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-electrolyte temperatures, change in viscosity, alumina solubility, electrical conductivity, and aluminium solubility.

Higher aluminium fluoride percentages have been proposed to substitute lower calcium fluoride contents to unlock full potential by lowering the electrolyte temperature, which enhances CE. However, can these two chemical additives, AlF_3 and CaF_2 be used interchangeably to control the electrolyte's physicochemical properties?

Use of higher AlF_3 concentrations can reduce the melting point and operating temperatures of the electrolyte. By using the latter approach, cell productivity can be improved [13, 14]. Yet, use of high concentrations of AlF_3 has been found to have detrimental effects on cathode life via the solubility of aluminium carbide in cryolite melts [6, 28, 29]. High-AlF_3 concentrations have also been described to have deleterious effects on electrolyte resistivity [11]. Some other adverse effects include cell instability during low ACD operations, the crystallization of the electrolyte, sludge deposition, and lower anode cathode distance, particularly for dissipative technologies. A dissipative system can exchange energy and matter spontaneously [15].

Based on these potential positive and adverse effects, it can be suggested that the AlF_3's properties act either in superposition with CaF_2, in opposition, or perhaps they interact with each other and with dissipative/non-dissipative systems. Currently, each smelter defines AlF_3 targets based on experience and heuristics, but heuristics are often non-logical mechanisms, they may lead to substandard solutions from normative principles. This research addresses this methodological gap.

3. The Purpose Statement

The study objectives are to answer the following questions:

Can a smelter exchange 1 % CaF_2 by 1 % AlF_3 to take advantage of higher productivity? What are the likely hidden or adverse effects of increasing AlF_3 concentration beyond a technology`s acceptable limit? Are these limits similar regardless of the dissipative/non-dissipative technologies? Can the AI enable a comprehensive depiction of the picture?

4. Literature Review

Electrolyte composition has impacts on the productivity of aluminium smelters and environmental performance. The published literature on the role of the electrolyte composition in the operating cells has primarily focused on a few specific elements, including AlF_3, CaF_2, MgF_2, LiF and NaCl, and their impact on the operating temperature and current efficiency [8, 9]. A more recent vision of profitable and sustainable smelter looks beyond the sole operating temperature and current efficiency; attention is given to all metrics such as cell stability, risk of lining failure, and specific energy consumption.

Antecedent research has proposed the electrolyte composition such as higher targets AlF_3 up to 13 % to lower its melting point and operating temperature, which improves plant current efficiency [1]. Higher aluminium fluoride percentages have also been proposed to substitute lower calcium fluoride contents to unlock the full potential of lowering the electrolyte temperature. However, depending on the composition of the electrolyte and its superheat, the set of parameters such as seasonality, the metal height, and the cathodic critical temperature can change the cell performance. Optimal electrolyte composition can not be investigated without integrating structural conditions (e.g., cathode design, the risk of crystallization, and dissipative conditions).

Both the cathode design and the heat dissipation pattern can influence material crystallization and deposition on the cathode surface [7]. A lower cathodic-surface temperature versus the electrolyte superheat can provoke spontaneous reactions at its boundary (e.g., entropy change; decrease in the system's free energy), increased precipitation of the cryolite and deposition on the cathode (see also the second law of thermodynamics) and Prigogine's Time, Structure and Fluctuations [24]. Entropy-change measures the dispersal of energy at a specific temperature and creates anisotropic pattern for the material deposit (see Figure 1).

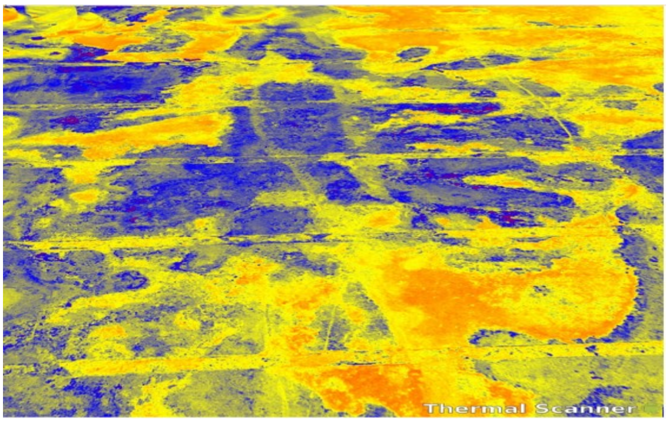


Figure 1. Anisotropic behaviour.

The magnitude of this anisotropic deposition is a function of the electrolyte composition, higher cathodic dissipative conditions, energy dispersal, lower superheat, and lower bath volume. For example, research shows that the addition of 1 % CaF_2 above the optimal concentration increases the cryolite viscosity by 3 %, which impacts the alumina solubility and material deposition on the cathode [8].

Lindsay and Welch [5] have investigated the kinetics and mechanism of the aluminium electrode reaction in cryolite melts with various alumina contents. Tkacheva et *al.* [9] conducted a similar investigation to find the dependence on alumina and calcium fluoride concentrations. These studies show that the upper concentration limit exists to avoid escalating the specific gravity of the electrolyte beyond an acceptable limit. The following questions may be asked: *What is the acceptable limit? Is the limit context-specific, or common for all cell technologies (dissipative and non-dissipative)? How do smelters ascertain these limits? What are potential interactions with other critical factors such as seasonality? What is the advised approach?*

Tkacheva et *al.* [3] investigated the CaF_2 effect on the liquidus temperature, electrical conductivity and alumina solubility in the potassium-sodium and potassium-lithium cryolite melts with cryolite ratio $(CR = (nKF+nMF)/nAlF_3$, M = Li, Na). The research found that the electrical conductivity in the KF-NaF-AlF_3-CaF_2 melt diminishes with building up the CaF_2 content [3]. In addition, the authors identified that the Al_2O_3 solubility in the KF-NaF-AlF_3 electrolyte improves with the rising KF content, but the opposite tendency is noted in the cryolite mixtures containing CaF_2 [3]. Noteworthy, the questions asked above can be reiterated in this section.

