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THERMO-CHEMO-MECHANICAL MODELING OF A HALL-HÉROULT CELL THERMAL BAKE-OUT

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Abstract

Start-up of a Hall-Héroult cell is a delicate task. Modern practices for high amperage cells involve preheating the lining before the molten electrolyte is poured in. The optimum preheating method for a rapid production of metal and a long pot life is elusive.

Numerical modeling is an invaluable tool to gain insights into the complex phenomena taking place during start-up. The adequate modeling of the mechanical response of the lining is critical to detect risks of cathode block cracking or the development of gaps where liquids could leak. Taking into account the ramming paste baking, the quasi-brittle nature of carbon and the contact interfaces are examples of key elements to consider.

A finite element demonstration cell slice model was built and simulations of different thermal bake-out scenarios were performed using the in-house code ***FESh++***. Potential industrial application of the model is discussed.

Introduction

It is well accepted that start-up and early operation have a strong influence on the performance and life of a Hall-Héroult cell [1]. Generally, a preheating phase is necessary during start-up to ensure a smooth transition to normal operation.

The requirements for preheating, summarized in [2], are the following:

- The cathode block temperature must be high enough to:
    - Minimize bath freezing when bath is poured in. Freezing leads to an uneven current distribution and a potentially harmful unstable early operation.
    - Avoid large thermal gradients in the cathode blocks before bath is poured in. Large gradients may induce cracks.
- If the preheating rate is too fast or not uniform enough, large thermal gradients within the cathode blocks will occur and may also induce cracks.
- The paste temperature must be sufficiently high to avoid flash pyrolysis when bath is poured in.
- The lining must be maintained in compression at all times to ensure no gap is present in the lining as this would allow bath or metal penetration.

Although preheating methods in the industry vary, thermal bake-out using gas-fired or oil-fired burners has been shown to provide the most uniform temperature distribution in the lining [1,3]. The desired heat-up curve also varies, using one or more surface temperature ramps, and sometimes ending with a soaking time at constant temperature [1,2,4].

An experimental study was carried out on VS Søderberg cells to determine the optimal thermal preheating cycle [2]. Surface and sub-cathodic temperature measurements were performed for different ramps and final temperature. It was concluded that the best results were obtained with a low heat-up rate and a high final block temperature.

Unfortunately in practice, the pressure to produce metal as fast as possible calls for the shortest possible preheating time. This results in less than optimal heat-up curves for the cathode blocks and lining, and the mechanical response of the cell then becomes a critical limiting factor.

Important Aspects of Cell Mechanical Behaviour

Complex phenomena are taking place during the start-up and early operation of a cell. Predicting its mechanical response is not a simple task.

There are several difficulties in this task. For example, the interaction of the lining with the pot shell, the intrinsic mechanical behaviour of the lining materials, the transformations within the materials, and the cell construction are important and are changing during the bake-out period.

Numerical modeling is therefore an interesting tool to help provide insights into these complex phenomena and help in designing the optimal procedure for a given cell.

Lining and Pot Shell Interaction

The pot shell does not only serves as a structural container for the lining, but is also an integral part of the cell design. In addition to its thermal purpose, it must also maintain the lining in firm compression without inducing cracks or excessive deformation.

It is observed that in operation the pot shell deforms. The problem is in reality *strain-driven*. The shell and the lining deformation and stresses result from the complex interaction of their expansion (thermal and chemical) and their stress-strain response. Although during preheating the shell is not likely to deform very much, this does not change the fundamental nature of the problem. The dilatometric response of the materials and their stress-strain behaviour must therefore be known accurately.

Lining Mechanical Behaviour

Several dense refractory materials are characterized by a *quasi-brittle* behaviour. That is they can still bear some load after their peak stress has been reached, their strength and ductility increases with confinement, they are permanently deformed at only a fraction of their peak stress, and they are significantly stronger in compression than in tension. Concrete, dense bricks and carbon [5] are all quasi-brittle materials.

