

AIPSim[®]: Simulation Software for Modeling of Aluminum Electrolysis Cell

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Abstract:

Due to a limiting number of operational parameters that can be measured in an operating cell, the process is not fully understood and cell operation based largely on experience. In this work, the principles of the Hall-Héroult process are presented and a mathematical model developed to predict the behavior of an aluminum reduction cell. AIPSim is a Simulating model which is used for calculation of aluminium electrolysis properties (same as Electrical Conductivity, Electrolyte Viscosity, Electrolyte Density, Aluminium Density, Max Alumina Solubility in Electrolyte, Max Aluminium Solubility in Electrolyte and Liquidus Temperature) in order to optimize operational parameter in aluminium production systems. AIPSim is a mathematical-experimental model with a static simulation base with ability to evaluate the effect of additive same as Alumina, Carbonate Sodium and Aluminium Fluoride on the electrolysis properties and cell voltage. Cell Voltage in this model separated to decomposition voltage, over voltage and ohmic voltage drops which is part of the ohmic voltage measured manually with operators and will be used as an input parameters.

Keywords: AIPSim; Mathematical Model; Aluminium Electrolysis; Mass & Energy Balance; Electrolyte Properties

Introduction

The objective of this work is to develop a mathematical model of a Hall-Héroult reduction cell as well as develop a better understanding of the reduction process itself and the effects of variations in operational parameters.

The predominant constituent of industrial electrolytes is cryolite (Na_3AlF_6) which is a double fluoride of aluminum and sodium, comprising at least 70% of the total electrolyte mass. Cryolite is the predominant solvent for alumina, with a maximum solvability of 15% by weight. The melting point of pure cryolite is 1011°C but with certain additives, such as excess aluminum fluoride (AlF_3) and calcium fluoride (CaF_2), the melting point can be lowered to $920\text{-}970^\circ\text{C}$, increasing the energy efficiency of the process. The three fluorides, Na_3AlF_6 , AlF_3 and CaF_2 form the basis of the electrolyte currently used by the industry, but an increasing number of reduction plants also introduce lithium fluoride (LiF) and magnesium fluoride (MgF_2) to the electrolyte for further benefits such as further lowering the melting point of the electrolyte and increasing the electrical conductivity of the electrolyte to decrease I^2R losses.

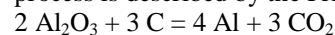
There are advantages and disadvantages of the various additives, so the composition of the electrolyte and the concentrations of the electrolyte constituents vary between plants. Each cell design and operating procedures defines the precise requirements and compromises have to be made between i.e. productivity, energy efficiency and the quality of the product.

Model Description

1- Principal Equations^[1,2,3,4]

Alumina (aluminum oxide or Al_2O_3) is decomposed in an electrolytic process to produce aluminum. At the positive electrode, the anode, oxygen (O_2) is formed which reacts immediately with the carbon anode (C) to carbon dioxide (CO_2). Aluminum (Al) is deposited at the negative electrode, the cathode, which is the already produced aluminum pool. This

process is described by the Principal Equation:



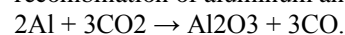
The Principal Equation means that two moles Al_2O_3 react with three moles C to production of four moles Al and three moles CO_2 .

The aluminum electrolysis process is governed by Faraday's law of electrolysis which is saying that:

✓ The amount of substances deposited or dissolved during an electrolytic process is proportional to the quantity of electricity passed through the electrolytic cell.

✓ One gram equivalent weight of matter is deposited or dissolved on each electrode for 96485 C (Coulomb) of electricity charge passed through the electrolyte.

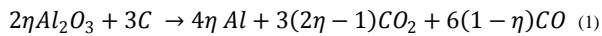
In reality the quantity of aluminum produced is lower than this theoretical value, mostly because of the internal recombination of aluminum and carbon dioxide:^[14]



The ratio of the actual quantity of aluminum produced to the theoretical quantity is referred to as the Faraday's Efficiency or Current Efficiency η (%CE if represented in percentage).

