Using ANSYS and CFX to Model Aluminum Reduction Cell since1984 and Beyond

> Dr. Marc Dupuis







4 Le Lingot, mardi, le 2 septembre 1980

Marc Dupuis Un stage qui portera ses fruits

par Christine Bernard

Marc Dupuis a récemment complété son baccalauréat en génie chimique à l'Université Laval. Il prépare sa maîtrise pour l'automne. Cet été, il a consacré son travail à la recherche pour le compte du Centre de recherche et de développement Arvida.

Pendant quatre mois, il a simulé, avec des modèles mathématiques, la circulation de l'air dans les salles de cuves. Ces modèles permettent d'aboutir plus rapidement à des solutions susceptibles d'améliorer les conditions de travail des employés.

Relations humaines

Il en est à sa première expérience à Arvida. C'est également la première fois qu'il travaille spécifiquement dans son domaine. Mais il voulait absolument voir ce qu'est le travail en usine. Il considère que l'école ne peut tout lui apprendre. Les relations avec les employés sont très importantes, et à ce titre sont essentielles à la formation. "On n'apprend que sur le métier", précisaitil.

Expérience à transmettre

"Je voulais absolument voir ce qu'est le travail en industrie." Marc Dupuis souligne également que les cours sont parfois très théoriques et, en cela, demeurent assez loin de la réalité. La théorie et la pratique font un complément, et c'est cela qu'il essaiera de transmettre aux plus jeunes étudiants, quand il retournera à Québec.



1980-84, 2D potroom ventilation model





1980-84, 2D potroom ventilation model







Best model results

The best results of my Ph.D. work: the 2D finite difference vorticity-stream function formulated model could not reproduces well the observed air flow regardless of the turbulence model used.



1984, 3D thermo-electric half anode model



2 PREP7 ELEMENTS

AUTO SCALING

That model was developed on ANSYS 4.1 installed on a shaded VAX 780 platform.

That very first 3D half anode model of around 4000 Solid 69 thermo-electric elements took 2 weeks elapse time to compute on the VAX.







1986, 3D thermo-electric cathode side slice and cathode corner model



ANSYS 4.2 AUG 28 1986 15:29:53 PLOT NO. 1 PREP7 ELEMENTS MNUM=1

XU=-1 YU=-1 ZU=1 DIST=1.75 XF=.701 YF=1.3 ZF=.673 ANGL=90 HIDDEN The next step was the development of a 3D cathode side slice thermoelectric model that included the calculation of the thickness of the solid electrolyte phase on the cell side wall.

Despite the very serious limitations on the size of the mesh, a full cathode corner was built next.



Design of 2 high amperage cell cathodes





1987: Apex 4

1989: A310

Comparison of the predicted versus measured behavior was within 5% in both cases, demonstrating the value of the numerical tools developed.



1988, 3D cathode potshell plastic deformation mechanical model



The new model type addresses a different aspect of the physic of an aluminum reduction cell, namely the mechanical deformation of the cathode steel potshell under its thermal load and more importantly its internal pressure load.



1989, 3D cathode potshell plastic deformation and lining swelling mechanical model



First "Half Empty shell" potshell model developed in 1989 and presented at a CRAY Supercomputing Symposium in 1990

GEN

1992, 3D thermo-electric quarter cathode model



With the upgrade of the P-IRIS to 4D/35 processor, and the option to run on a CRAY XMP supercomputer, the severe limitations on the CPU usage were finally partially lifted.

This opened the door to the possibility to develop a full 3D thermo-electric quarter cathode model.



1992, 3D thermo-electric "pseudo" full cell and external busbars model

As a first step toward the development of a first thermo-electromagnetic model, a 3D thermo-electric "pseudo" full cell and external busbars model was developed.

That model was really at the limit of what could be built and solved on the available hardware at the time both in terms of RAM memory and disk space storage.



1992, 3D cathode potshell plastic deformation and lining swelling mechanical model



The empty quarter potshell mechanical model was extended to take into account the coupled mechanical response of the swelling lining and the restraining potshell structure.

That coupling was important to consider as a stiffer, more restraining potshell will face more internal pressure from the swelling hining material.

1992, 3D cathode potshell plastic deformation and lining swelling mechanical model



A numerical scheme external to the ANSYS solver must be setup, starting from an assumed initial internal load. The task of that external numerical scheme is to converge toward that cathode block equilibrium condition pressure loading for each element face of the carbon block/side lining interface.



1992, 3D cathode potshell plastic deformation and lining swelling mechanical model



1993, 3D electro-magnetic full cell model



The development of a finite element based aluminum reduction cell magnetic model clearly represented a third front of model development.

Because of the presence of the ferro-magnetic shielding structure, the solution of the magnetic problem cannot be reduced to a simple Biot-Savard integration scheme.



1993, 3D electro-magnetic full cell model



1993, 3D electro-magnetic full cell model



1993, 3D transient thermo-electric full quarter cell preheat model

The cathode quarter thermo-electric model was extended into a full quarter cell geometry in preheat configuration and ran in transient mode in order to analyze the cell preheat process.

The need was urgent, but due to its huge computing resources requirements, the model was not ready in time to be used to solve the plant problem at the time.



1993's Model Extension to Stress Analysis



Equivalent stress in the cathode panel at 36 hours – standard coke bed



1993, 2D CFDS-Flow3D potroom ventilation model





1993, 2D CFDS-Flow3D potroom ventilation model



2D "Reynolds flux" model results vs. physical model results



1998, 3D thermo-electric full cell slice model



As described previously, the 3D half anode model and the 3D cathode side slice model have been developed in sequence, and each separately required a fair amount of computer resources.