On the contrary, steel has the same response in tension and compression, regardless of the confinement. Therefore, it is unrealistic to assume a steel-like behaviour for the cell lining, as it will not provide an adequate tool to predict cracking.

Also, although the temperature is normally always increasing during preheating, it is still possible to undergo a local unloading. For example the load would decrease in the region surrounding a growing crack, or when a material experiences a contraction. For instance, this is the case with ramming paste as it is baked.

Therefore, it is important to account for thermally-, chemically- or mechanically-induced irreversible deformations in a material in order to capture the potential opening of gaps in the lining and to predict correctly the stresses.

Material Transformation and Time Response

During preheating, it is assumed that liquid bath is not present, so the effect of sodium and the associated chemical reactions within the refractory lining can be ignored.

However, castables will cure and ramming paste will start to bake and will undergo irreversible transformations of their microstructure. This will affect their thermal and mechanical behaviour. In general, these reactions also cause an irreversible volume change.

Ramming paste is undoubtedly a critical part of the cell, as it should seal the lining while accommodating some of the cathode blocks expansion. It is also difficult to characterize and to model. It was reported that during baking, most pastes first expand and then shrink. A plausible explanation is that the initial swelling is caused by a build-up of reaction gases while the subsequent shrinkage is due to the cokefaction of the binder phase [6,7].

The strength and stiffness of the paste increases by more than an order of magnitude during baking while its ductility decreases in the same proportion. Its behaviour evolves from being almost incompressible and plastic to that typical of quasi-brittle materials.

Ramming paste has also been shown to continue to deform under a constant load, a phenomenon known as creep [6]. Some of this additional deformation is recovered over time when the load is removed, but the rest of it is permanent. Creep relaxes the stresses in the material but also increases the risks of opening gaps, since it increases the deformation for a given load.

Cell Construction

Some of the lining materials are laid dry while mortar is used to join others. However, most interfaces cannot be assumed to be completely cohesive. Joint behaviour has a profound effect on the stiffness of the structure, and it is of paramount importance to characterize this correctly for the accurate prediction of a possible gap opening in the lining.

For most interfaces, the most conservative assumption is to neglect cohesion altogether. This means that this interface cannot sustain a tensile stress and that a gap will open under a tensile loading.

Finite Element Demonstration Model

For demonstration purposes, a realistic prebaked point-fed 300 kA cell design inspired from a VAW publication [8] was used. The thermo-electrical results, using ANSYS, are presented in [9] for normal steady-state operation.

Geometry, Assumptions and Simplifications

As a first step, a fully coupled cathode slice model was built using the finite element toolbox ***FESh++*** [10] to illustrate the effect of the heating rate at the center of the cell. The slice mesh represents a quarter cathode and its corresponding lining, shell and cradle, as shown in Figure 1. The shell and cradle are discretized using large rotation shell elements while the lining is discretized using 3D brick elements. The semi-graphitic cathode blocks (~30% graphite) are glued together, as can be seen from the absence of a small joint.

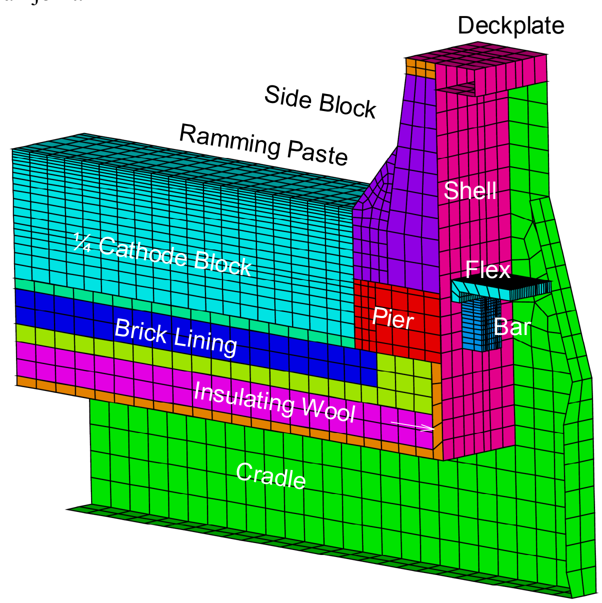


Figure 1 -Thermal slice mesh.

