Analysis of aluminum-air battery by physics-based mathematical model

Chong Zhou
ABSTRACT

ANALYSIS OF ALUMINUM-AIR BATTERY BY PHYSICS-BASED MATHEMATICAL MODEL

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The demand of electrical energy system is increasing rapidly these days for diverse applications from portable electronics and electrical vehicles to grid-scale energy storage. Lithium-ion battery has been utilized for most of those applications, but due to high cost (about $600/ kWh) and lower energy density (0.37 kWh/kg), the advent of low-cost and high-performing battery system is required. In this study, we will revisit aluminum-air battery as a promising system which has excellent features such as high energy density of 2.8 kWh/kg, low cost, and safe in nature, but it was abandoned due to challenging issues. One of the key issues is the parasitic corrosion of aluminum anode to evolve hydrogen gas, which significantly decreases the aluminum-air battery’s efficiency.

This research focused on building physics-based mathematical model to define the key controlling parameters for the performance of aluminum-air battery. Especially, the side reaction (i.e., self-corrosion of aluminum to generate hydrogen gas) was analyzed in detail to understand its effect on mass-transfer boundary layer, conductivity of electrolyte, surface concentration of reactive species, and reactive surface area of electrode. Fraction of electrode
surface area occupied by the H2 gas bubble was calculated by combing physics-based analytic relations with experimental results. The relations include the physical components such as contact angle formed by bubble on the electrode surface; critical diameter of bubble detached from the surface, which was calculated from the force balance among gravity; buoyancy, drag, and surface tension forces; bubble generation rate; and Jacob numbers. And also, the effect of bubble coverage on kinetics was considered by modifying active reactive area in Butler-Volmer equation.

It was found that the effect of side reaction on the cell performance was significant. Due to the self-corrosion of aluminum electrode, open-circuit voltage was decreased significantly from theoretical value of 2.7 V to 1.9, and the side reaction was found to be decreased as main cell current increased. The effect of bubble coverage was significant in the kinetic loss, and it could be reduced by minimizing contact angle formed by gas bubble on the electrode by using hydrophilic material or by using higher flow rate of electrolyte. In the presentation, all the detailed research works conducted for this project were addressed along with analysis of key results, and it is expected that the results from this fundamental research will not only advance knowledge of bubble dynamics and two-phase flow in the battery system but also guide future research in this field.
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ANALYSIS OF ALUMINUM-AIR BATTERY BY PHYSICS-BASED
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BY

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Chapter 1 — INTRODUCTION

1.1 Background

1.1.1 History

Aluminum-air batteries (Al-air batteries) generate electricity when oxygen in the air reacts with aluminum. As a type of battery with very high energy density, the study of aluminum-air batteries that were mechanically rechargeable started from as early as 1960s. At that time, the efforts were mainly made on researching into and solving material problems at the air electrode, thermal management and different kinds of problems associated with the anode. Moreover, an evaluation of 2500 Al alloys in NaCl was performed during the 1960s. However, due to the great anode cost issue, Al-air battery was not widely used at that time. Then in the 1970s, Al-air batteries with wedge anodes were developed, and later the 120W saline Al-air batteries were put into military use by Norwegian Defense Research Center. Also, during this period, aluminum-air technology had been applied to electric vehicle propulsion. During the 1980s, the US Department of Energy began to study Al-air batteries for traction use.

Shortly afterwards, Aluminum Company of Canada started the research with subsidiary Alupower. The company obtained a patent for AB50V, Al/0.6 Mg/0.1 Sn/0.05 Ga for saline and Al/0.1 In/0.8 Mg/0.1 Mn for alkaline at 60°. During the 1980s to 1990s, aluminum-air battery was further used for military application and portable wireless devices. In early 1990s, Al-air batteries were used in filter and crystallizer by Eltech Systems. Meanwhile, more and more
companies started their research and development in Alupower and Al-air batteries, including Renault & LEMPI in France and ENER-TEK. From 2000 to 2010, the Al-air batteries technology had already had a wide range of applications. AT&T and Bell Canada had used this system to increase the reserve backup from lead acid battery to over 60 hours. Now some companies, including Aluminum Power attempted to produce small aluminum-air cells for portable applications. Moreover, researchers have found that electric cars with aluminum batteries have the potential for as many as eight times the range of a lithium-ion batteries while the total weight is much lower. However, today there are still some issues remaining in terms of the application of Al-air batteries, including alloys, unwanted wastes and necessary recycle processes.

1.1.2 Advantages

There are several advantages of aluminum-air batteries. First, since aluminum is the third most abundant element on earth, there are very few issues regarding the supply of materials. Second, Al-air batteries have the second highest theoretical energy density among all kinds of batteries, meaning that while the energy potential is great, the total weight of the batteries is much lower. Third, the theoretical cell voltage of Al-air batteries is 2.7V, an amount that is higher than most other batteries. Overall, Al-air batteries have the advantages of high energy density, silence and low infrared.
1.1.3 Challenges

However, there are also several challenges for aluminum-air batteries. First, the anode may experience rapid degradation. In other words, the energy storage has been an issue that has not been addressed yet. Second, Al-air batteries have a short shelf life as a result of the reaction between the aluminum and the electrolyte. Such reaction produces hydrogen when the battery is not in use. However, the problem has already been relieved with modern designs in which electrolyte is stored in a tank outside the battery. Third, the Al-air batteries have a short operational life as a result of electrolyte leakage. Although the problem could be solved with modern air cathodes, which consist of a reactive layer of carbon, a catalyst such as a cobalt, and a porous hydrophobic PTFE film, the costs are huge. As a result, the cost of Al-air batteries remains high.

1.2 Literature review

Almando J. Leon from Florida Atlantic University in Boca Raton, Florida, has conducted a modeling and analysis of aluminum-air fuel cell that considered Ohmic losses and mass transfer but ignored the parasitic effect (Leon, 2013). Shao et al. analyzed the performance of the aluminum-air battery and took the kinetics of the anode, cathode, and parasitic reactions into consideration but did not mention the pH effect corrosion rate in “Modeling the performance of an aluminum-air cell” published in the Journal of Power Sources (Yang, 2003). Young-Cho et al. researched into the influences of aluminum purity in Al-air battery model but did not consider different concentration effects in the article, “Aluminum Anode For Aluminum-Air
Battery” (Young-Joo Cho et al., 2015). Yisi Liu et al. presented the fundamentals, challenges and the recent advances in Al-air battery technology from aluminum anode and air cathode but did not consider bubble coverage effect in the Al-air battery model in the article “A Comprehensive Review on Recent Progress in Aluminum-air Batteries” (Yisi Liu, 2017).

