

# Scientific computing for aluminum production

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This work was partially financed by Alcan-Péchiney Company.  
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The manufacturing process in the industry for aluminum production is to inject alumina  $Al_2O_3$  in an electrolytic cell in order to obtain the chemical reaction:  $2Al_2O_3 + \text{electric energy} \rightarrow 4Al + 3O_2$ . The oxygen is burnt up by anodes:  $C + O_2 \rightarrow CO_2$  and the aluminum is collected at the cathodic bloc at the bottom of the cell. Two liquids are present in a cell. At the top, close to the anodes, there is the electrolytic bath in which the chemical reaction occurs. In the bath the dissolution of particles of alumina as well as the convection-diffusion of the dissolved alumina has to be considered. At the bottom of the cell, the liquid aluminum is deposited on the cathodic bloc. The temperature gradient in the cell leads to the formation of solid ledges on its walls.

A very strong electric current density  $\vec{j}$  flows through conductors into the hall which contains about a hundred electrolytic cells ( $\sim 6000$  A/m<sup>2</sup> in a cell). This current produces a strong magnetic induction field  $\vec{B}$  ( $\sim 1000$  Gauss) which is absorbed in part by a steel shell supporting the device. It is important to consider the ferromagnetic screen effects when we want to know the magnetic induction field  $\vec{B}_i$  inside the cell. This field, combined to the internal current density  $\vec{j}_i$  give rise to Lorentz forces  $\vec{j}_i \wedge \vec{B}_i$  which are responsible of hydrodynamic effects leading to a velocity  $\vec{u}$  of the fluids which can reach 0.5m/s. The knowledge of the motion and the stability of the bath-aluminum interface is very important for obtaining a good working of the cell. Among the different approaches found in the literature in order to study this phenomenon, let us mention Fourier analysis of linear models (see for instance [1]), linear stability of MHD stationary solutions (see for instance [2],[3]), or numerical modeling of the dynamic MHD equations (see [4] and its references).

In this talk we present a numerical modeling in order to compute the current density  $\vec{j}_i$ , the magnetic induction field  $\vec{B}_i$  with the screen effects of the steel shell, the motion of the fluids  $\vec{u}$  and its interface. The dissolution of alumina and its distribution in the cell are considered as well as the thermal effects.

To do this, we numerically solve a system of coupled partial differential equations:

- An elliptic equation for the potential  $V$  to obtain the current  $\vec{j}_i = \sigma(-\vec{\nabla}V + \vec{u} \wedge \vec{B}_i)$  which flows through the cell, where  $\sigma$  is the electric conductivity of the fluids,

- Maxwell equations to obtain  $\vec{B}$  from the current density  $\vec{j}$  and the equations modeling the magnetization effects of the steel shell,
- Incompressible Navier-Stokes equations with free surface to obtain the pressure  $p$  and the velocity  $\vec{u}$  from the gravity forces  $\rho \vec{g}$  and the electric forces  $\vec{j}_i \wedge \vec{B}_i$ ,
- A kinetic transport equation to describe the dissolution of alumina particles and a convection-diffusion equation to obtain the distribution of liquid alumina,
- Heat equation with phase change (temperature and enthalpy) for the computation of the solid ledges which are formed on the wall of the cell.

All these equations are numerically solved with finite elements methods in space and splitting methods in time. The magnetic induction field and the magnetization of the steel shell are obtained from a domain decomposition method (see [6] and [5]). The free interface between liquid aluminum and the electrolytic bath is obtained from a level set technique coupled to a stabilized finite element method for solving Navier-Stokes equations (see [7]). The transport equation for the particles of alumina is solved by a characteristic method coupled to a streamline upwind technique for the convection-diffusion of dissolved alumina (see[8]). Finally the heat equation is solved with a Chernoff scheme which allows to obtain the enthalpy and the solid fraction of the bath (see [9]).

## References

- [1] R. Moreau, D. Ziegler: *Stability of aluminum cells, a new approach, Light Metals, 1986, 359-364.*
- [2] J. Descloux, M. Flueck, M. V. Romerio: *Spectral aspects of an industrial problem. In Spectral analysis of complex structures. Hermann éditeurs des sciences et des arts, Paris, 1995, 17-33.*
- [3] J. Descloux, M. Flueck, M. V. Romerio: *A modelling of the stability of aluminum electrolysis cells. In Nonlinear partial differential equations and their applications. Collège de France Seminars, Vol XIII. D. Cioranescu and J.L. Lions editors, Pitman Research Notes in Mathematics Series 391. Addison Wesley Longman 1998, 117-133.*
- [4] J.-F. Gerbeau, C. Le Bris, T. Lelièvre: *Mathematical methods for the magnetohydrodynamics of liquid metals. Numerical Mathematics and Scientific Computation Series. Oxford Science Publications 2006.*

- [5] J. Rappaz, G. Steiner: *On a domain decomposition method for numerically solving a magnetic induction problem. Scientific report in Analysis and Numerical Analysis, EPFL. To appear.*
- [6] M. Flueck, T. Hofer, A. Janka, J. Rappaz: *Numerical methods for ferromagnetic plates. Scientific report Nr.08.2007, Institut d'Analyse et Calcul Scientifique EPFL 2007 and to appear in ECCOMAS Springer Series.*
- [7] M. Flueck, A. Janka, C. Laurent, M. Picasso, J. Rappaz, G. Steiner: *Some mathematical and numerical aspects in aluminum production. Proceedings of INSF2007, Journal of Scientific Computing, Springer Verlag. To appear.*
- [8] Th. Hofer: *Scientific report in Analysis and Numerical Analysis, EPFL. In preparation.*
- [9] M. Flueck, J. Rappaz, and Y. Safa: *Numerical simulation of thermal problems coupled with magnetohydrodynamic effects in aluminium cell. Accepted in Appl. Math. Modelling, to appear in 2008.*