Contact mechanics is used between different parts of the lining, as can be seen from the non-concordant mesh at the interfaces between different parts (Figure 2).

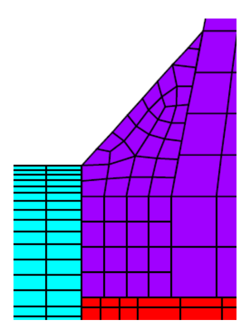


Figure 2 – Slice mesh detail: non-concordant interface mesh.

An additional thermal contact resistance (constant or contact pressure-dependent) can be used at an interface, for example to emulate the effect of a mortar joint. Thermal conductance values were estimated from [11]. The interfaces are assumed to be non-cohesive, *i.e.* they cannot sustain a tensile stress.

The cradles are welded to the shell, and the steel plate thicknesses were estimated from experience [12]. The collector bar is rodded with cast iron, and a simple geometry was assumed, as shown in Figure 3. At ambient temperature, an air gap is present between cast iron and carbon, and as the assembly heats up, thermal expansion of the parts eliminates this air gap.

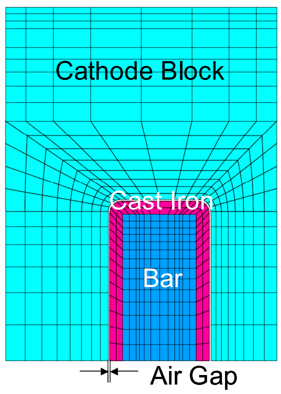


Figure 3 - Collector bar, cast iron and half-cathode block detail.

The brick lining under the cathode block is assumed to have no bending stiffness because in this design there is a layer of insulating refractory fibre wool that will absorb its thermal expansion in the horizontal plane. Therefore, the brick lining under the cathode does not contribute significantly to the mechanical response of the cell during preheating and is accordingly not solved in the mechanical problem. Conceptually, the cathode block and the pier are assumed to rest on springs of equivalent stiffness to the underlying brick lining. This is implemented in the finite element model by using contact mechanics to connect the shell floor to the bottom of the collector bar and pier. The mechanical mesh is shown in Figure 4. Note that the whole slice is solved for temperature (see Figure 1).

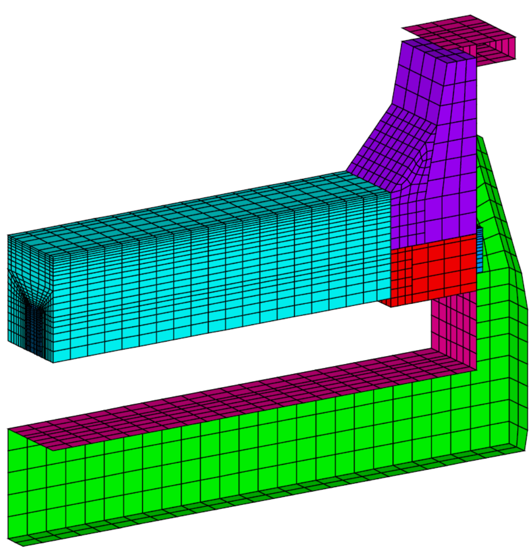


Figure 4 - Mechanical slice mesh.

Material Properties

The thermal properties were obtained from [9]. The mechanical constitutive laws are summarized in Table 1.

Table 1 - Assumed mechanical material models.

Material	Material Model	Reference
Cathode Block	Quasi-Brittle	[5]
Collector Bar	Elastic	[13]
Cast Iron	Elastic	[13]
Pier	Elastic	[13]
Ramming Paste	Reactive Quasi-Brittle	[6]
Side Block	Quasi-Brittle	[5]
Castable	Quasi-Brittle	[5]

Boundary Conditions and Loads

The only external mechanical load considered is gravity. It must be included to stabilize the problem, since the lining is mostly free to move in the upward vertical direction.

