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MATHEMATICAL MODEL FOR CONTINUOUS DETECTION OF CURRENT EFFICIENCY IN ALUMINUM PRODUCTION①

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ABSTRACT A mathematical model called "three parameter model" which can be used to detect current efficiency continuously in aluminium production has been developed. The model includes: (1) calculation of physical fields in the cell; (2) calculation of temperature, anode-cathode distance, Al-electrolyte interfacial tension and aluminium concentration factor; (3) comprehensive mechanism model of aluminium loss. The current efficiency and current distribution of 160 kA prebaked cells were measured. Experimental results show the "three parameter model" is valuable in aluminium electrolysis.

Key words current efficiency mathematical model aluminium electrolysis

1 INTRODUCTION

The mathematical models for calculation of current efficiency in alumina reduction have been reported by many investigators, most of which belong to mechanism model or empirical model. The mechanism models commonly used can well explain experimental results of both laboratory and factory[1-3]. But Grjotheim *et al*[4] thought that it was because some parameters in those models were so selected in order to agree with the results. The empirical models were kinds of relations between the current efficiency and some operating parameters, which were developed by use of statistical analysis of much measured data. None of present models can be applied to continuous detection of current efficiency in alumina reduction cell, therefore we develop a mathematical model called " three parameter model".

2 COMPREHENSIVE MECHANISM MODEL OF ALUMINUM LOSS

Analyzing the flow feature of melt in cell, and its effect on current efficiency, we can derive comprehensive mechanism model that includes all mass transfer process. On the basis of Lillebuen's model, and by redefinition or recalculation of some variables in his model, it can be done easily. In Lillebuen's model, $f = C_m / C_m^*$, C_m is the metal concentration in bulk melt. He neglected the mass transfer in bulk, and didn't take the interfacial tension into account when he calculated diffusivity. If we fully consider the factors that Lillebuen neglected, we can develop the mechanism model as Eqn. (1), which includes all factors in whole mass transfer processes[5],

$$\left.\begin{aligned} CE\% &= 100 - 219A \times I^{-1} D_{me}^{0.67} \cdot \\ &\quad \mu^{-0.5} U_e^{-0.83} d^{-0.17} \rho_c^{1.5} \cdot \\ &\quad w(\mathrm{Al})(1-f) \\ f &= C_m / C_m^* \\ D_{me} &= D_m^{il} (\sigma_r / \sigma)^{0.5} \end{aligned}\right| \qquad (1)$$

where D_{me}—metal diffusivity corrected for interfacial tension, m^2/s; σ_r—interfacial tension corresponding to diffusivity, D_m; u_a—mean electrolyte flow velocity referred to the cathode-

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aluminum surface, m/s; d —anode-cathode distance, m; μ —viscosity of electrolyte, Pa · s; ρ_e —density of electrolyte, kg/m^3; f —fraction of metal saturation; I —cell current, kA; A —cathode Al surface area, m^2; w (Al) —mass fraction of Al (equivalent) in electrolyte at saturation

By further investigation of variables included in mechanism model we got, it can be known that they are mainly determined by six operating parameters, which are temperature (T), current density(d_c), melt flow velocity(u), anode-cathode distance(d), interfacial tension(σ), fractional factor(f). Unfortunately, most of the variables are unable to be measured continuously, so the comprehensive mechanism model is not suitable to continuous supervision of current efficiency. If these variables can be defined by the equations that only include the parameters which can measured continuously, the continuos detection of current efficiency can be realized. Fortunately, d_c, u can be calculated by solving the equation of electric field, magnetic field and flow filed; and T, d, σ, f can be calculated by semiempirical relationships derived behind.

3 MATHEMATICAL MODEL FOR CONTINUOUS DETECTION OF CURRENT EFFICIENCY

3.1 Selection of variables

If some parameters can be found out, and meet the following three conditions:

(1) they can be continuously measured and processed by computer conveniently;

(2) their change can reflect the change of current efficiency precisely;

(3) the stable and quantitative relation can be established between the selected variables and current efficiency. Then we can get the continuous detection model of current efficiency.

Analyzing the physical and chemical process occurred in cell, electrolytic technology and the cell construct, combining the previous research works by others and us, we selected three parameters, which are: ①voltages on anode rods; ②cell voltage; ③voltages on cathode aluminium ribbon, and used the three parameters to calculate the variables in Eqn. (1), thereby, relation of current efficiency with selected parameters would be built.