Kisza, Kazmierczak, Thonstad, and Hiveš [4] investigated the kinetics and mechanism of the aluminium electrode reaction in two cryolite-based melts containing cryolite with either 11 % AlF_3 or 5 % CaF_2 and varying alumina contents at 1000 °C. Results show that the exchange current density of the cathodic reaction was conditional on the AlF_3 [4]. *Can a smelter increase this concentration indefinitely? Can a smelter replace* CaF_2 *by* AlF_3 *at a 1/1 ratio?*

5. Theoretical Framework

5.1 Comparing CaF_2 and AlF_3 Impacts on Electrolyte Melt's Physicochemical Properties

Calcium fluoride and aluminum fluoride are both ionic compounds that are used as additives in molten electrolytes. These compounds can influence both the activity, the conductivity, and the capacity of the electrolyte to dissolve alumina and metallic aluminium; but their impacts differ based on several factors; here are a few:

5.2 Electronegativity: Theory and Application

Electronegativity serves as a useful indicator of a chemical element's bonding capability in chemical reactions. The electronegativity values are determined using the Pauling scale, with fluorine having the highest value of 3.98. Here are the electronegativity values for calcium (Ca), fluorine (F), and aluminum (Al):

Figure 2. Electronegativity of the elements [19].

Implications:

5.2.1 CaF_2 (Calcium Fluoride)

In the Mendeleev-Periodic Table, calcium, an alkaline earth metal in Group 2, combines with fluorine to produce calcium fluoride. The difference in electronegativity between fluorine and calcium $\Delta\chi = |3.98-1| = 2.98$ and the weighted average electronegativity $\sum\chi = \left(\frac{1+3.98\times2}{3}\right) = 2.99$. Based on the Van Arkel-Ketelaar triangle of bonding (see Figure 3), this molecular leads to a near-ionic bond with a high ionic character of (>90.8 %). In an ionic bonding, charged ions are held together by electrostatic forces; these forces need huge amount of energy to break the bond. The literature shows that negative Gibbs free energy is generated when CaO converts to CaF_2 (via a reaction with AlF_3) in the electrolyte melt [5].

5.2.2 AlF_3 (Aluminium Fluoride)

The electronegativity difference between aluminum and fluorine in aluminum fluoride is also significant, though lower than in CaF_2, leading to $\Delta\chi = |3.98-1.61| = 2.37$, and average electronegativity $\sum\chi = \left(\frac{1.61+3.98\times3}{4}\right) = 3.39$ resulting in a polar covalent bond with an ionic character (>72.2 %). The relative position of these additives in the Van Arkel-Ketelaar Triangle of Bonding is given in Figure 3.

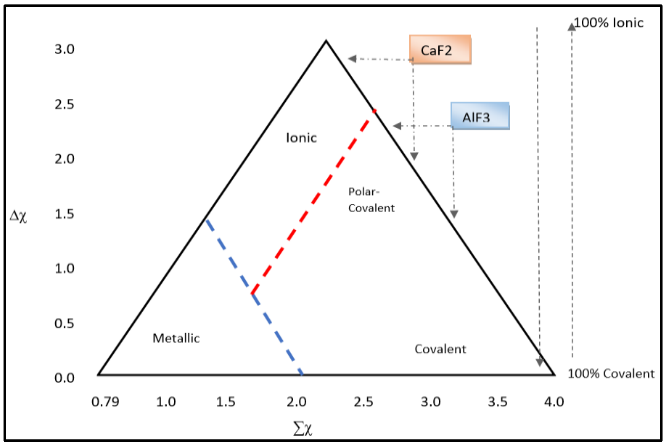


Figure 3. Van Arkel-Ketelaar Triangle of bonding type: CaF_2 vs. AlF_3.

In summary, while both CaF_2 and AlF_3 involve polar covalent bonds due to high electronegativity differences between elements, the specific electronegativity values contribute to variations in the degree of ionic character in these compounds; higher in CaF_2 than AlF_3.

5.3 Electrolyte Conductivity and Other Physical Properties

The introduction of either chemical component into the cryolite electrolyte results in reduced electrical conductivity, with differing magnitudes. The building-up of CaF_2 lowers the electrical conductivity and alumina solubility but also affects the vapour pressure, the viscosity and specific gravity of the molten electrolyte [3]. Crust softness is positively correlated with higher CaF_2 contents [17]. On the flip side, an excessive concentration of AlF_3 results in the formation of complex chemical structures with other ions, causing agglomeration in the electrolyte and reducing the efficiency of ionic transport [16].

5.4 Atomic/Ionic Size

The approximate ratio of the ionic radii of Ca^{2+} to Al^{3+} is about 1.67 (see Figure 4). Ionic radii represent the sizes of ions in a crystal lattice. It is agreed that the size of a metal atom plays a role in determining the efficiency of metallic bonding, structural packing, and electron density. These properties affect the electrical conductivity and ions mobility.

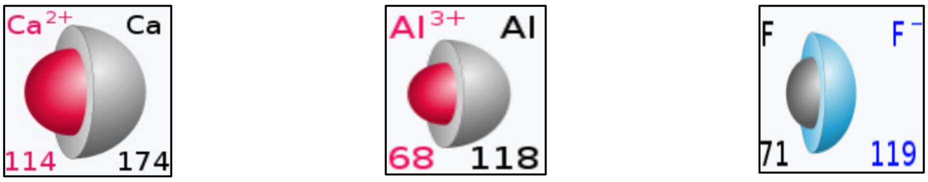


Figure 4. Relative radii of atoms and ions [18].

5.5 Aluminium Solubility

All metals are proven to be soluble in their molten salts. In particular, the electrolyte that contains aluminium cations dissolves aluminium. A factor that can reduce current efficiency is a specific situation of back reaction. Both CaF_2 and AlF_3 have been proven to reduce back reaction [1]. Increasing content of CaF_2 has been proven to have a positive effect on current efficiency according to some tests conducted in the laboratory [21].

5.6 Alumina Solubility

Both CaF_2 and AlF_3 have been proven to have negative effects on alumina dissolution with different magnitudes. For example, studies suggest that when AlF_3 is overly concentrated, it forms intricate chemical structures with other ions, leading to diminishing the efficiency of ionic transport [16].

Research by Skybakmoen *et al*. [26], corroborated by Peng *et al.* [27] showed that the saturated solubility of alumina in the electrolyte depends on the amperage-to-feeder ratio. Higher ratios lead to increased local agglomeration. Agglomeration is one of the most important contributors to slow dissolution [24, 25].

