their simple formulation, all the three models (WLE [68], UIP [69], and the \( \varepsilon \) formalism by Ma et al. [72]) presented are computationally light and require only minimal programming effort. In view of the results of Hay et al. [49], the apparent theoretical weaknesses of the WLE formalism in comparison to the UIP formalism have little bearing on the simulation results in the context of mathematical modeling of the EAF process. Meanwhile, the description of the thermodynamic properties of the solid scrap has received much less attention. In the model of Arnout et al. [62], solid fcc, and solid bcc solutions were described using the sublattice model.

### 6.2.2. Activity Models for Slag

From thermodynamics point of view, silicate slags can be viewed as ionic liquids with a complex network structure. A detailed overview of the application of thermodynamic models for molten slags in thermodynamic databases was published by Jung. In addition to those, simpler descriptions are used frequently in mathematical modeling of processes.

As shown in Table 4, the main models used in contemporary EAF modeling are the regular solution model (RSM) [75], cell model [76], and modified quasichemical model (MQM) [69,77]. The simplest of the models is the RSM, which assumes that all the cations contained by the silicate melt are distributed evenly in a matrix formed by oxygen anions. [75] The activity coefficient of species \( i \) is expressed as follows [75]

\[
RT \ln \gamma_i = \frac{N}{j} \sum \sum \alpha_j X_j^2 + \sum \sum \sum \left( \alpha_j + \alpha_k - \alpha_{jk} \right) X_j X_k + \Gamma
\]

where \( \alpha \) denotes the interaction energy between the cations, \( X \) is the cation fraction, and \( \Gamma \) is the conversion factor between hypothetical regular solution and a real solution. Tabulated values for the interaction energies and conversion factors in systems relevant to steelmaking [78] and stainless steelmaking [79] are available in the literature. The interaction energies derived by Kho et al. [33] for CaO–MgO and CrO\(_{1.5}\)–MgO based on the data of Pei and Wijk [79] were not reported.

The cell model proposed by Kapoor and Frohberg [76] assumes that the slag melt is a mixture of cells formed by two cations.

---

**Table 3. Description of scrap melting in EAF process models.**

| Study             | Year | Modeling approach | Notes |
|-------------------|------|-------------------|-------|
| Köhle [30]        | 1982 | TE                |       |
| Linninger et al.  | 1995 | DF                |       |
| Deneyes/Peaslee/Shah [31] | 1997 | TE Pseudodynamic in predefined stages |
| Matson/Ramirez [32] | 1998 | Differential equation for melting/heating |
| Bekker et al. [33] | 1998 | DF Based on scrap and bath temperature |
| Morales et al. [34] | 2000 | Empirical equation 100% DRI, empirical melting rate equation |
| Nyssen et al. [35] | 2002 | Multiple zones with individual melting/heating rates |
| Rathaba [36]      | 2005 | DF Based on scrap and bath temperature |
| MacRosty/Swartz et al. [37] | 2005 | DF Based on temperature and melting point of scrap |
| Kleimt et al. [38] | 2005 | TE                |       |
| Arnout et al. [39] | 2006 | TE                |       |
| Natschläger et al. [40] | 2007 | DF                |       |
| Clerici et al. [41] | 2008 | DF                |       |
| Logar et al. [42] | 2011 | DF Based on temperature and melting point of scrap |
| Brooks et al. [43] | 2012 | TE Linear relationship of TE supplied and scrap melted |
| Meier [44]        | 2016 | DF Based on temperature and melting point of scrap |
| Optiz [45]        | 2016 | Multiple zones with TE approach for each zone |
| Fathi et al. [46] | 2017 | DF Based on temperature and melting point of scrap |
| Hay et al. [47]   | 2019 | DF Based on temperature and melting point of scrap |

*TE, total energy (for heating and melting); DF, division factor (dividing total heat flow into heating and melting).*
Table 4. Description of the activities of metal and slag phases in EAF models.

| Study          | Year     | Calculation method       | Metal phase                           | Slag phase                            |
|----------------|----------|--------------------------|---------------------------------------|---------------------------------------|
|                |          |                          | Model(3)                              | Notes                                 |
|                |          |                          | RSM                                   | Notes                                 |
| Cameron et al. | 1998     | Gibbs free energy minimization | UIP                                   | First- and second-order interactions |
|                |          |                          |                                       |                                       |
| Modigell et al.| 2001     | Gibbs free energy minimization | UIP                                   | –                                     |
| Morales et al. | 2001     | NA                       | WLE                                   | –                                     |
| Morales et al. | 2002     | Equilibrium constant method | None                                  | –                                     |
| MacRosty and  | 2005/2007| Gibbs free energy minimization | UIP                                   | –                                     |
| Swartz         |          |                          |                                       |                                       |
| Arnout et al.  | 2006     | Gibbs free energy minimization | Sublattice formalism (solid), WLE (liquid) | Data from FACT | M/M, RSM, WLE, UIP | First-order interactions | RSM FeO, Fe2O3, MnO, CaO, MgO and Al2O3 considered |
| Kho et al.     | 2010     | Gibbs free energy minimization | WLE                                   | First-order interactions              | RSM Interaction energies for CaO-MgO and CrO3-MgO estimated based on experimental data(79) |
| Hay et al.     | 2019     | Equilibrium constant method | WLE, UIP                              | First-order interactions, comparison of methods | RSM, CM Comparison of methods |

