Essential Readings in Light Metals: Aluminum Reduction Technology.
Edited by Geoff Bearne, Marc Dupuis and Gary Tarcy.

2. MODELING

Hall-Héroult cells are very challenging to model. This is true now and it was especially true half a century ago. The aluminum industry has invested huge resources in the development of mathematical models especially to support its cell design activities. Today the use of mathematical models is considered indispensable to the successful design of efficient high current cells. However, there was a time when it was not clear if the investment in modeling would ever become beneficial.

The papers included in this section present the work that made the difference. They have established that it is possible to develop reliable mathematical models of the cell thermo-electric behavior in order to correctly predict the cell heat balance, and the very complex magneto-hydrodynamic (MHD) cell behavior in order to correctly predict the cell stability. Today, it would be unthinkable to design efficient high amperage cells without the help of those two types of models.

A third type of model has more recently become the focus of intensive R&D, namely the bath bubble flow models used to support the effort to minimize the bubble layer electrical resistance below the anodes. This type of model has not yet reached maturity and so only a partial story will be presented here.

Of course, many more types of models have been developed than these three categories. Papers on these others, such as potroom ventilation models, pot shell mechanical deformation models and smelter logistic models are also presented.

Models more specifically representing the anode or the cathode behavior are not presented here as they are more appropriately included in *Electrode Technology for Aluminum Production* (Volume 4 of this *Essential Readings in Light Metals* collection).

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SIMULATION OF THERMAL, ELECTRIC AND CHEMICAL BEHAVIOUR OF AN ALUMINUM CELL ON A DIGITAL COMPUTER

A. Ek and G. E. Fladmark

Abstract

Part one of the paper presents a method for calculating the temperature and electric potential in the cathode of a reduction cell. The time-independent temperature and potential fields are described by two coupled quasi-linear partial differential equations of elliptic type in two dimensions with appropriate boundary conditions. Box-integration is used for constructing the difference equations. Because of the temperature dependent coefficients a special strategy of inner-outer iterations is used for solving the system of equations. Part two of the paper presents a model for the energy and mass balance of a complete reduction cell. The model takes into account energy production and consumption in all parts of the cell. The dynamic solution requires the integration of 16 coupled non-linear first-order differential equations. A stationary solution of the energy balance is found by solving a set of 15 non-linear algebraic equations. The model has been tested against measurements from a real cell, and good results have been obtained.

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Preface

The purpose of this paper is to present some of the work concerning aluminum production which has been carried out at Institutt for Atomenergi during the last two years. The institute has, with its background in nuclear reactor calculations, developed powerfull numerical competence which is now also being used in industrial process modelling.

The presented work has been done in cooperation with, and is paid by A/S Årdal og Sunndal Verk.

The paper presents two different numerical techniques, and is therefore divided in part I and II.

Part I

Numerical Calculation of Temperature and Electric Potential in the Cathode of a Reduction Cell

by

G. E. Fladmark

1. INTRODUCTION

This part of the paper presents a numerical method for calculating the stationary temperature and potential fields in the cathode of an aluminum reduction cell. With the cathode, we here also mean the side lining, the frozen cryolite at the side and the melted aluminum in the cell.

Results from the calculation are also the heat flux and the electric current density. The heat flux and the temperature distribution are used to study the thermic balance of the cell. The current distribution in aluminum is necessary, along with the magnetic fields, if one wants to calculate the convection of the metal. This is shown in the paper of Müller & Solberg (3).

In the calculations, conduction is assumed to be the mechanics of heat transfer. However, surface radiation is taken into account. The calculation will be done in a two-dimensional cartesian geometry. Leakage of heat or electric current in the third direction is taken care of either by leakage coefficients or internal boundary conditions.

The author wishes to thank Mr. I. Martinussen, who has done most of the programming work.

2. BASIC EQUATIONS

2.1 Heat Transfer

The basic equation for the heat transfer is written:

$$- \nabla \kappa(\vec{r},T) \nabla T(\vec{r}) + L_h(\vec{r},T)\, T(\vec{r}) = q \qquad (2.1)$$

with

$$q = \sigma(\vec{r},T) \left(\nabla \phi(\vec{r})\right)^2 \qquad (2.2)$$

where

$\vec{r}$: position vector in space (x,z)
T : temperature (^{o}C)
κ : heat conduction coeff. $(W/m\ ^{o}C)$
L_h : heat leacage coeff. $(1/m^2)$
q : heat source (W/m^3)
ϕ : electrical potential (V)
∇ : Laplacian operator

The following types of boundary conditions may appear:

A ; prescribed temperature on the boundary
B ; prescribed temperature outside the boundary and heat transfer coefficients
C ; prescribed heat current density on the boundary
D ; symmetrical boundary conditions

Surface radiation is approximated by letting:

$$a = a_1 + a_2\, T \qquad (2.3)$$

where

a : total heat transfer coeff. $(W/m^2\ ^{o}C)$
a_1 : partial heat transfer coeff. $(W/m^2\ ^{o}C)$
a_2 : partial heat transfer coeff. rate $(W/m^2\ ^{o}C)$

2.2 Electric Current Transfer

The electric potential is given by:

$$- \nabla \sigma(\vec{r},T) \nabla \phi(\vec{r}) + L_e(\vec{r},T)\, \phi(\vec{r}) = 0 \qquad (2.4)$$

where

L_e : electric current leacage coeff.

