MATHEMATICAL MODELLING OF BUBBLE DRIVEN FLOWS IN A NOVEL ALUMINUM ELECTROLYSIS CELL ①

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ABSTRACT A mathematical model describing fluid flow stirred by the bubble in a novel aluminum electrolysis cell was presented. Based on SIMPLER algorithm, the turbulent momentum equations closed by k-ε model were solved. The regularities of bath circulations in a water model cell were obtained. The results showed that the flow rate in the lower compartment was much larger than that in the upper one, which was in agreement with the experimental data.

Key words mathematical modelling fluid flow aluminum electrolysis cell k-ε model

1 INTRODUCTION

At present, although some improvements are possible to realize in the monopolar cells of aluminum electrolysis by means of increasing the capacity of design, the advantages of this kind of larger cells are approaching to limits[1]. In order to reduce energy consumption and increase equipment productivity, it is necessary to use multicompartment cell instead of monopolar cell. Many experts have pointed out that the ultimate aluminum electrolysis cell probably would have bipolar electrodes using Al_2O_3 as the raw material[1-3].

Besides a series of electrochemical reactions, many heat and mass transfer processes also happened in the aluminum cell. To let aluminum cell run stably and efficiently, it is necessary to design the cell structure rationally. Since these processes are related to the bath circulation, many attentions[4-7] have been paid to the flow of the electrolyte, but nearly all focussed on the monopolar cell, while our studies aimed at the explanation of regularities of bath circulations in multicompartment cell using mathematical model.

2 BASIC HYPOTHESIS AND MATHEMATICAL MODEL

The structure of the bipolar model cell is shown in Fig. 1(a). In this model, the electrodes are laid horizontally and stacked vertically. On the two sides of the electrodes, there are two passages for dropping of aluminum and draining of anode gas; on the other two sides, the electrodes contact closely with the cell wall, so that the electrolyte can not pass through, and the electrolyte flow in the cell can be considered as two-dimensional. In the industrial cell, the electrolyte flow is driven by three kinds of forces: MHD effects, temperature and concentration gradients and bubble motion. Because in the multicompartment cell with inert electrodes, liquid aluminum will not accumulate on the cathode, MHD effects become unimportant, bubble motion becomes the major force, and others can be neglected. The problem studied is two-phase flow of gas and liquid, which can be described by many models; since the homogenous flow model has been successfully used to study the argon agitation in the ladle[8], it can be also used here.

There are two two-phase areas near the

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anode surface and in the gas lift passages. Suppose at the bottom of anode, the thickness of bubble layer is the same everywhere, then the bubble fraction α can be calculated iteratively by the formula of $\alpha = \frac{q \cdot L}{u_b \cdot S}$, while the bubble fraction in the gas lift passage must be obtained from measurement.

Suppose fluid properties are constant, and the flow is incompressible and steady, the turbulence viscosity can be described by using k-ε turbulence model.

2.1 *Basic Equations*

The equation governing the motion of the flow is:

$$\mathrm{div}(\rho \vec{V} \Phi) - \mathrm{div}(\Gamma \,\mathrm{grad}\, \Phi) = S_\Phi$$

where Φ, Γ, S_Φ are listed in Table 1.

Table 1 Differential equations

Name of Eqs.	Φ	Γ	S
Eq. of continuity	1	1	0
Eq. of x direction momentum	u	μ_e	$\alpha\rho_l g_x - \frac{\partial P}{\partial x}$
Eq. of y direction momentum	v	μ_e	$\alpha\rho_l g_y - \frac{\partial P}{\partial y}$
Eq. of turbulent kinetic energy	k	$\frac{\mu_e}{\sigma_k}$	S_1
Eq. of dissipation rate of turbulent kinetic energy	ε	$\frac{\mu_e}{\sigma_\varepsilon}$	S_2

Here

$$S_1 = \mu_t[2(\frac{\partial u}{\partial x})^2 + 2(\frac{\partial v}{\partial y})^2 + (\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})^2] - \rho\varepsilon$$

$$S_2 = \frac{\varepsilon}{k}\{c_1 \mu_t[2(\frac{\partial u}{\partial x})^2 + 2(\frac{\partial v}{\partial y})^2 + (\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x})^2] - c_2 \rho\varepsilon\}$$

$\mu_e = \mu + \mu_t$, $\mu_t = c_\mu \rho k^2/\varepsilon$;

$g_x = g\sin a$, $g_y = g\cos a$;

$\rho = \alpha\rho_g + (1-\alpha)\rho_l$;

$c_1 = 1.43$, $c_2 = 1.92$, $c_\mu = 0.09$,

$\sigma_k = 1.0$, $\sigma_\varepsilon = 1.33$.

2.2 *Boundary Conditions*

(1) On the free surface

$$v = 0,\ \frac{\partial u}{\partial y} = \frac{\partial k}{\partial y} = \frac{\partial \varepsilon}{\partial y} = 0$$

(2) At the walls

At the walls of the cell and electrodes, the non-slip condition was applied, where $k = \varepsilon = u = v = 0$; but in the boundary layer near the wall, the turbulence is not isotropic, and the flow is matched with the outer solution by wall functions[9].