1.3 Motivation

Aluminum-air battery is one of the cheap battery sources. It has high theoretical energy density, high theoretical cell voltage, high theoretical volumetric capacity and high specific energy, but due to the aluminum corrosion, it has some challenging issues like anode quickly degradation, short shelf life and short operational life. I focus on the main reason of the Aluminum Air Battery challenging issue: parasitic reaction. I use theoretically compare other experiments to find a way to reduce these issues.

1.4 Objectives

The overall research objective is to develop a physics-based mathematical model of aluminum-air battery. In specific, the research analyzed the effect of H2 evolution on cell current, electrolyte conductivity, ionic species flux (boundary layer thickness), and active area of electrode (bubble coverage). The research also analyzed the parameters to control H2 evolution, including the pH condition, flow rate, cell gap, and length of electrode. Additionally, the research analyzed the cell parameters and operating conditions, including cell gap, height, concentration, flow rate, etc, for the best performance.
Chapter 2 — RESEARCH METHOD

2.1 Al-Air Battery Schematic

We used pure aluminum as the anode and porous material for cathode in our model. This battery model relies on anode aluminum oxidation and cathode oxygen reduction to generate electrical energy. From Figure 1, we can see at anode, when aluminum material combined with hydroxide from electrolyte, aluminum will oxidize and get aluminum hydroxide and three free electrons. This anodic reaction got 2.328 voltage, and electrons will pass the electric wire to the cathode.

In the cathode, these electrons are combined with oxygen and water to make oxygen reduction and got hydroxide ions. This cathodic reaction got 0.401 voltage. The hydroxides from cathode can transfer through the membrane and electrolyte to the anode, joining anode oxidation reaction.

Because we used alkaline solution to be electrolyte (potassium hydroxide), we need to consider material corrosion. This reaction will consume aluminum to produce hydrogen and aluminum hydroxide, but there are no electrons transferred through the electric wire, so it is a side reaction. That reaction we called parasitic reaction in anode. Aluminum oxidation reaction is called main reaction in anode and cathode reaction.
Figure 1 Al-air battery schematic
2.2 Polarization Performance

Based on battery fundamentals, we know there are three mean losses dominant that affect on open-circuit voltage; their relation we can show in current VS. voltage graph (Figure 2).

\[ V_{cell} = E_{ocv} - \eta_{act} - \eta_{ohm} - \eta_{conc} \]

![Figure 2 Polarization performance](image-url)
2.3 Governing Equations

2.3.1 Model Simple Schematic

Concentration is a very important parameter in batteries, it is depending on the total species flux. So, we can use governing equation to drive it.

In the geometry of Al-air battery graph (Figure 3) we can see this is two electrode battery; $S$ is the cell gap and $H$ is the cell height, and cell height should be much larger than cell gap. We put two direction coordinates on the model ($X$ and $Y$). The electrolyte enters from the bottom in laminar flow with developing boundary layer (i.e., the boundary layer thickness increases with height). The electrochemical reactions occur only on the electrode surfaces. Based this, we will control a couple basic parameters for building the model.

Figure 3 Model simple schematic
2.3.2 Fundamental Equations

The flux equation of species will include migration, diffusion and convection.

\[ N_i = -z_i u_i F c_i \nabla \phi - D_i \nabla c_i + v c_i \]  \hspace{1cm} (1)

The mass conservation is

\[ \frac{\partial c_i}{\partial t} = -\nabla N_i + R_i \]  \hspace{1cm} (2)

Because all the electrochemical reactions are on the anode, that means no reaction on electrolyte, so we can remove \( R_i \) from the equation.

Solution is electrically neutral. We can use the electrical neutral equation

\[ \sum_i z_i N_i = 0 \]  \hspace{1cm} (3)

The current density equation is depending on the motion of charge:

\[ i = F \sum_i z_i N_i \]  \hspace{1cm} (4)

In flowing electrolyte, we can use Navier–Stokes equation for the velocity relation with the pressure and time:

\[ \rho \left( \frac{\partial v}{\partial t} + v \nabla v \right) = \nabla p - \mu \nabla^2 v + \rho g \]  \hspace{1cm} (5)

When we put flux equation in mass conservation equation (Eq. [1] in Eq. [2]) we can get

\[ \frac{\partial c_i}{\partial t} + v \nabla c_i = D_i \nabla^2 c_i + z_i u_i F c_i \nabla^2 \phi + z_i u_i F (\nabla c_i) \cdot \nabla \phi \]  \hspace{1cm} (6)
When we put flux equation in current density relation (Eq. [1] in Eq. [4]) we can get

\[ i = -k \nabla \phi - F \sum z_i D_i \nabla c_i \]  

(7)

where \( k = F^2 \sum z_i^2 u_i c_i \)

From the Eq. 6 we can get an equation for charge conservation equation:

\[ -\nabla i = 0 = k \nabla^2 \phi + (\nabla) k \ast \nabla \phi + F \sum z_i D_i \nabla^2 c_i \]  

(8)

In the electrolyte bulk medium, due to the large Peclet number \( \text{Pe} = \frac{U L}{D_R} \gg 1 \), we can get \( V \gg D \); potential is linear and bulk solution concentration is constant. So, we can update Eqs. 6 and 7:

\[ v \nabla c_i = 0 \]
\[ -\nabla i = \nabla \ast k \nabla \phi = 0 \]  

(9) (10)

In the diffuse layer, the approximation of concentration will be linear (Figure 4).

Figure 4 Concentration in double layer
We can identify species concentration equation is

\[ c_i = c_{i0} + \frac{(c_{lb} - c_{i0})}{\delta} x \]  

(11)

When we update Eq. 1 with Eq. 11 and no convection in diffusion layer, we can get total flux equation related with current, concentration and bounder layer thinness:

\[ N_i = -z_i u_i F c_i \left( \frac{l_m}{k} \right) - D_i \frac{(c_{ib} - c_{i0})}{\delta} \]  

(12)

2.3.3 Boundary Conditions

In my model, there are two reactions on the anode, but from fundamental equation we only can get total flux with the cell current. So, we need to use boundary conditions which consider parasitic reaction.