In modern industrial cells the average current efficiency for metal production generally varies between 90 and 95%, assuming that only aluminum is deposited at the cathode. The current efficiency depends greatly on the cell's design as well as a number of other variables including temperature, current density, inter-polar distance (distance between the electrodes), etc.^[7]

With assumption that the loss in current efficiency is only due to the internal recombination of aluminum and carbon dioxide, By modifying the two principal equations with this assumption, considering that a $(1-\eta)$ fraction of aluminum is lost if an η fraction is produced, results in the modified electrolysis equation:



Taking the current efficiency into account, the actual production and consumption rate of components can be expressed as follows:

$$\frac{dm_{Al_2O_3} (Consumption)}{dt} = 1.761 * 10^{-7} * I * \eta \quad (2)$$

$$\frac{dm_C (Consumption)}{dt} = 3.111 * 10^{-8} * I \quad (3)$$

$$\frac{dm_{Al} (Production)}{dt} = 9.322 * 10^{-8} * I * \eta \quad (4)$$

$$\frac{dm_{CO} (Production)}{dt} = 1.452 * 10^{-7} * I * (1 - \eta) \quad (5)$$

$$\frac{dm_{CO_2} (Production)}{dt} = 1.140 * 10^{-7} * I * (2\eta - 1) \quad (6)$$

These equations are theoretical rate of consumption and production but Real Consumption of Alumina and Carbon because of below reasons are differ from above relations so in the model some input data (same as alumina impurities, Alumina Moisture, carbon excess consumption because of air burn) has been considered as a correction value.

There are various additional loss mechanisms for carbon consumption that contribute to the overall consumption, such as air burning and detachment of anode carbon particles from the blocks. According to Grjotheim and Welch, the total excess carbon consumption to the theoretical consumption can be expected to be in the range of 7-18%. Furthermore, the anodes are not made up of pure carbon.

The anodes used in industrial aluminum cells are made from paste consisting of 70-80% aggregate coke and 30-20% pitch as a binder, with about 98-99% carbon concentration. The anode consumption rate is thus considerably higher in practice than expressed by equation 3.

The theoretical consumption of Alumina is about 1.89 kg of pure alumina per kilogram of aluminum produced.

Smelter grade alumina is not pure, so the total amount of alumina that is required for the reduction process is thus higher in practice than the theoretical consumption. Up to 1% of the alumina mass is natural impurities and about 2-3% of the mass is moisture. The main impurity is sodium oxide, while calcium, silicon, iron and titanium oxides are also present. Furthermore, when using dry scrubbers for

removing fluorides from the effluent pot gases and bag filters for the particulates, the alumina is used as a gas absorbent before it is fed to the cell. A part of the feed material is thus recycled fluoride which exists in the alumina bulk material mainly as aluminum fluoride. When using dry scrubbers, the fluoride content can range from 1.0 to 1.5% of the mass, depending on the absorbability of the alumina used. This means that only about 94-95% of the raw feed material mass is in fact pure alumina so the actual bulk consumption of alumina can be expected to be around 5-6% higher than expressed by equation 2.

2- Cell Emissions

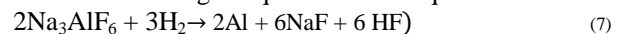
The evolution of gases from the anodes provides a transpiring medium for volatile materials as well as entraining particulate matter. The amounts of gases, dust or fumes emitted vary for different cell types.

The fine particulate fluorides and gaseous hydrogen fluoride are of greatest concern in relation to the material balance, since fluorides are lost from the electrolyte. These are present in the anode gases as a result of:

- Gaseous fluoride evolution
- Particulate emission
- Entrainment of particulate materials

Approximately half of the cell fluoride emissions, predominantly hydrogen fluoride (HF), leaving the cell are gases. The sources of the hydrogen (H) can be from the anode carbon or from moisture present in the air or in the alumina feed.

Hydrogen absorbed or entrapped in the anode carbon matrix can be electrochemically oxidized to either water or hydrogen fluoride because the reaction requires less operating potential than the alumina electrolysis. Part of the hydrogen reacts with cryolite to produce hydrogen fluoride according to equation below equation:



According to Haupin, the total rate of the gaseous fluoride evolution in kilograms per metric ton of aluminum can be estimated with equation 8:

$$E_G = 1.4537 * 10^7 * e^{(0.7812 * R^2 - 3.173R - \frac{8444}{T})} * \left(\frac{462-191R}{P*\eta}\right) * \left(\frac{C_{H_2O}}{37.44} + \frac{C_H}{21.5}\right)^{0.5} * \left(\frac{C_{Al_2O_3}}{C_{Al_2O_3 Max}}\right)^{-0.462} \quad (8)$$

