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Editorial

Special Issue on "Process Modeling in Pyrometallurgical Engineering"

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This Special Issue on "Process Modeling in Pyrometallurgical Engineering" consists of 39 articles, including two review papers, and covers a wide range of topics related to process development and analysis based on modeling in ironmaking, steelmaking, flash smelting, casting, rolling operations, etc. The approaches include small-scale experiments and experimental design, first-principles modeling, detailed modeling based on CFD or DEM, and statistical and machine-learning-based methods. In the following paragraphs the issue is briefly scanned, presenting the papers in the order roughly following the route from raw materials processing to rolling and heat treatment.

1. Coal

Lignite is a low-grade coal with the lowest carbon content. Liu et al. [1] studied the structural changes of Huolinhe lignite when it was modified by microwave and ultrasound treatment and reported the chemical composition of the products.

2. Sintering

Sintering is an important agglomeration process that is a prerequisite for downstream processing. Liu et al. [2] studied the combustion kinetics during sintering at a partial replacement of coke powder by anthracite and found improvements in the combustion rate. Two combustion models, the volumetric and random pore models, were compared and the latter was demonstrated to yield better agreement with the measurements.

Wang et al. [3] studied a partial replacement of coke with biomass in sintering. The results indicated a higher combustion rate using charcoal due to a higher surface area, in spite of a lower fixed carbon content. It may therefore be viable to partially replace coke by charcoal in the sintering process.

Cheng et al. [4] investigated the removal of arsenic from iron ore through roasting in air and nitrogen. They reported higher removal ratios using a reducing atmosphere.

3. Blast Furnace

The ironmaking blast furnace (BF) is an extremely complicated industrial unit process, and this is a reason why many computational approaches have been made to study its behavior or to predict its performance under new operation conditions.

An analysis of the process based on a state-of-the-art 3D static model is presented by Kou et al. [5], addressing the problem of estimating the extent of the solution loss, or Boudouard, reaction. The model is applied to shed light on how operation factors, such as blast oxygen enrichment and scrap charging, affect the solution-loss in the furnace. Another global study of the BF is provided by Ouyang et al. [6], with the goal of detecting abnormal events in the process. This entirely data-driven approach is based on a multidimensional Gated Recurrent Unit (GRU) neural network that, using its feedback nodes, can consider temporal evolutions of signals.

The charging of burden is treated in three papers. Wei et al. [7] studied the fundamental features of BF burden materials, including the angles of repose and bed porosity, by small-scale experiments in combination with computational analysis based on the Discrete Element Method (DEM). Mio et al. [8] used a unique 1:3 pilot model of the BF top to study the radial distribution of the rings of burden materials and used the results for validation of a DEM-based model of the system. Li et al. [9] outlined a model of the burden distribution in the BF by considering the falling trajectories, layer formation, and descent. Radar measurements of the burden profile provided supporting evidence.

The flow of molten iron and slag in the coke bed of the lower BF is very complex and traditional modeling techniques cannot describe the flow patterns. Natsui et al. [10] presented an interesting attempt based on smoothed particle hydrodynamics (SPH) simulation, demonstrating the role of wettability on the arising flow rivulets of iron and slag, shedding light on the complex liquid flow patterns. The role of the dead man, and how it influences the conditions in the lower part of the BF, is reviewed by Shao et al. [11], presenting approaches to model the dead-man state and the way in which it affects hearth performance, e.g., the flow paths of hot metal, lining wear, and liquid levels.

The combustion region, or raceway, formed in front of the tuyeres is studied in two papers. Peng et al. [12] developed a three-dimensional transient Eulerian multiphase flow model of the raceway to study how the raceway size, pressure distribution, and flow field are affected by the blast parameters. The use of natural gas as auxiliary reductant is studied by Okosun et al. [13] using a CFD model of the furnace from the raceway to the top. Special attention is focused on means to counteract the cooling of the raceway associated with high injection rates of natural gas.

