# ON THE IMPORTANCE OF FIELD VALIDATION IN THE USE OF CELL THERMAL BALANCE MODELING TOOLS

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**Abstract**

Mathematical models have become essential for the design of modern, efficient high-amperage reduction cells, but the models are only one part of the cell design process. Since many of the inputs to a thermal balance model are difficult to evaluate, a process for validation of the predictions of the model is essential.

The validation process typically includes two sources of feedback: from operational pots and from post-mortem examination. Measurements of temperatures, heat fluxes and ledge shape must be made on the operating pots. In addition, prototype pots are shut down for post-mortem examination (cell autopsy) which is the only way to evaluate transformations of materials.

The transformation of materials during operation is one of the major reasons why model predictions do not match real operation. The risk of using unvalidated models to carry on design work is highlighted through the presentation of a real example from the past.

## Introduction

As described in the introduction to the modeling section of Essential Reading in Light Metals Vol. 2 [1], modeling of Hall-Héroult cells went from essentially non-existing, to being very expensive and mostly fruitless, to finally becoming a big success story, finally becoming indispensable in the process of designing modern, efficient high-amperage cells [2]:

"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".

In order to be successful, the design of high amperage cells must be conducted using the "cell development cycle" method [3]. The method comprises several steps, from modeling to measurement campaigns that must be used in repetitive cell design improvement cycles:

1) Cell design through modeling
2) Cell engineering and prototype cells construction
3) Prototype cells operation
4) Prototype cells measurement campaigns
5) Prototype cells postmortem autopsy
6) Model calibration and validation

This cycle is required for two reasons, one is to measure the behavior of cell prototypes that are testing innovative design ideas, for example the replacement of carbon side blocks with SiC or collector bars with copper inserts.

The second reason is the collection of data to be used for model validation. This is very important because models are only as good as the quality of the inputs used to set them up, hence the famous expression: "garbage in, garbage out".

The temperature dependent material properties used in models are such critical model inputs. In models, those properties are set to be temperature dependent but this image is misleading as it is not the complete picture.

For example, refractory brick manufacturers do provide temperature dependent thermal conductivity data obtained by testing their bricks at different operating temperatures.

However, in a Hall-Héroult cell, the cathode lining is exposed to chemical degradation that will significantly affect its properties. Those affected properties are the ones that need to be used as inputs in models and those properties are especially difficult to assess [4, 5].

Only data obtained from cell prototypes in steps 4 and 5 of the cell development cycle can be used in order to get reliable predictions from cell thermal balance models.

## Prototype cells heat balance measurement campaigns

The first way to verify the accuracy of cell heat balance model predictions is to directly compare them with data obtained from prototype cell heat balance measurement campaigns [6, 7].

This technique consists of measuring the heat flux on enough locations of the external surface of the cell to be able to calculate the global heat loss of the cell such as the one presented in Table 1.

Cell heat balance models will generate equivalent cell heat balance predictions that can be compared at posteriori to the cell heat balance measurements. Considering the accuracy of individual cell measurements of +/- 5% in the best cases, several such cell heat balance measurements are required to ensure that the model is calibrated using reliable data.

Comparison of the global heat loss and the heat loss partition will tell if the model predictions were right or not but will not directly tell what need to be adjusted if the predictions were not perfect.

Figure 1: Measurement of the heat flux on the crust and the anode yoke using heat flux probes from Japan in the 70's

Table I: Measured cell heat loss from Hirakud HSS 55 kA cell, table II in [7]

