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Editorial

Advancing Extractive Metallurgy: Computational Approaches for a Sustainable Future

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Extractive metallurgy, combined with mineral processing, is at the heart of modern industry, facilitating the transformation of raw mineral resources into valuable metals essential for infrastructure, technology, and energy systems. As global priorities shift toward decarbonization and the rapid expansion of renewable energy technologies, the field of extractive metallurgy has gained renewed prominence. This resurgence is driven by the urgent need for critical metals, such as lithium, cobalt, nickel, rare earth elements, and other metals [1–4], which are indispensable in the manufacturing of batteries, wind turbines, and electric vehicles [5,6]. This is in addition to a massive transition in the steel industry [7], modernizing and/or moving away from traditional blast furnace operations [8,9] and, eventually, toward hydrogen-driven reduction and DRI [10–13]. A key element in addressing the new engineering challenges posed by this demand is the integration of advanced computational approaches into extractive metallurgy, opening exciting new avenues for research and development.

Computational fluid dynamics (CFD) is one such powerful tool that can revolutionize how metallurgical processes are designed and optimized [13–16] at the level of individual unit operations, i.e., the individual furnaces. Traditionally, extractive metallurgy has relied on empirical data and physical experimentation to model fluid flow, heat transfer, and mass transport within reactors, furnaces, and smelters. Plant- and pilot-level studies are now extrapolated as the basis for CFD simulations. These simulations provide detailed insight into these phenomena by numerically solving the governing equations of fluid mechanics, thermodynamics, and chemical kinetics. In the context of metallurgical processes, the representation of multiphase simulations, which often intercouple physical phenomena remains a critical issue in the design of reactors [17], often considered multiphysics simulations [18,19]; for example, magnetohydrodynamics is the foundation for magnetic stirring, which controls impurities within molten charges [19]. Other critical issues include adapting dynamic meshing techniques to represent free surfaces of slags [20], which realistically have varying viscosity levels as well as inhomogeneous compositions and nonideal solution chemistry. By simulating complex metallurgical environments, researchers can predict how molten, gaseous, and solid charges will behave under varying conditions, allowing for more efficient process design, optimization of energy consumption, and minimization of emissions. For example, in steelmaking, CFD models can help to optimize the gas flow and slag behavior inside a metallurgical furnace, reducing gas emissions (e.g., carbon and sulphur dioxide) while improving metal yield. For researchers in chemical and metallurgical engineering, the ability to fine-tune processes through CFD simulations is not only intellectually rewarding, but also of immense societal value, contributing directly to global decarbonization efforts.

Beyond CFD, computational optimization techniques offer another exciting dimension for the advancement of extractive metallurgy. The complexity of metallurgical processes, which involve multiple variables such as temperature, pressure, reaction kinetics, and resource inputs, are at the level of individual unit operations, and thus beckon techniques that globally optimize the coordination of several operations, i.e., to integrate the unit

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operations [21]. Specially designed algorithms that combine mathematical programming and metaheuristics can explore vast parameter spaces and identify optimal operating conditions that balance efficiency, environmental impact, and cost [22,23]. Computational approaches have contributed significantly to geometallurgy [24,25], which is the linkage of geological compositions and attributes to metallurgical outcomes. Geometallurgically oriented computations are important in the representation of metallurgical processes within strategic mine planning [26–28], and also are vital at the operational timescale. Real-time adjustment of processes in response to fluctuating conditions maximizes the recovery of valuable metals while minimizing waste [29,30]. For instance, the optimization of hydrometallurgical processes for the extraction of metals from low-grade ores or electronic waste can dramatically enhance the sustainability and economic feasibility of recycling technologies, which are critical for the circular economy.

In addition, logistical simulations are becoming increasingly relevant as extractive metallurgical operations grow in complexity. Modern metallurgical facilities must operate within an interconnected supply chain [30], where the availability of raw materials, transportation costs, and market fluctuations can have a significant impact on production efficiency. Simulation models, such as discrete event simulations or agent-based models [29–32], enable metallurgical engineers to assess the performance of supply chains, evaluate the impact of operational disruptions, and devise strategies for enhancing the resilience of their operations. These tools may become valuable in the context of energy transition metals [5,6,32], where supply disruptions could have consequences on renewable energy deployment.

For process engineering researchers with chemical and metallurgical backgrounds, the integration of these computational approaches into extractive metallurgy represents a new frontier for innovation. Not only do computational methods enable more sustainable and efficient production processes, they also offer opportunities to explore complex systems in unprecedented detail, from geological and mineralogical attributes to global supply networks. The combination of traditional metallurgical knowledge with cutting-edge computational techniques is poised to transform the field, and researchers with expertise in computational modeling and optimization are well-positioned to lead this transformation. As the world faces increasing demand for critical metals and stringent requirements for environmental stewardship, the contributions of researchers in extractive metallurgy will be crucial to ensuring a sustainable future.

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