The last stage of ironmaking in the BF is the tapping operation. The complex flow patterns in the main trough were studied by Ge at al. [14], using transient 3D CFD based on the volume of fluid (VOF) model. As for the outflows of iron and slag, Roche et al. [15] developed a strategy for compressing the information about the outflow rates from a large BF by principal component analysis.

4. Iron Smelting

Alternative ironmaking technologies have also been developed and some are analyzed in this Special Issue. Xie et al. [16] carried out water modeling experiments to study the mixing time in a smelter as a function of nozzle position, nozzle diameter, nozzle immersion depth, gas flow rate, and liquid properties. Applying dimensional analysis, the authors derive expressions for the mixing time and compare the results with practical findings.

Many studies of the burden distribution in the blast furnace have been undertaken, but much less work has been reported for the COREX process, which has a more complex charging system. Li et al. [17] reported results from mathematical modeling of burden distribution in the COREX melter–gasifier. Based on experimental results from a pilot rig, the model was found to accurately predict the DRI/coal ratio as a function of the radial position.

Sun et al. [18] described a mathematical model predicting the raceway geometry in the melter–gasifier as a function of time and gas velocity. By dynamic simulations, the authors concluded that the final shape is reached in a short time (<1 s). Increasing the velocity of the gas increases the depth of the raceway. For a normal blowing speed of 250 m/s and a tuyere angle of 4°, a raceway depth of 950 mm was predicted.

5. Copper Smelting

Smelters used for other metals, e.g., copper and nickel, are also complex processes, where mathematical modeling can provide valuable information used for enhancing the process or for improved control. Jylhä et al. [19] developed a CFD–DEM model to study the settling of copper particles in a flash smelter settler, applying a population balance model to describe the settling and coalescence of the droplets. The modeling confirmed that small particles (< 100 mm) remain in the slag, suggesting that an operation with a thinner slag layer would increase the yield of the process.

Wang et al. [20] found a higher elimination rate of arsenic in copper smelters by controlling the oxygen/sulfur potential, reporting a decrease in As from 0.07% to 0.02%.

Navarra et al. [21] discussed the application of sensors and process control systems for process automation of copper smelters, and stressed the potential of data-driven models and discrete-event simulation for smelter optimization.

6. BOF

The basic oxygen furnace that converts hot metal into liquid steel is also characterized by harsh conditions that justify model-based analysis. Jiang et al. [22] introduced a novel hybrid model integrating multiple linear regression (MLR) and Gaussian process regression (GPR) to predict the oxygen consumption for optimization of the energy requirement of the BOF. The model was validated with actual data collected from a steel factory in China.

Rahnama et al. [23] reported correlations between the operating parameters and rate of decarburization (dc/dt) in a pilot plant. A positive correlation was found between the decarburization rate and the oxygen flow as well as the temperature and CO_2 content in the waste gas, while a negative correlation was found with the lance height. A neural network was trained to predict the decarburization in a full-scale plant, yielding satisfactory performance.

Dering et al. [24] described a first principles-based dynamic model of the BOF. The model considers an energy balance, slag formation, as well as decarburization rate. The authors estimated a set of parameters to adapt the model to data reported in the literature and from a reference BOF, and the model was demonstrated to capture the dynamics of the process.

7. EAF

The high temperatures and complex melting phenomena in the electrical arc furnace are reasons why many model-based studies of the process have been undertaken. Carlsson et al. [25] determined the effect of scrap shape and density on the energy consumed to melt the scrap in the EAF by using a statistical model and process optimization algorithms validated through plant trials. The results provide significant evidence that a well-chosen scrap categorization is important to predict the electric energy demand.

A simulator of an EAF based on a dynamic model was developed by Hay et al. [26], to be used as an automatic control tool for assessment of multiple scenarios in the operation. The model can also be used for training furnace operators.

Chen et al. [27] developed a 3D mathematical model of the interaction of the supersonic coherent jet with the steel bath. The model predicts the decarburization kinetics, including the distribution of the in-bath components, flow patterns, and bath temperatures, and can be used to optimize the refining process.