Heat Balance Results

| | | | |
|---|---|---|---|
| date: | 5-Nov-03 | Cell: | Cell 265 |
| **Cathode Heat Losses** | **W / m2** | **kW** | **%** |
| Shell side coverplate | 821 | 2.26 | 2.00 |
| Shell side spacer between boxes | 1796 | 3.59 | 3.18 |
| Shell side bottom box | 3105 | 6.41 | 5.69 |
| Collector bars to air | 1337 | 7.96 | 7.06 |
| Collector bars to flexible | | 2.40 | 2.13 |
| Shell side wall collector bar level | 625 | 0.57 | 0.50 |
| Shell side wall insulation level | 981 | 1.80 | 1.60 |
| Shell side vertical boxes | 918 | 1.97 | 1.75 |
| Shell side floor perimeter section | 1172 | 9.56 | 8.48 |
| Shell side floor center section | 1884 | 8.14 | 7.22 |
| Shell end coverplate | 809 | 2.21 | 1.96 |
| Shell end spacer between boxes | 1789 | 3.55 | 3.15 |
| Shell end bottom box | 3065 | 6.29 | 5.58 |
| Shell end wall collector bar level | 623 | 0.81 | 0.72 |
| Shell end wall insulation level | 969 | 1.82 | 1.61 |
| Shell end vertical boxes | 1150 | 2.16 | 1.92 |
| Shell end floor perimeter section | 1165 | 6.34 | 5.62 |
| **Total for the cathode part** | | **67.82** | **60.17** |
| **Anode Heat Losses** | | | |
| Crust | 306 | 2.85 | 2.53 |
| First side channel | 4002 | 12.11 | 10.74 |
| Second side channel | 2037 | 6.16 | 5.47 |
| Third side channel | 1206 | 3.65 | 3.24 |
| Forth side channel | 739 | 2.24 | 1.98 |
| Above forth side channel | 594 | 1.70 | 1.51 |
| Anode top | 552 | 4.13 | 3.67 |
| Studs | | 12.06 | 10.70 |
| **Total for the anode part** | | **44.9** | **39.83** |
| **Total for the cell** | | **112.7** | **100.00** |
| **Cell internal heat** | | **117.8** | |
| **Blitz closing** | | **95.71%** | |

**Prototype cells postmortem autopsy**

The only way to directly obtain the required used material properties required as inputs in models is to stop the prototype cells, dig out samples and measure the properties of those samples at a range of operating temperatures.

This is typically done in parallel with postmortem cell autopsies which more typically are carried out to determine the mechanism of failure of cells that tapped out or had to be stopped just before it happened [8]. Yet, it is not uncommon to stop some prototype cells for the purpose of obtaining the type of data presented in Figure 2 for example. This is very costly, of course, illustrating well the importance of using a properly validated model in order to come up with an optimum cell design using a minimum of cell development cycles.

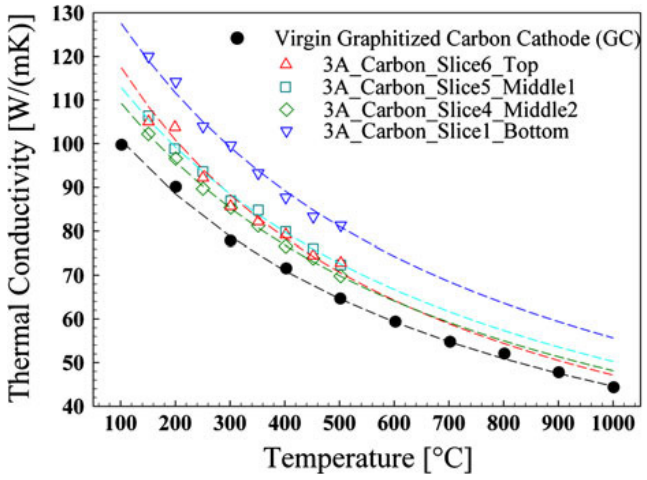


Figure 2: Example of thermal conductivity of spent cathode blocks obtained from pot autopsy, Figure 12 in [5]

**The over insulated cathode example**

Very often, technical papers and training courses discuss the importance of respecting certain guidelines having in mind some past mistakes and failures without actually discussing any of those mistakes and failures.

In this paper, such a practical example from the recent past will be presented in detail in order to clearly highlight the consequences of using an unvalidated cell heat balance model to come up with a cathode lining design.

This practical example is quite well covered in the literature [8, 9, 10]. It is the case of the over insulated Alcoa P155 cathode lining as explicitly specified in [10]. Notice that the original Alcoa A697 lining design is essentially the same. The original lining design is presented in Figure 3 taken from Figure 1 in [10]. There are 2 very thick layers of calcium silicate slabs just above the potshell floor. Calcium silicate is a fairly good thermal insulator; typical temperature dependent thermal conductivity of that material is presented in Figure 4.