Haupin suggests that the average concentration of moisture in the alumina feed material is approximately 2.8% and the concentration of hydrogen in the anode carbon 0.093%.

$$\Delta m_{Al} = 0.01155 * E_G \quad (9)$$

$$\Delta m_{Al_2O_3} = 0.8726 * E_G \quad (10)$$

$$\Delta m_{AlF_3} = -1.473 * E_G \quad (11)$$

Studies have established that sodium tetrafluoroaluminate (NaAlF₄) is the most volatile species existing above cryolite-alumina melts. The vapor exists both as the monomer NaAlF₄ and the dimer Na₂Al₂F₈, from the reaction of sodium fluoride with aluminum fluoride, according to equation 12:



For vaporization to be a significant factor, it must have a driving force for removing the electrolyte vapors from the cell. In an operating cell this is provided by the gases from the anodes, which are mostly carbon dioxide and carbon monoxide. The rate of loss of vapors is thus dependent on the saturation vapor pressure as well as the number of moles of the transpiring gases. The total vapor pressure PT (kPa) which is equal to the sum of the partial pressures of the individual gases can be expressed as a function of bath composition and temperature.

The mechanism when liquid droplets or solid particulates are entrained in a flowing gas is known as entrainment. The transpiring anode gases have sufficient gas velocity for electrolyte droplets to be entrained. There will also be some entrainment of condensed phases in the anode gases. When the liquid electrolyte entrained in the anode gas cools it forms particulates. Haupin developed an empirical model for estimating the rate of fluoride evolution due to entrainment, given by equation 13. The model was based on the theory that the difference between measured total fluoride losses and the calculated estimate of the gaseous fluoride evolution and the particulate emissions would be the result of electrolyte being entrained by the effluent gases.

$$E_E = \frac{1}{\eta} * (-17030 + 29800R - 13000R^2 + 67C_{Al_2O_3} - 173\tau - 0.389\tau^2 + 141.6R\tau) \quad (13)$$

Since Haupin's model can only be considered as a mean for correcting the total amount of fluorides lost by entrainment, it cannot be used to account for the loss of other constituents making up the entrained electrolyte droplets.

$$\Delta m_{AlF_3} = -1.473 * C_{AlF_3} * E_E * \frac{1}{E_E + E_G} \quad (14)$$

$$\Delta m_{NaF} = -2.210 * C_{NaF} * E_E * \frac{1}{E_E + E_G} \quad (15)$$

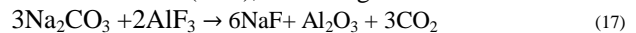
$$\Delta m_{Al_2O_3} = -C_{Al_2O_3} * \Delta m * \frac{1}{E_E + E_G} \quad (16)$$

3- Corrective Fluoride Addition

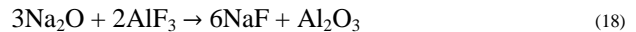
When using dry scrubbers for removing fluoride from the effluent pot gases, the fluoride losses are almost completely recycled to the cells. The recycled fluoride exists in the alumina bulk material mainly as aluminum fluoride, but also as sodium fluoride and cryolite.

The amount of fluoride required for correcting the electrolyte composition is mainly determined by the so-called bath ratio Rb , which is the mass ratio of NaF to AlF_3 . Most of the electrolyte characteristics are closely related to the bath ratio, such as the volatility, melting point, electrical conductivity and density. Maintaining a stable bath ratio is thus of major importance in the alumina reduction process. Another obvious reason for corrective additions is to maintain sufficient electrolyte volume. To increase the ratio, sodium fluoride is added to the electrolyte in the form of sodium carbonate

(Na_2CO_3), which reacts with aluminum fluoride to form sodium fluoride (NaF), according to the reaction:



As can be seen from equation 17, by adding sodium carbonate instead of adding NaF directly to the electrolyte, the bath ratio can be varied more with less addition, since the AlF_3 is reduced at the same time. Sodium fluoride also enters the cell as the natural occurring impurity, sodium oxide (Na_2O) in the feed material, which reacts with aluminum fluoride to form sodium fluoride:



According to Grjotheim and Welch, the sodium dioxide makes up of around 0.3% of the feed material mass. Correspondently, the bath ratio can be decreased by adding aluminum fluoride, but aluminum fluoride is however added directly. Adding aluminum fluoride also reduces sodium deposition, since excess AlF_3 reacts with sodium to form cryolite, according to the reaction:



4- Electrolyte Properties

The physical properties of the electrolyte are strongly influenced by its composition and temperature. In the following, expressions for various properties involved in modeling the aluminum reduction cell will be given.

