

# Simulation of Electro-Thermal Processes

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## Abstract

Hall-Héroult cells, also known as aluminum reduction cells or ARCs, have been studied at industry research labs for many years. An ARC is a type of electro-chemical furnace used to separate aluminum from bauxite ore (alumina). Oxygen ions are driven off by passing an electrical current through an electrolytic bath containing the ore. The internal temperature of the molten mixture stratifies into a layer of pure metal and a highly corrosive material called cryolite. A compound of cryolite, alumina, and other trace materials accumulates and solidifies along the walls of the cell near the surface of the bath, forming a protective coating over the cell's refractory lining. System efficiency is affected as well.

Controlling the formation of the so-called *side ledge* or *side freeze* is a primary operational concern. If the side ledge is allowed to become too thin, the cryolite will quickly corrode the lining of the containment vessel and can even perforate the shell itself (steel). If the side ledge is allowed to become too thick, processing efficiency drops dramatically [LST96]. Since cell operation is naturally biased away from catastrophic failure, the industry suffers from a sort of inefficiency by design. Indeed, data submitted to Congress in 1988 suggests that the efficiency of contemporary ARCs is something less than 50% [SA88].

Inside of the cell, intense energy levels and the cryolite combine to form an extremely hostile environment. Actual measurements of the electrical and thermal fields are difficult and expensive to obtain and consequently, simulations of internal reactions are indispensable. Commercial research efforts benefit from access to realistic data, but they are equally hindered by the usual secrecy agreements found in industry, but our experience has shown that these labs often rely on outdated simulation technologies that are incapable of achieving the level of resolution required to accurately model such a complex process.

A transient model in two dimensions has been developed by one of the investigators. Its three-dimensional counterpart is well underway. Upon completion, a new approach for solving large, coupled systems of equations based on a multiscale finite element method (MFEM) will be implemented. A posteriori error analysis routine will be incorporated for validation purposes and also as a step in the direction of a self-adaptive computer model.

Other enhancements including the replacement of a direct solver with a generalized conjugate gradient solver and parallel preconditioner are planned. In the final stages of development, a threads-based port of the entire model will be completed and evaluated prior to beginning work on the end product message passing code. Both of these efforts will rely on a new source translator called CAPTools maintained by the University of Greenwich, London, UK. Versions that embed OpenMP directives and write MPI source will be tested. Scaling studies of the resultant codes will be performed on a number of shared memory and distributed memory supercomputers.

## Mathematical Model

Multidisciplinary analysis of Hall-Héroult cells generally revolves around two basic models. Magneto-hydrodynamics models are used to study fluid motion in the melted region. Electro-thermal models focus on optimal sizing of the side ledge. As a first step, we will consider an expansion of the latter type that includes the determining mechanisms of latent heat and the effects of superheating and supercooling.

The cell model includes temperature,  $T$ , the electric potential,  $P$ , and the rate of internal heat generation,  $Q$ , due to electrical resistance. Temperatures in the cell range from about 100° C to 960° C, thus the incorporation of material dependent properties such as electrical and thermal conductivities is essential. The mathematical model is represented in the following equations:

$$\begin{aligned} \text{Temperature, in the cell:} \quad & -\nabla \cdot (k(T)\nabla T) + Q(\nabla P) = \mathbf{r}(T)C_p(T)\left(\frac{\partial T}{\partial t}\right) \\ & \text{with appropriate boundary conditions} \end{aligned}$$

$$\begin{aligned} \text{Electric Potential, in the cell:} \quad & -\nabla \cdot (\mathbf{s}(T)\nabla P) = 0, \\ & P = P^* \text{ for the anode and collector bars} \end{aligned}$$

where  $k$ ,  $\mathbf{r}$ ,  $C_p$ , and  $\mathbf{s}$  are (respectively) the thermal conductivity, density, heat capacity, and electrical conductivity of the materials, and  $t$  is time. Note the dual coupling between the thermal and electrical equations through the dependence of specific heat ( $Q$ ) on the electric potential ( $P$ ) and the dependence of electrical conductivity ( $C_p$ ) on temperature ( $T$ ).

Nonlinearities in  $k$  and  $\mathbf{s}$  have been recovered by the investigators using cubic interpolation of experimental data for each of the different materials comprising a cell. Since the cells are driven by current flow through them, the system is modeled as a boundary value problem driven by the drop in potential between the anode and cathode. Rather than simply lagging the nonlinearities, an extrapolation method that retains second-order accuracy in the model is applied [R73].

Multiscale discretization methods developed by Xu [X96] for elliptic boundary value problems and by one investigator [AL96 and LL96] for fluid flow problems are promising approaches that serve to reduce the computational requirements of models represented in large, coupled, nonlinear systems. A basic two-scale method alternates between the application of a coarse mesh to determine a global solution envelope followed up by the application of a refinement based on the original mesh to resolve detailed structures. The ratio of element diameters between the scaled meshes must be implemented as a function of the approximate linearization used. See [AL96] for examples of these algorithms.

## Resource Requirements

Requirements for code development have been estimated at basic C90 and T3E award levels (10 and 500 BUs, respectively).

A sequence of production runs will be initiated on both platforms upon completion of this work. Problems will be designed such that the longest run on a dedicated C90 machine will require no more than 1 hour of CPU time. Optimistic (and convenient) assumption of perfect scaling efficiency implies that a sequence of C90 benchmarking runs (1, 2, 4, 8, and 16 CPUs) will require  $5 \times 16 = 80$  C90 BUs. Use of a realistic assumption that the performance of one C90 CPU will be matched by 16 T3E processors implies that a similar sequence (1, 2, 4, 8, ..., 512 PEs) of T3E bench runs will consume  $10 \times 16 \times 16 = 2560$  T3E BUs.

Finally, a discovery effort involving at least one "real" physical problem will be undertaken on the T3E. The estimate for this work must be based on the the size of the targeted problem and the results of the performance tests described above and therefore, requirements for experimentation will be handled at a later date by an amendment to this proposal.

Therefore, the total allocation request is for 90 C90 BUs and 3060 T3E BUs. Please find attached account applications for two investigators, one faculty and one graduate assistant.

## Acknowledgements

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## References

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## Attachments

Graphical output produced by two-dimensional ARC model (coarse mesh).

PSC account request forms.