Model(3) = Comparison of methods

For example, the system M–SiO2 can be described using cells M–O=M, M–O=Si, and Si–O=Si, for which the network breaking reaction can be presented as follows(70)

\[(M–O=M) + (Si–O=Si) = 2(M–O=Si) \tag{5} \]

for which the corresponding free energy change is defined by

\[\Delta G = 2W_{Si-M} \text{ where } W_{Si-M} \text{ is the cell formation energy. The model is used as main parameters, the cell formation energy (}W_{Si-M}\text{ and the cell interaction energy (}E_{Si-M}\text{, which are defined as a function of composition and temperature.} \tag{70} \]

The MQM proposed by Pelton and Blander(69) is based on the quasichemical theory of Guggenheim.(80) Similar to the cell model, the MQM model explicitly accounts for the ordering behavior of silicate melts in the composition-dependent properties of the melts.(70) The main model parameter is the Gibbs energy of the network breaking (depolymerization) reaction, which is defined using an empirical polynomial function of composition and temperature. In later publications, the MQM has been improved(81) and extended to multicomponent solutions(82) and two sublattice systems with nearest- and second-nearest-neighbor interactions.(83,84) The MQM has been used extensively in thermodynamic software and databases.(70) In the model by Arnout et al.,(62) for example, the MQM was implemented using the ChemApp routine library. In their study the solution monoxide and (Ca,Mg)2SiO4 were modeled using the asymmetric Kohler–Toop extrapolation technique. The choice of this approach highlights the complex behavior of silicon in slags.

6.3. Gas Phase Equilibria in the Freeboard

Both homogeneous and heterogeneous reactions take place in the EAF atmosphere. These include combustion of methane, homogeneous and heterogeneous water–gas shift (WGS) reactions, the Boudouard reaction, and oxidation of carbon by oxygen. A compilation on the treatment of gas phase reactions in mathematical models for the EAF process is shown in Table 5. It should be noted that many of the publications do not provide enough details to assess how the reactions are treated mathematically.

The calculations of Linninger et al.(137) suggest that the volumetric flow rate and composition of the exhaust gas vary significantly during the EAF process, while the temperature of the exhaust gas increases gradually toward the end of the process. The fluctuations in the exhaust gas flow rate are related mainly to the use of burners and oxygen lances as well as leakage air.(137) The main components of the exhaust gas are N2 and CO.

The approaches for calculating the equilibria in the freeboard are varied. The models by Matson et al.(64) and Frittella et al.(86) as well as the model by Meier et al.(138,139) and its further development by Hay et al.(88,89) use the equilibrium constant method. Dienes et al.,(131) Shah et al.,(63) Cameron et al.,(90) Matson et al.,(91,92) MacRosty and Swartz,(54,55,93,94) Arnout et al.,(62) and Kho et al.(13) all use Gibbs energy minimization to determine gas phase equilibria in the freeboard.

6.4. Kinetic Treatments

One of the challenges for modeling the EAF process is the difficulty of determining reaction areas and suitable “geometric simplifications” for their mathematical expression. For this reason, the proposed models mostly make use of the reaction volume approach, in which the process kinetics are described by modeling mass exchange between equilibrium volumes. Figure 6 shows a typical example of the definition of different zones and the exchange between them. Unfortunately, this approach does not account for the effect of the microkinetic mass transfer resistances on the local thermodynamic equilibrium.
### Table 5. Description of gas phase equilibria in the freeboard in EAF models.