In the main reaction at the anode:

\[ \sum s_{im} M_{li}^{z_l} \rightarrow n_m e^- \]

at \( x \rightarrow \delta_i \) \( c_i \rightarrow c_{lb} \)

\[ N_{im} = -\frac{s_{im} l_m}{n_m F} \]  

(13)

In the parasitic reaction at the anode:

\[ \sum s_{ip} M_{li}^{z_l} \rightarrow n_p e^- \]

at \( x \rightarrow 0 \) \( N_{ip} = -\frac{s_{ip} l_p}{n_p F} \)  

(14)

Based on this, total flux should be sum of the Eqs. 13 & 14:

\[ N_i = N_{im} + N_{ip} = -\frac{s_{im} l_m}{n_m F} - \frac{s_{ip} l_p}{n_p F} \]  

at \( x = 0 \)  

(15)
Right now we have two flux equations (12 and 15). The flux should be the same in the battery; we can get surface concentration rate:

\[
\begin{align*}
C_{i0} &= \left[ 1 + \frac{F \, i_m}{2RT \, k} \, \delta_i \right] - \frac{s_{im} \, i_m}{n_m \, F} - \frac{s_{ip} \, i_p}{n_p \, F} \\
C_{ib} &= \frac{D_i - C_{ib}}{\delta_i} \left[ 1 - \frac{F \, i_m}{2RT \, k} \, \delta_i \right]
\end{align*}
\]

From this equation we can see relation of surface concentration with respect to main reaction current, parasitic current, conductivity, and boundary layer thickness.

### 2.4 Effect of Gas Bubble Generation

My research focuses on the parasitic reaction, so hydrogen bubble generation is very important parameter effect of battery performance. During my research, hydrogen bubble will affect battery boundary layer thickness, conductivity, surface concentration and bubble coverage of electrode (Figure 5).
2.4.1 Boundary Layer Thickness

For battery boundary layer thickness, we normally used convection from electrolyte flow to calculate (Pickett, 1979):

$$\delta_c = 1.08Sc^{-1/3}Re_y^{-1/2}y^{0.95}S^{0.05}$$  \hspace{1cm} (17)

where $\delta_c$ denotes convection from diffusion boundary layer thickness, $Sc$ denotes Schmidt number and $Re$ denotes Reynolds number.

$$Re = \frac{UL\rho}{\nu}$$  \hspace{1cm} (18)
where \( \rho \) denotes density, \( U \) denotes velocity, \( L \) denotes linear dimension and \( V \) denotes kinematic viscosity.

\[
S_c = \frac{\mu}{\rho D}
\]  
(19)

where \( \mu \) denotes dynamic viscosity \( \text{kg/m}^2\text{s} \), \( \rho \) denotes density and \( D \) denotes mass diffusivity \( \text{m}^2/\text{s} \).

If we consider there are some bubbles in the diffuse layer adhering on the electrode surface, we need to think about micro-convection effect from gas evolution (Janssen, 1973):

\[
\delta_b = \alpha \dot{V}_g^m = 0.0103 \star | t_p |^{-0.36}
\]  
(20)

\( \delta_b \) denotes boundary layer thickness due to micro-convection near a bubble generation surface, \( m \) denotes empirical constant and \( \dot{V}_g \) denotes rate of bubble generation.

For the final boundary layer thickness, we should use root mean square to combine the boundary layer thickness from electrolyte flow convection and boundary layer thickness from gas evolution micro-convection (Vogt, 1978):

\[
\frac{1}{\delta_i} = \sqrt{\left( \frac{1}{\delta_c} \right)^2 + \left( \frac{1}{\delta_b} \right)^2}
\]  
(21)

Final form of the boundary layer thickness should be

\[
\delta_i = \frac{\delta_c \delta_b}{(\delta_c^2 + \delta_b^2)^{1/2}}
\]  
(22)

2.4.2 Conductivity

For the conductivity, if we consider hydrogen bubble, that means there are some gas bubbles in the electrolyte flow. These bubbles will be decreased by ion movement (Figure 6).
We should use Bruggeman relation for define gas fraction effect on conductivity (Bruggemann, 1935):

\[
k(y) = k^0[1 - f(y)]^{1.5}
\]  

(23)

where \( k(y) \) denotes effective conductivity at height \( y \), \( k^0 \) denotes conductivity of gas-free electrolyte and \( f(y) \) : axial position-dependent gas fraction of the electrolyte (Tobias, 1959):

\[
f(y) = \frac{\rho_{gas}^{-1} S n F V_b}{\int_0^h i_p(y) dy}
\]  

(24)

\( \rho_{gas} \) denotes density of the generated gas, \( h \) denotes height at which the void fraction is evaluated, \( i_p \) denotes function of the electric field, that is affected by \( f(y) \) and \( V_b \) denotes rising velocity of the bubbles in flowing electrolyte:

\[
V_b = v_b + v
\]  

(25)

\( v \) denotes fluid velocity and \( v_b \) denotes bubble rising velocity in stagnant by Stoke’s law:

\[
v_b = \frac{\rho g d_{bubble}^2}{18 \mu}
\]  

(26)
2.4.3 Surface Concentration

In the battery, electrolyte solution should be separated to two parts: one of the parts is bulk solution and another part is diffuse layer. In the bulk solution, species concentration is constant value. In diffuse layer, due to mass transfer, surface concentration should be smaller than bulk concentration (Figure 7). Relation shown in Eq. (11).

In Eq. (11), we can see surface concentration will depend on bulk concentration and boundary layer thickness. From Eq. (20) and Eq. (22) we can know boundary layer thickness will depend on the parasitic current density. So, in different current density, surface concentration should be different.

From Eq. (16) we can see relation of surface concentration with respect to parasitic current density. Based on the kinetic equation for the side reaction:

\[ i_p = i_{po} \left[ -\exp\left(-\beta_p n_p \left( \frac{F}{RT_p} \right) \eta_p \right) \right] \]
\[ \beta_p \] denotes Cathodic transfer coefficient, \( n_p \) denotes Number of electrons transferred, and \( \eta_p \) denotes Overpotential of the parasitic reactions. Parasitic current density is due to the parasitic exchange current density. That means when the exchange current density changes, surface concentration will be changed. But in the different surface concentration, exchange should be different. Most people fixed corrosion rate in the battery model, but it’s not correct. Because surface concentration will be changed with the current density, that means exchange current density and corrosion rate should affect each other.

I used a former student’s experiment result to update the relation between the surface concentration and corrosion rate (Kaustubh, 2017).