5.7 Cathodic Wear Rates Depending on Electrolyte Compositions

Based on Odegard's research [28] and Wang *et al.*'s study [29], changes in bath composition affect the solubility of Al_2O_3, as well as the viscosity and density of the bath, resulting in different Al_4C_3 solubility and mass transfer factors. Although higher bath acidity has benefits for enhancing the CE, it also has downsides, like increased Al_4C_3 solubility and cathode wear rates [29].

5.8 Heat Capacity and Thermodynamic Functions

Figure 5 summarises the heat capacity, standard enthalpy, and entropy of reaction for each substance, provided by the Shomate equation [20]. Interpreting the main thermodynamic functions shows a statistically significant disparity between the two primary electrolyte additives.

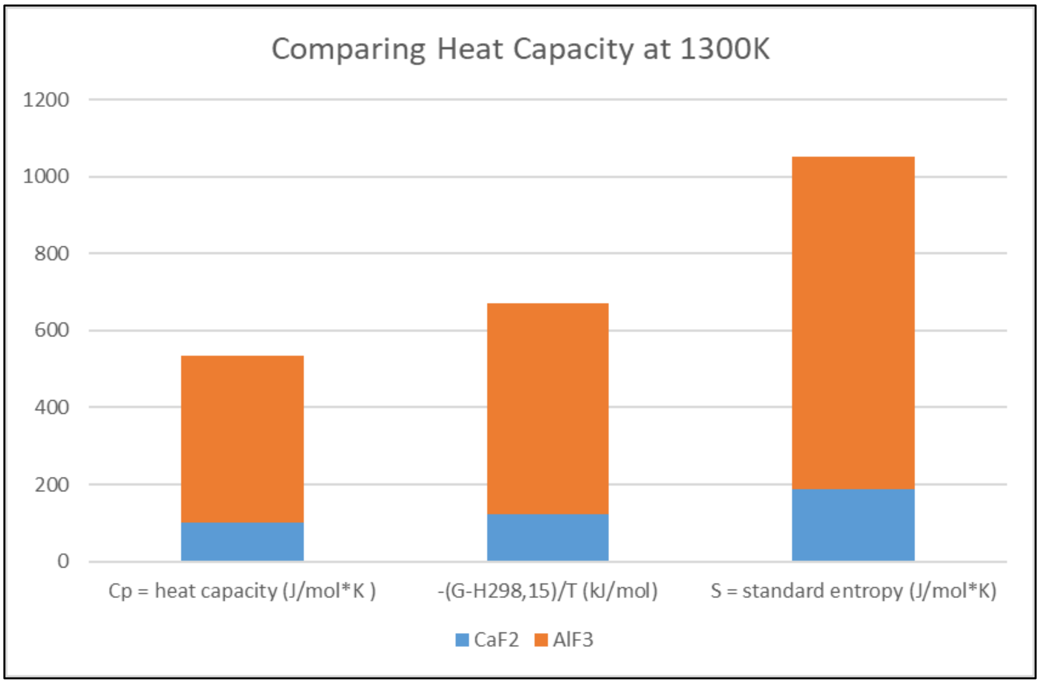


Figure 5. Comparing critical thermodynamic functions; Reproduced from the NIST Webbook.

6. Theoretical Summary

The temperature dependence is typically observed in the conductivity of molten electrolytes. CaF_2 and AlF_3 exhibit different conductivity impacts at various temperatures. The dopant element's electronegativity also plays a role in influencing this conductivity and activity. The increase in ionic radius and decrease in electronegativity typically result in higher conductivity, such as in high basicity compared to high acidity. Most physicochemical properties and thermodynamic functions of these two chemical substances are distinct.

7. Our Approach

7.1 Artificial Neural Networks (ANNWs)

One of the primary applications of AI in chemical engineering is process optimization. Chemical processes can be complex, requiring constant adjustments of multiple variables for optimal efficiency. Various parameters, including concentration of additives and cell resistance, can be adjusted using AI algorithms in a multi-objective optimization problem.

Can AI-driven solutions effectively determine minima and maxima, apply the substitutional rule, and suggest actions that lead to the best trade-off? Optimal solutions suggest reducing reoxidation of metallic aluminium, minimizing annual production loss, selecting the best option to decrease pot life loss, mitigating voltage instability, and minimizing emissions.

Multiple simulations were performed on (CaF_2, AlF_3) and the critical KPIs were analyzed for sensitivity. There are often competing criteria for optimizing several responses. The desirability for all responses was computed as the geometric mean of the desirability functions for the individual responses.

Denote the individual desirability functions of equal weight for n responses Y_i by $d_1(y_1)$, $d_2(y_2)$, ..., $d_n(y_n)$, then the overall desirability function is

$$D = d_1^{\frac{1}{n}}.d_2^{\frac{1}{n}} \dots d_n^{\frac{1}{n}} \tag{1}$$

Should the importance of individual desirability differ, then the overall desirability is computed as a weighted geometric mean of the individual desirability functions with the weights(wi)

$$D = d_1^{w1}.d_2^{w2} \dots d_n^{wn} \tag{2}$$

The desirability functions d_i assign numbers between 0 to 100 % to the possible values of Yi, with $d_i = 0$ representing undesirable performance of Yi and $di = 100$ % representing an ideal response [23]. Here is an example (shown in Figure 6) of competing desirability where higher AlF_3 improves current efficiency (CE) but deteriorates pot noise, leading to higher energy use, an increase in superheat that deteriorates ledge and pot life.

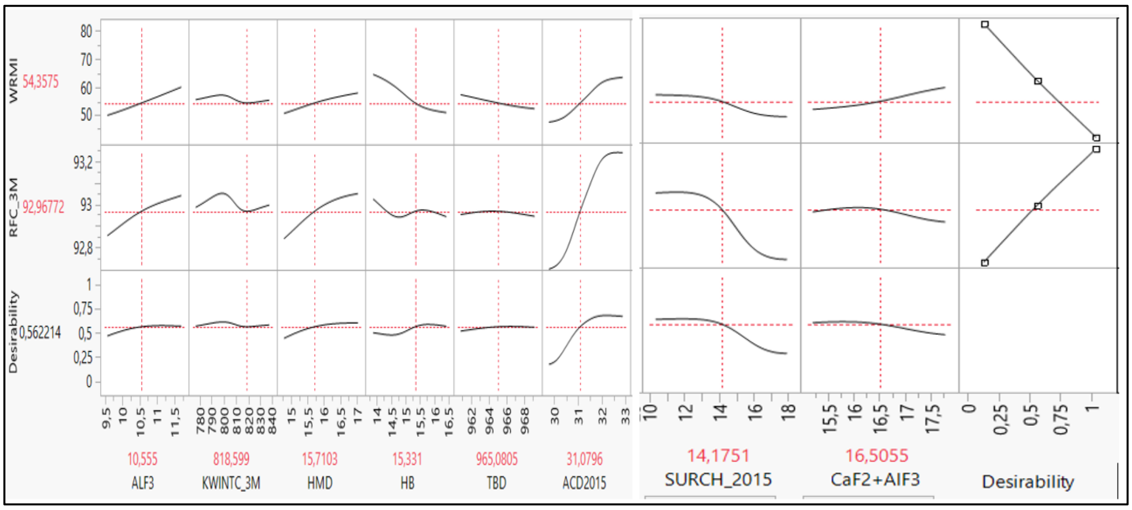


Figure 6. Competing desirability and decision trade-offs.