The dashed lines in Figure 5 represent planes S1, S2 and P3 on which symmetry conditions could be applied.

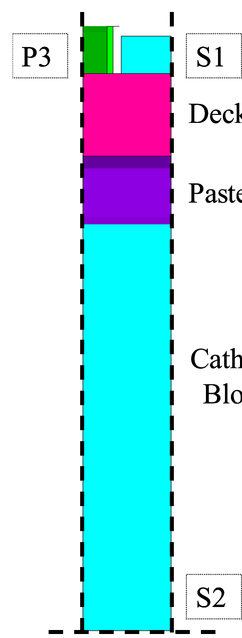


Figure 5 - Slice symmetry planes, top view.

Planes S1 and S2 are true symmetry planes. For the shell and cradle, P3 is obviously a true symmetry plane as well. However, the conditions for the lining on plane P3 are difficult to evaluate. It reality, the confinement on this plane is the result of the interaction between the lining and the shell along the length of the pot. For this study, the two extreme cases were considered for the lining on plane P3: symmetry conditions, and free to move.

The thermal boundary conditions for all external surfaces take into account natural convection and grey body radiation, using well-known semi-empirical correlations, and were taken from [9]. The surface of the ramming paste and the sidewall are insulated by crushed bath. A convection coefficient of 1 W/m^2K was used.

Given that the objective is not to design a gas-preheating burner system, but rather to study the transient mechanical response of the cell during preheating, the boundary conditions on the top surface of the cathode block were kept very simple. A heat transfer coefficient of 650 W/m^2K was assumed, with a gas temperature following a linear ramp-up to 955ºC in 12, 24, 36 or 72 hours.

Results and Discussion

Thermal

Final temperatures at the top surface of the block in the center of the cell are within 20ºC for all simulations. As expected, the thermal gradients within the cathode blocks are decreasing with the increasing preheating time. For instance, Figure 6 represents the difference between the surface and sub-cathodic temperature at the end of the cathode block (adjacent to the ramming paste, between the collector bars).

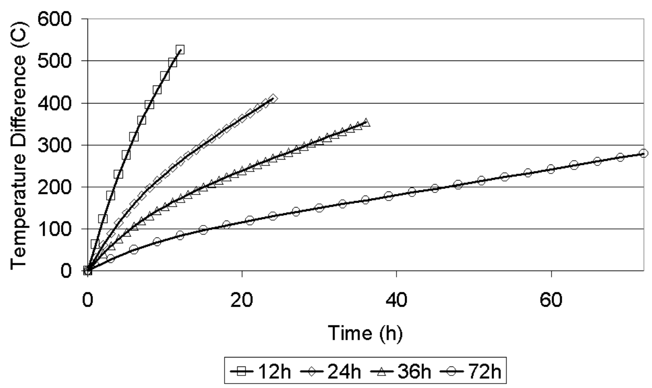
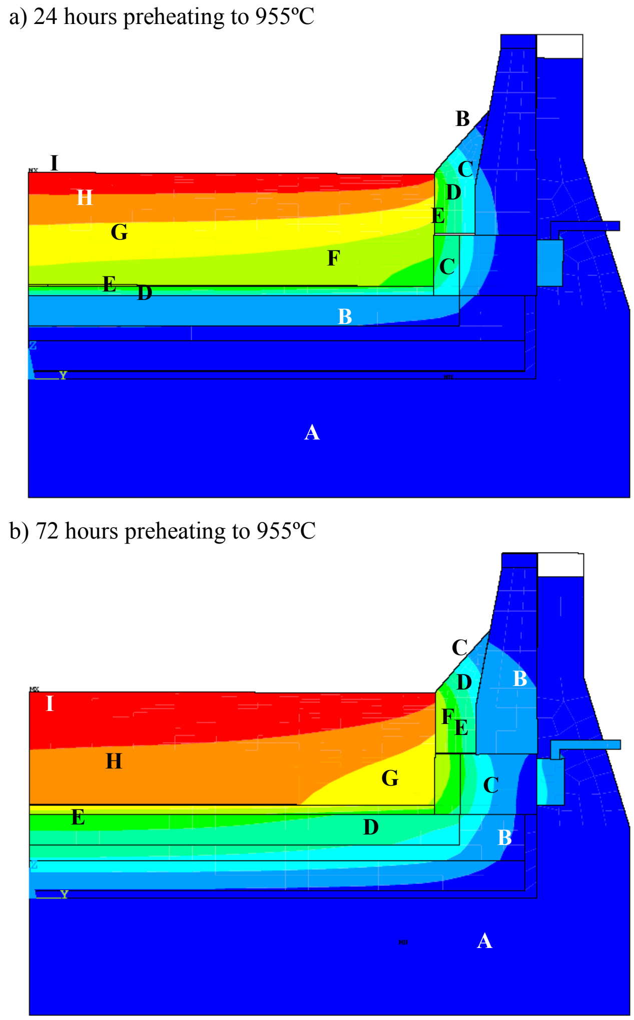