| Study                                | Year | Species                  | Reactions                                                                 | Calculation method                                                                 |
|--------------------------------------|------|--------------------------|---------------------------------------------------------------------------|----------------------------------------------------------------------------------|
| Linninger et al.[37]                 | 1995 | O₂, CO₂, CO, H₂O, H₂, N₂, C₆H₁₀ | Combustion of C, CH₄, H₂ and CO; WGS reaction[a]                          | Combustion reactions are treated in algebraic manner, kinetics of WGS reaction are accounted for |
| Hayman et al.[114]                   | 1997 | O₂, CO, CO₂              | Postcombustion of CO                                                      | NA                                                                               |
| Deneyes and Peaslee[31]              | 1997 | O₂, CO, CO₂, H₂, H₂O, N₂, (CH₄) | Combustion of CO and H₂ by oxygen                                         | No process kinetics; chemical equilibrium calculated using Gibbs energy minimization (Pyrosim simulation software), gas phase treated as an ideal gas |
| Shah et al.[35]                     | 1998 | O₂, CO, CO₂, H₂, H₂O, N₂, (CH₄) | Combustion of CO and H₂ by oxygen                                         | Pseudodynamic calculation with five calculation steps; chemical equilibrium calculated using Gibbs energy minimization (Pyrosim simulation software), gas phase treated as an ideal gas |
| Cameron et al.[90]                  | 1998 | O₂, CO, CO₂, possibly also others | Combustion of CO                                                          | Kinetics accounted with the boundary layer theory. Gibbs energy minimization for the equilibrium contents |
| Bekker et al.[52,103,106]            | 1998/1999 | CO, CO₂, N₂                | Combustion of CO                                                          | First-order rate expression for formation of CO. All O₂ of leak air consumed directly for postcombustion of CO |
| Matson et al.[64]                   | 1997 | O₂, CO, CO₂, H₂O, H₂, N₂   | Combustion of CO and H₂                                                   | Equilibrium constant method                                                        |
| Matson et al.[91,92]                 | 1998 | O₂, CO, CO₂, H₂O, H₂, N₂   | NA                                                                        | No kinetics; chemical equilibrium calculated using Gibbs energy minimization (RAND algorithm) |
| Modigell/Traebert[103,104]           | 1999/2001 | NA[a]                       | NA                                                                        | Postcombustion zone and burner                                                     |
| Morales et al.[85,126]               | 2001/2002 | CO                           | CO production from slag                                                   | No kinetics                                                                       |
| Nyssen et al.[28,147,161]            | 2002/2004/2011 | NA                          | Primary postcombustion of CO in the slag, secondary postcombustion of CO in the inlet of the exhaust shaft | Calculation divided into primary combustion in the slag and secondary combustion at the shaft inlet |
| MacRosty and Swartz[14,53,91,94]     | 2005/2007 | O₂, CH₄, CO, CO₂, H₂O, H₂, N₂, C₆H₁₀ | NA                                                                       | No kinetics; chemical equilibrium calculated using Gibbs energy minimization (HSC Chemistry ver. 5.1). |
| Rathaba[38]                          | 2005 | CO, CO₂, N₂, O₂, H₂, CH₄, C₆H₁₀ | Calculation divided into primary combustion in the slag and secondary combustion at the shaft inlet | Efficiency factors |
| Arnout et al.[82]                   | 2006 | NA                        | NA                                                                        | No kinetics; chemical equilibrium calculated using Gibbs energy minimization |
| Frittella et al.[178]               | 2009 | NA                        | Postcombustion of CO                                                      | NA                                                                               |
| Kho et al.[35]                       | 2010 | O₂, CO, CO₂, Mn (g), MnO (g) | Postcombustion of CO                                                      | No kinetics; chemical equilibrium calculated using Gibbs energy minimization (HSC Chemistry ver. 5.1). |
| Frittella et al.[39]                 | 2011 | H₂, H₂O, CO₂, O₂, CO       | Postcombustion of CO, WGS reaction                                        | Equilibrium constant method                                                        |
| Logar et al.[34,54]                  | 2012 | CO, CO₂, N₂, O₂, CH₄, C₆H₁₀ | CO combustion with leak air, postcombustion of CO, combustion of CH₄      | Total combustion of CH₄ assumed (no CH₄ present in the gas phase) |
| Meier et al.[73,87]                  | 2016/2017 | CO, CO₂, N₂, O₂, CH₄, H₂, H₂O, C₆H₁₀ | Reaction of CH₄ with O₂, CO and CO₂, reaction of C₆H₁₀ with C, Boudard reaction, homogeneous and heterogeneous WGS reaction, oxidation of H₂ and C by O₂ | Equilibrium constant method. Equilibrium constants precalculated with MediumModel equilibrium toolbox (MATLAB) |
| Fathi et al.[39]                     | 2017 | CO, CO₂, N₂, O₂, CH₄, C₆H₁₀ | CO combustion with leak air, postcombustion of CO, combustion of CH₄      | Total combustion of CH₄ assumed (no CH₄ present in the gas phase) |
First-order kinetics have been used by several authors to describe metal–slag mass transfer; these include the models by Cameron et al.,[90] Hay et al.,[49] and MacRosty and Swartz.[34,53] In these models the reactions are determined via the composition at the reaction interface. Consequently, the mass change of species $i$ is described simply by