7.2 Study Design

The ANNWs use the hyperbolic tangent in the hidden nodes to transform weighted inputs from the first layer and calculate outputs based on a sigmoid-nonlinear mapping.

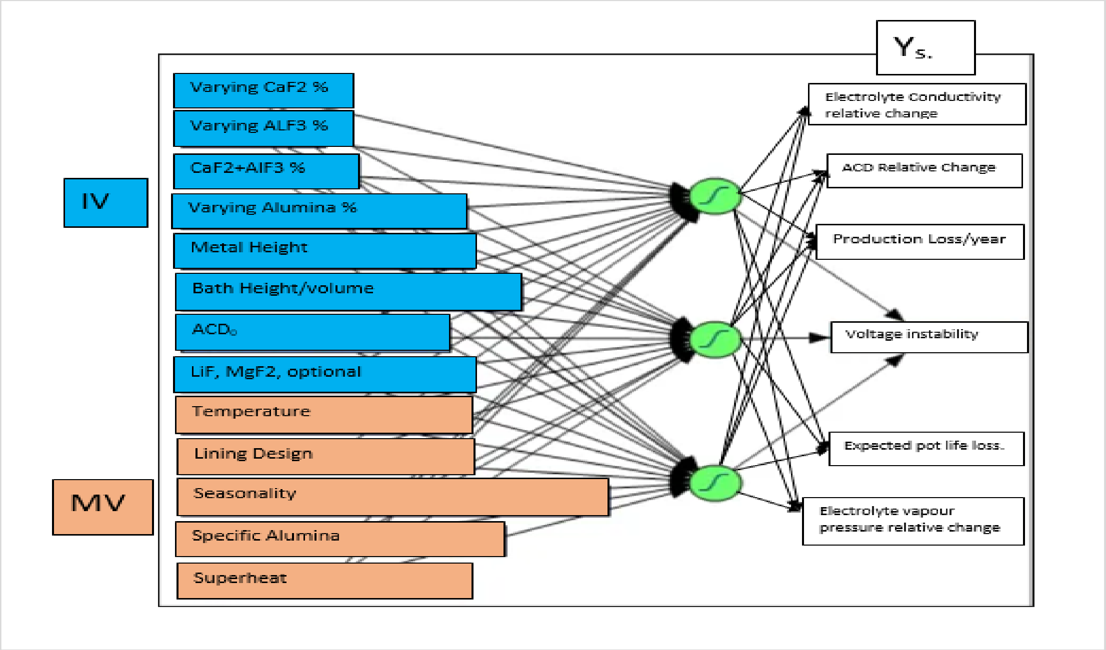


Figure 7. The Neural networks design.

In a geographic region like Canada, ***seasonality*** matters, as it has a significant impact on heat dissipation.

A dissipative design differs from a non-dissipative. A dissipative system (DS) can exchange energy and/or matter spontaneously with the outer environment [15].

8. Results and Interpretations

8.1 Cases Description and the Unit of Analysis

In most Rio Tinto smelters in Canada, the CaO/Na_2O ratio decreased from 10-12 % to 3-6 % between 2019 and 2023 given the change in alumina sourcing and reduced calcite additions in the Bayer process.

During this period, the CaF_2 reduced from 6.4 to 3.8 % and 5.3 % in Case1 and Case 2 respectively. In Case 1, there were two smelters employing a similar pot lining technology, except that the smelters had different alumina handling systems. The handling-methodology difference provoked differing attrition index, cathodic lining drop, and cell instability. Therefore, the alumina attrition was considered as a moderating variable in this study.

8.2 Use of ANNWs

AI was used in an investigation to determine the best operating point by varying (CaF_2, AlF_3) concentrations. The data depth spanned 2 years, capturing all pot line thermoelectrical variations. Earlier investigations of this topic analyzed the electrolyte set point using either heuristics or linear methodology to set the limit threshold of $AlF_3+CaF_2 \leq 17$ % [5]. It was a surprising finding that the twin-lining technologies showed varying electrolyte compositional patterns, with a difference of up to 0.7 % AlF_3. The only difference that was obvious and acknowledged was the alumina attrition index. One important lesson to learn is to never compare the performance of two pot lines without integrating their context, even if they are using a similar technology.

Analyses also suggest that higher CaF_2 combined with high AlF_3 content was detrimental to low-frequency noise (refer to Figures 8 and 9). The second important lesson is that CaF_2 concentration is correlated with a U-shaped pattern of voltage instability and productivity loss (see Figure 10). This study is breaking new ground by establishing this nonlinear relationship, to the best of our knowledge.

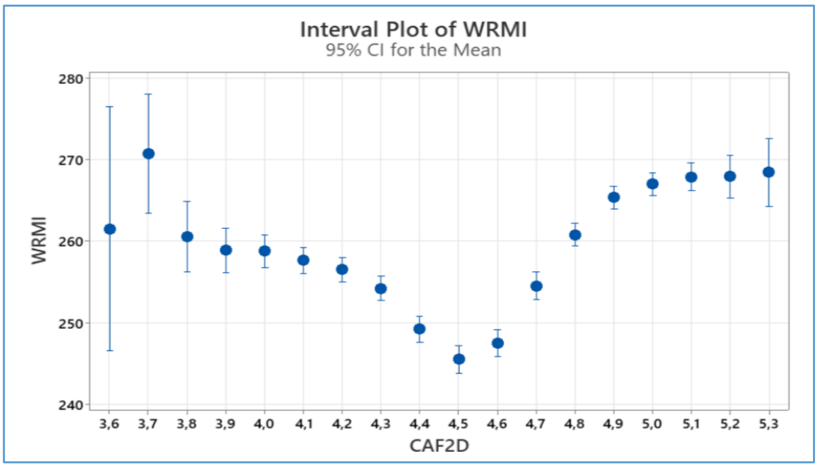


Figure 8. Low-frequency noise and CaF_2 relationship.