Merging them together was clearly not an option at the time, yet it would have been a natural thing to do. Many years later, the hardware limitation no longer existed so they were finally merged.



1998, 2D+ thermo-electric full cell slice model



2D+ version of the same full cell slice model was developed. Solving a truly three dimensional cell slice geometry using a 2D model may sound like a step in the wrong direction, but depending on the objective of the simulation, sometimes it is not so.

The 2D+ model uses beam elements to represent geometric features lying in the third dimension (the + in the 2D+ model).



1999, 2D+ transient thermo-electric full cell slice model



An interesting feature of that model is the extensive APDL coding that computes other aspects of the process related to the different mass balances like the alumina dissolution, the metal production etc.

As that type of model has to compute the dynamic evolution of the ledge thickness, there is a lot more involved than simply activating the ANSYS transient mode option.



2000, 3D thermo-electric cathode slice erosion model



Cathode erosion rate is proportional to the cathode surface current density and that the initial surface current density is not uniform, the erosion profile will not be uniform.

Furthermore, that initial erosion profile will promote further local concentration of the surface current density that in turn will promote a further intensification of the non-uniformity of the erosion rate.



Base Case Model Solution





2001, 3D CFX-4 potroom ventilation model





2001, 3D CFX-4 potroom ventilation model



Temperature fringe plot, back plane



2002, 3D thermo-electric half cathode and external busbar model





Relationship between Local Heat Transfer Coefficient of the Liquid/Ledge Interface and the Velocity Field





2002, 3D thermo-electric half cathode and external busbar model





2003, 3D thermo-electric full cathode and external busbar model

A P4 3.2 GHz computer took 16.97 CPU hours to build and solve that model



2003, 3D thermo-electric full cathode and external busbar model







2004, 3D thermo-electric full cell and external busbar model

Initial 585,016 elements mesh Coarser 329,288 elements mesh



2004, 3D thermo-electric full cell and external busbar model

.2247

.4495

.6743

.8991

1.124

1.349

1.574

1.798

2.023







Thermo-Electric Design of a 740 kA Cell, Is There a Size Limit?

Thermo-Electric Design of a 740 kA Cell Using a Complete Full Cell Quarter Thermo-Electric Model



2004, 3D thermo-electric full cell and external busbar erosion model



Once the geometry of the ledge is converged, a new iteration loop start, this time to simulate the erosion of the cathode block as function of the surface current density



2005 Weakly coupled 3D thermo-electric full cell and external busbar and MHD model







First Weakly Coupled Solution Between Thermo-Electric and MHD Models: 500 kA Cell Design



Velocity fields and turbulent effective viscosity distribution in liquid aluminium for the 500 kA cell as predicted by the MHD model

First Weakly Coupled Solution Between Thermo-Electric and MHD Models: 500 kA Cell Design



 $h_{\text{metal/ledge (W/m2K)}} = 1684 + 2000 V_{(m/s)}^{1/2}$

 $h_{\text{bath/ledge (W/m2K)}} = 1121 + 2000 V_{(m/s)}^{1/2}$

First Weakly Coupled Solution Between Thermo-Electric and MHD Models: 500 kA Cell Design

The obtained ledge profile geometry is transferred to the MHD model and the MHD cell stability analysis is computed again





2006 Weakly coupled 3D thermo-electric full cell model and mechanical quarter cell model





2006 Weakly coupled 3D thermo-electric full cell model and mechanical quarter cell model



Temperature Loading for the Fine Mesh Model



2006 Weakly coupled 3D thermo-electric full cell model and mechanical quarter cell model



Relative Vertical Displacement for the Fine Mesh Model



500 kA Cell Mechanical Model Results

Base Case.

With Cooling Fins.

With Forced-Air Cooling.



Temperature distribution for the studied 500 kA cell configurations.

500 kA Cell Mechanical Model Results



Comparison of the relative vertical displacement on the long axis of the 500 kA cell.

2007 Weakly coupled thermo-electromechanical model and magneto-hydrodynamic full cell and external busbar model







2009, "Half Empty Shell" Potshell Model



Took 103842 CPU seconds or 1.2 CPU days which is 3.8 times more than what was required to solve the "almost empty shell" potshell model.

2009, "Improved Half Empty Shell" Potshell Model



2010, Thermo-Electro-Mechanical Anode Stub Hole Model



Pressure and temperature dependent contact resistance model results



2010, Thermo-Electro-Mechanical Anode Stub Hole Model





2010, Thermo-Electro-Mechanical Anode Stub Hole Model





Horizontal voltage 40 mm under the anode carbon surface

Instrumented Anode: Anode Stud Voltage Drop Comparison



Future developments

Currently, we can fit Hall-Héroult mathematical models into three broad categories:

- Stress models which are generally associated with cell shell deformation and cathode heaving issues.
- Magneto-hydro-dynamic (MHD) models which are generally associated with the problem of cell stability.
- Thermal-electric models which are generally associated with the problem of cell heat balance.





Future developments

Yet, to be rigorous, a fusion of those three types of model into a fully coupled multi-physics finite element model is required because:

- MHD is affected by the ledge profile, mostly dictated by the cell heat balance design.
- local ledge profile is affected by the metal recirculation pattern mostly dictated by the busbars MHD design.
- shell deformation is strongly influenced by the shell thermal gradient controlled by the cell heat balance design.
- steel shell structural elements like cradles and stiffeners influence the MHD design through their magnetic shielding property.
- global shell deformation affects the local metal pad height, which in turn affects both the cell heat balance and cell stability



3D fully coupled thermo-electro-mechanicomagneto-hydro-dynamic full cell and external busbar model weakly coupled with a 3D potroom ventilation model