In his experimental (Figure 8), he used aluminum foil in the different concentration KOH solution; the hydrogen will be collected by drum. He controls the time and calculates the hydrogen volume flow rate:

\[
\frac{I}{A} = \frac{2PVF}{RTA}
\]  

(28)

\( P \) denotes Pressure, \( V \) denotes Volume rate, \( F \) denotes Faraday’s constant, \( R \) denotes ideal gas constant, \( T \) denotes temperature and \( A \) denotes electrode area. We can use Eq (28) to get the relation between parasitic current density and KOH concentration (Figure 9).
Experimental setup

Al foil (4cm x 4cm) + 20 ml electrolyte

Figure 8 Kaustubh experimental setup

Experimental results

Figure 9 Experimental results

$$y = 0.0924e^{0.4761x}$$
Because his experimental is based on open-circuit voltage condition, we can calculate parasitic overpotential by equilibrium potential different between the parasitic reaction and main reaction:

\[ \eta_p = E_p^{eq} - E_m^{eq} \]  

This means except for parasitic current density and parasitic exchange current density, other values in Eq. (27) are constants. We can get exchange current density in different KOH concentrations from this experimental result:

\[ i_p = i_{po}[\text{Constants}] \]  

2.4.4 Bubble Coverage

From the parasitic reaction equation, we know when aluminum corrodes, there is some hydrogen product. When the hydrogen goes of the aluminum, it forms bubbles in the electrolyte.

For the micro-condition (Figure 10), bubbles have four process stages: nucleation, growth, detachment and rise. When the bubble forms before detachment from the electrode, it will adhere on the electrode surface and cover the electrode surface; we call this is bubble coverage. Bubble detachment will be due to a couple different force balance.
If we want to calculate bubble coverage, we should use number of bubbles on the electrode surface times each bubble occupy area and then divide electrode area:

$$\Theta = \frac{Z \times \pi \times R_0^2}{A} \quad (31)$$

First, we need to focus on the one bubble on the electrode. Due to the bubble growing with the time, $R(t)$ denotes bubble radius of the function of $t$; $R_0$ denotes the occupy circle area radius; $Z$ denotes number of bubbles (Figure 11).
From Figure 12, we can easily define the relation between the bubble radius and occupy area radius:

\[ R_0 = R \sin(\theta) = RK \]

(32)

\[ K = |\sin(\theta)| \]
If we put Eq. (32) into the Eq. (31) and calculate average time with integral area, we can get

$$\Theta = \frac{z}{Atr} \int_0^{t_r} \pi * [KR(t)]^2 dt$$

(33)

Because bubble radius’s square increases with the time, we can use Fourier number to be the relation between the bubble radius and time (Vogt, 2017)

$$F_o = \frac{Dt}{R^2}$$

(34)

After putting Eq. (34) into Eq. (33) we can get

$$\Theta = \frac{\pi}{2} K^2 * R^2 * \frac{z}{A}$$

(35)

Right now, we need to define the number of the bubbles. Because total hydrogen volume is equal to the number of bubbles times each bubble volume, and bubble shape is a sphere:

$$V_G = z * \frac{v_{bubble}}{t} = z * \frac{1}{6t} \pi d^3$$

(36)

Because I used steady-state condition in my modeling, so I replaced time to be the Fourier number, which means putting Eq. (34) and Eq. (36) in Eq. (35) get the final form equation of the bubble coverage:
\[ \Theta = 3K^2 \times \left( \frac{R_r}{d} \right)^4 \times d \times \frac{V_G}{A} \times \frac{F_0}{D} \]  

(37)

In this equation we can see there are five different parameters to define the bubble coverage (Table 1):

### Table 1

**Bubble Coverage Effect Parameters**

<table>
<thead>
<tr>
<th></th>
<th></th>
<th>Contact angle $\Theta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>$K = \sin(\Theta)$</td>
<td></td>
</tr>
<tr>
<td>(2)</td>
<td>$\frac{d}{R_r} = \left[ 2 \times (1 + \cos\theta)^2 (2 - \cos\theta) \right]^{\frac{1}{2}}$</td>
<td>Bubble volume balance</td>
</tr>
<tr>
<td>(3)</td>
<td>$d = \sqrt{C_1 \times \left[ \sqrt{1 + \left( \frac{C_{d,1}}{1 + \sqrt{\Theta}} \right)^2 - \frac{C_{d,2}}{1 + \sqrt{\Theta}} \right]^2}$</td>
<td>Detachment diameter determined by force balance</td>
</tr>
<tr>
<td>(4)</td>
<td>$PV = nRT \quad n = \frac{i}{p} \quad \frac{V_G}{A} = \frac{i_{p} \text{ RT}}{F} \quad (\text{cm/s}) \quad i_{p} = 0.255 + 0.04^{<em>}\exp(1.13^{</em>}C_{D}^{<em>}A^{</em>})$</td>
<td>Bubble generation rate/ electrode area</td>
</tr>
<tr>
<td>(5)</td>
<td>$F_0 = \frac{\pi}{2a} \left( \frac{L}{4 - \pi} \right)^{\frac{1}{2}}$</td>
<td>Fourier number $F_0$ /diffusion coefficient</td>
</tr>
</tbody>
</table>

$\Theta$ is the contact angle.
2.5 Bubble Coverage Calculation

2.5.1 Contact Angle

Contact angle is the geometry of the liquid and solid angle which is determined by three phases (liquid, gas and solid) of interfacial tensions. For the normal contact angle, we also used a liquid drop on the solid surface (Figure 13).

![Figure 13 Liquid drop contact angle](image)

From Young equation:

\[
\gamma_{SG} - \gamma_{SL} - \gamma_{LG} \cdot \cos \theta = 0
\]  

(38)

\(\gamma_{LG}\) denotes liquid-gas, \(\gamma_{SL}\) denotes solid-liquid and \(\gamma_{SG}\) denotes solid-gas. In my modelling, it is the gas bubble on the solid surface.

Interfacial tensions force relation is (Figure 14).

\[
cos \theta = \frac{\gamma_{SG} \cdot \gamma_{SL}}{\gamma_{LG}}
\]  

(39)
Because I used flowing electrolyte, I need to consider bubble inclination angle, advancing angle and receding angle. I used Herry's experimental result (Herry, 1986; Figure 15). Herry's (1986) measurement bubble inclination angle in different velocity as this result.