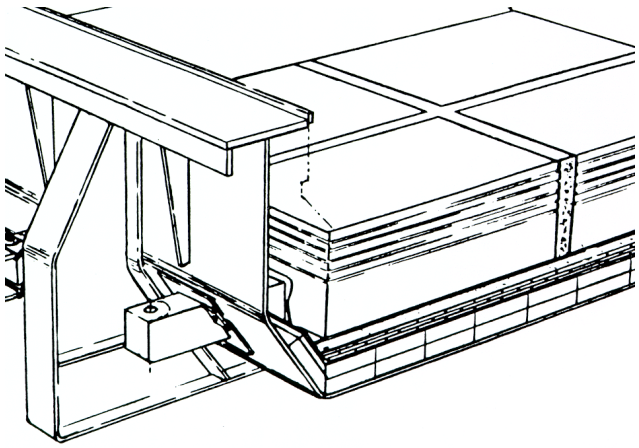

Figure 3: Original lining design of the Alcoa P155 cell, Figure 1 in [10]

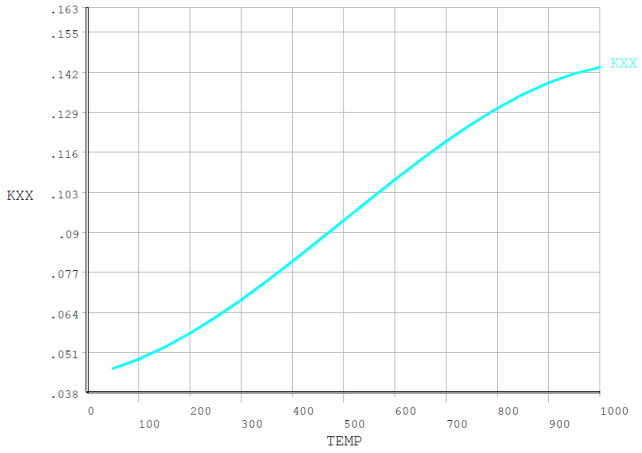


Figure 4: Temperature dependent thermal conductivity of new calcium silicate material

In [10] several types of cathode models were presented; Figure 5 shows the cathode side slice model. The navy blue material above the potshell floor is the calcium silicate.

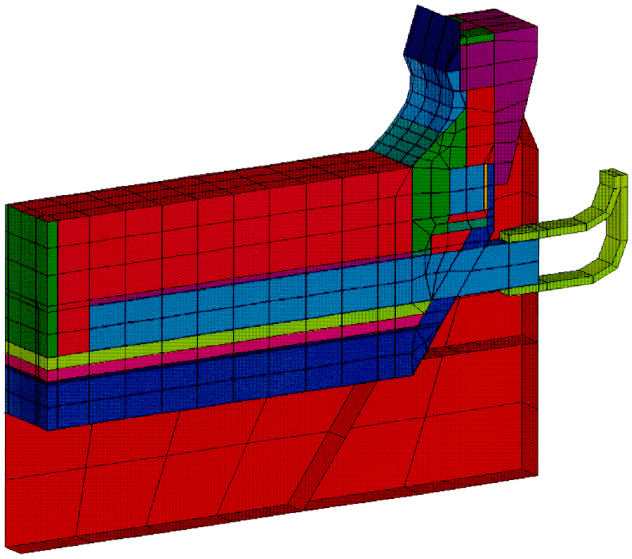

Figure 5: P155 cathode side slice model mesh as developed in 1993, Figure 5 of [10]

That model is no longer available to the authors but a full cell slice of the A697 developed by GeniSim and presented in Figure 6 is available instead. In that model, the calcium silicate is gold.

That A697 full cell slice model was run first using the new calcium silicate temperature dependent thermal conductivity presented in Figure 4. The obtained temperature solution is presented in Figure 7. Notice that contrary to the cathode slice model presented in [10], the full cell slice model presented in here calculates first the cell internal heat from that anode-to-cathode distance (ACD) specified by the user as input and converged in parallel the cell superheat and the ledge thickness so that the presented converged solution is in thermal balance i.e., the cell dissipates exactly the calculated cell internal heat.