3.2 Mathematical model on continuous detection of current efficiency

3.2.1 Construction of the model

The supervision of CE (current efficiency) by computer can be done if the relation of current efficiency with time, not with the operating parameters measured difficultly, was established. Based our comprehensive mechanism model, CE can be calculated by the “three parameters” we selected. The whole model consists of four parts: (1) time-varied model of “three parameters”; (2) calculation models of electric field, magnetic field, force field, fluid velocity field; (3) calculation of temperature, anode-cathode distance, interfacial tension and fraction factor; (4) comprehensive mechanism model of aluminium loss.

3.2.2 Mathematical expression of model[6]

The mathematical model for continuous detection of current efficiency in alumina reduction cell can be expressed by a group of equations as follows.

$$\Delta u = f'(t) \tag{2a}$$

$$\boldsymbol{J} = -\sigma \nabla \boldsymbol{E} \tag{2b}$$

$$\Sigma \boldsymbol{J} = 0 \tag{2c}$$

$$\boldsymbol{B} = \mu_0/(4\pi) \int [(\boldsymbol{J}_{\text{electro}} \times \frac{\boldsymbol{r}^0}{r^3} \mathrm{d} V_{\text{electro}}) + (\boldsymbol{M}_{\text{iron}} \frac{r_1^0}{r_1^3} \mathrm{d} V_{\text{iron}})] \tag{2d}$$

$$\boldsymbol{F} = \boldsymbol{J} \times \boldsymbol{B} \tag{2e}$$

$$\rho \boldsymbol{v} \cdot \nabla \boldsymbol{V} = -\nabla P + \langle \kappa \varepsilon \rangle + p\boldsymbol{F}(g) \nabla \cdot \boldsymbol{V} = 0 \tag{2f}$$

$$\nabla \cdot \boldsymbol{V} = 0 \tag{2g}$$

$$T = T(\Delta U) \tag{2h}$$

$$d = \mathrm{d}(\Delta U) \tag{2i}$$

$$\sigma = \sigma(\Delta U) \tag{2j}$$

$$f = f(\Delta U) \tag{2k}$$

$$\left.\begin{array}{l} CE\% = 100 - 219A \times \\ I^{-1} D_{\text{me}}^{0.67} \mu^{-0.5} \times \\ U_e^{-0.83} d^{-0.17} \rho_e^{1.5} w(\text{Al})(1-f) \\ f = C_{\text{m}}/C_{\text{m}}^* \\ D_{\text{me}} = D_{\text{m}}(\sigma_r/\sigma)^{0.5} \end{array}\right| \tag{2l}$$

where (2a) is time-varied model of “three parameters"; (2b) differential formula of Ohm's law; (2c) Coulomb's law; (2d) equation for calculation of magnetic flux; (2e) equation for calculation of electric-magnetic force; (2f) time averaged Reynolds' equation; (2g) fluid continuous equation; (2h), (2i), (2j) and (2k) expression for calculation of temperature, anode-cathode distance, interfacial tension and fraction factor respectively; (2l) comprehensive mechanism model of aluminium loss, $\langle \kappa\varepsilon \rangle$ means it is solved by κ-ε two equations.

3.3 Estimation of parameters

Because of the difference of parameters in different positions, we use weighted average method to determine the cell parameters.

3.3.1 Calculation of temperature

The temperature of alumina reduction is related to current, voltage and heat circumstance for a long period of time. Because all of the factors vary with time, the calculation of temperature is very complex, although it can be done by the temperature at one time and the relation of electric power with time for that period[7]. But for normal electric cell, if the current doesn't change quickly with time, we can neglect some non-linear factors and adopt the second power function of current to compute the temperature, that is[6]

$$T = A + BI^2 + CI$$

where A, B and C are constants which can be determined from practical measure.

For 160 kA prebaked cell, the model for special period is expressed by

$$T = 965 + 0.65 d_e (d_e - 3) \qquad (3)$$

where d_e is the average current density in electrolyte(A/m^2). Eqn. (3) is not suitable for the zone where anode has been just changed.

3.3.2 Calculation of anode-cathode distance

When calculation of anode-cathode distance, it is assumed that there is equal electric potential on anode busbar, also equal in aluminium cathode. Let L_i be anode-cathode distance under the anode, I_i be the current it passes, Δu be voltage between busbar and cathode aluminium, and we get

$$I_i = (\Delta u - \Delta u')/(R_{\text{anode}} + R_{\text{electrolyte}})$$

For $R_{\text{anode}} \ll R_{\text{electrolyte}}$

$$I_i = (\Delta u - \Delta u') \times S_i/(\rho L_i) \approx C_i/L_i \qquad (4)$$

where $\Delta u'$ is voltage needed for alumina reduction, S_i is conduct area corresponding to the anode.

The constant can be calculated by design parameters or by measured value. For 160 kA prebaked cell, $C_1 = 81$.

