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CURRENT EFFICIENCY PREDICTIVE MODEL AND ITS CALIBRATION AND VALIDATION

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Abstract

Current efficiency is one of the most important technical and economic parameters. Current efficiency loss is due to dissolved aluminum reacting with the anode bubbles by the back reaction, which is assumed to be responsible for the largest part of current efficiency loss in Hall-Héroult aluminum reduction cells. The magnetichydrodynamics flow in cells can be seen as a gas-liquid-liquid flow by neglecting the mina effect of alumina particles. An current efficiency predictive model (CEPM) was developed based on multiphase multicomponent flow. The model takes the flow in cells as a three-phase(the bath, the metal, and the anode bubbles) and multicomponent problem(the bath phase: bath species and dissolved Al species; the anode-bubble phase:CO_2 and CO), which is able to incorporate the mechanism of current efficiency loss in cells. The model was calibrated by a 160kA cell and validated by a 300kA cell. This study provides a new approach for predicting current efficiency of aluminum reduction cells.

Introduction

Primary aluminum is obtained by a complex process of electrochemical reduction of alumina. Direct current flows through the anode, the bath, the metal pad and the cathode carbon. The bath floats on the surface of the metal because of density difference. Both the bath and the metal are driven by the magnetic force. The anode bubbles are generated on the anode surface and escape from the bath surface. As a result the flow in cells can be treated as a gas-liquid-liquid three-phase flow by neglecting the mina effect of alumina particles.

The published papers about numerical simulation of flow field in cells mostly treated the flow as a two-phase flow [1-6] or "shallow layer model"[7,8]. For the first case, the multiphase flow in the cells was simplified as a gas-liquid [1,2] or liquid-liquid[3-6] flow. The gas-liquid model took the interface of bath-metal as symmetry or moving wall by representing the metal flow. Homogeneous or inhomogeneous two-phase flow was developed to track the interface of bath-metal. The liquid-liquid model neglected the driven force of the anode bubbles. The "shallow layer model" partitioned the flow field as two/three layers to simplify the flow as a single phase or two-phase flow [7,8]. The "shallow layer model" assumed that the horizontal dimensions were much larger than the typical depth for each of the layers and the interface deformation was small relative to the depth.

The effect of the anode bubbles, the bath and the metal as well as the inter-phase moment exchange is important for the flow in cells.

As the development of Computational Fluid Dynamics (CFD), some researchers focus on the three-phase flow in cells. Dagoberto et al [9] compared various methods for modeling the bath-metal interface which presented a three-phase homogeneous model. The three-phase model took the flow in cells as an open box problem, which was able to track both the air-bath interface and the bath-metal interface. The effect of anode bubbles is ignored and the model is in fact a two-phase flow. Feng et al [10] introduced moment source to take into account the driven force of the anode bubbles. Li et al [11] developed an inhomogeneous three-phase flow to model the complex flow.

Current efficiency is one of the most important technical and economic parameters. The metal will dissolve and reacts with the carbon dioxide by the back reaction, which is assumed to be responsible for the largest part of the current efficiency loss in modern Hall-Héroult aluminum reduction cells. Many researchers focus on the parameters affecting the current efficiency and strive to model the current efficiency of aluminum reduction cells. Zeng et al [12] developed a comprehensive mathematic model to describe the relationship between the current efficiency and the current distribution based on the viewpoint of zone current efficiency. Simões et al [13] studied the impact of bath ratio on current efficiency and a statistical regression analysis method was adopted to develop a model of current efficiency. Sterten et al [14] developed a current efficiency model based on the mechanism of current loss. The model didn't take into account the effect of the melts flow and the deformation of the metal-bath interface. Haarberg et al [15] introduced the effect of the anode bubbles and developed a current efficiency model as a function of cell geometry defined by the side ledge based on surface renewal theories. Li et al [11] improved the current efficiency model based on surface renewal theories, which related turbulence eddy dissipation of the metal-bath interface with local current loss.

In this paper a current efficiency predictive model (CEPM), based on multiphase multicomponent flow, was calibrated by a 160kA cell and validated by a 300kA cell. This study provides a new approach for predicting current efficiency of aluminum reduction cells.

Governing Equations and Conditions

As mentioned above the flow in cells can be treated as a gas-liquid-liquid three-phase flow. The flow can be simulated by Euler-Euler model, which treats the bath and the metal as continuous phases and the anode bubbles as a dispersed phase. The flow in cells is assumed to be isothermal. The Euler-Euler model solves one set of continuity and N-S (Navier-Stokes) momentum governing equation for each phase, the bath, the melt and the anode bubbles. Their couple is achieved through inter-phase momentum exchange terms.