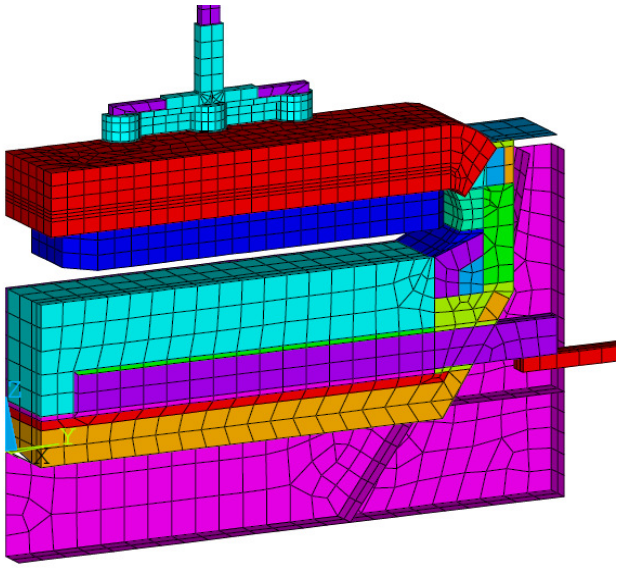

Figure 6: A697 full cell slice model mesh used in this study

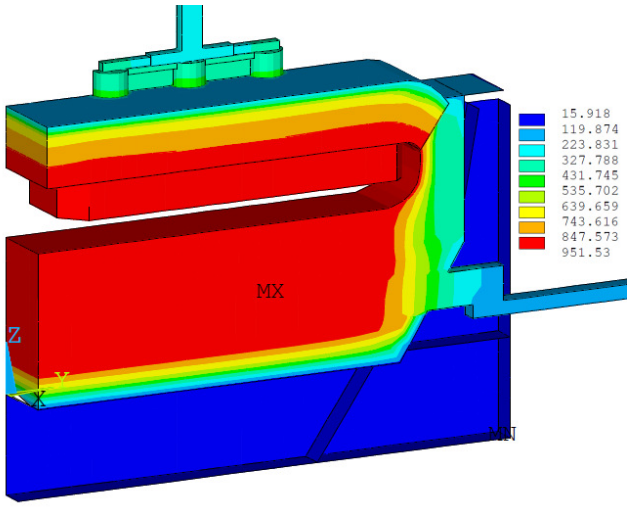


Figure 7: A697 full cell slice model temperature solution using new calcium silicate property

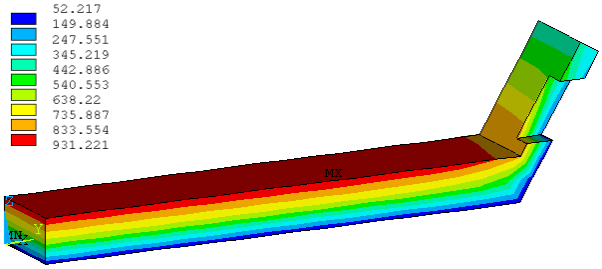


Figure 8: Calcium silicate temperature solution using new calcium silicate property

The temperature solution of only the calcium silicate material is presented in Figure 8, we can see that the top section is reaching above 900 °C.

In the operating cell, the light insulating materials are exposed to degradation both by high temperatures and by reaction with bath chemicals. It has been shown that above about 700 °C, these materials will lose much of their insulating property as first presented in [11] and reproduced in Figure 9. In addition, cathodic bath components, including sodium, permeate the lining materials. If these components reach the insulation in liquid form, they will penetrate the porous structure of the insulation, destroying the insulating value.

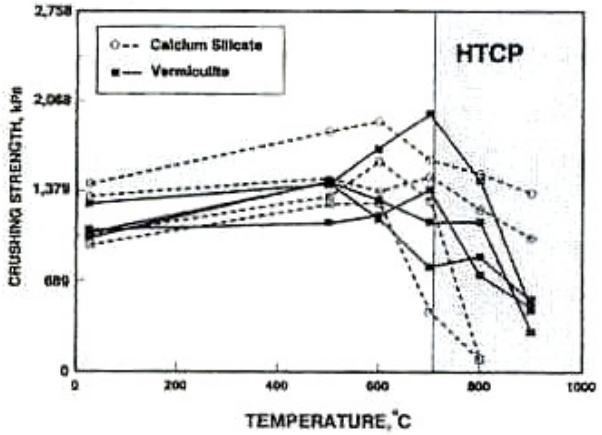


Figure 9: Observed degradation of insulating material properties above about 700 °C from [11]

As noted in [10] the sign of that degradation was seen in a cell autopsy but those autopsy results for the P155 cell were not presented in [10]. Fortunately, very similar autopsy results were presented in [8] for the A697 cell, those autopsy results confirm the chemical degradation of very large portion of the thick insulation layer as presented in Figure 10.