Lesson number three: To prevent increased losses, it is important that the total of the two additives is above 13.5 % but not exceed 16.5 %. The limitation at 16.5 % is potentially constrained to the KA-to-the number of feeder ratio. Consensus is that high concentrations develop sludge, influence the cathodic lining drop and wear pattern. On the flip side, higher temperatures can occur with lower concentrations and lead to the reoxidation of metallic aluminum. The model exhibited strong correlation and consistency between the training and validation (R-*Square 0.71, MAD 4.25).*

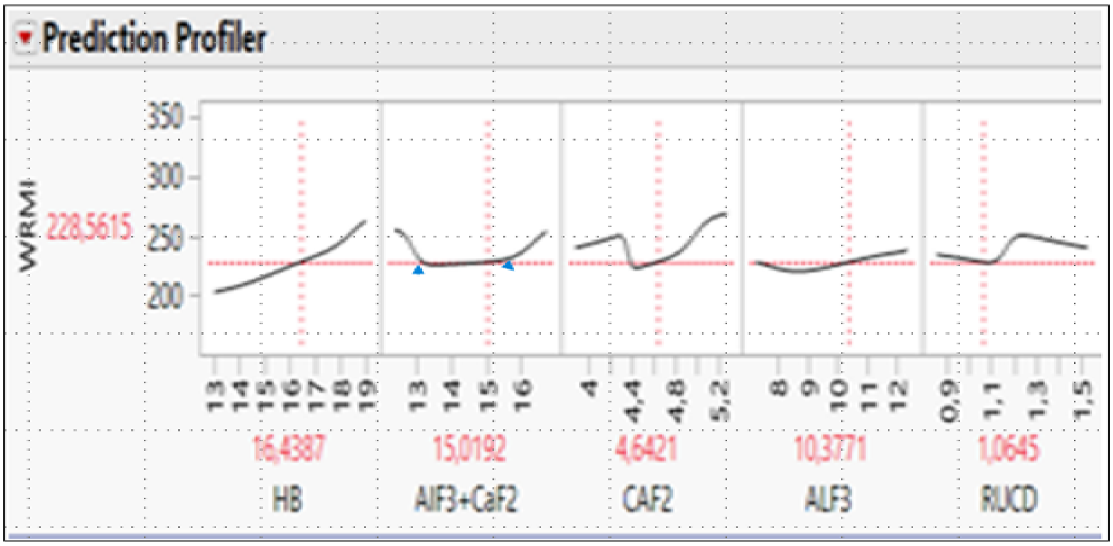


Figure 9. Finding the optimal CaF_2, AlF_3, and (CaF_2+AlF_3).

9. Business Case Study 1

While CaF_2 content dropped by over 1 %, a decision was made to compensate the drop by (+1 % AlF_3), but pot instability increased forcefully by over 7-10 %. High instability may develop from higher-electrolyte resistivity by AlF_3 (e.g., reduced ACD) and sludge formation because of poor dissolution (refer to Figures 10, 11, and the Theoretical Framework section). The Skybakmoen's theory of KA/Nb of feeder ratio [26] suggests that the alumina solubility saturation will worsen if additional AlF_3 dumps are added at the same location with constant bath volume.

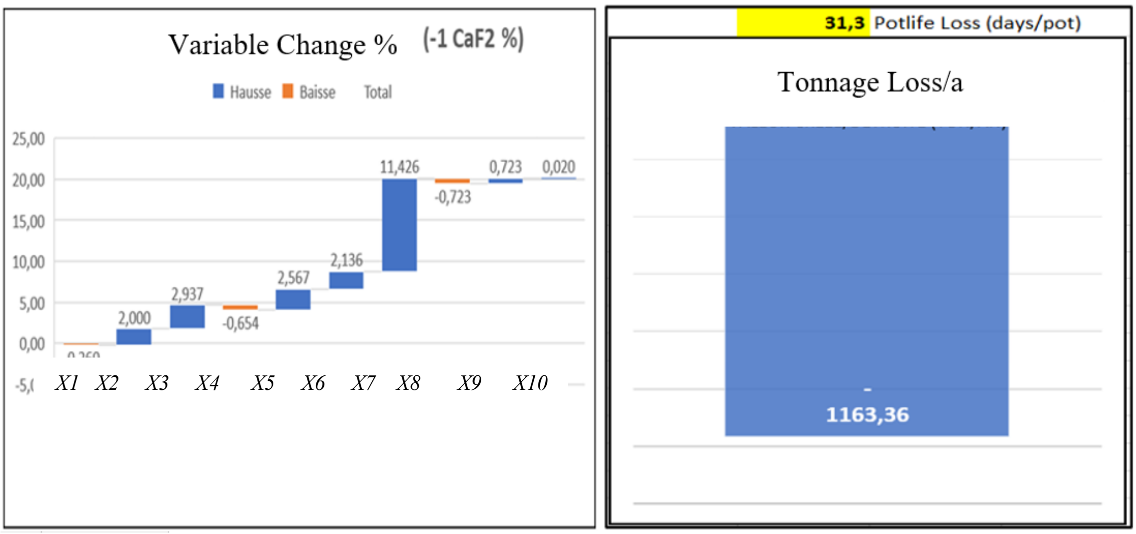


Figure 10. (a) Downsides and advantages of low CaF_2 in electrolyte: (b) Note. These results are contextual.