Figure 14 Gas bubble contact angle

Figure 15 Inclination angle experimental
I used this result (Figure 16) to get the relation between the velocity and inclination angle as

\[
\text{Inclination angle} = 107.922 - \frac{998.3894}{\text{velocity}} + 9.251839
\]  

(40)

When the bubble is in flowing fluid, the largest contact angle is advancing angle \( \theta_a \), and the smaller contact angle is the receding angle \( \theta_r \). The inclination angle hysteresis is \( \theta_a - \theta_r \) (Figure 17).
We can show the relation by:

\[ \theta_a - \theta_r = \theta_{in} \]  \hspace{1cm} (41)

When the bubble is in stagnant fluid, advancing angle and receding angle are the same with contact angle:

\[ \theta_a + \theta_r = 2\theta_c \]  \hspace{1cm} (42)

After combining Eq. (41) and Eq. (42) we can get the advancing angle and receding equation with respect to contact angle and inclination angle:

\[ \theta_a = \theta_c + \frac{1}{2} \theta_{in} \]  \hspace{1cm} (43)

\[ \theta_r = \theta_c - \frac{1}{2} \theta_{in} \]  \hspace{1cm} (44)

I used the Jacob and Krevelen drives in the Young’s equation (Jacob, 1985-2004; Krevelen, 1976):
When I put Eq. (43) and Eq. (44) in the Eq. (45), I can solve the contact angle with respect to fluid velocity (Figure 18).

\[
\theta_c = \arccos \frac{r_a \cos \theta_a + r_r \cos \theta_r}{r_a + r_r}
\]

\[
r_a = \left( \frac{\sin^3 \theta_a}{2 - 3 \cos \theta_a + \cos^3 \theta_a} \right)^{\frac{1}{3}}
\]

\[
r_r = \left( \frac{\sin^3 \theta_r}{2 - 3 \cos \theta_r + \cos^3 \theta_r} \right)^{\frac{1}{3}}
\]

When I put Eq. (43) and Eq. (44) in the Eq. (45), I can solve the contact angle with respect to fluid velocity (Figure 18).

![Figure 18 Bubble coverage VS. velocity](image)

In the graph, we can see bubble contact angle will increase with velocity. I used fundamental equation to explain that (Figure 19):

\[
\gamma_{LG} \cos \theta = \gamma_{SG} - \gamma_{SL}
\]

(46)
In the stagnant fluid, Eq. (46) is the three interfacial tensions relations. If we add the velocity in the fluid, that means there is drag force on the bubble (Figure 20).

And interfacial tension force relations should be

\[
\gamma_{LG} \cos \theta = \gamma_{SG} - \gamma_{SL} - \gamma_F
\]  

(47)

Where \( \gamma_F \) denotes tension force from the drag force. Compare Eq. (46) and Eq. (47), if three-phase tension forces do not change and the tension force from the drag is large than 0, we can
find \( \cos \theta \) will be smaller. That means flow fluid \( \theta \) should be larger than stagnant fluid \( \theta \) (0 < \( \theta < 90 \)).

2.5.2 Bubble Volume Balance

From Eq (37), we know if we want to calculate bubble coverage we need to know \( R/d \); \( R \) is radius and \( d \) is detachment diameter. We can use volume balance to calculate this relation.

I used integral horizontal section area by bubble vertical direction to calculate bubble volume with contact angle. The schematic graph is Figure 21.

![Figure 21 Bubble volume with contact angle](image)

From the graph, we can used \( \pi x^2 \) to denote section area, and the vertical direction basic on the geometry calculation, we can know it is \([-r \cos \theta, r]\). We can write the volume of bubble equation as
We can replace x by the sphere expression equation:

$$x^2 = r^2 - y^2$$  \hspace{1cm} (49)

So, the final equation form of volume of bubble with contact angle is

$$V = \frac{\pi}{3} r^3 (1 + \cos \theta)^2 (2 - \cos \theta)$$  \hspace{1cm} (50)

That volume can be used to calculate bubble right before detachment (Figure 22).

![Figure 22 Bubble before detachment](image)

When the bubble is right after detachment (Figure 23), bubble volume can be defined by the sphere volume equation:

$$V = \frac{4}{3} \pi \left( \frac{d}{2} \right)^3 = \left( \frac{1}{6} \right) \pi d^3$$  \hspace{1cm} (51)
When we consider the moment on the bubble detachment, that means at the
detachment equilibrium, volume before the detachment should approximate the volume after
the detachment [Eq. (50) = Eq. (51)].

After solving we can get the detachment diameter divided before detachment radius
relation with the contact angle:

$$\frac{d}{R} = \left[2 \times (1 + \cos \theta)^2(2 - \cos \theta)\right]^\frac{1}{3} \quad (52)$$

2.5.3 Detachment Diameter Determined by Force Balance

When the bubble in the electrolyte adheres on the electrode surface, there is a lot of
force acting on it. But there are couple of main forces (Vogt, 2000); first is difference between
gravitational force and buoyancy force:

$$F_1 = F_{Buoy} - F_{Grav} \quad (53)$$
We can use gravity constants times density of the liquid and volume of bubble for buoyance force:

$$F_{Buoy} = g\rho_L V_{bubble}$$  \hspace{1cm} (54)

And with almost the same equation we can get gravitational equation:

$$F_{Grav} = g\rho_G V_{bubble}$$  \hspace{1cm} (55)

Putting Eq. 54 and 55 in Wq. 53 and replacement volume by Eq. 50 we can get the final form:

$$F_1 = g(\rho_L - \rho_G)\frac{1}{3}\pi R^3 (1 + \cos\theta)^2 (2 - \cos\theta)$$  \hspace{1cm} (56)

The second force is drag force:

$$F_D = C_D \frac{\rho v^2}{2} A_S$$  \hspace{1cm} (57)

Area $A_S$ can be calculated by the sphere projection area with contact angle; from the graph (Figure 24) we can know the shadow read is

$$\pi r^2 \left( \frac{\theta}{\pi} - \frac{\sin\theta \cos\theta}{\pi} \right)$$  \hspace{1cm} (58)
The sphere projection area with contact angle can use circle area $\pi r^2$ subtract to shadow area:

$$A_S = \pi r^2 - \pi r^2 \left( \frac{\theta}{\pi} - \frac{\sin \theta \cos \theta}{\pi} \right)$$

(59)

After replay $C_D$ to be drag number and $A_S$ in the equation:

$$F_2 = \xi \frac{\rho L V^*}{2} \pi R^2 \left( 1 - \frac{(\theta - \cos \theta \sin \theta)}{\pi} \right)$$

(60)

The drag number is

$$\xi = \frac{20}{Re} \left( \frac{1}{1 + \sqrt{\Theta}} \right)$$

(61)

The average flow velocity at the adhering bubble can be

$$V^* = \frac{1}{H} \int_0^H \nu \ dy$$

(62)

$H$ denotes the bubble height:
At laminar flow the mean velocity $\bar{v}$ in an rectangular flow channel is

$$\frac{v}{\bar{v}} = \frac{y}{Y}$$  \hspace{1cm} (64)

$Y$ is the electrode-membrane distance, $v$ is local velocity and $y$ is the distance from the electrode surface. When we put Eq. (63) and Eq. (64) into Eq. (62):

$$V^* = 3\bar{v} \frac{R}{Y} (1 + \cos\theta)$$  \hspace{1cm} (65)

Rewriting Eq. (60) by Eq. (61) and Eq. (65):

$$F_2 = \frac{15\pi R^2 \eta L^p}{Y} \left( \frac{1}{1+\sqrt{\theta}} \right) (1 + \cos\theta) \left( 1 - \frac{(\theta - \cos\theta \sin\theta)}{\pi} \right)$$  \hspace{1cm} (66)

The third force is interfacial tension force at the electrode surface (adhesive force).

