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The mathematical simulation of an electrolytic cell for aluminium production

Andris Buiķis and Harijs Kalis, Institute of Mathematics of Latvian Academy of Sciences and University of Latvia, Rīga, Latvia *

Aluminium extraction from the corresponding oxide is generally performed through an electrolytic procedure. Running through aluminum and steel bars, the electric current I (see fig.1) spreads into the anodes, builds in graphite and generates the electric and magnetic fields in the electrolytic bath [1]. Total electric current in modern aluminium reduction cell reaches the magnitude $300kA$ and higher. There are two liquid layers (electrolyte, aluminium) and some solid layers (carbon, steel and other) in the electrolytic bath. The electromagnetic force in two liquid layers causes circulation of melt and oscillation of interface between aluminium and electrolyte. The typical Reynolds number in this case is $Re \sim 10^5 - 10^6$. Special influence on the process has distribution of joule heat.

Investigation of the control processes of aluminium reduction cells requires development of effective algorithms and numerical methods for solving following $3-D$ hydrodynamical and heat transfer equations in the form

$$\partial\vec{v}/\partial t + (\vec{v}\text{grad})\vec{v} = -\rho^{-1}\text{grad}\, p + \nu\Delta\vec{v} + \rho^{-1}\vec{F}, \tag{1.1}$$

$$\text{div}\ \vec{v} = 0, \tag{1.2}$$

$$\rho c_p \partial T/\partial t + (\vec{v}\text{grad})T = \text{div}(\lambda\text{grad}\, T) + q, \tag{1.3}$$

where $\vec{F} = \vec{j}\times\vec{B}$ – a vector of electromagnetic force; $\vec{j}$, $\vec{B}$ – vectors of electric current density and induction of magnetic field determined by Ohm's law and from Maxwell's equations; $q = j^2/\sigma$ – joule's heat source; σ, ρ, ν, λ, c_p – coefficients of conductivity, density, kinematic viscosity (dynamic viscosity $\eta = \nu\rho$), heat transfer, specific heat capacity at constant pressure.

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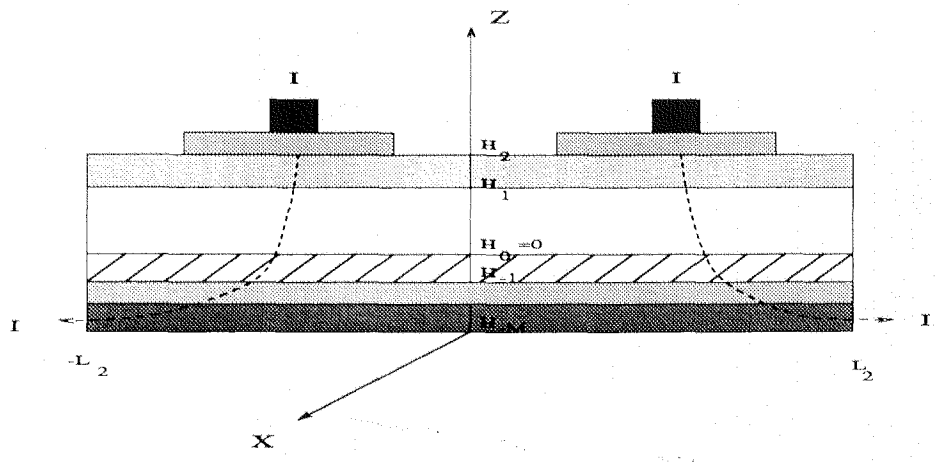

Figure 1.1 Cross section of a cell

Unknown quantities in system $(1-3)$ are velocity vector $\vec{v}$ (components u, v, w), pressure p, temperature T, which in general are functions of spatial coordinates x, y, z and time t. The movement of liquid is described by the full Navier-Stokes equations system $(1,2)$ for viscous incompressible flow.

The equations $(1,2)$ are determined in two liquid layers of parallelepiped form (see fig.1):

$$\Omega_1 = \{(x,y,z) : |x| \le L_1, |y| \le L_2, 0 < z < H_1\},$$

$$\Omega_2 = \{(x,y,z) : |x| \le L_1, |y| \le L_2, H_1 < z < H_2\}, \tag{1.4}$$

where L_1, L_2 – half-length and half-width of electrolytic bath, H_1 - – height of aluminium layer, $l_2 = H_2 - H_1$ – height of electrolyte layer. Here $z = H_1$ is the flat interface between metal and electrolyte.