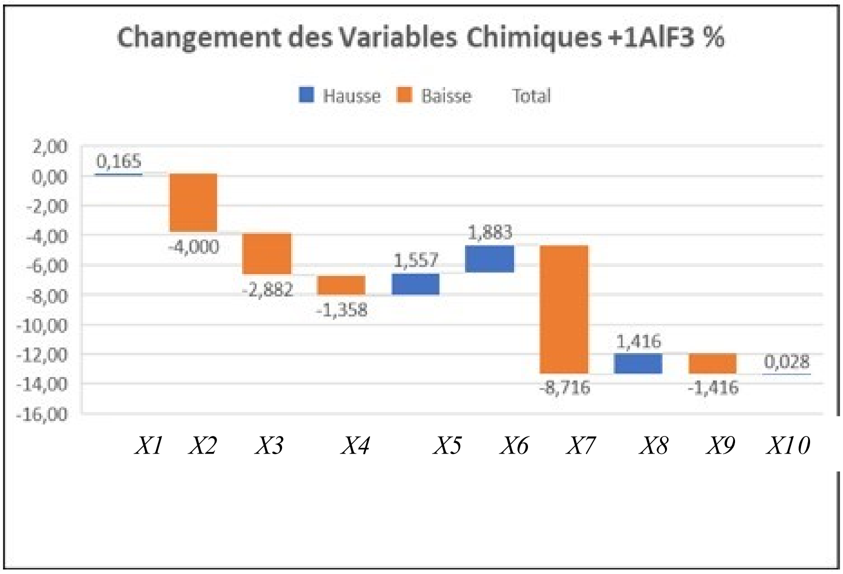


Figure 11. Downsides and advantages of additional 1 AlF_3 in electrolyte: Note. These results are contextual.

The AI recommends increasing 0.5 % instead of 1 % AlF_3 to substitute a reduction of (-1 % CaF_2). This finding agrees with the thermodynamic functions derived from the Shomate equations by Chase in the NIST Web book [20].

AI also identifies a poor performing setting when running below 4 % CaF_2. In some simulations, results show, operating at 3 to 4 % CaF_2, smelters may lose over 800 to 1200 t Al/a, and up to 37 days pot life; an EBITDA of USD 3.5-5 million each year was estimated. A business case was launched, and the decision was made to start adding fluorspar to uplift the CaF_2 in both the electrolyte (see Figures 13 a) and the anode cover material.

The target was 4.5-5 % and an additional 0.5-0.6 % AlF_3 percentage was planned. A test was initially done in a group of cells to establish the change in CaF_2. Figure 12 shows the CaF2 trend after the addition of 22 kg of fluorspar.

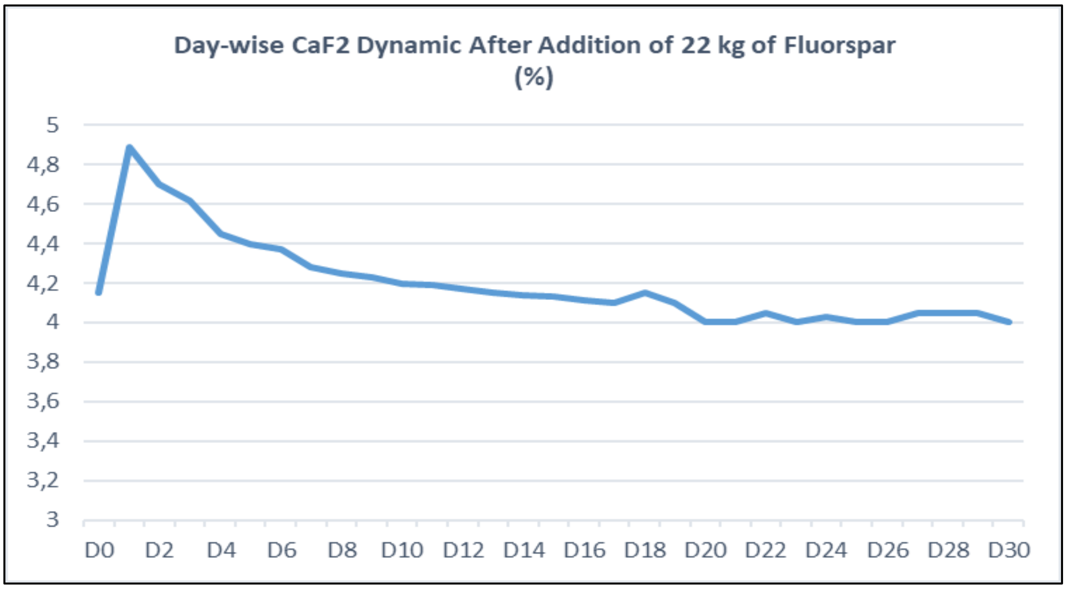


Figure 12. CaF_2 dynamic in the electrolyte after additions of 22 kg fluorspar.

Four factors contributed to dropping this trend including (a) the dilution, (b) anode changing and covering, (c) electrolyte transfer from cell-to-cell, and (d) continuous feeding of alumina at low CaO/Na_2O ratio (3%).
The fourth lesson learned: AI showed that, not only independent and moderating factors had main effects on the cell instability, but these factors interacted strongly among each other to amplify instability. The main and interaction effects of factors in cell instability are shown in Figure 13. This part of the reality was overlooked in the previous investigations.

10. Case 2: Description

Two lining designs, D1 and D2 were analyzed in this context. Based on the energy and matter exchange patterns, we characterize them as dissipative for the former and non-dissipative for the latter. The alumina employed and CaF_2 content were identical in both designs. The erosion of CaF_2 was linked to the decrease in the CaO/Na_2O ratio caused by reduced calcite additions during alumina calcination. The assumption was that the substitution of (-1 % CaF_2) with (+1 % AlF_3) would lead to improved electrolyte performance, considering the previous heuristic assumptions.

10.1 Methods.

The literature is abundant in modeling electrolyte electrical and chemical properties; we have made the choice to use the Solheim's [6] electrolyte liquidus equation, Ødegård's [29] solubility and electrochemical behaviour of aluminium and aluminium carbide formation, Wang et al.'s cathodic erosion model [30], Solheim, Sterten, and Skybakmoen's [28] alumina solubility model, electrolyte density model by Haupin [31], aluminium density by Handbook [33], Wang [30] for bath resistivity, and vapour pressure by Haupin and Kvande [32].