3.3.3 Calculation of average Al-electrolyte interfacial tension

The difference of Al-electrolyte interfacial tension is caused by the unevenness of electrolyte composition, predominately of Na^+. The Al/electrolytes interfacial tension is decreased with increase of Na^+ concentration, and the function is nearly linear[5]. Furthermore, Na^+ concentration on interface is defined by current density. For that reason the higher density, the larger Na^+ concentration. Because 99% current in melt is carried by Na^+, it can be true that Na^+ concentration is directly proportional to current density, so we can use the following formula to express the relation between them

$$\sigma_{\text{interf}} = C_0 - C_2 d_c \qquad (5)$$

where σ_{interf} is interfacial tension of Al/electrolyte, mN/m; d_c is zone average current density of cathode, A/cm^2.

The constants were determined by referring to Utigard's[8] work, $C_0 = 550$, $C_2 = 110$.

3.3.4 Calculation of fraction factor coefficiency f

According to $f = C_m / C_m^*$, the larger current density of anode, the more CO_2 produced, and the less metal concentration in the bulk, which results in the decrease of f, thereby current efficiency decreases. By the replacement of the data Lillebuen suggested in the definition of f, we get

$$f = f' - C_3 \cdot C_{m2}$$

where f' is the fractional coefficiency in Lillebuen's model, C_{m2} metal concentration of bubble/electrolyte interface.

Because C_{m2} is very small, it doesn't cause much difference that we estimate C_{m2} linearly by anode current density. Therefore, f can be calculated by this expression

$$f = f_0 - C_4 \cdot d_a \quad (6)$$

where d_a is anode current density, A/cm^2, the constants were defined by previous works made by others, which are $f_0 = 0.5$; $C_4 = 0.5$.

3.4 The computer program for continuous supervision of current efficiency

The diagram of calculation program is shown in Fig. 1.

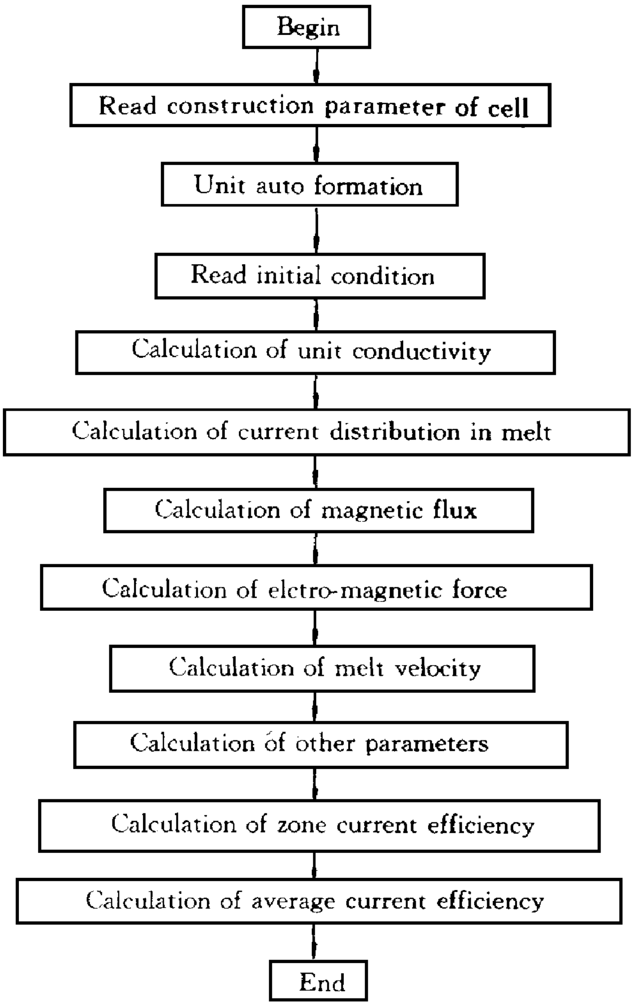

Fig. 1 Diagram of the computer program for continuous supervision of current efficiency

4 CORRECTION OF MATHEMATICAL MODEL

4.1 The used method and measured parameters

What we measured in site are the equal distant voltage and surface temperature of anode bars and cathode aluminum ribbons, the composition of anode gas, temperature of electrolyte, the shape of furnace chest, cell current and cell voltage. The method we adopted in measurement is what workers usually practice in production, but simultaneous measurement is required. The main technical conditions for the period of test are CR= 2.8, bath level 13 cm, average operating temperature is 966~ 972 ℃, current intensity 130~ 150 kA, cell voltage 3.8~ 4.4 V, MgF_2 2%~ 4%, CaF_2 3%~ 5%.