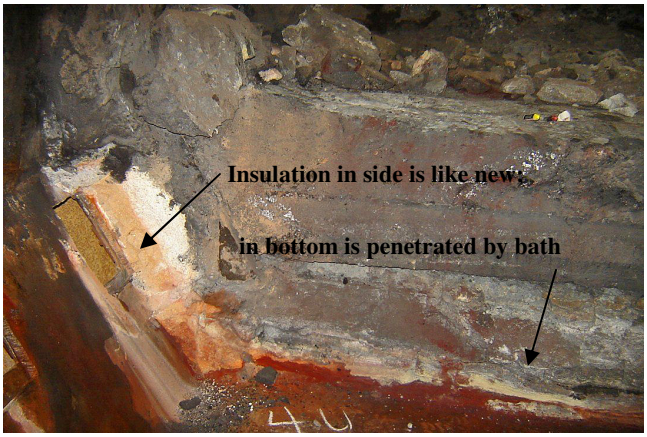


Figure 10: Picture from a A697 cell autopsy showing the chemical degradation of the insulation layer from [8]

Since it is not that easy to observe from that picture the chemical degradation of the insulation layer, the sketch describing the state of the cell lining prepared during another autopsy is presented in Figure 11.

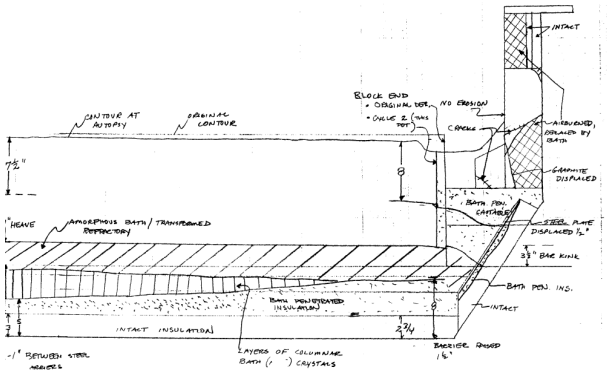

Figure 11: Sketch from a A697 cell autopsy describing the chemical degradation of the insulation layer from [8]

As discussed in [10], in order for the model to take into account that chemical degradation that occurs in the calcium silicate exposed at high temperature, the temperature dependent thermal conductivity needs to be adjusted as presented in Figure 12.

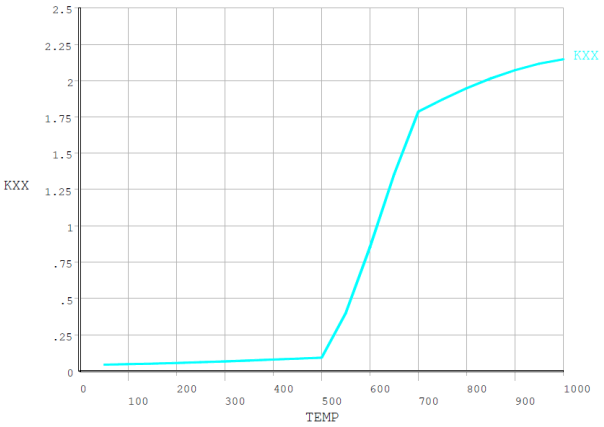


Figure 12: Temperature dependent thermal conductivity of calcium silicate material used in cell lining