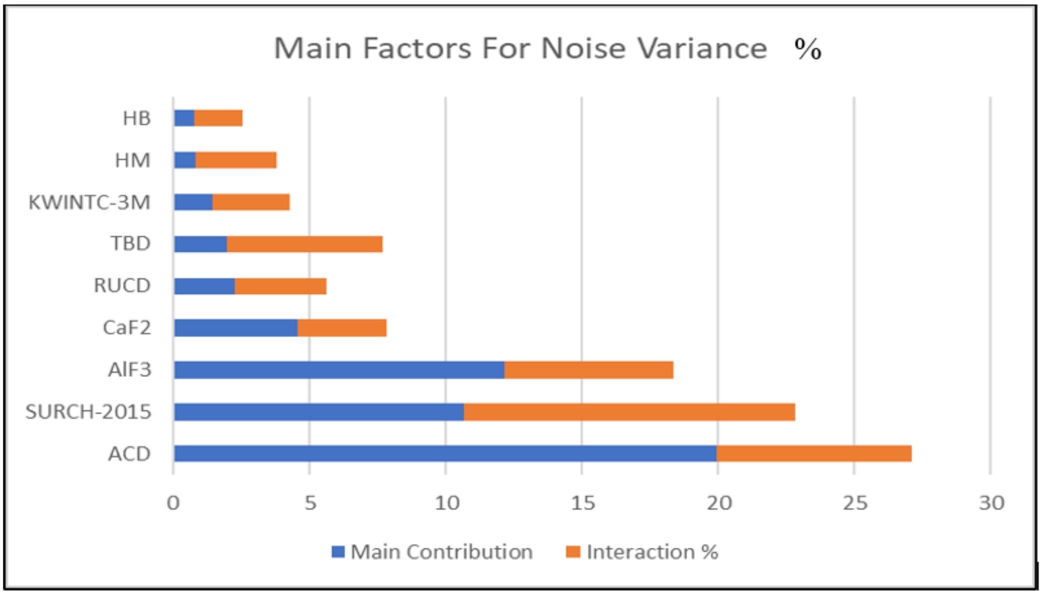


Figure 13. Main and interaction effects of factors in cell instability.

10.2 Optimal Chemical Settings for Productivity Improvement

The ANNW model was applied to operating variables for optimization. Figures 14 and 15 illustrates the range of critical parameters that allow meeting the goal. *Please read Figure 15 in a reverse order.*

The results prove that the dissipative design needed lower levels of AlF_3+CaF_2 to maintain acceptable pot line stability, in contrast to the least-dissipative design; the difference ranged from 0.4 to 0.5%. AI also factored in the cell age when suggesting AlF_3 patterns.

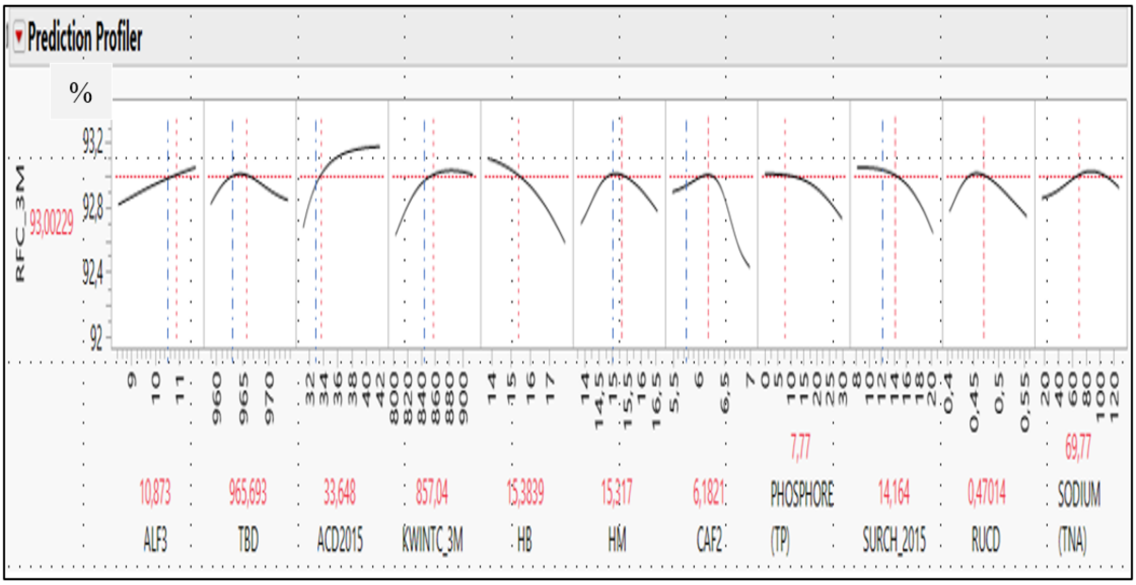
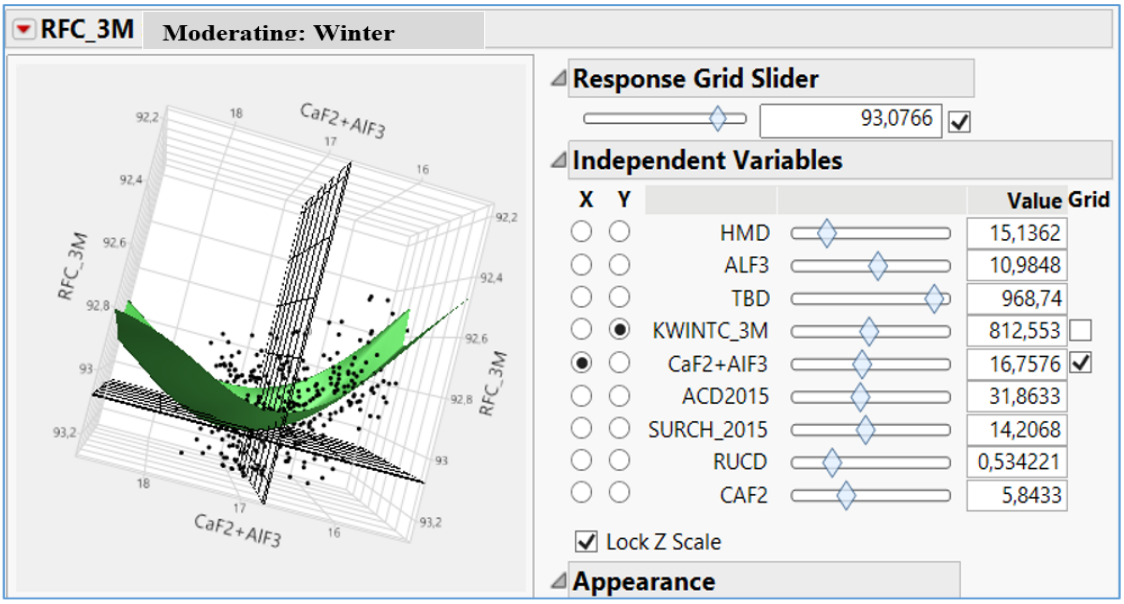