$$\frac{dm_i}{dt} = -\dot{m}(y_i - y'_i)$$

where $\dot{m}$ is the total mass flow between reaction volumes. This kind of formulation assumes that the rate is controlled by mass transfer but does not take a stand on what factors might affect it. As metal–slag reactions are heterogeneous reactions, they are usually controlled by mass transfer owing to the high temperatures involved. For the purposes of mathematical modeling, it is usually permissible to assume that the mass transfer resistance lies entirely in the diffusion boundary layer between phases; this approach was first proposed by Nernst[95] in 1904. In some cases, the reaction resistances in both phases are of the same magnitude and both need to be accounted for. The overall resistance of mass transfer constraints in two phases can be solved analytically by making use of the two-film theory by Lewis and Whitman,[96] which may be extended also for competing mass transfer controlled reactions.[97] Nevertheless, it is oftentimes much simpler and more flexible to opt for a numerical solution approach; a detailed discussion on available approaches has been presented by Järvinen et al.[98] A major challenge for the boundary layer approach is the uncertainty related to the interfacial area. Morales et al.[65] defined the metal–slag interfacial area based on the stirring energy correlation of Themelis and Zhao.[99] For most other models, the interfacial area is implicitly contained within empirical model parameters.

So far, there have been little attempts to model reactions inside the foam in the EAF process. In principle, descriptions similar to those used in recent BOF models[100–102] could be adopted. Nevertheless, more information is still required for the formation of foam in the EAF process.
6.4.2. Kinetic Treatment of Gas Phase Reactions

Both homogeneous reactions and heterogeneous gas phase reactions take place in the EAF. The models by Deneys and Peaslee,[31] Sha et al.,[63] Matson et al.[91,92] Modigell et al.[103,104] MacRosty and Swarz,[53,54,93,94] Arnout et al.[62] and Kho et al.[33] do not account for the kinetics of gas phase reactions at all. Cameron et al.[90] used the boundary layer theory to determine mass flow rates between equilibrium zones. Bekker et al.[52,105,106] assumed that all oxygen contained within the leak air reacts completely in the postcombustion of CO; this means the only kinetic constrains for the gas phase reactions were the formation rate of CO (which was assumed to follow first-order kinetics) and the air leakage rate. Similarly, Logar et al.[48,54] consider the CO postcombustion in the freeboard and assume total combustion of the CH₄ added through the burners. Meier et al.[13,87,107] and based on that Hay et al.[49,89] assume infinitely fast reactions for the burning of CH₄ in oxyfuel burners and kinetically limited reactions inside the freeboard as well as limited heterogenous reactions such as the Boudouard reaction based on empirical parameters and equilibrium constants. The different reactions of CH₄ considered by Meier[13] are shown in Figure 7.

6.4.3. Kinetic Treatment Carbon and Oxygen Injection

When injected into a foaming slag, carbon particles react with CO₂ inside the gas bubbles surrounding them, forming CO. Part of this CO then reduces oxides from the slag (e.g., iron oxides) producing CO₂ which, in turn, can react with the carbon particle again, as shown in Figure 8.

The conversion of the carbon particles depends on various process conditions, including size and residence time of the carbon particles, injection conditions, slag chemistry, and temperature.[21] An overview of reaction models and experimental studies regarding the injection of carbon into EAF slags have been given by King[108] and Zhu.[109]

Most of the EAF models proposed in the literature assume a full conversion of the injected carbon. At simplest, as implemented in the models by Bekker et al.,[106] Rathaba,[108] and Logar et al.[48,54] this means that the injected carbon is consumed entirely for the reduction of FeO. A detailed description of the reduction kinetics of FeO by carbon injection was proposed by Morales et al.,[22] who accounted also for the related jet penetration in the liquid and coupling–uncoupling characteristics between carrier gas and solid particles. Later, Morales et al.[65] used the FeO reduction model as a part of their fundamental mathematical model for DRI melting in an EAF. In the models by Matson et al.,[64,91,92] Modigell et al.,[103] MacRosty and Swarz,[53] Arnout et al.,[62] and Kho et al.[33] a full conversion of carbon is also assumed, but the carbon injection is considered as an input stream to an equilibrium reactor, thereby allowing the carbon to react with species other than FeO.

As with the injection of carbon into the slag, the reactions resulting from injecting oxygen into the metal bath present a complex phenomenon. Logar et al.[48,54] used fixed oxygen distribution coefficients to determine the distribution of injected oxygen to species dissolved in the metal bath. The downside of this approach is that part of the process dynamics is inevitably lost when the oxygen distribution coefficients are held constant over time. Furthermore, the constants are unlikely to be valid for different data sets. Bekker et al.[106] assumed that all oxygen injected is first converted to FeO, which acts as an intermediary
reaction product and is later reduced partially or completely by subsequent reactions. This approach has also been employed in BOF modeling.[110] Similar to carbon injection, oxygen injection is considered as an input stream to an equilibrium reactor in the models by Matson et al.[64,91,92] Modigell et al.,[103] MacRosty and Swartz,[14] Arnout et al.,[62] and Kho et al.[13]

7. Validation

Training and validating an EAF model present a challenging task due to limited availability of online information. The high temperature of the furnace atmosphere, incandescent radiation from the electric arc, high magnetic currents, and constant vibration of the furnace shell limit the utilization of measurement sensors in the vicinity of the furnace. Most of the available continuous data are related to the boundaries of the EAF model, namely, temperature and composition of the off-gas, side panel cooling water temperature gradient, and electrical supply parameters. The composition and temperature of the steel melt and slag can be acquired through routine probe sampling, which offer discrete information especially useful in validating the end results of the process model.