Boundary conditions to be considered are:

A : prescribed potential on the boundary
B : prescribed potential outside the boundary and current transfer coeff.
C : prescribed electric current density on the boundary
D : symmetric boundary conditions

3. METHOD OF SOLUTION

3.1 General

Assuming the temperature dependent material data given in a tabulated way or as functions defined on the actual temperature range, the solution of the temperature and the potential is performed in the following steps:

i) A temperature field is assumed.

ii) Calculate the potential from Eq. (2.4) with the material properties based on the last temperature.

iii) Calculate the source in Eq. (2.1) from the last potential and temperature.

iv) Calculate the temperature dependent heat transfer coefficients in the boundary conditions for Eq. (2.1).

v) Calculate the temperature from Eq.(2.1) with the material properties based upon the last temperature.

vi) Make a jump to:

a) item iv) and perform a new set of inner iterations in v).

b) item ii) and perform a new outer iteration.

The outer iterations are stopped when a convergence criterion on the temperature is met. Inner iterations are used for solving the potential and the temperature when the coefficients and the source are given. In order to get a fast all-over convergence and low computing times, the convergence criteria in the inner iterations should depend in some way on the outer iterations.

This way of using an outer iteration loop has the advantage that either by solving the temperature or the potential we have to solve the same mathematical problem, namely:

Calculate the function $\psi(\vec{r})$ when s, α, β, γ and δ (all depending on the space point) are given where

$$- \nabla \beta \nabla \psi + \delta \cdot \psi = s \qquad (3.1)$$

with the boundary conditions:

$$\beta \frac{\partial \psi}{\partial n} + \alpha \psi = \gamma \tag{3.2}$$

Here $\partial/\partial n$ denotes the normal derivative operator,
s is the electric or thermic source,
α is the electric current or the heat transfer coefficient on the boundary,
β is the electric current or the heat conduction coefficient and
δ is the leakage coefficient.

In Eq.(3.2) the values of α, β and γ depend on the type A, B, C or D boundary conditions discussed earlier.

3.2 Finite Difference Equations

We consider a plan through the cathode and divide this into a set of rectangular and triangular cells (Fig. 1). In each cell we assume constant material properties. The cell corners constitute the nodes were we want the solution.

Two types of nodes exist, the internal and the boundary nodes. We treat them separately.

Internal nodes

Fig. 2 shows a node surrounded by cells with different material properties. We integrate Eq.(3.1) on the domain A with the boundary L_ℓ, $\ell = 1, 2, 3, 4$. By use of the divergence theorem we have:

$$-\int_A \nabla \beta \nabla \psi \, dA + \int_A \delta \psi \, dA = -\oint_L \beta \frac{\partial \psi}{\partial n} dL + \int_A \delta \psi \, dA = \int_A s \, dA \tag{3.3}$$

Assuming the following approximations:

$$1) \quad \psi(\vec{r}) \approx \psi(\vec{r}_o) \; ; \; \vec{r} \in A$$

$$2) \quad \frac{\partial \psi(\vec{r})}{\partial n} \approx \frac{\psi(\vec{r}_\ell) - \psi(\vec{r}_o)}{|\vec{r}_\ell - \vec{r}_o|} \; ; \; \vec{r} \in L_\ell, \; \ell = 1,2,3,4 \tag{3.4}$$

we get the following five point difference equation:

$$a_{0_{i,j}} \psi_{i,j} - a_{1_{i,j}} \psi_{i-1,j} - a_{2_{i,j}} \psi_{i,j-1} - a_{1_{i+1,j}} \psi_{i+1,j} - a_{2_{i,j+1}} \psi_{i,j+1} = s_{i,j} \tag{3.5}$$

with

$$\left.\begin{aligned} a_{1_{i,j}} &= \frac{1}{2 h_{i-1}} (\beta_{q_{12}} k_j + \beta_{q_{21}} k_{j-1}) \\ a_{2_{i,j}} &= \frac{1}{2 k_{j-1}} (\beta_{q_{22}} h_{i-1} + \beta_{q_{31}} h_i) \\ a_{0_{i,j}} &= \sum_{\ell=1}^{4} a_{\ell_{i,j}} + F_{i,j}(\delta) \end{aligned}\right\} \tag{3.6}$$

$$s_{i,j} = F_{i,j}(s) \tag{3.7}$$

The function $F_{i,j}$ is defined as:

$$F_{i,j}(x) = \frac{1}{8}\left((x_{q_{11}} + x_{q_{12}}) h_{i-1} k_j + (x_{q_{21}} + x_{q_{22}}) h_{i-1} k_{j-1} + (x_{q_{31}} + x_{q_{32}}) h_i k_{j-1} + (x_{q_{41}} + x_{q_{42}}) h_i k_j\right) \tag{3.8}$$

Here $q_{\ell m}$ denotes the material property in cell no ℓm.