4.2 Comparison of calculation with measurement

The results of current efficiency of cell 76$^\#$ is shown in Fig. 2, and that of cell 77$^\#$ is shown in Fig. 3.

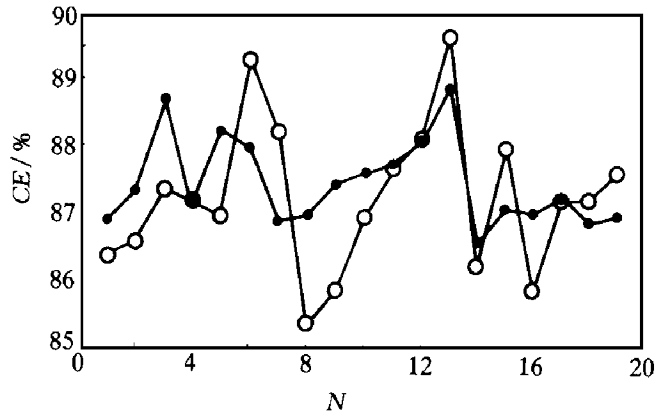

Fig. 2 Comparison of calculated data with measured ones for cell 76$^\#$
○—Measured; ●—Calculated

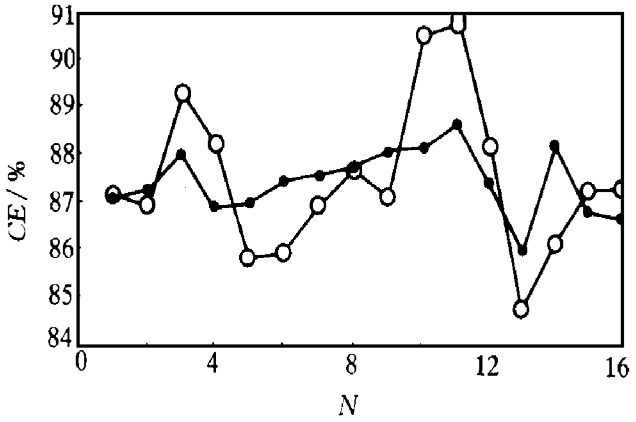

Fig. 3 Comparison of calculated data with measured ones for cell 77$^\#$
○—Measured; ●—Calculated

5 DISCUSSION

From the above figures we can conclude: (1) the error in some points is relative large; (2) the calculated average current efficiency for the period of test (one month) is well in agreement with measured one (relative error is 0.2% for cell 76$^{\#}$, −0.1% for cell 77$^{\#}$); (3) measured value fluctuates more sharply than calculated one. Why does the phenomena exist?

5.1 Problem in measurement

Because of its complex and difficulty, the measurement of parameters can not be simultaneous exactly; there is a little disclosure when the anode gas is fetched, it is hard to tell how much the gases fetched in one zone is mixed with other zones; and the temperature is not the same in different position of the cell, so the measured values differ with the real average one.

5.2 Problem of data treatment

The expression from Ref. [9] and [10], which is $CE\% = 50 + 1/2 \times \varphi(CO_2) + 4.0$, was used to treat the data we got (no better one). From the source we know the correction item 4.0 was got by statistics of a great number of data measured for long term, and its derivation is ±2. Therefore we can think the expression should be

$$CE\% = 50 + 1/2 \times \varphi(CO_2) + (2 \sim 6)$$

if it is used to calculate short-term current efficiency, for the sake of which, the measured value well agrees with calculated one. Perhaps it is true that short-term current efficiency can not be measured precisely, but it can be calculated out more precisely.

5.3 Problem of our model

From the process that our model was derived, it is obvious some equations are semiempirical and they should be corrected by experiments. There are also errors in our model.

6 CONCLUSIONS

(1) Comprehensive mechanism model of aluminium loss was derived on the bases of Lillebuen's model and by reference of some previous works.

(2) The three parameters, which are equal distant voltage in anode bar, voltage in cathode aluminium band and cell voltage, were selected as variables, by which mathematical model on continuous detection of current efficiency was developed.

(3) The calculation models for electrolysis temperature, anode-cathode distance, average interfacial tension and metal fractional factor were got on the case of practical production.

(4) The computer program of detection of average current efficiency was compiled.

(5) The current efficiency and current distribution of some 160 kA prebake cell were measured in site, and compared with value calculated by our model. The results showed that relative error is less 0.5% for one month average current efficiency.

(6) It should be indicated that the model we derived cannot reflect the change of current efficiency with electrolyte composition, and it cannot be suitable when temperature fluctuate obviously. The electrolyte composition and operating temperature must be measured at given time and put in computer. This is a problem that will be solved in the near future.

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