The approach on validating EAF models depends on the purpose of the model. EAF models intended for educational purpose are not validated or the validation results are not presented.[33,111,112] Likewise, for many commercially used models the data used for their validation are not disclosed.[37,113–122] In some studies,[49,88,89] the data used are normalized, which complicates the comparison of model accuracy.

Typically, the main parameters to be adjusted or fitted are related to the kinetics of the process. The most basic type of a validation is to conduct a case study, in which a heuristic comparison between simulated heats and selected heats from validation is to conduct a case study, in which a heuristic comparison between simulated heats and selected heats from validation is to conduct a case study, in which a heuristic comparison between simulated heats and selected heats from validation.

A common validation approach utilized in the majority of the presented noncommercial models[27,33,38,42,43,48,54,62,65,103,104,125] is to formulate a physical model with the literature data and validate it using point data from the refining period or tapping of industrial EAF. While steel and slag temperature and composition have high relevance to EAF operations, the lack of continuous variables in model training and validation makes it harder to analyze the sources of errors and makes it very challenging to validate the results during the heat. Furthermore, separate datasets are not often used or at least not specifically published for training and validation, obscuring the procedure how the model was adjusted and the validation dataset was selected.

The lack of continuous data for steel and slag composition poses a challenge also for other processes in the primary and secondary metallurgy of steelmaking, and only rarely the data are public to the extent that it can be used for validation by other authors. For example, recent multiphysics models for the BOF process have been criticized for relying too much on the same dataset in their validation.[113] In case of the EAF modeling, even using such a public reference dataset would be a significant step forward in making the model results more comparable.

Utilizing models for different EAF regions has enabled validation of the model also with the continuous data.[13,36,48,49,52,61,87–90,106,107,115–117] The most widely used continuous data are the off-gas temperature or composition. It can be used for validating models intended for optimizing of burners, injection systems, or postcombustion.[13,30,36,52,87,90,106,107,115,116,142,143] The models intended for that overall EAF energy balance calculations presented by Logar et al.[35,48,54] Meier at al.[13,30] Hay et al.[49,88,89] and Opitz[89] were also validated using the predicted and measured temperatures of the side panel and roof cooling water. Most of the EAF models consider at least some electric supply parameters as input variables, but few predict values such as voltage, current, or consumption of electric energy and consider them in the model validation. Meier developed an algorithm for the automatic generation of operation charts based on the input of scrap, slag formers, and coals as well as the desired endpoint conditions.[143] The development of this algorithm was continued by Hay at al.[89] In both studies, the predicted power profiles were compared with values measured for heats with similar inputs.[89] Meanwhile, Logar et al.[35,48,54,111,132] and Opitz et al.[29,40,41,44,144] include sophisticated models of the electrical system in their process models, capable of predicting the arc current and voltage based on the selected transformer tap. Both have validated their electrical models with continuous electric data.[29,131]

Some researchers also use novel continuous measurements to validate their models. Morales et al.[65,126] utilized the arc distortion parameter measured with acoustic sensor in validation of dynamic foaming index. Kleint et al.[61,137–141] performed validation of the bath temperature by comparing the model results to online temperature measurement with optical fibers. Nyssen et al.[28,145–148] took imaging measurements of slag tapping stream that were used to validate the amount of slag calculated by the process model. In addition, Nyssen et al. included distance measurements performed on the melting scrap to evaluate the validity of the calculated melt temperatures.

The compilation of the different sources of validation data utilized is shown in Table 6. The validation data sources have been interpreted as they have been published and, where applicable, several publications concerning the same model have been combined.

An example of the validation using continuous data can be seen in the measured and simulated CO content of the off-gas as published by Meier,[13] as shown in Figure 9.

8. Discussion

Apart from the areas discussed so far, the various models differ in other aspects such as the number and definition of zones, the solver algorithm, and their specific focus and purpose. While the approach of using lumped zones is common to process models, the precise definition of the different zones, the system boundaries, and additional sinks or sources of mass or energy varies widely. Models aimed predominantly toward the estimation of overall energy consumption or endpoint control may use just a single zone and empirical parameters to define energy losses. Others use additional zones with separate heat and mass balances allowing more detailed tracking of energy losses, phase
changes, or distribution of energy and mass to different phases. Solver algorithms range from simple fixed timestep methods\(^\text{[30,62,123]}\) to adaptive multistep methods.\(^\text{[39,142]}\) The reported computing time for the simulation is between \(\approx 40\) min\(^\text{[144]}\) and below 1 min,\(^\text{[49]}\) although a direct comparison often is not possible because the specifications of the computers used to obtain those results are usually not given. While some of the proposed models have been published recently and in detail, allowing a comprehensive evaluation, others, especially those used commercially, were only described superficially and during the earlier stages of their development, making it difficult to compare them with each other.