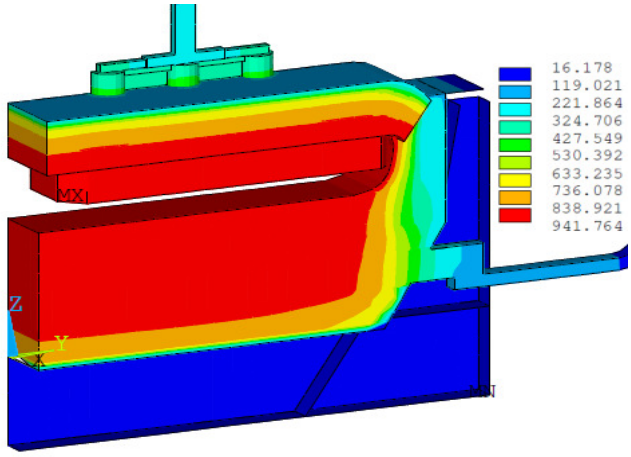


Figure 13: A697 full cell slice model temperature solution using the modified calcium silicate property

The thermal conductivity curve presented in Figure 12 essentially assumed that below a temperature threshold, 500 °C in this case, the new calcium silicate properties remain intact and that above a second temperature threshold, 700 °C in this case, we are dealing with a completely different new material. The ramp between the 2 temperature threshold transition zones is numerically required to ensure that the finite element (FE) solver will be able to converge that very non-linear problem.

Since the cell internal heat was kept the same, the converged cell heat loss remained the same but the heat loss partition is now very different: the cell bottom floor dissipates more heat while cell side wall now dissipates less heat due to the predicted decrease of the cell superheat and the corresponding predicted increase of the ledge thickness. This change in ledging results in changes in the operational behavior of the cell, and may require additional energy input to maintain stability. In any case the cell behaves quite differently than predicted by the model prior to the corrections made as a result of the validation process. The obtained temperature solution is presented in Figure 13, while the temperature solution of only the calcium silicate material is presented in Figure 14.

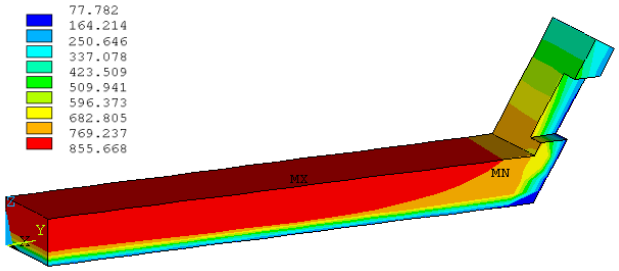


Figure 14: Calcium silicate temperature solution using the modified calcium silicate property

That change of repartition of the cathode heat loss would be quite easy to observe as it significantly affects the potshell temperature. Figure 15 presents the potshell temperature solution of the first case when using the new calcium silicate property while Figure 16 presents the potshell temperature solution of the second case when using modified calcium silicate property.

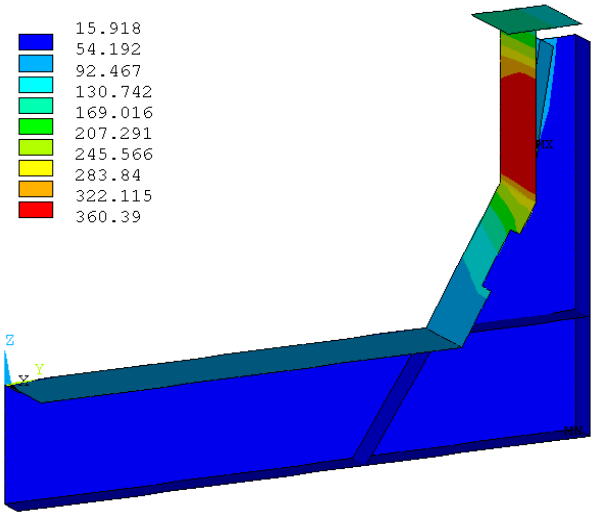


Figure 15: Potshell temperature solution using new calcium silicate property

Of course this change would not occur overnight, the first case would be representative of the condition a few weeks after startup when cell operations have stabilized while the second case would be representative of the condition after full penetration of the bath constituents into the cathode lining.