The equation (3) for temperature is determined additionally in M-finite number of solid layers Ω_j with heights l_j, where

$$\Omega_j = \{(x,y,z) : |x| \le L_1, |y| \le L_2, H_{j-1} < z < H_j\}, \tag{1.5}$$

$$(l_j = H_j - H_{j-1}, j = -M+1, \ldots, -1, 0; H_0 = 0).$$

The electromagnetic force $\vec{F}$ distribution in the fluid is generated by an electric current density $\vec{j} = -\sigma \mathrm{grad}\,\varphi$ (φ – electric potential) and the integral magnetic field $\vec{B}$, which is a superposition of the fields $\vec{B}_i$ due to the internal current $\vec{j}$ within the cell itself, and $\vec{B}_e$ due to the current in the external circuit (leads, bars, etc.). The internal current $\vec{j}$ is computed dividing the cell into a number of layers of different electrical conductivity σ ($\sigma = 2 \cdot 10^4$ in anodes, $\sigma_{Al} = 3 \cdot 10^6$, $\sigma_{el} = 200(1/ohm)$), for each of these the Laplace equations $\Delta\varphi = 0$ is solved numerically. According to the numerically determined $\vec{j}$ distribution, the internal magnetic field $\vec{B}_i$ is found from Biot-Savart law by integrating the corresponding singular volume integrals. The external magnetic field $\vec{B}_e$ is computed integrating Biot-Savart law over approximately $200 - 500$ linear current-elements, constituting the external circuit of the single cell. The integral $3 - D$ magnetic field $\vec{B}$ and the corresponding force $\vec{F}$ are evaluated within the two layers of liquid aluminium and electrolyte in spatial grid points. That requires the greater part of the computer time.

Heat removal at outer boundary is represented with boundary condition of third type [2]

$$-\lambda \partial T/\partial n = \alpha(T - T_B), \tag{1.6}$$

but liquid adhesion condition as follows

$$\vec{v} = 0. \tag{1.7}$$

The condition (7) is set on the bottom of metal ($z = 0$) and at the surface of electrolyte $z = H_2$, but at part of free surface

$$\eta_2 \partial u_2/\partial z = \eta_2 \partial v_2/\partial z = 0, \quad w_2 = 0. \tag{1.8}$$

At interface $z = H_j$ conjugacy (continuity) condition

$$T_j = T_{j+1}, \quad \lambda_j \partial T_j/\partial z = \lambda_{j+1} \partial T_{j+1}/\partial z, \quad j = \overline{-M+1, 1}$$

$$u_1 = u_2, \eta_1 \partial u_1/\partial z = \eta_2 \partial u_2/\partial z, v_1 = v_2, \eta_1 \partial v_1/\partial z = \eta_2 \partial v_2/\partial z, \tag{1.9}$$

is set together with impenetrability condition through surface with $z = const$

$$w = 0. \tag{1.10}$$

Quantities H_2/L_2 and H_2/L_1 are small (≈ 0.05) and operation of averaging may by used to reduce dimensionality of the problem. The equations of system are averaged along the heights of layers Ω_j and quadratic approximation of functions along z-coordinate in following form is used [3]

$$s_j = S_j + m_j(z - Z_j) + e_j G_j l_j^{-2}[(z - Z_j)^2 + l_j^2/12], j = \overline{-M+1, 2} \quad (1.11)$$

where

$$G_j = l_j/\gamma_j, Z_j = (H_j + H_{j-1})/2, \quad S_j = l_j^{-1} \int_{H_{j-1}}^{H_j} s dz,$$

as a variable s we can take u, v, w, p, T, but for γ-η (the coefficient of viscosity) or λ (the coefficient of heat conductivity); $e_j = 0$ for variable p. The variables m_j, e_j are the unknown coefficients of the spline-function, S_j – the averaged values of s_j. After averaging along every layer Ω_j the system $(1-3)$ is in the initially form, only at the right side the derivatives of $\gamma \partial^2 s/\partial z^2$ are replaced by the term

$$l_j^{-1}\gamma_j(s_z(H_j) - s_z(H_{j-1})) = 2l_j^{-1}e_j, \quad (1.12)$$

$$(s_z(H) = \partial s/\partial z, z = H_j),$$

and in the third equation and in continuity equation spline (11) coefficient m appears.

All $2M + 18$ spline coefficients (11) m_j, e_j are uniquely determined by the help of averaged quantities U, V, W, P, T and instead of initial equations $(1-3)$ we have a system of $M + 10$ equations in layers, which do not depend on z-coordinate. As long as continuity equation remains valid, we can introduce the averaged stream function ψ and separate determination of quantities U, V from P.

As an example which shows the uniquely solvability of the system of algebraic equations for spline-coefficients e_j, dependent on averaged temperatures T_j we have the following system

$$A_j e_{j-1} + C_j e_j + B_j e_{j+1} = a_j(T_{j+1} - T_j) - b_j(T_j - T_{j-1}), \quad j = \overline{k, 2} \quad (1.13)$$

where

$$e_{-M} = e_3 = 0, A_j = G_j G_{j-1}/(G_j + G_{j+1}), B_j = G_j G_{j+1}/(G_j + G_{j+1}),$$

$$C_j = A_j + B_j + D_j, \quad D_j = G_j,$$

$$a_j = 3G_j/(G_j + G_{j+1}) > 0, \quad b_j = 3G_j/(G_{j-1} + G_j) > 0,$$

$$G_{-M} = 2/\alpha_k, G_3 = 2/\alpha_2, T_{-M} = T_{Bk}, T_3 = T_{B2} \ (k = -M + 1).$$