Table 6. Validation data used in the different EAF process models.

| Author          | References | Bath temperature | Slag composition | Steel composition | Cooling water temperature | Off-gas data | Electric data | Note                                      |
|-----------------|------------|------------------|------------------|-------------------|--------------------------|--------------|--------------|------------------------------------------|
| Boland/Billings| [28,29]    | x                | x                | x                 | x                        | x            |              | Validated to refining time               |
| Köhle           | [30]       |                  |                  |                   |                          |              |              |                                          |
| Cameron         | [40,41]    | x                | x                |                   | x                        |              |              | Carbon content, tap weight               |
| Bekker et al.   | [42,44–46] | x                | x                |                   | x                        |              | x            | Carbon content and oxygen activity       |
| Rathaba/Coetzee | [48,49]    | x                |                  |                   |                          |              |              | Mass of slag, off-gas and steel           |
| Modigell et al. | [50,51]    |                  |                  |                   |                          |              |              | Acoustic measurements                     |
| Morales         | [52,53]    |                  |                   |                   |                          |              |              | Slag flow in tapping stream               |
| Nyssen et al.   | [54–58]    |                  |                   |                   |                          |              |              | Continuous melt temperature measurement  |
| MacRosty/Swartz et al.| [60–64] | x                | x                |                   |                          |              |              |                                         |
| Kleirnt et al.  | [65–70]    | x                |                  |                   |                          |              |              | Compositions also during heat             |
| Wendelstorf     | [71,72]    |                  |                  |                   |                          |              |              |                                          |
| Arnout          | [73]       | x                | x                |                   |                          |              |              |                                          |
| Logar et al.    | [20,89–93] | x                | x                | x                 | x                        | x            |              | Prediction of electrical data (voltage, current, etc.) |
| Fathi/Saboohi   | [94–97]    | x                | x                | x                 |                          |              |              | Electric energy consumption only          |
| Meier           | [12,98–102]| x                | x                | x                 | x                        | x            |              | Melt temperature and gas phase results compared to Logar et al.\(^{[25,48,54,131,132]}\) prediction of electrical data (voltage, current, etc.) |
| Opitz           | [106–110]  | x                |                  |                   |                          |              |              |                                          |
| Hay             | [103–105]  | x                | x                | x                 | x                        | X            | x            | Electric energy consumption only          |

Figure 9. Simulated and measured CO content of the off-gas for two heats. Reproduced with permission.\(^\text{[13]}\) Copyright 2016, Mainz Verlag.
8.1. Relation to Modeling of Other Metallurgical Processes

Many of the challenges and resulting solutions encountered in modeling the EAF can also be found in other metallurgical processes such as the basic oxygen furnace, argon/vacuum oxygen decarburation (AOD/VOD), hot metal desulfurization, and other refining processes. In some cases, a model can be adapted for several of these processes, retaining a common basic model structure. This can be found, for example, in the models for EAF, VOD, and AOD proposed by Swinbourne et al.[33,149,150] or Modigell et al.[103,104] modeling both the EAF and BOF.

In other cases, complete models may not be transferable but specific phenomena can be found in several processes and under similar conditions. The injection of solid reagents, for example, is also relevant in the desulfurization process, and detailed models for the description of the resulting interfaces as well the kinetics of reactions along these interfaces have been developed.[151] Other than Morales et al.[21,22,65] who developed a similar complex model for the injection of carbon particles into EAF slags and incorporated it into their EAF process model, EAF process models do not include a detailed description of these reaction kinetics. The injection of oxygen both from top-lances and tuyeres underneath the bath surface is a significant part of the BOF, VOD, and AOD processes. The description of the gas–liquid interface itself and the formation of slag droplets carried into the metal phase and vice versa found in many process models for the AOD,[152,153] VOD,[154] BOF,[134] and CAS-OB[155,156] is more detailed than what is implemented in those for the EAF. The impact of the injection of gases and solids on mixing and reaction kinetics has also been studied thoroughly through physical models and CFD modeling.[151,157,158] Regarding the equilibrium at the metal–slag interface in other processes, the approaches are generally similar to those found in EAF process models. Some models of refining processes, however, include more detailed descriptions of the mass transport and the resulting reactions kinetics,[151,159,160] Overall, the mass transfer limitations, interface conditions, and reaction kinetics are often modeled in less detail in the EAF and there is less information available about the conditions such as the flow, exact form, and surface area of the interfaces or the mixing conditions, making more simplifications and assumptions necessary. The gas phase, on the contrary, is not usually modeled in detail for other processes while it has significant influence on the EAF process. Especially postcombustion and burners are not used in the other processes and are therefore specific to modeling the EAF and, to some extent, the BOF where partial postcombustion may occur within the converter vessel.[134] For this reason, descriptions of gas phase reactions and additional reaction zones for postcombustion and burners implemented in EAF process models are usually more comprehensive when compared with the other processes.