- **Density:** Several empirical equations have been published for calculating the density of the molten electrolyte. The empirical relationship given by Haupin^[8] was considered to be the one best suited for the electrolyte composition at Al-Mahdi and Hormozal, which is given by:

$$\rho_{EL} = 100 \left/ \left(\frac{C_{Na_3AlF_6}}{3.305 - 9.37 * 10^{-4}T_b} \right) + \left(\frac{C_{NaAlF_2}}{1.987 - 3.19 * 10^{-4}T_b + 0.094C_{NaAlF_3}} \right) + \dots \right. \\ \left. + \left(\frac{C_{CaF_2}}{3.177 - 3.19 * 10^{-4}T_b + 0.0005C_{CaF_2}} \right) + \left(\frac{C_{Al_2O_3}}{1.449 + 0.0128C_{Al_2O_3}} \right) + \dots \right. \\ \left. + \left(\frac{C_{MgF_2}}{3.392 - 5.24 * 10^{-4}T_b + 0.01407C_{MgF_2}} \right) + \left(\frac{C_{LiF}}{2.358 - 4.9 * 10^{-4}T_b} \right) * 10^3 \right. \quad (20)$$

- **Viscosity:** The viscosity of the electrolyte influences several hydrodynamic processes in the cell such as the convection in the electrolyte, movement of metal droplets and dissolution and sedimentation of alumina particles. The viscosity of the electrolyte can be expressed by the following simplified equation, given by Grjotheim and Welch^[2]:

$$\mu_{EL} = 11.557 - 9.158 * 10^{-3} (T_b - 273) - 1.587 * 10^{-3} C_{NaAlF_3} \\ + (-2.094 * 10^{-3} + 1.853 * 10^{-5} (T_b - 1273)) C_{NaAlF_3}^2 - 2.168 * 10^{-3} * C_{Al_2O_3} \\ + (5.952 * 10^{-3} - 1.938 * 10^{-5} (T_b - 1273)) C_{Al_2O_3}^2 \quad (21)$$

- **Maximum Alumina Solubility:** The maximum amount of alumina that can be dissolved in the electrolyte depends on both the electrolyte composition and temperature. The maximum alumina solubility can be expressed by the following equation, given by Skybakmoen, et al^[10]:

$$C_{Max}^{Al_2O_3} = A \cdot \left(\frac{T_b - 273}{1000} \right)^B \quad (21)$$

Where

$$A = 11.9 - 0.062 C_{xs AlF_3} - 0.0031 C_{xs AlF_3}^2 - 0.20 C_{CaF_2} - 0.50 C_{LiF} - 0.30 C_{MgF_2} + \frac{42 C_{xs AlF_3} C_{LiF}}{200 + C_{xs AlF_3} C_{LiF}} \quad (22)$$

$$B = 4.8 - 0.048 C_{xs AlF_3} + \frac{2.2 C_{LiF}^{1.5}}{10 + C_{LiF} + 0.001 C_{xs AlF_3}^3} \quad (23)$$

When the concentration of alumina reaches the maximum alumina solubility, the electrolyte becomes saturated with alumina, and all excess alumina sinks to the bottom of the cavity, where it can form sludge.

- **Electrical Conductivity:** The electrical conductivity of the cryolite electrolyte is an important factor in cell voltage and therefore in power efficiency. The unit of the electrical conductivity is Siemens per meter (S/m or S/cm). Siemens (reciprocal Ω or eventually mho) is the unit of electrical conductance^[11].

$$K = -1.66 X_{AlF_3} - 0.942 X_{AlF_3} X_{Li_3AlF_6} - 0.76 X_{CaF_2} - 1.805 X_{CaF_2} X_{Al_2O_3} - 2.53 X_{Al_2O_3} - 2.59 X_{Al_2O_3} X_{MgF_2} + 0.97 X_{Li_3AlF_6} - 1.07 X_{MgF_2} - 0.206 X_{KF} \quad (24)$$