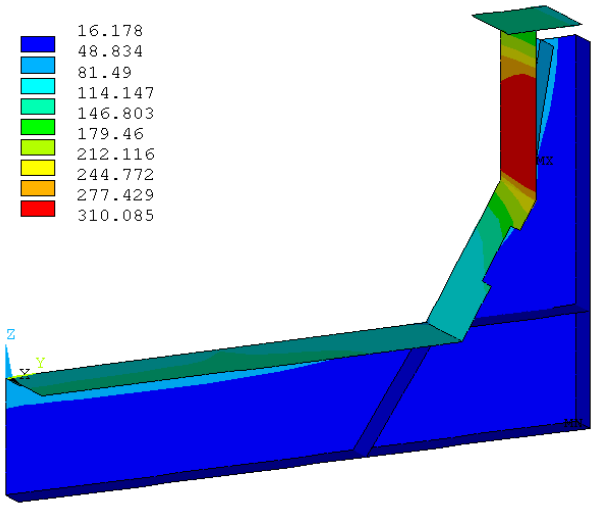


Figure 16: Potshell temperature solution using the modified calcium silicate property

In fact, that type change of the potshell floor temperature have been measured and reported in [4] on a 155 kA cell, those measurements are presented in Figure 17.

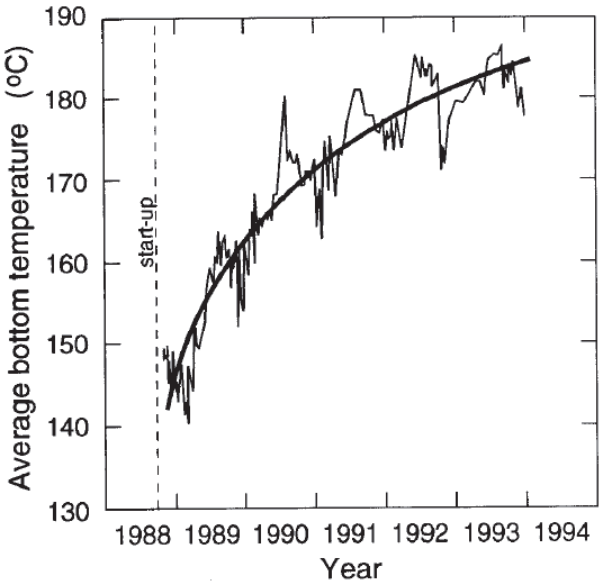


Figure 17: Averaged measured change of the potshell floor temperature of 16 155 kA prebaked cells, Figure 17 of [4]

**The need for more field validation work**

In retrospective the story of the over insulated cathode lining with a too thick layer thickness of calcium silicate that could not possibly avoid chemical degradation regardless of the type of physical barrier put in place to try to protect it is quite instructive as it is not unique.

Calcium silicate is not the only material that is susceptible to chemical attack and significant properties changes when put in cell operating conditions. Anode cover material is another example of equal importance that also has been the object to significant studies over the years including quite recently: [12, 13].

On the other hand some material would need more characterization work, for example the dry barrier material extensively use in Chinese lining designs. Despite the recent work done [14], there is certainly a need for more work in order to come up with a validated temperature dependent thermal conductivity property to be used in cell thermal balance modeling.

## Conclusions

In order to be successful, the cell design of high amperage cells must be conducted using the "cell development cycle" method [3]. The method comprises several steps, from modeling to measurement campaigns that must be used in repetitive cell design improvement cycles:

1) Cell design through modeling
2) Cell engineering and prototype cells construction
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Only data obtained from cell prototypes in steps 4 and 5 of the cell development cycle can be used in order to get reliable predictions from cell thermal balance models.

The first way to verify the accuracy of a cell heat balance model predictions is to directly compare them with data obtained from prototype cell heat balance measurement campaigns [6, 7].

The only way to directly obtain the used material properties required as inputs in models is to stop the prototype cells, dig out samples and measure the properties of those samples at a range of operating temperature [8, 14].

For example, it is well known that above about 700 °C, light insulating materials such as calcium silicate will get exposed to chemical degradation and will lose much of its insulating property.

In order for the model to take into account the chemical degradation that occurs in the insulation exposed at high temperature, the temperature dependent thermal conductivity needs to be adjusted.

The thermal conductivity of other materials such as the dry barrier material used in Chinese lining designs also must be characterized after exposure to high temperatures and penetration by cathodic bath materials.

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