Heat transfer also plays less of a role in modeling the refining processes, and assumptions such as isothermal phases or constant heat losses are common without any extensive description of specific heat transfer phenomena. The BOF is an exception in this regard as the heating and melting of scrap is essential to modeling the process. The kinetics of scrap melting have been modeled in detail for the BOF,[134] and while additional challenges such as the direct heating of scrap through burners and arcs remain for the EAF, the modeling of the submerged scrap could potentially be improved based on these solutions developed for the BOF.

8.2. Application in Contemporary Industrial Practice and Future Trends

While many EAF models use relatively simplistic descriptions for metal–slag and gas phase equilibria for reasons of model speed and robustness, there are also many models that use complex Gibbs energy minimization routines and slag models that are virtually the same as those used in computational thermodynamics software. As for the model accuracy, the differences between models with simplistic descriptions and those with more complex descriptions (e.g., MQM for slag species) are not substantial. Consequently, it appears unlikely that thermodynamic descriptions would be limiting the accuracy of current models or that major improvements in model accuracy could be attained by improving them.

A major area for further improvement of the EAF models is the description of the process kinetics. Especially in reaction volume models, the kinetic parameters related to mass exchange between the volumes are essentially empirical constants. The more such parameters are used, the more dependent the model becomes from the datasets used for training and validation.

As for the metal–slag reactions, major uncertainties are related to the foaming slag practice. Nyssen et al.[28,146,147,161] related the apparent foaming slag density to CO generation rate. A popular and mathematically simple approach is to describe the foaming slag using the concept of foaming index, for which the most common definition is that given in ref. [162] which has been used, e.g., by Logar et al.[54] and the models based on that. Other definitions are also available. Morales et al.[126] use the foaming index as formulated by Ghag et al.[163] However, an exhaustive validation of the foaming index approach for the conditions of an industrial EAF is yet to be conducted.

As mentioned earlier a more detailed description of the kinetics of reactions during the injection of reactants, at the interface of slag and melt, and the melting of scrap may be possible based on solutions developed and used for other processes. However, for some of these, more information about local conditions as well as flow and mixing within the EAF would be necessary, making the process models more complex and computationally demanding.

To the knowledge of the authors, none of the published EAF process models provide a detailed description of the local gradients and differences inside the EAF. The proposed models either assume simplified geometries or consider specific phenomena such as the heat transfer or chemical reactions only for the whole furnace and not for smaller, local scales, apart from the definition of additional zones to describe specific reactions or the melting of the scrap pile somewhat more accurately in some models. These assumptions significantly increase the calculation speed, which is in many cases required for the use in online applications. The drawback of the approach is the limited accuracy and applicability of such models due to the omission of localized phenomena of smaller scales. Such local phenomena are highly relevant to most aspects of EAF modeling. Due to
the injection of gases and carbon through lances as well as burners, for example, local temperatures and compositions may be significantly different from those in the averaged, homogenous zone used in modeling. While detailed models exist for specific phenomena such as the local heat transfer conditions around burner flames,[164] the melting of scrap submerged in liquid metal,[160] or the injection of reactants as discussed in the previous section, the necessary simplifications in EAF process modeling prevent the accurate description of the exact local conditions and resulting phenomena such as the formation of hot spots, localized melting or freezing of the steel, or certain chemical reactions.

Another significant shortcoming of the current EAF process models is how the plasma heat transfer is considered. Many of the models require assumption of arc length, which is difficult to define correctly as it changes constantly based on electrical supply voltage. Arc models could be improved using the empirical correlations between the voltage and arc length to extract the arc length based on voltage. Furthermore, in all the presented models containing plasma submodels, the heat transfer from the arc plasma is based on assuming the plasma surface as a black body. From the physical point of view, this assumption is inaccurate because the heat transfer in arc plasma occurs through movement of electrons and photons. A more detailed description of heat transfer from plasma could be achieved by utilizing a model that calculates the radiative heat transfer from the arc plasma based on plasma composition and excitation conditions. In the modeling of arc welding, the radiative emission coefficients have been utilized to model the effect of metal vapors on the welding plasma.[165] In the field of electric arc smelting, such a model was developed by Sevastayenko and Bakken[166] for a ferrosilicon production furnace. The advantage of the radiative emission models is that they make it possible to describe the relation between emission power and wavelength more accurately, which can be coupled to the absorptivity model of the transmitting medium in the EAF. The wavelength of the plasma emission is important in calculation of heat transfer because the absorption behavior of the dust and gases in the EAF atmosphere is wavelength dependent. The black body assumption of plasma surface is limiting the accuracy of the absorptivity models of the EAF atmosphere, especially in the areas close to the arc. To achieve more accurate modeling of the heat transfer, the wavelength-dependent arc emissivity model could be utilized with a weighted-sum-of-gray-gases model for the EAF atmosphere as proposed by Opitz et al.[144]