The perimeter (Figure 25) of the occupied is:

$$2\pi R \sin\theta$$  \hspace{1cm} (67)

Figure 25 Occupied bubble perimeter
The surface tension force is

\[ 2\pi R \sin \theta \gamma \]  \hspace{1cm} (68)

So, the surface tension force in parallel to surface is

\[ 2\pi R \sin \theta \gamma \cos \theta \]  \hspace{1cm} (69)

Because we used flowing electrolyte, we need to consider advancing angle and receding angle.

Net surface tension force in parallel to surface (Figure 27)

\[ 2\pi R \sin \theta \gamma (\cos \theta_r - \cos \theta_a) \]  \hspace{1cm} (70)

Figure 26 Inclination angle

After we consider the Y component (Figure 27), net surface tension force is

\[ F_3 = 2\pi R \sin \theta \gamma (\cos \theta_r - \cos \theta_a)K \]  \hspace{1cm} (71)
Figure 27 Y component

At detachment equilibrium:

\[ F_1 + F_2 = F_3 \]  \hspace{1cm} (72)

Putting Eq. 56, 66 and 71 in Eq. 72 and calculating detachment diameter of the bubble:

\[ d = \sqrt{C_1} \times \left[ 1 + \left( \frac{c_2V}{1+\theta} \right)^2 - \frac{c_2V}{1+\theta} \right] \]

where

\[ C_1 = 12 \frac{R_r g(\rho_L - \rho_G)}{\sin \theta (\cos \theta_r - \cos \theta_a)K_2} \]

\[ C_2 = \frac{45 \eta_L}{\sqrt{C_1} (\rho_L - \rho_G)} \left( \frac{R_r}{d} \right)^2 \left( 1 + \cos \theta \right) \left( 1 - \frac{\theta - \cos \theta \sin \theta}{\pi} \right) \]

### 2.5.4 Bubble Generation Rate

From the ideal gas law and Faraday constant equation:

\[ PV = nRT \ (n \text{ is mole/s}) \]  \hspace{1cm} (74)

\[ I = nF \]  \hspace{1cm} (75)

Because each hydrogen ion has two electrons, so Eq. (75) can written:

\[ I = 2nF \]  \hspace{1cm} (76)
Combine Eq. (74) and Eq. (76) to get parasitic current density:

\[
\frac{I}{A} = \frac{2PV_G F}{RTA}
\]  

(77)

Rewrite Eq. (77), we can get bubble generation rate with respect to the parasitic current density:

\[
\frac{V_G}{A} = \frac{i_p RT}{F p}
\]  

(78)

2.5.5 Fourier Number

From Vogt paper (2005), I know empirical relation between Fourier number and Jacob number:

\[
F_0 = \frac{\pi}{3J_a^3 \left[ 1 + \left( \pi \frac{\ln 4}{3} J_a \right)^{0.5} \right]^2}
\]  

(79)

and Jacob number can be expressed by supersaturation:

\[
J_a = \frac{R_m T}{p} \Delta C
\]  

(80)

From Vogt’s (2017) experimental result we can know the supersaturation changed with the parasitic current density (Figure 28):
Figure 28 Supersaturation VS. current density

Complete result of Fourier number in different parasitic current densities is (Figure 29):

Figure 29 Fourier number VS. current
2.5.6 Validation of Bubble-Coverage Calculation

After putting all the parameters in Eq. (37) we can get final bubble coverage data with different velocity (Figure 30).

![Velocity VS bubble coverage when $i_p = 0.02$ A/cm$^2$](image)

**Figure 30** Bubble coverage VS. velocity

I compared my result with Vogt’s experimental result (2000) and it matched up will.
2.5 Numerical algorithms

2.5.1 Flow Chart of Model

Figure 31 Flow chart of model
2.5.2 Convergent Parasitic Current Density Flow Chart

Control $i_c(i_{cell}) = 0.01\, A$

Assume $i_p = -0.2\, A$

Parasitic current density ($i_p$) convergent loop start

Calculate velocity speed between bubble and electrode

Calculate Boundary layer thickness:
- Diffusion boundary layer thickness
- Boundary layer thickness due to bubble generation surface

Conductivity calculation depend on parasitic current density

Calculate surface concentration

Overpotential of the main reactions

Calculate overpotential of the parasitic reactions

Got new parasitic reactions from Botler-Volmer eq

Parasitic current density ($i_p$) convergent loop end

Figure 32 Convergent parasitic current density flow chart
5.5.3 Convergent Surface Concentration Flow Chart

Figure 33 Convergent surface concentration flow chart
5.5.4 Two convergent Loop Result

I checked concentration effect over potential convergent loop first. From the Figure 34, we can see when this loop is running around 15 times, parasitic current density almost convergents. That means this loop works well.