Figure 14. Optimisation of the pot line parameters



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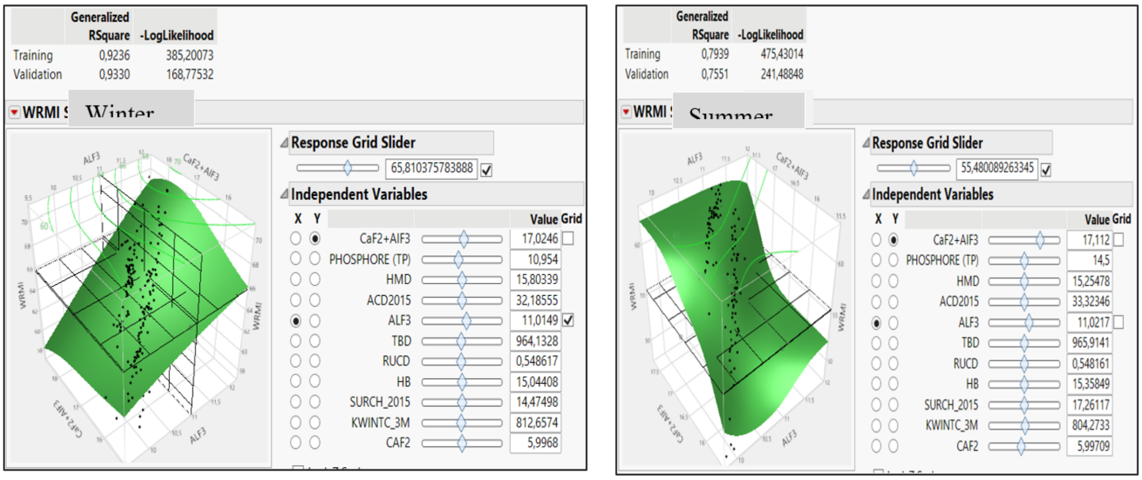
○	○	ALF3	10,9848	
○	○	TBD	968,74	
○	●	KWINTC_3M	812,553	☐
●	○	CaF2+AlF3	16,7576	☑
○	○	ACD2015	31,8633	
○	○	SURCH_2015	14,2068	
○	○	RUCD	0,534221	
○	○	CAF2	5,8433	

☑ Lock Z Scale

Figure 15. Current efficiency optimisation Vs chemical composition: Moderating factor seasonality

10.3 Seasonality’s Impact on the Optimal Chemical Composition.

The maximum AlF_3% that could be tolerated was lower for both designs during the winter compared to the summer. Figures 16a and 16b exemplify this result, showcasing two distinct patterns and the varying degree of instability. The results suggest that, if the chemical composition remains unchanged, there could be an increase of 10 to 20 % in instability during the winter. In summer, the temperature and superheat could experience a 1 to 2 ºC rise.



(a) Winter

	Generalized RSquare	-LogLikelihood
Training	0,9236	385,20073
Validation	0,9330	168,77532

Response Grid Slider: 65,810375783888 ☑

Independent Variables

X	Y		Value	Grid
○	●	CaF2+AIF3	17,0246	☐
○	○	PHOSPHORE (TP)	10,954	
○	○	HMD	15,80339	
○	○	ACD2015	32,18555	
●	○	ALF3	11,0149	☑
○	○	TBD	964,1328	
○	○	RUCD	0,548617	
○	○	HB	15,04408	
○	○	SURCH_2015	14,47498	
○	○	KWINTC_3M	812,6574	
○	○	CAF2	5,9968	

(b) Summer

	Generalized RSquare	-LogLikelihood
Training	0,7939	475,43014
Validation	0,7551	241,48848

Response Grid Slider: 55,480089263345 ☑

Independent Variables

X	Y		Value	Grid
○	●	CaF2+AIF3	17,112	☐
○	○	PHOSPHORE (TP)	14,5	
○	○	HMD	15,25478	
○	○	ACD2015	33,32346	
●	○	ALF3	11,0217	☐
○	○	TBD	965,9141	
○	○	RUCD	0,548161	
○	○	HB	15,35849	
○	○	SURCH_2015	17,26117	
○	○	KWINTC_3M	804,2733	
○	○	CAF2	5,99709	

Figure 16. (a) (winter), (b) (summer): Seasonality-based instability with varying AlF_3 and CaF_2.

The chemical composition of the electrolyte and internal heat interact and affect productivity. The productivity of the cell seemed to exhibit a reversed U-shaped pattern. Lower AlF_3 content resulted in higher losses, but this relationship is not linear.

11. Discussions and Business Implications

This study aimed to provide a deep explanation and differences of the physicochemical properties of the two major electrolyte additives. The following served as the primary research question: What are the likely hidden or adverse effects of increasing AlF_3 concentration beyond the technologically acceptable limits? Are these limits comparable regardless of the technology and seasonality? Is it technically feasible for a smelter to trade 1 % CaF_2 for 1 % AlF_3 to maximize productivity? Can AI-driven solutions effectively determine minima and maxima, apply the substitutional rule, and suggest actions that lead to the best trade-off?

Two case studies and three different technological designs were examined. In each case, we could integrate both dependent, independent, and moderating variables to determine the optimal electrolyte composition that enables maximum value creation (e.g., CE and energy consumption).

Through contextual analysis, the AI could discern the combined Xs and moderating factors, resulting in the identification of optimal settings. It was a surprising finding that twin-lining technologies showed varying electrolyte compositional optima, with a difference of up to 0.7 % AlF_3. The only recognized distinction was the alumina attrition index.

Likewise, the AI can show the variations in electrolytes between a dissipative and non-dissipative lining. In both dissipative and non-dissipative designs, the maximum AlF_3 that could be tolerated was lower in winter compared to summer. Instability increased by up to 10-20 % during the winter when the chemical composition remained unchanged. Conversely, during summer, the temperature and superheat rose by 1 to 2 ºC, with everything else remaining constant, except possibly the heat dissipation capability.

Both AlF_3 and CaF_2 can play different roles in different electrolysis processes, and their effects on temperature are intertwined with their impact on the overall efficiency of the cell. When comparing the effects, it's important to consider both their primary and interaction effects. The specific heat capacity calculated using Shomate equations implies that the influence on the operating variables was expected to be more pronounced with 1 % AlF_3 in comparing to 1 % CaF_2.

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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