While several of these issues could, in principle, be solved through comprehensive CFD models of the EAF process, these are, as mentioned earlier, still too computationally expensive to be used as a substitute for process models.[160] Therefore, the further development toward more detailed but still fast and efficient process models, partially replicating some of the CFD models’ abilities, can still be expected for the foreseeable future. Unlike CFD models, existing process models can already be utilized in scenario analysis to predict what effects the various changes in the EAF process have on parameters such as the time needed to melt down the scrap or the melt temperature evolution. The increasing complexity of the models, such as the introduction of off-gas models for the optimization of post-combustion within the EAF or the modeling of the properties and foaming of the slag, accordingly allows more detailed scenario analysis and optimization.[124,133,143,148] It is important to note that the increase in complexity of process models has not caused excessive increase in computation time.[89] This enables the current process models to be utilized also in online computations,[127,131,115–122,141,147,148,167] although the reported applications of such models are still scarce. Most of the published online applications include the prediction of melt temperature[121,113,115–122,141,147,167] or control of burners as well as carbon and oxygen injections.[113,115–122,147,148,167] In the melt temperature prediction application, the process model continuously predicts the melt temperature and the model result is calibrated with the temperature measurements. Most of the presented online applications have been achieved with commercial models, which makes it difficult to objectively assess their performance. Publishing and utilizing an EAF reference dataset would be a step forward in comparing the performance of the proposed models. Furthermore, unit test could be used to independently validate submodels such as the calculation of view factors, radiative heat flows, or equilibrium compositions and therefore quantifying and possibly eliminating the errors introduced by these into the overall process model results.

It is likely that online applications of EAF process models will increase in the future, due to increased pressure to optimize costs and emissions as well as the increased complexity of the optimization problem due to additional materials and energy carriers used in the process.[11] The advantage of online process models is that they can be conveniently linked to the online measurements because both measurements and process models deal with physical quantities of the process. This allows constant readjustment of empirical model parameters and accurate extrapolation of results based on the measured data. The development of fundamental EAF process models is getting closer to the stage where they can be applied to extensive off-line and online process optimization as well. Due to the high number of scenario evaluations necessary in optimization, the model needs to be highly efficient and fast for this purpose. While some optimization has been performed with somewhat reduced and simplified models,[124,133,143,148] both the fast or even online optimization of control strategies for specific heats and the automatic adjustment of empirical parameters offer significant challenges in EAF process modeling.

To become more widely used in the industry, the more complex models need to overcome these and other challenges. Sufficient speed and efficient optimization algorithms are needed to allow automated adjustment of model parameters, avoiding the complex readjustment of the model to account for slight changes in the furnace environment or the process conditions and to make online optimization of operation strategies feasible. Appropriate user and data interfaces are needed to integrate models into the control systems of a steel plant. Furthermore, plausibility checks of both model results and inputs are necessary to detect false inputs and possible failures of the model to make meaningful predictions in specific and unusual cases. While some or all of these conditions may be fulfilled by several existing commercial models, there are several detailed and comprehensive process models reported in mostly academic settings that need further development to bring these advances into industrial use. Furthermore, the accurate calibration and validation of complex EAF models would benefit from additional and more accurate
measurements. Some desirable measurements such as the continuous analysis of the off-gas composition and temperature, the sound and vibrations levels as an indicator of the progression of the melt down and foaming slag quality, the continuous determination of the melt temperature, or the composition of the arc plasma, are only available for some furnaces or still in development. With more widespread use of such systems and better quality control applied to the acquisition and handling of process data, the accuracy and applicability of process models could be improved significantly.

9. Conclusion

The existing models are generally capable of describing all the main aspects of the process. The fundamental process models supplement the information obtained from other types of models such as CFD models and statistical models, by providing a tool for understanding and simulating all the main aspects of the EAF process with specific advantages and drawbacks compared with these other classes of models. Modern fundamental process models can predict the distribution of electric and chemical energy in the furnace as well as dynamic changes in metal, slag, and off-gas compositions and are sufficiently fast and stable to be used for model-predictive control.

Thermodynamic descriptions are fairly sophisticated and can reproduce the metal–slag and gas phase equilibria with reasonably good accuracy. The description of kinetics, however, could be improved based on approaches developed for other metallurgical processes and by making use of information that can be extracted from more detailed phenomenon-based models or laboratory scale experiments. The same is true for more detailed descriptions of local phenomena such as the melting of scrap, the formation of hot spots, or the description of the electric arc that cannot be predicted using the current, simplified heat and mass transfer models. Furthermore, new measurement techniques can be incorporated as information sources for input and validation as they become available.

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Conflict of Interest

The authors declare no conflict of interest.

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