And then I checked Concentration effect exchange current density loop. From Figure 35, we can see this loop running only 5 times when parasitic current density is almost convergent. This loop works.
Figure 35 Concentration convergent loop result
## Chapter 3 — RESULTS AND DISCUSSION

### 3.1 Basic Equation and parameters Used in the Modeling

Table 2 Main Equation Used in Model

<table>
<thead>
<tr>
<th>Overall equation</th>
<th>Open circuit voltage</th>
<th>Activity loss</th>
<th>Concentration loss</th>
<th>Omics loss</th>
</tr>
</thead>
<tbody>
<tr>
<td>( V_{cell} = E_{OCV} - \eta_{act} - \eta_{conc} - \eta_{ohm} )</td>
<td>( E_{OCV} = E_{eq}^c - E_{m} + E_{p}^q )</td>
<td>( \eta_{act} = \eta_{m} - \eta_{p} + \eta_{c} )</td>
<td>( \eta_{conc} = \eta_{conc,k} + \eta_{conc,N} )</td>
<td>( \eta_{ohm} = i_{cell} \times \frac{V}{R} )</td>
</tr>
<tr>
<td>Equilibrium potential of Anode</td>
<td>( E_{eq}^c = E_{eq}^c - E_{p}^q )</td>
<td>( i_p = i_{pol} \times \exp(-\beta_{p} \eta_{p} \eta_{p}) )</td>
<td>( \eta_{conc,k} = \frac{1}{anf} \ln(1 - \frac{j}{J_{lim}}) )</td>
<td>Conductivity</td>
</tr>
<tr>
<td>Equilibrium potential of Cell</td>
<td>( E_{eq}^c = E_{eq}^c - E_{eq}^A = E_{OCV} )</td>
<td>( i_{lim} = \frac{F D C_{eq}^1}{\delta_{A} (1 - \frac{\delta_{f}}{\delta_{A}}) \eta_{A}} )</td>
<td>( \eta_{conc,N} = \frac{1}{nf} \ln(1 - \frac{j}{J_{lim}}) )</td>
<td>Cell current density</td>
</tr>
<tr>
<td>Open circuit voltage</td>
<td>( C_{OH}^{-} )</td>
<td>( C_{A}^{\text{eq}}_{ion} )</td>
<td>( i_{lim} = \frac{F D C_{eq}^1}{\delta_{A} (1 - \frac{\delta_{f}}{\delta_{A}}) \eta_{A}} )</td>
<td>( i_{cell} = i_{lim} + i_p )</td>
</tr>
<tr>
<td>Activity loss</td>
<td>Concentration loss</td>
<td>Omics loss</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Boundary layer thickness</td>
<td>( C_{OH}^{-} = 1 - \frac{i_p + 4i m}{F \delta_{OH}} )</td>
<td>( \delta_{c} = 1.08SC^{-1/3}Re_{y}^{-1/2}y_{0.95} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Limiting current</td>
<td>Conductivity</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( C_{OH}^{-} = 1 - \frac{i_p + 4i m}{F \delta_{OH}} )</td>
<td>( \delta_{b} = 0.0103 )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Boundary layer thickness</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Equations Explained

- **Open circuit voltage**:
  \( E_{OCV} = E_{eq}^c - E_{m} + E_{p}^q \)

- **Activity loss**:
  \( \eta_{act} = \eta_{m} - \eta_{p} + \eta_{c} \)

- **Concentration loss**:
  \( \eta_{conc} = \eta_{conc,k} + \eta_{conc,N} \)

- **Omisión loss**:
  \( \eta_{ohm} = i_{cell} \times \frac{V}{R} \)

- **Equilibrium potential of Anode**:
  \( E_{eq}^c = E_{eq}^c - E_{p}^q \)

- **Equilibrium potential of Cell**:
  \( E_{eq}^c = E_{eq}^c - E_{eq}^A = E_{OCV} \)

- **Limiting current**:
  \( i_{lim} = \frac{F D C_{eq}^1}{\delta_{A} (1 - \frac{\delta_{f}}{\delta_{A}}) \eta_{A}} \)

- **Boundary layer thickness**:
  \( \delta_{c} = 1.08SC^{-1/3}Re_{y}^{-1/2}y_{0.95} \)
### Table 3

Parameter Used in Model

<table>
<thead>
<tr>
<th>Parameters used in the modeling for pure aluminum in B300 cell</th>
<th>Main</th>
<th>Parasitic</th>
<th>Cathode</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature = 333K</td>
<td>$i_{mo} = 1.371 \times 10^{-2} \text{A/cm}^2$</td>
<td>$i_{po} = 1.119 \times 10^{-2} \text{A/cm}^2$</td>
<td>( \eta_c ) = (-0.29279 )</td>
</tr>
<tr>
<td>$C_{OH^-} = 5 \text{M}$</td>
<td>$\beta_m = 0.9804$</td>
<td>$\beta_m = 0.0591$</td>
<td>(-0.025096 \log(i_c \times 1000) )</td>
</tr>
<tr>
<td>$C_{Al(OH)_4} = 0.5 \text{M}$</td>
<td>$\alpha_m = 0.07956$</td>
<td>$\alpha_m = 0.9409$</td>
<td>(-0.203429 \times i_c )</td>
</tr>
<tr>
<td>$D_{OH^-} = 5.26 \times 10^{-5} \text{cm/s}$</td>
<td>$\lambda_m = 0.5$</td>
<td>$\lambda_m = 1$</td>
<td>( i_c \text{ in A/cm}^2; \ \eta_c \text{ in V} )</td>
</tr>
<tr>
<td>Electrolyte conductivity = 0.8 (Ωcm)$^{-1}$</td>
<td>Height = 17cm</td>
<td>Density = 1.15 g/cm$^3$</td>
<td></td>
</tr>
<tr>
<td>Viscosity = 0.008 g/(cm*s)</td>
<td>Cell gap = 0.2cm</td>
<td>Electrolyte velocity = 8.5 cm/s</td>
<td></td>
</tr>
<tr>
<td>Density = 1.15 g/cm$^3$</td>
<td>$\delta_m = 1$</td>
<td>$n_m = 1$</td>
<td></td>
</tr>
<tr>
<td>Viscosity = 0.008 g/(cm*s)</td>
<td>$n_m = 1$</td>
<td>$n_m = 1$</td>
<td></td>
</tr>
<tr>
<td>$\delta_m = 1$</td>
<td>$n_m = 1$</td>
<td>$n_m = 1$</td>
<td></td>
</tr>
<tr>
<td>$E_{eq}^{m} = -2.4403$</td>
<td>$E_p^{eq} = -0.9058 \text{V}$</td>
<td>$E_c^{eq} = 0.2857$</td>
<td></td>
</tr>
<tr>
<td>$E_a = 0 \text{V}$</td>
<td>$\Delta U_p = 1.5345$</td>
<td>$\Delta U_c = 2.726$</td>
<td></td>
</tr>
</tbody>
</table>
3.2 Validation of Developed Model

In my research, I separate three stages. For the first stage I developed a basic Al-air battery model (no bubble effect) and then include parasitic reaction in the model by considering change of boundary layer thickness and conductivity. For the second stage, I implemented the effect of OH\(^-\) concentration on side reaction through experimental results, finding the best concentration for the cell performance. At the third stage, I implemented the bubble coverage effect into the model by combining stagnant model and flowing electrolyte effect. Final goal is conducting the effects of cell design variables (cathode electrode material, electrolyte flow rate, cell gap and height, and concentration) to provide guideline to the cell developer.