Boundary nodes

The equation may be constructed from Eq.(3.5) by making the following corrections:

1) Add to $a_{0_{i,j}}$ and $s_{i,j}$ the quantities $\Delta_{i,j}$ resp. $\varepsilon_{i,j}$, which are the results when taken the line-integral along the external boundary of the cell.

2) Let $\beta = \delta = s = 0$ for cells outside the boundary.

As an example we consider the boundary node given in Fig. 3. The contribution to the line integral is:

$$-\int_{L_1+L_4} \beta \frac{\partial \psi}{\partial n} dL = (\alpha_{q_{31}} \psi_{i,j} - \gamma_{q_{31}}) \tfrac{1}{2} \sqrt{h_i^2 + k_{j-1}^2} + (\alpha_{q_{12}} \psi_{i,j} - \gamma_{q_{12}}) \tfrac{1}{2} \sqrt{h_{i-1}^2 + k_j^2} \tag{3.9}$$

assuming piecewise constant coefficients.

Then

$$\Delta_{i,j} = H_{i,j}(\alpha)$$
$$\varepsilon_{i,j} = H_{i,j}(\gamma) \qquad (3.10)$$

with

$$H_{i,j}(x) = x_{q_{31}} \frac{1}{2}\sqrt{h_i^2 + k_{j-1}^2} + x_{q_{12}} \frac{1}{2}\sqrt{h_{i-1}^2 + k_j^2} \qquad (3.11)$$

The finite difference equations are written in the following way:

$$A_i \vec{\psi}_i - B_i \vec{\psi}_{i-1} - B_{i+1} \vec{\psi}_{i+1} = \vec{s}_i \quad ; \quad i = 1,2,\cdots, I \qquad (3.12)$$

with the matrices and the vectors of order J(i). Matrix A_i is three-diagonal and B_i is diagonal. $\vec{\psi}_i$ then denotes the solution ψ at the nodes along line i.

The method of successive overrelaxation is applied to Eq.(3.12). Let t denote the iteration index, then:

$$A_i \hat{\vec{\psi}}_i(t) = B_i \vec{\psi}_{i-1}(t) + B_{i+1} \vec{\psi}_{i+1}(t-1) + \vec{s}$$
$$\vec{\psi}_i(t) = \omega \left(\hat{\vec{\psi}}_i(t) - \vec{\psi}_i(t-1)\right) + \vec{\psi}_i(t-1) \quad ; \quad i = 1,2,\cdots,I \qquad (3.13)$$

The first equation is solved by matrix factorization (1) and the optimum ω is calculated according to an algorithm of Varga (2).

3.3 Inner-outer Iterations

A total convergence is obtained by doing a certain number of inner iterations during each outer iteration. In order to decrease the error by a factor of at least δ_m during the m'th outer iteration, the number of inner iterations to be performed is:

$$N_m = \frac{\ln \delta_m}{\ln(\omega-1) + \ln q} \qquad (3.14)$$

The parameter q depends on the properties of the iteration matrix. In general we have $q \geq 1$. However, numerical experiments have shown that the value on q have a very small influence on the total convergence.

The outer iterations are stopped when

$$||\vec{T}_m - \vec{T}_{m-1}|| \leq \varepsilon$$

where $||\ ||$ denotes the maximum norm and ε is the wanted accuracy.

4. EXAMPLES FROM A CALCULATION

In Fig. 4 is shown the temperature distribution in the cathode as resulting from a calculation. The liquidus temperature of cryolite is 957°C, and symmetri has been assumed.

In the electric potential calculation, a uniform current density of 7.05 kA/m^2 is supplied from the anode to the top of aluminum. Let us define the positive y-direction from the centerline towards the side, and the positive z-direction from the top towards the bottom of the cell. Fig. 5 then shows the y- and z-components of the current density in the metal. The curves represent the average values over the height of 20 cm aluminum, and may serve as input for the calculation of the convection in the metal. Experiments show that the computed current densities may be uncertain. The reason for this is the insufficient knowledge of the properties of the materials in the cell.

5. CONCLUSION

The presented method allows a very detailed calculation of the thermic and electric state in the cathode of the cell. Since material properties may differ from one node to the next, the fine-structure in the cell construction may easily be studied. The number of nodes is restricted only by computer space and computing time.

The size and shape of the cryolite freeze must be pre-specified and kept constant in the calculations. Since the shape of the freeze is in reality a function of the temperature distribution, a sort of manual trial-and-error method must often be applied to achieve good results.

A method for calculating the shape of the cryolite freeze have now been developed by the author.

6. REFERENCES

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