8. Ladle Furnace

Ladle treatment is an important step for adjusting the final composition and temperature of the metal before it is cast. Two papers deal with the simultaneous optimization of mixing and slag open-eye area in ladle furnaces. Jardón-Pérez et al. [28] validated a CFD model against PIV measurements and applied the model to analyze the mixing time and open-eye area in gas-stirred ladles using two plugs with equal (50%/50%) or differentiated (75%/25%) flows. Yang et al. [29] applied a physical model to measure the mixing times and interface slag entrainment under different conditions, including the injection modes, gas flow rates, and top slag thicknesses. The authors suggested an optimum argon flow rate between 36 m^3/h and 42 m^3/h with two plugs.

Zhao et al. [30] reported fundamental research on a water–oil–air physical model to study the dynamics occurring when bubbles pass through the liquid–liquid interface for different oil viscosities at various gas flow rates. They found that bubble movement is greatly influenced by the viscosity of the oil and that the water-oil interface stability was enhanced with increased viscosity of the oil phase.

Lei et al. [31] computed, based on the Ion-Molecule Coexistence Theory, the titanium distribution ratio in ladle furnace slags ($CaO–SiO_2–Al_2O_3$– $MgO–FeO–MnO–TiO_2$) at 1853 K for tire cord steel production, and found a good agreement of the model with the measurements. The structural unit CaO was found to play a pivotal role in the slags.

Finally, Conejo [32] presented an extensive and exhaustive review of physical and mathematical models of mass transfer in gas-stirred ladles, stressing the effects of the process variables on the mass transfer coefficient. The review noted that currently there is a lack of means to simultaneously keeping both liquid phases (steel and slag) well mixed in the ladles.

9. Casting and Solidification

The solidification of a metal is a complex and gradual process that is difficult to control. Niaz et al. [33] reported numerical predictions of the Horizontal Single Belt Casting (HSBC) process, which avoids multiple hot-rolling steps by directly producing a thin sheet. Results from an experimental rig were compared with findings from a CFD model, and the latter was applied to study non-uniformity and other undesired conditions, as well as means to address these, e.g., by appropriate design of the metal feeding system.

Precipitation behavior of inclusions was studied by both Wang et al. [34] and Li et al. [35], the former for titanium nitride (TiN) during solidification and the latter for chromium spinels in stainless steel slags. A systematic study was made to clarify the mechanism of TiN precipitation to guide the development of ultra-high strength grade steels. The stability of chromium in stainless steel slag was found to have a positive correlation with spinel particle size and a negative correlation with the calcium content of the spinel. However, both groups of authors stress that further experimental work and theoretical analysis are needed to understand the precipitation behavior of the inclusions to improve the quality of the finished steel.

10. Rolling

Most steel products are manufactured by hot rolling, because it is one of the most efficient plastic-forming processes. On the basis of comparative studies on the temperature distribution during hot plate rolling and rod rolling, Hwang [36] concluded that the temperature distribution and variation of a rod during shape rolling are different from those of a plate during flat rolling. The higher variation in effective stress of the rod along the circumferential direction induces a higher temperature difference of the rod. The same author [37] also investigated the effect of roll design on the strain distribution of the flat surface, lateral spreading, and the strain inhomogeneity of a flat-rolled wire, proposing a new strategy for fabricating high-quality flat-rolled wires through a cambered roll of a small radius.

Hu et al. [38] developed an optimization model for hot rolling based on the time-of-use (TOU) electricity pricing using a genetic algorithm. Jumps between adjacent slabs in width, hardness, and thickness were avoided by including penalties in the objective function. The method was verified on batch results from the hot rolling of 240 slabs of different sizes and was demonstrated to reduce the cost of power required for rolling.

Chen et al. [39] found that the hot working ability of a nickel-based GH4698 alloy markedly decreased under lower temperatures and higher strain rates in isothermal compressions: this alloy is extremely sensitive to thermal processing parameters and cracking may easily occur. An Arrhenius model was used to estimate the flow stresses and profiles for processing under various thermal conditions.

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