Figure 6 – Difference between surface and sub-cathodic temperature for different preheating times to 955ºC.

Figure 7 shows the isotherms at the end of preheating to 955ºC in 24 and 72 hours. The large thermal inertia of the lining is such that even after 72 hours of preheating, the shell floor and most of the shell sidewall are still cold (Figure 7b). Note that the discontinuity in the isotherms is a result of the thermal resistance of the interface between the parts.

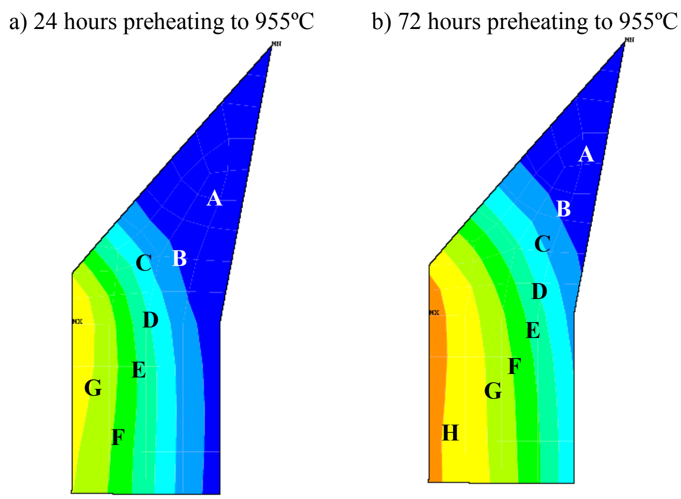
An interesting effect of the transient diffusion of heat into the lining is that the extent of baking of the ramming paste changes dramatically with the preheating time, as shown in Figure 8. Note that the local baking index is defined as the paste local compressive strength normalized to its strength at full baking (refer to [6] for more details).

After 24 hours of preheating, some of the paste in the line of action of the cathode block expansion is still completely green (Figure 8a), *i.e.* it is still plastic. This is not the case for a preheating of 72 hours (Figure 8b). The baking of the paste must be taken into account in the design of a start-up method. Green paste deforms to accommodate the expansion of the cathode blocks, but it also shrinks when it starts to bake. The timing of this process must be such that no gap will open where bath could leak into the lining when the bath is poured in the cell after the preheating is completed.



A:20 B:133 C:246 D:359 E:473 F:586 G:699 H:812 I:925 (ºC)

Figure 7 – Isotherms at the end of preheating.



A: Green B:13 C:24 D:35 E:45 F:56 G:67 H:78 I:89 (%)

Figure 8 – Ramming paste baking index at the end of preheating.