The solution of system (13) we seek in the form

$$e_j = \sum_{i=k}^{3} \alpha_{j,i}(T_i - T_{i-1}) = \sum_{i=k}^{2} a_{j,i}T_i + \alpha_{j,3}T_3 - \alpha_{j,k}T_{-M},$$

where the unknown variables $\alpha_{j,i}$ do not depend on T_j:

$$A_j\alpha_{j-1,i} + C_j\alpha_{j,i} + B_j\alpha_{j+1,i} = \tilde{F}_{j,i}, j = \overline{k,2} \tag{1.14}$$

$$\alpha_{-M,i} = \alpha_{3,i} = 0, i = \overline{k,3}$$

$$\tilde{F}_{j,i} = -\delta_{j,i}b_j + \delta_{j+1,i}a_j, \quad a_{j,i} = \alpha_{j,i} - \alpha_{j,i+1},$$

$\delta_{j,i}$ - Kronecher's symbol. In the new variables $\beta_{j,i} = (-1)^{i+j+1}\alpha_{j,i}$ the system of difference equations (14) is of the form

$$A_j\beta_{j-1,i} - C_j\beta_{j,i} + B_j\beta_{j+1,i} = F_{j,i}, \ \beta_{-M,i} = \beta_{3,i} = 0, \tag{1.15}$$

where

$$F_{j,i} = (-1)^{i+j}\tilde{F}_{j,i}.$$

These are the finite-difference equations and from the inequalities $F_{j,i} \leq 0$, $A_j > 0$, $B_j > 0$, $C_j > A_j + B_j$ and from maximum principle it easy follows the nonnegativity $\beta_{j,i}$ and apriory estimation.

$$\max \beta_{j,i} \leq \max(3/(G_j + G_{j-1})).$$

For difference $\tilde{a}_{j,i} = \beta_{j,i} - \beta_{j,i+1} = (-1)^{i+j+1}a_{j,i}$ we have a system of equations (15), where

$$F_{j,i} = (-1)^{i+j+1}(-\delta_{j,i}b_j + \delta_{j+1,i}a_j + \delta_{j,i+1}b_j - -\delta_{j+1,i+1}a_j) \leq 0,$$

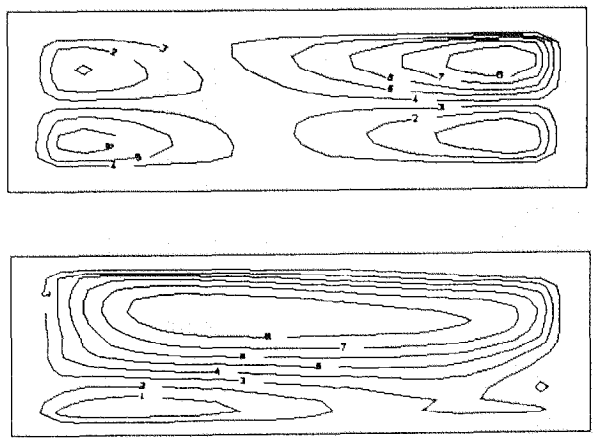

Figure 1.2 Circulation of the melt ($\psi = const$, $v \sim 10cm/sec$)

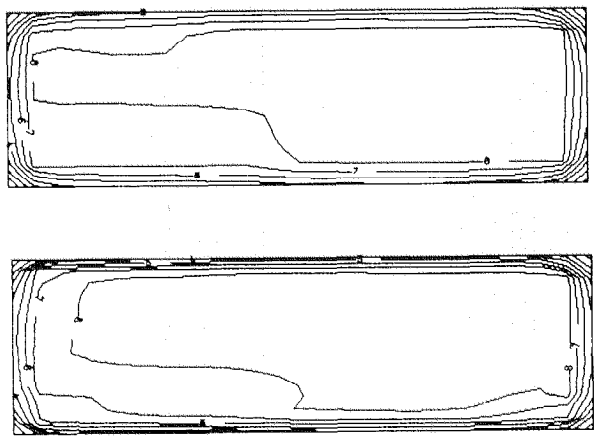

Figure 1.3 Temperature distributions in (x, y) – plane ($T = const$)

otherwise we have estimation

$$0 \leq \tilde{a}_{j,i} \leq \max(6/(G_j + G_{j-1})).$$

The system of averaged $2-D$ equations is discretized on general irregular meshes and special monotone finite-difference schemes are used [4]. The equations were solved by a modification of the finite-difference method using an integro-interpolation approximation of the second order accuracy in space and the first order in time.

The results of numerical experiments were obtained for two layers, in the case $M = 0$. In the fig.2 we can see the velocity distributions in (x, y)-planes of electrolyte (upper) and aluminium (lower) layers, where ψ is the averaged stream function.

The maximum of the averaged temperature T in the layers $(997^0C, 979^0C)$ is not in the coordinate center anymore (see fig.3).

There is a special complex of programs for industrial aluminium cell simulation in the University of Latvia.

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