The two-equation k - ε turbulence model is used for the bath, the metal and the anode bubbles, which is applicable for most of the industrial flow phenomena.

The anode bubbles' mass source S_{MSi} is determined by the Faraday's law:

$$S_{MSi} = \frac{IM_o}{4F} \tag{1}$$

Where: I is the current density. M_o is the molecular weight for the anode bubbles. F is the Faraday constant.

The inter-phase force is used to represent the momentum exchange.

- The inter-phase force between the bath and the metal. The bath and the metal are separated by a free surface, which can be regarded as a free surface flow. The bath and the metal can entrain each other by the inter-phase momentum exchange and the magnetic force. So the bath and the metal are both treated as continuous phases and a free surface flow with the inhomogeneous model is adopted to allow entrainment of one phase within another. The drag force coefficient $C_D = 0.44$.
- The inter-phase force between the anode bubbles and the bath. The inter-phase force includes drag force and non drag force. The drag force is modeled by the Ishii and Zuber drag force model, which is applicable to general fluid particles. The non-drag force includes the lift force, the virtual mass force, the wall lubrication force and the turbulence dissipation force.
- The inter-phase force between the anode bubbles and the metal. The anodes bubbles and the metal will react by the back reaction as they meet each other. As a result the inter-phase force can be neglected.

The computational zone mesh of 160kA is shown in Figure 1 and the mesh of 300kA is not shown here.

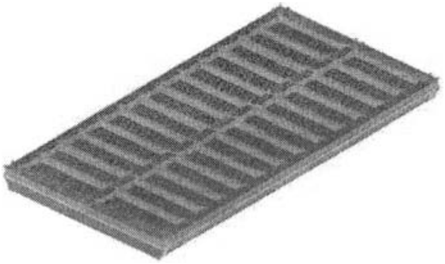

Figure 1. Physical model of the 160kA aluminum reduction cell

The Current Efficiency Predictive Model

The CEPM is based on the mechanism of current efficiency loss. From the point of current efficiency loss the possible phase or species includes: the bath phase(CO2 species, Al species and bath species), the metal phase, and the anode bubbles phase (CO2 species and CO species).

The possible back reaction includes:

1) CO2 of the anode bubbles is dissolved as a species of the bath. CO2 species of the bath reacts with Al species of the bath or the metal.

2) CO2 of the anode bubbles reacts with Al species of the bath or the metal.

Dissolvability of CO2 is as small as about 1e-6 kg/kg and the back reaction that CO2 of the bath participates could be neglected [17]. The mechanism of current efficiency loss is shown as Figure 2.

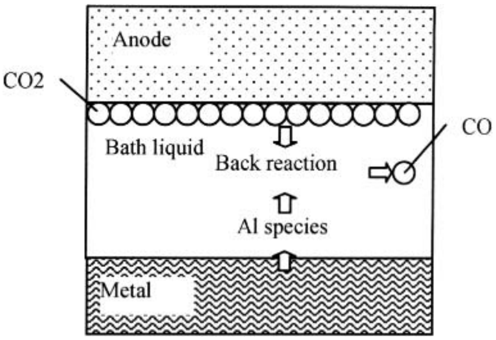

Figure 2. Process of current efficiency loss

The process of current efficiency loss can be described as follows:

1) The metal is dissolved as a species(Al species) of the bath at the bath-metal interface

This step is the law-speed step [17]. The metal dissolution rate can be expressed as:

$$Al(species) = k_c * k_f * A * (c^* - c) \tag{2}$$

Where: k_c is a constant for calibration. k_f is a dimensionless variable dependent on the turbulent flow. A is the interface area density of the bath and the metal. c^* is the saturation mass concentration. c is the mass concentration.

2) The dissolved Al species of the bath diffuses through the interface layer of the bath and the metal under the gradient of concentration difference.

3) The dissolved Al species diffuses into the bath by convective mass transfer and diffusion mass transfer. The diffusion mass transfer coefficient is as in [11].

4) The dissolved Al species and the metal react with the anode bubbles by the back reaction with quick reaction rate, which causes the current efficiency loss.

$$Al + CO_2 = CO + Al_2O_3 \tag{3}$$

According to the mentioned process the anode bubbles after back reaction is composed of CO_2 and CO. Three-phase flow as well as the mechanism is incorporated into the CEPM and solved by CFD method. As a result the current efficiency of Hall-Héroult aluminum reduction cells can be expressed as in [17]:

$$\mathrm{CE} = \frac{1}{2}\mathrm{vol.\%}CO_2 + 50 \tag{4}$$

Results and Discussion

The CEPM is based on the work of magnetic field and magnetic hydrodynamic flow field. The magnetic field was finished by ANSYS, which was not described in details. The CEPM was in corporate into the magnetic hydrodynamic flow field study. The CEPM was calibrated by the industrial current efficiency data of a 160kA cell and validated by a 300kA cell.