- **Liquidus Temperature:** The liquidus temperature (T_L) is the temperature at which solid material is precipitating when a liquid is cooled. The bath temperature (T_B) is the temperature of the liquid electrolyte in a electrolysis cell that is measured during normal pot operation. The difference between bath temperature and liquidus temperature is called Superheat (ΔT).

$$\Delta T = T_B - T_L \quad (25)$$

The electrolyte is a multi-component system of cryolite (Na_3AlF_6) with additions of alumina (Al_2O_3), aluminum fluoride (AlF_3), calcium fluoride (CaF_2) and eventually lithium fluoride (LiF), magnesium fluoride (MgF_2) and potassium fluoride (KF). In the literature several relations of the cryolite liquidus temperature for this multicomponent system are found:^[19]

$$T_L = 1011 + 0.50 C_{AlF_3} - 0.13 C_{AlF_3}^{2.2} - \frac{3.45 C_{CaF_2}}{1 + 0.0173 C_{CaF_2}} + 0.124 C_{AlF_3} C_{CaF_2} - 0.00542 (C_{AlF_3} C_{CaF_2})^{1.5} - \frac{7.93 C_{Al_2O_3}}{1 + 0.0936 C_{Al_2O_3} - 0.0017 C_{Al_2O_3}^2 - 0.0023 C_{Al_2O_3} C_{AlF_3}} - \frac{8.90 C_{LiF}}{1 + 0.0047 C_{LiF} + 0.0010 C_{LiF}^2} - 3.95 C_{MgF_2} \quad (26)$$

5- Cell Voltage

The total voltage drop over a reduction cell is referred to as the cell voltage and is measured between the busbars connected to the electrodes. Although it is usually not a design parameter, the cell voltage is one of the most important operating parameters in aluminum reduction cells, and is often the only parameter measured in real-time. The cell voltage is closely related to both the alumina concentration in the electrolyte and the bath temperature and is thus generally, one of the bases for computer control of the Hall Héroult process. The total cell voltage is composed of three different types of contributions^[13]:

- The decomposition voltage.

(Theoretical minimum potential required for the decomposition of alumina)

- The overvoltage

(The excess voltage due to electrode polarization)

- The ohmic voltage drops

(Voltage drops due to the resistance of various sections in the cell)

The decomposition voltage for alumina is around 1.1-1.2V, but due to electrode polarization and the electrical resistance of various sections of the cell, the cell voltage is typically in the range of 4.1-4.5 volts. The difference between the theoretical energy requirements and the energy generated by the electric current is manifested as heat, so the primary cause for the low energy efficiency of the Hall-Héroult process is the high cell voltage. The reduction cell must operate in thermal balance, so the cell voltage cannot be dramatically decreased without accounting for the change in balance by either a change in design or operating conditions.

Under normal operating conditions, the cell voltage does not deviate far from the optimal cell voltage for the given cell design. However, when the anode effect occurs, which is an abnormal operating condition, the cell voltage can reach up to 80 V, which is the primary cause of sidewall erosion as well as lowering the cell's production efficiency.

For the primary reaction, the decomposition voltage can thus be written as:

$$E_0 = E^0 - \frac{R \cdot T}{n \cdot F} * \ln \left(\frac{a_{Al}^4 * a_{CO_2}^3}{a_{Al_2O_3}^2 * a_C^3} \right) \quad (V) \quad (27)$$

Where the standard electrode potential becomes:

$$E^0 = \frac{\Delta G}{n_e F} = \frac{1098.9 - 0.33143 T}{6 * 96485} = 1.898 - 0.0005725 T_b \quad (V) \quad (28)$$

The excess voltages due to polarization at the electrodes interfaces have to be considered, to determine the total voltage required for the decomposition. This includes over voltages due to concentration gradients around the electrodes as well as a reaction overvoltage close to the surface of the anodes. The three over voltages are all derived from the Nernst equation and are proportional to the electrolyte temperature.

Concentration Overvoltage

During the electrochemical reactions, the reactants around the electrodes are consumed, thus lowering the concentration in that area. The random motion of molecules causes a net transfer of mass from an area of high concentration to an area of low concentration, which balances the concentration. In an aluminum reduction cell, the electrochemical reactions are more rapid than the mass transport of the reacting species, so a concentration gradient is built up around the electrodes.