Mehanical

The boundary conditions on the lining surface on plane P3 (Figure 5) have a small impact on the overall displacements along the width of the cell, but have a large impact on the stress-strain behaviour of the lining. This aspect will be covered later on.

The deformed shape of the lining at the end of the preheating can provide a strong indication on the formation of gaps where bath could potentially leak. For example, Figure 9 shows the final deformed shape for a 24 hours preheating to 955ºC (corresponding to the temperature distribution in Figure 7a), with displacements amplified by a factor of 10. As expected, the cathode blocks are bending up and compress the ramming paste.

A gap opens between the ramming paste and the pier as the cathode block pushes up the paste (Figure 9, *A*). The thermally induced deformation of the shell also opens up a gap between the side block and the sidewall near the deckplate (Figure 9, *B*).

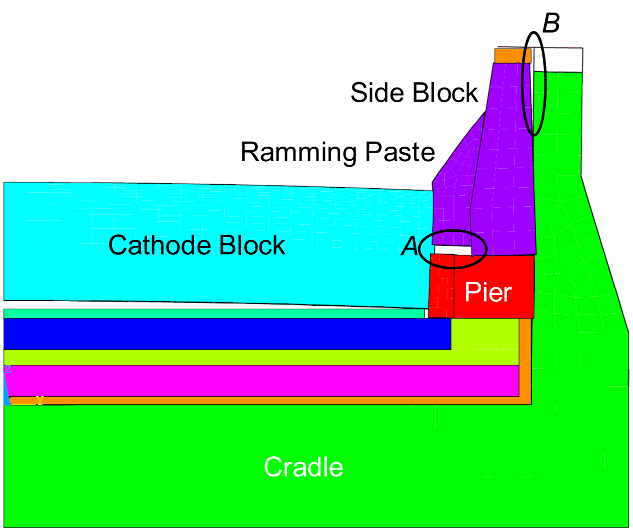


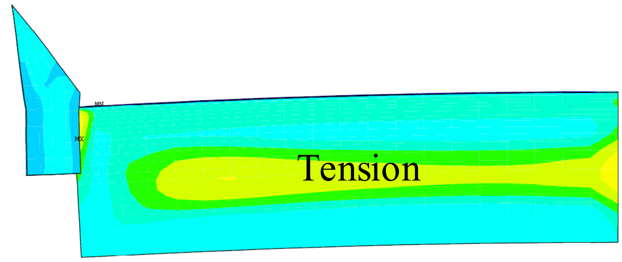
Figure 9 - Exaggerated deformed shape at the end of a 24h preheating to 955ºC.

The impact of the boundary conditions on the lining on plane P3 (Figure 5) on the response of the cathode block was investigated. Two extreme cases were simulated: full symmetry and free to move. This corresponds respectively to an infinitely rigid shell, and to a perfect expansion joint along the length of the pot.

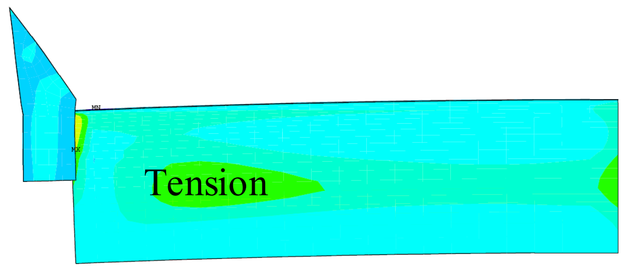
Faster preheating rates mean larger thermal gradients in the cathode blocks, which leads to tensile stresses as shown in Figure 10. For the studied cases where the lining surface on plane P3 is free to move, these stresses were not sufficient to crack the block.

