Improving Cell Performance with Artificial Intelligence Multi-Objective Optimisation of Bath Composition

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Abstract

Highly demanding environment of the aluminium production often requires the optimisation of chemical processes for sustainable operations. Multiple, often conflicting objectives arise when striving to find the suitable electrolyte composition to enhance cell performance. The influence of CaF_2, AlF_3, or CaF_2 + AlF_3 on cell performance has been studied in both, laboratory and field settings. Many smelters, regardless of the lining design and context of aluminium processing variables, adhere to heuristics rules and use similar chemical compositions and limits for CaF_2, AlF_3, or (CaF_2 + AlF_3) concentrations. Heuristic-based decisions in complex systems or technical uncertainty may not capture the entire scope, as there is no one-size-fits-all solution for all designs and contexts. These decisions, influenced by representativeness and anchoring heuristics, may disregard significant interactions and result in either overestimating or underestimating the interaction effects. Despite plentiful studies, there is no expert consensus on the best method for determining the ideal electrolyte composition for maximizing smelter performance. By leveraging artificial intelligence (AI) and thermoelectric equilibria, this research paper proposes an approach to determine the best electrolyte compositions for enhanced voltage stability, current efficiency, and minimal cell-life decline. The AI uses desirability functions to recommend design-specific optimum values (minimum and maximum) for CaF_2, AlF_3, or (CaF_2 + AlF_3) concentrations, based on characteristics and operating conditions such as dissipative/non-dissipative design, seasonality, alumina attrition index, etc. By incorporating precise quantities of calcite in the Bayer process, refineries can alter (CaO/Na_2O) ratios to fulfill smelter process demands, achieve maximum economic benefits, and minimize ecological consequences.

Keywords: Aluminium electrolysis, Electrolyte efficiency, Cell performance, Aluminium and calcium fluoride concentrations, Artificial Intelligence.

1. Introduction

Electrolyte process for metallic aluminium production still suffering from a high energy loss. A huge part of the energy inefficiency is mainly dependent on the melt composition [12]. One of the current trends in technological research is to try to substitute CaF_2 content by AlF_3 to further lower operating temperatures. The benefits commonly evoked are multiple: increasing cell productivity, reducing energy consumption and the global environmental footprint.

Knowledge of the physicochemical properties of cryolite-based melt is thus essential for technological progress and smelter performance. The published literature on the role of the electrolyte composition in the operating cells has primarily focused on specific elements, such as AlF_3, CaF_2, LiF and their impacts on the operating temperature and current efficiency, which are only some metrics of good performance.

A more recent and holistic vision of profitable and sustainable smelters is now considering performance beyond the sole operating temperature and current efficiency (CE) outputs. For instance, attention is given to such metrics as energy consumption, electrolyte conductivity, crystallization, and deposition; voltage stability, heat balance, and risk to lining failure.

Finding the optimal electrolyte composition pattern has then become crucial for smelters to increase cell productivity, particularly when operating at low anode cathode distance (ACD). The composition of the electrolyte in modern smelters includes cryolite, calcium fluoride, aluminium fluoride, and aluminium oxide. At times, other chemical elements have been used including LiF and MgF_2 to enhance electrolyte performance. Research shows that additives to produce these products are no longer in use at most smelting locations [5], therefore, this study sets their concentration to zero in the model that has been developed to predict the optimal electrolyte composition in each smelter. Yet, the program provides options to use any combination of concentrations including LiF, MgF_2.

Alumina is the primary impurity source for the electrolyte bath. Large quantities of calcium carbonate (calcite) are needed in multiple process reactions to produce alumina from bauxite through the Bayer process [2]. The CaF_2 in the bath is heavily dependent on the quantity of calcite added during the Bayer process.

Extensive research has been conducted in various brownfield-smelters and laboratories to calculate these electrolyte properties and guide the smelters on optimal choices. However, most of this research uses a linear approach to determine the impacts of CaF_2, AlF_3, or (CaF_2+AlF_3). Applying linear methods to complex systems with unpredictable cause-and-effect relationships may introduce biases and lead to flawed decisions in optimizing pot performance.

By following a 1/1 substitutional rule, these investigations propose that electrolyte with higher AlF_3 can replace electrolyte with lower CaF_2, allowing smelters to achieve their maximum productivity. Unlike in an ideal world, complex processes in real life often involve interactions rather than linearity.

The typical operational risks evoked when increasing AlF_3/CaF_2 ratio cover alumina dissolution, sludge formation, voltage stability, pot life, and high-energy consumption. What then are the optimal substitutional ratios? The transferability ratio of AlF_3 from CaF_2 is an important productivity factor.

In the remaining part of this study, we will first give an overview of the problem statement and the current technical challenges. Next, the paper outlines the study's purpose, objectives, and business implications. Furthermore, the paper offers a concise literature review of the subject and builds upon the initial reflection on challenges, biases, and lessons learned. Third, the paper discusses in depth the theories that analyse the impact of CaF_2 and AlF_3 on the physicochemical properties of the electrolyte melt. The key principles involve analysing electronegativity using the Pauling scale and the Van Arkel-Ketelaar Triangle of bonding and examining the effect of atomic and ionic size on the mobility and conductivity of charges. We then explain our approach to solving this multi-objective optimization problem using artificial neural networks.

2. The Problem Statement

Refineries are working towards significant cost savings and calcination improvement by decreasing the amount of calcite present in the Bayer process, resulting in lower CaO/Na_2O ratios and correspondingly, lower CaF_2 in the bath. High concentrations of impurities in the solution can considerably cause problems in the alumina production cycle [22]. A decrease in CaO/Na_2O ratios in alumina has implications for the electrolyte's properties. Some implications include high-

12. Conclusions

The temperature dependence is typically observed in the conductivity of molten electrolytes and dissolution of materials. CaF_2 and AlF_3 exhibit different conductivity and dissolution effects at various temperatures, as most physicochemical properties, and thermodynamic functions of the two additives were distinct. Scalable percentages of CaF_2 and AlF_3 revealed conflicting levels of desirability. Research shows that increasing bath acidity (AlF_3) can lead to greater solubility of Al_4C_3 and mass transfer coefficient, ultimately leading to increased carbon loss and higher rates of cathode erosion.

Smelters must be mindful of the opportunity cost and downsides involved in every operational decision. The trade-offs are context specific and will be determined by the risk to the lining failure, cost, and efficiency output. Use of these additives cannot be accomplished interchangeably in a symmetric pattern. AI allowed to depict optimal settings in terms of both temperature control, process efficiency, energy consumption, and pot life. Different economic and process factors would affect the decision on the levels of the two additives; we provide a few of them hereafter.

a) Both the lining and cell design play a role in the alumina dissolution process and heat-transfer. The constraints consist of the cathodic heat-dispersal pattern, superheat condition, and decreased free energy near the cathodic surface,
b) The kA/feeder ratio (requires more feeders to minimize material agglomeration issues).
c) The opportunity for the refinery to save cost by improving processes while reducing calcite concentrations, good alignment with (a)+(b) would be beneficial.
d) Minimize aluminium reoxidation in the cell.
e) Trade-off between high efficiency and reduced pot life and
f) The operations at low or high ACD.

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