The decomposition voltage is determined at zero current flow, with the concentration of the bulk solution as a reference point, which means that a concentration gradient would result in a potential difference. The

potential difference, which is generally known as the concentration overvoltage or polarization, is necessary to make the electroactive species migrate against the gradient concentration.

- Anode Concentration Overvoltage^[6]

The anode concentration overvoltage occurs at the boundary between the anodes and the electrolyte. Based on the Nernst equation, Haupin introduced an equation for determining the anode concentration overvoltage:

$$\eta_{AC} = \frac{RT}{nF} * \ln\left(\frac{j_{cr}}{j_{cr} - j_A}\right) \quad (V) \quad (29)$$

where j_A is the anode current density and j_{cr} is the so-called critical current density, which is the maximum current density attained before the normal anode reaction is superseded by the anode effect

$$j_{cr} = \frac{(a * C_{Al2O3} + b * C_{Al2O3}^2)}{(a * C_{Al2O3}^{AE} + b * (C_{Al2O3}^{AE})^2)} * j_A \left(\frac{A}{m^2}\right) \quad (30)$$

- Cathode Concentration Overvoltage

To migrate against concentration gradients at the boundary between the electrolyte and the metal pad cathode, a potential difference occurs at the boundary, which can be expressed by the cathode concentration overvoltage, η_{CC} , given by:

$$\eta_{CC} = \frac{RT}{nF} * \ln\left(\frac{j_c}{0.283} * \left(\frac{1.375 - 0.125R}{1.5}\right)\right) \quad (31)$$

Where j_c is the cathode current density and $n = 2$. Regarding to the relationship between the bath ratio and the cathode concentration overvoltage, the cathode concentration overvoltage is normally small and is close to being linearly dependant on the bath ratio. Unlike the anode concentration overvoltage, the cathode concentration overvoltage is independent of the critical alumina concentration.

Ohmic Voltage drops

Ohmic voltage drops due to the electrical resistance of various cell components, contribute to the overall cell voltage. The ohmic voltage drops, as well as the electrode polarization, are manifested as heat. Within the cell, the only resistance that can be varied independently and freely at constant current density is the electrical resistance of the electrolyte, which can be achieved by either altering the composition of the electrolyte, or by reducing the inter-polar distance. The other resistances are subject to the cell design. The primary conductive regions within the cell are the anode, the electrolyte and the cathode assembly. The insulating materials have very low electrical conductivity, so their contribution will be neglected.

Electrolyte Voltage Drop

The voltage drop over the electrolyte is considered to exist between the anode and the cathode, and is due to the electrical resistivity of the bath. Assuming a uniform current density, the electrical resistance of the electrolyte follows the basic law of electrical resistance:

$$R_{EC} = \frac{d}{k * A} \quad (32)$$

Where the distance d is the inter-polar distance, A is the total surface area of the anodes and k the electrical conductivity of the electrolyte. Ohm's law then combines the electric current and the electrical resistance of the electrolyte to determine the electrolyte voltage drop:

$$U = I * R_{EC} \quad (33)$$

Bubble Voltage Drop^[15]

The horizontal orientation of the anodes in a reduction cell causes gas accumulation beneath the anode surface. The gas volume beneath the working anode surface forms an insulating layer of bubbles, reducing the cross-sectional area of the electrolyte in that zone. This effect causes an increase in the effective resistivity of the electrolyte, resulting in a voltage drop generally known as the bubble voltage drop. Hyde and Welch introduced the following expression for determining the bubble voltage drop:

$$V_{Bubble} = \frac{d_{Bubble} * j_A}{K} * \frac{\phi}{1 - \phi} \quad (v) \quad (34)$$

where d_{bubble} is the bubble layer thickness and ϕ the surface coverage.

Cathode Voltage Drop

The cathode is made up of three parts, the aluminum metal pad, carbon cathode blocks and steel collector bars. The voltage drop over the cathode lining due to the electrical resistance of its components is an important indicator of the cathode's condition. As the cell gets older, the cathode-voltage drop increases in a more or less regular way mainly due to deposition of sodium in the lining. The rate of the increase depends on many factors including the quality of the cathode blocks and insulating materials, but operational factors are also important.

Typically, the voltage drop may increase by approximately 0.1 V over the lifetime of cells. In the following, an expression will be given for determining the voltage drop over a new cathode.

Other voltage drop same as anode butt, Yoke, Connecting Rod and Contact Resistance should be measured by the operator and input to the model.