2.3 *Solution Procedure*

In order to compare with experimental results, the flow field in a hydraulic model cell was first simulated. The following constants of flow properties were used: density of liquid= 1024.5 kg/m^3; viscosity= 0.0011 Pa·s[10]; density of gas= 1.205 kg/m^3.

There are two difficulties to solve equations by numerical methods: one is the nonlinearity of momentum equations, the other is that for the pressure there are only equations coupled with velocity. Many differential schemes can not fulfill the incompressible condition, here the SIMPLER algorithm[11] based on staggered grids system was used. The discretization equations were deduced by volume controlling method, and the continuity equation was changed into pressure revised equation. The iterations of the line-by-line technique were used to speed convergence. To promote convergence, the under relaxation was adopted, and the different relaxation factors were selected for the different variables. The employed main grid was 18 × 12 for the monopolar cell, and 18 × 20 for the bipolar cell. The actual computation was done on the IBM-486 microcomputer.

3 COMPARISON OF CALCULATED RESULTS WITH EXPERIMENTAL DATA

3.1 *Monocompartment Cell*

The anode in the model cell was submerged under bath, see Fig. 1(b). The velocity fields calculated are shown in Fig. 2(a). It can be seen that the electrolyte circulates mainly around the anode; only in the lower corner of the bubble lift passage is there a local small circulation. The velocity near the anode surface is the largest, and that near the cathode the smallest, which is beneficial to bubble drainage and aluminum entrainment.

3. 2 *Bipolar Cell*

The velocity vector distribution simulated in the bipolar cell is plotted in Fig. 2(b). The electrolyte circulates unidirectionally around end-anode and bipolar electrode, and there is no stagnant area in the interpolar gap and side passages.

Fig. 1 Plot of electrolysis cell models
(a) —bipolar cell; (b) —monopolar cell

Fig. 2 Calculated velocity fields of monopolar and bipolar cells
($\alpha = 7.5°$, ACD= 25 mm, $W_1 = W_2 = 30$ mm, $H = 40$ mm, $i = 0.5$ A/cm^2)
(a) —monocompartment cell; (b) —bipolar cell

3. 3 *Comparison With Experimental Results*

In order to verify the correctness of the mathematical model, a series of experiment were carried out in designed hydraulic model cell. The velocity in the interpolar gap was measured by electrochemical method[12], and the gas fraction by electric conduct probe. In the measurement of gas fraction, data sampling about sixty thousand times per second was done by microcomputer. The gas fraction could be gained by judging the electric level of the samples. The effects of ACD, electrode tilt, current density on the velocity in interpolar gap were studied respectively. Here the change of current density can be got by adjusting gas flow rate, according to the formula: $q = iRT/(4FP)$. The results of comparison are shown in Fig. 3. From Fig. 3, it is clear that the results of calculation are in accord with the experimental data, indicating that the mathematical model established is correct.

4 CONCLUSIONS

The mathematical model describing the flow field in two-compartment cell has been presented. A special treatment has been done to the two-phase region. The calculated results agree well with the experiments, showing the correctness of the mathematical model, and providing experimental foundation for the model to be applied in bipolar cell with multicompartments.

From the calculated results in bipolar cell, it can be found that the flow rate in lower compartment is much larger than that in upper one, which provided important information for the structure design of bipolar cell.

Symbols

α —void fraction;
q —gas formation rate, m^3/s·m^2;
L —distance from the lower end of the anode, m;
u_b —bubble velocity, m/s;
S —thickness of the bubble layer, m;
k —turbulent energy, m^2/s^2;
ε —dissipation rate of turbulent energy, m^2/s^3;
ρ —density of the bubble-liquid mixture, kg/m^3;
μ_t —turbulent viscosity, Pa·s;

Fig. 3 **Comparison of calculated and experimental results**

(Δ—experimental; ●—calculated)

(a) —effect of ACD(*d*) (α = 7.5°, $W_1 = W_2$ = 30mm, H = 40mm, i = 0.5A/cm^2); (b) —effect of electrode tilt (ACD = 25mm, $W_1 = W_2$ = 30mm, H = 40 mm, i = 0.5A/cm^2); (c) —effect of current density (α = 5°, ACD= 30mm, $W_1 = W_2$ = 30mm, H = 30mm)

μ_e —effective viscosity, Pa·s;
α —angle of inclination(horizontal), (°);
ACD —anode-cathode distance, mm;
H —electrode immersion depth, mm;
W_1 —passage width of gas lift, mm;
W_2 —passage width of aluminum entrainment, mm;
i —current density, A/m^2;
g —acceleration of gravity, 9.81 m/s^2;
V —velocity vector, m/s;
Φ —universal variable;
Γ —diffusion coefficient;
S_Φ —source;
u, v —velocity components in x, y directions, m/s;
μ —molecular viscosity, Pa·s;
R —universal gas constant, 8.314 J/(mol·K);
T —absolute temperature, K;
F —Faraday constant, 96 500 C;
P —pressure, Pa;
ρ_l —density of electrolyte, kg/m^3;
ρ_g —density of gas, kg/m^3;

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