In the Figure 36, **Stage 1** is effect of parasitic current that was included; **Stage 2** is effect of OH\(^-\) surface concentration on parasitic current that was included into stage 1 model; **Stage 3** is bubble coverage on anode that was included into stage 2 model.

If we compare stage 1 and stage 2, we can find cell performance is increased, because we include OH\(^-\) surface concentration is lower than the bulk solution. This means corrosion rate is decreased when we consider surface concentration effect parasitic current.

When we see stage 3, we can find cell performance is decreased a lot. Because bubble coverage is blocks part of the electrode reaction, but stage 3 matches the experimental results well (Savinell and Chan, 1991).
Figure 36 Different stage I, V graph
3.3 Performance Analysis with Respect to Ideal Case

When we compare with base model (no corrosion effect) and final model (Figure 37), we can see cell performance is decreased a lot. We can use polarization performance to explain this decrease: open-circuit voltage, kinetic losses, Ohmic losses and mass transfer losses.
3.3.1 Open-Circuit Voltage

For the basic open-circuit voltage calculation, we used equilibrium potential difference between anode (main reaction) and cathode:

\[ E_{ocv} = E_{c}^{eq} - E_{m}^{eq} \]  \hspace{1cm} (81)

But when we consider corrosion reaction, we need to use equilibrium potential difference between main reaction and parasitic reaction to be anode equilibrium potential:

\[ E_{ocv} = E_{c}^{eq} - (E_{m}^{eq} - E_{p}^{eq}) \]  \hspace{1cm} (82)

That is the main reason for the cell voltage decrease.

3.3.2 Kinetic Losses

If we compare basic model kinetic losses and final model kinetic losses, we can see final kinetic losses are larger than basic. This difference is due to the bubble coverage (Figure 38).
Figure 38 Compare Kinetic losses

When I used final model, kinetic losses subtract base model kinetic losses (Figure 39), and we can find when current density increases, their difference is decreased. Its means bubble coverage is decreased when current density increases.
From bubble coverage Eq. (37), we know $K$ & $\frac{d}{R_r}$ is determined by contact angle; $d$ and $F_0$ determined by flow velocity and $V_G$ is determined by parasitic current density. So, we can say bubble coverage is determined by contact angle, bubble generation and flow velocity (Figure 40).
Figure 40 Effect bubble coverage
3.3.2.1 Contact angle

I fixed another perimeter, only control contact angle, and got the bubble coverage in different contact graph (Figure 41). When contact angle is smaller, that means material is hydrophilic and bubble coverage decreases. When contact angle is larger, that means material is hydrophobic and bubble coverage increases.

Figure 41 Contact angle effect bubble coverage
3.3.2.2 Bubble Generation and Flow Velocity

I checked bubble coverage in different current density and fluid velocity. From the graph (Figure 42), when velocity increased, bubble coverage decreased. When current density increased, bubble coverage decreased, because parasitic current density will decrease when current density increases (Figure 43).

Figure 42 Velocity and current density effect bubble coverage
And from equation (78) we can know the relation between the bubble generation and parasitic is direct proportion.
3.3.3 Ohmic losses

Final model Ohmic losses are larger than basic model because as hydrogen bubble impedes ion movement, conductivity decreases (Figure 44).

![I, V graph](image.png)

Figure 44 Ohmic losses VS. current density

I also checked the Ohmic losses difference between the final model and basic model (Figure 45), when the current density was smaller than 0.28 A/cm²; their difference is increased with current density. When the current density is larger than 0.28 A/cm², their difference is decreased with current density. The reason of decrease is parasitic current density
is decreased when current density increases, which means bubble generation is decreased and conductivity decreased slower. The reason for increase needs further study.

**Figure 45** Difference Ohmic losses
3.3.4 Mass Transfer Losses

Due to the micro-convection effect from gas evolution, boundary layer thinness will be thinner. That means mass transfer flux should be larger and surface concentration will be larger (Figure 46). That is the reason final model mass transfer is smaller than basic model mass transfer.

![Graph showing mass transfer losses versus current density](image)

**Figure 46** Mass transfer losses VS. current Density
3.3.5 Current Efficiency

We calculate current efficiency by

\[
Efficiency = \frac{cell \ current - parasitic \ current}{cell \ current}
\]  \hspace{1cm} (83)

In the efficiency graph (Figure 47), we can know when cell voltage larger cell current is decreased, and parasitic current is increased. Parasitic current will be the maximum at OCV condition and decreased as cell current increased. High current efficiency will be in the low cell voltage because at low cell voltage, cell current density is larger and parasitic current density is smaller.

Final model (velocity = 8 cm/s, cell gap = 0.2 cm, height = 17 cm)

Figure 47 Current and cell efficiency
4.1 Summary and conclusions

In this research, I developed a physics-based mathematical model of aluminum air battery. This model includes all the equations drive progress; it is easy to control parameter and to find each factor relation. I used experimental results data in my model and I also compared my main result with experimental data, in specific, the research done by analyzing the effect of hydrogen evolution on corrosion reaction, electrolyte conductivity, ionic species flux (boundary layer thickness), and active area of electrode (bubble coverage). The research also analyzed the parameters to control hydrogen evolution, including the pH condition, flow rate, cell gap, and length of electrode. Additionally, the research analyzed the cell parameters and operating condition, including cell gap, height, concentration, flow rate, etc, for the best performance.

For my analysis result, I find hydrogen generation rate affects battery performance a lot and bubble coverage is the main factor. Based on my modeling result, there are three ways to reduce bubble coverage for increase in battery performance. First is we can use high-velocity flow rate; second is to use low-concentration electrolyte, and third way to use hydrophilic anode material (make contact angle smaller).
4.2 Future Work

Based on my analysis result, we can use three ways to reduce bubble coverage for increase in battery performance, but these ways still need to consider side effect. If we used high-velocity flow rate, that means we need to use more power from pump; it will decrease total battery efficiency. If we used low-concentration electrolyte, bubble generation is decreased, also main reaction is decreased. Using hydrophilic anode material can make contact angle smaller, but that means we need to consider new reaction between anode and electrolyte.

In the future work I will find optimization for different battery materials, like aluminum alloys anode, different electrolyte and corrosion-protection additives. And base on these material change, I will also find operating condition (velocity of electrolyte, concentration of electrolyte, cell current).
REFERENCES