Results and Discussions

In order to Validation of this static model two method has been selected, one of them is with data gathering from Al-Mahdi poor point feeder cell and the other way is compare result of this model with other static model.

AIPSim is a model with 7 tabs and 5 sub tabs for prediction of electrolysis properties and cell voltage.

In this model analysis of electrolyte and amount of alumina, Sodium Carbonate, Sodium Oxide and Aluminium Fluoride addition are as an input values and Electrolyte Properties same as Liquidus Temperature, Electrical Conductivity, Density, Viscosity, Alumina Solubility in electrolyte, Aluminium Solubility in electrolyte are as output data although over voltages, ohmic voltages and total cell voltage will be calculated.

Figure 1 illustrated the GUI of AIPSim Model.

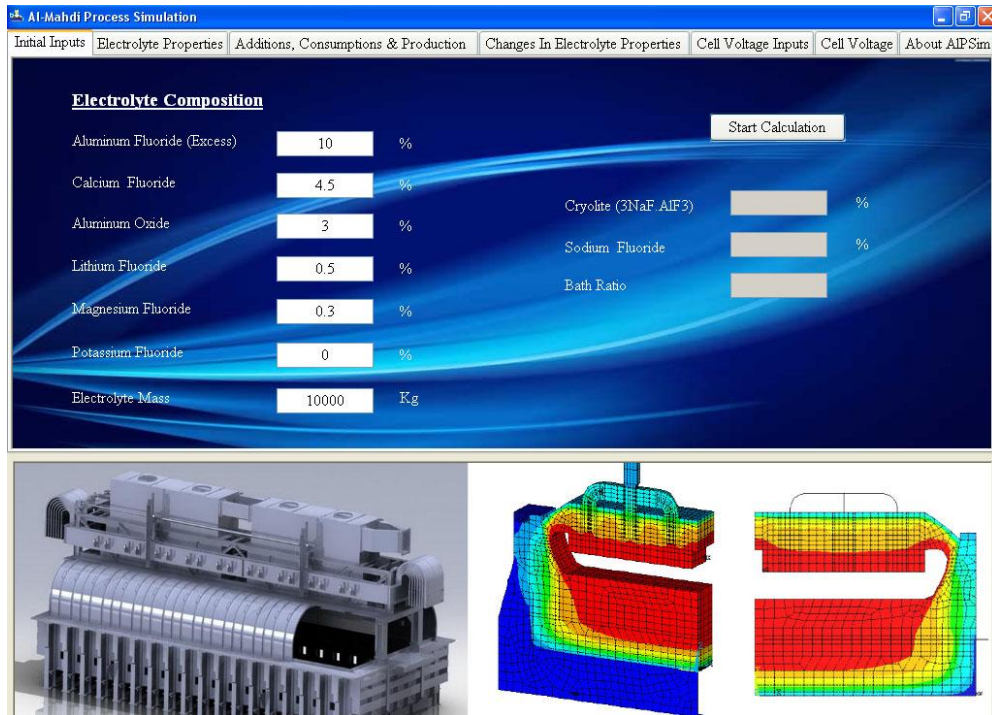


Figure 1 – AIPSim GUI

In the first method of validation electrolyte analysis of Poor Point Feeder pot used for model validation.

According to the values of table 1 output data from AIPSim model has been generated in tables number 2-6

	Input Parameter	Value	Unit
1	Excess Aluminum Fluoride	8	%
2	Calcium Fluoride	5	%
3	Aluminum Oxide	3	%
4	Lithium Fluoride	0	%
5	Magnesium Fluoride	0	%
6	Potassium Fluoride	0	%
7	Super Heat	5	°C
8	Anode Cathode Distance	4.5	cm
9	Current Intensity	175	KA
10	Aluminum Fluoride Addition	90	Kg
11	Sodium Carbonate Addition	0	Kg
12	Sodium Oxide Addition	0	Kg
13	Alumina Addition	6	Kg
14	Alumina Impurity	5	%
15	AlF ₃ in Feed Alumina	1	%
16	Excess Carbon Consumption	10	%
17	Current Efficiency	95	%