Assuming a full symmetry boundary condition on plane P3, it was found that for all our studied cases, the cathode block is permanently deformed and cracks occur in the collector bar slot. A typical cracking pattern is shown in Figure 11. When the lining surface on plane P3 is free to move, no such crack develops.

a) 12 hours preheating to 955ºC



b) 24 hours preheating to 955ºC



c) 72 hours preheating to 955ºC

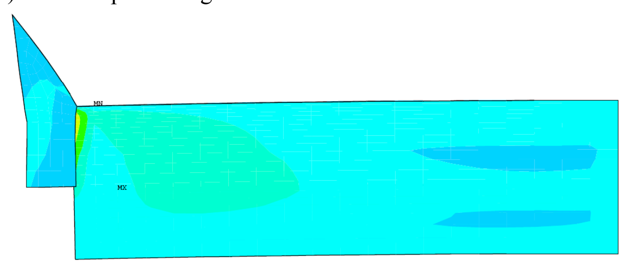


Figure 10 – First principal stress in cathode block and ramming paste at the end of preheating.

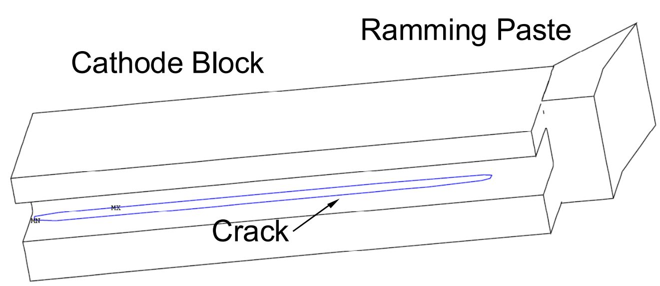


Figure 11 – Cathode block cracking for 24h preheating to 955ºC, full symmetry conditions on plane P3.

It had been previously demonstrated that a slice model might be used for the thermo-electric design of a cell [14]. Given the significant difference of behaviour of the cathode block with the change in boundary conditions on plane P3, it is clear that a slice model cannot be trusted to accurately predict cathode cracking during preheating unless the shell provided no confinement along the length of the pot, or otherwise if it was infinitely rigid. As this is rarely the case in practice, at least a quarter cell should therefore be modeled. Obviously, this is also required to study the corner of the cell.

However, these results do show that a proper amount of expansion relief along the length of the cell must be built-in the design. Ramming paste small joints between cathode blocks will partially play that role. Predicting the resulting effect is not trivial. Further, to avoid leaks into the lining, the end walls must also provide an adequate confinement.

Conclusion

A finite element model of a Hall-Héroult cell slice was built using the in-house code ***FESh++***. Key features of the model include the baking of ramming paste, the quasi-brittle nature of carbon and contact interfaces.

The transient fully coupled thermo-mechanical solution on an Opteron 850 64-bit machine required approximately 2.6 GB of RAM and 2.9 to 3.3 hours of wall clock time per time step. The total wall clock time then varied between 35 and 120 hours.

Faster preheating rates mean larger thermal gradients in the cathode blocks. For the modeled configuration, this leads to a horizontal tensile stress zone in the cathode block. For the cases studied these stresses were not sufficient to crack the block but this highlights one of the possible cathode failure mechanisms.

From this work, it was shown that a slice model is not sufficient to detect cracking of the cathode blocks for practical cell designs. At least a quarter cell needs to be modeled to accurately represent the confinement of the lining along the length of the cell. However, it is possible to obtain valuable information with a slice model about the extent of ramming paste baking and the opening of gaps that would allow bath infiltration into the lining and possibly reduce pot life.

To help determine the optimal final cathode surface temperature and ramming paste baking profile, it is now necessary to study what happens when the bath is poured in the cell. The timing of the cathode block expansion and ramming paste shrinkage is critical to ensure no gap will form which would allow liquid to leak into the lining. Thermal shock of the cathode blocks and flash pyrolysis of the ramming paste must also be avoided. The desired conditions at the end of preheating could then be reverse engineered.

From the work presented here, it can be seen that a numerical model is an invaluable tool to gain insights into the complex response of a cell during start-up. Once validated with experimental measurements, it can be used in the optimisation of the heat-up practices. The results of the model could also be used to determine some control metrics in the operation, for example by relating the evolution of cathode bar temperature to the risks of cathode block cracking.

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