1) Flow Field

Velocity of middle metal pad of 160kA is shown in Figure 3. The average velocity of metal is 1.476E-1 m/s and the maximum velocity is 2.879E-1 m/s. The average velocity of the bath is

1.165E-1 m/s and the maximum velocity is 2.866E-1 m/s. The velocity of metal was validated by the measured values [18].

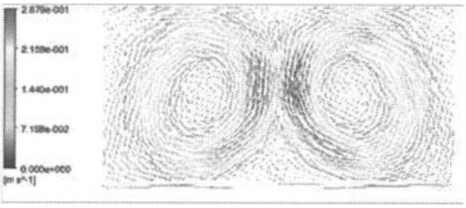

Figure 3. Velocity of the middle metal pad of 160kA

The bath-metal interface of 160kA is shown in Figure 4.

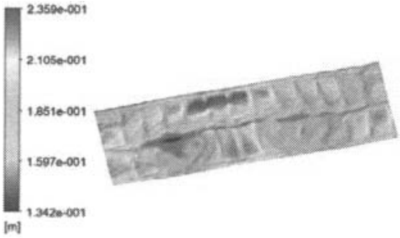

Figure 4. The bath-metal interface deformation of 160kA

The interface deformation is between –6.58e-2 m and +3.59e-2 m, which is beneficial for the stable operation and the Anode Cathode Distance (ACD) may be shortened for energy saving. It can be seen that the presence of the anode affects the bath-metal deformation.

The constant k_c in equation (5) was calibrated by industrial current efficiency date and a 160kA Hall-Héroult aluminum reduction cell. The predictive CE is 91.90% after calibration as shown in Figure 5. The industrial CE of 160kA is 91.32% by statistics and the calibration error is 0.58%.

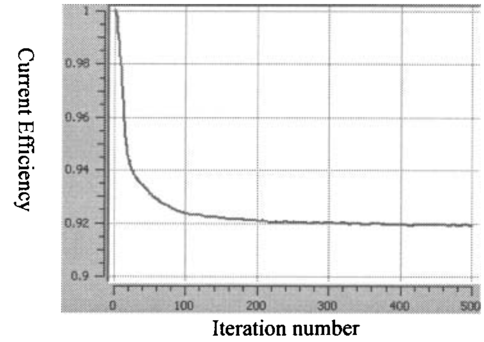

Figure 5. CE congvegence history of 160kA

The CEPM model after calibration was used to predict the current efficiency of a 300kA cell. The 300kA CE convergence history is shown in Figure 6. The predictive CE is 93.83%. The industrial CE of 300kA is 94.22% by statistics and the prediction error is 0.39%.

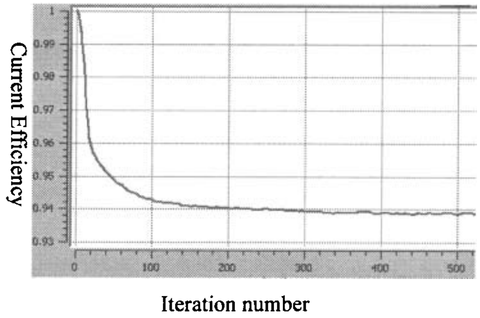

Figure 6. CE congvegence history of 300kA

Current efficiency is dependent on many factors such as bath temperature, bath properties, alumina concentration, magnetic field, flow field and so on. The most important factor is magnetic field, which affects the flow field. The published papers focused on the evaluation method of MHD instability, which was an indirect criterion. The direct judgment standard is current efficiency. The CEPM provide a direct evaluation criterion to judge the cells by current efficiency, which is one of the most important technical and economic parameters.

The CEPM is based on the mechanism of current efficiency loss and is a theoretical model. As discussed above the effect factors include many other parameters which are not included in the CEPM. To predict current efficiency more accurately more industrial current efficiency data are needed to calibrate the CEPM model. On the other hand the parameters such as temperature and bath properties can be included to coupledly solve the heat field and flow field, which needs further study.

Summary

A CEPM based on multiphase multicomponent flow was developed according to the mechanism of current efficiency loss. The CEPM was calibrated by a 160kA cell and validated by a 300kA cell.

The CEPM provides a new approach for determining the current efficiency of aluminum reduction cells and is an effective tool for test the results of optimization.

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