Table 1 – Input Data from Al-Mahdi Poor Point Feed Cell

	Electrolyte Properties	Value	Unit
1	Liquidus Temperature	970.445	°C
2	Electrolyte Density	2.1406	gr/cm ³
3	Aluminum Density	2.3025	gr/cm ³
4	Electrolyte Viscosity	2.4584	mPa.s
5	Max Alumina Solubility	9.3533	%
6	Max Aluminum Solubility	0.0478	%
7	Electrical Conductivity	2.2749	S/cm
8	Bath Temperature	975.445	°C
9	Bath Ratio	1.2115	-

Table 3 – Electrolyte Properties with first Composition

	Electrolyte Production	Value	Unit
1	Aluminum Production	970.445	°C
2	Carbon Consumption	2.1406	gr/cm ³
3	CO Production	2.3025	gr/cm ³
4	CO ₂ Production	2.4584	mPa.s
5	Duration of Alumina Consumption	9.3533	%

Table 4 – Effect of Alumina addition in Production and Consumption of basic elements of main reaction

Table No.3 show the electrolyte properties which is calculated base on first electrolyte analysis that is measured with operators.

Table No.4 show the amount of Aluminum, Carbon monoxide and Carbon dioxide which is produced by addition of 6 kg alumina to the cell.

	Electrolyte Properties	Value	Unit
1	Liquidus Temperature	963.8242	°C
2	Electrolyte Density	2.1252	gr/cm ³
3	Aluminum Density	2.3025	gr/cm ³
4	Electrolyte Viscosity	2.4545	mPa.s
5	Max Alumina Solubility	8.6952	%
6	Max Aluminum Solubility	0.0438	%
7	Electrical Conductivity	2.1954	S/cm
8	Bath Temperature	968.8242	°C
9	Bath Ratio	1.1560	-

Table 5 – Change of Electrolyte Properties with additions

Table No.5 show the electrolyte properties after addition of 6 kg Alumina and 90 kg of Aluminum Fluoride to 4500 kg Electrolyte in order to correct the bath ratio to proper amount.

	Cell Voltage	Value	Unit
1	Anode Conc. Over Voltage	0.0260	V
2	Cathode Conc. Over Voltage	0.0456	V
3	Electrolyte Voltage Drop	1.4930	V
4	Anode Voltage Drop	0.2640	V
5	Cathode Voltage Drop	0.2790	V
6	Decomposition Voltage	1.2274	V
7	Bubble Voltage Drop	0.2579	V
8	External Voltage Drop	0.180	V

Table 6 – Cell Voltage Drop

Conclusion

All generated data from model compared with poor point feeder cell in Al-Mahdi aluminum production plant and following differences in table No.7 are observed.

	Difference of Electrolyte Properties	ΔX	Percent
1	Electrolyte Density	0.04281	- 2 %
2	Aluminum Density	0.02993	- 1.3 %
3	Electrolyte Viscosity	-	-
4	Electrical Conductivity	0.02502	1.1 %
5	Bath Temperature	2	0.2 %
6	Bath Ratio	0.0012	0.1 %

Table 7–Inaccuracy between AIPSim Data and Plant Data

Data

All other Static value compared with AIPrg[®][21] and because these two models are base of same fact so all generated values from AIPSim is Completely same of AIPrg but in AIPSim Model some other values same of Cell Voltage calculated which is in the AIPrg these values didn't Considered.

	Electrolyte Properties	Value	Unit
1	Liquidus Temperature	970.445	°C
2	Electrolyte Density	2.1406	gr/cm ³
3	Aluminum Density	2.3025	gr/cm ³
4	Electrolyte Viscosity	2.4584	mPa.s
5	Max Alumina Solubility	9.3533	%
6	Max Aluminum Solubility	0.0478	%
7	Electrical Conductivity	2.2749	S/cm
8	Bath Temperature	975.445	°C
9	Bath Ratio	1.2115	-

Table 8 – Electrolyte Properties From AIPrg Model

	Electrolyte Production	Value	Unit
1	Aluminum Production	970.445	°C
2	Carbon Consumption	2.1406	gr/cm ³
3	CO Production	2.3025	gr/cm ³
4	CO ₂ Production	2.4584	mPa.s
5	Duration of Alumina Consumption	9.3533	%

Table 9 – Effect of Alumina addition in Production and Consumption in AIPrg Model

So Given the above it can be concluded that AIPSim Model with max 2 percent inaccuracy is a suitable static model for simulation aluminum electrolysis cell and completely useful for operator of aluminum production companies to get more familiar with basic facts and relations in electrolysis systems.

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