A New 3D Transient Thermoelectric Modelling Approach for an Aluminium Electrolysis Cell Considering Bath Chemistry Variations

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Abstract

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A novel approach is introduced to model the transient thermoelectric behaviour of an aluminium electrolysis cell using a 3D finite-element cell-slice model developed in Ansys and coupled with a Python submodel. This approach solves the model one timestep at a time, using nodal results from the previous step as initial conditions for the next. A moving interface between the molten liquids (electrolytic bath and aluminium) and the ledge was adopted, enabling variation of heat transfer over its height, thus representing the variation of the heat transfer coefficient with height by assigning different thermal contact conductances along the interface. Additionally, a simple yet extensible mass balance submodel was developed in Python and coupled with the finite-element model, accounting for the influence of bath melting/freezing and also the bath film (between the metal and ledge) on bath chemistry. A power modulation scenario with electrolyte freezing and melting periods was simulated using the coupled model, and results were compared to those obtained with a calibrated cell-slice model with no submodel accounting for chemistry change. Accounting for bath chemistry changes caused by freeze movement results in restrained solidification, and melting. For instance, at the end of the melting period, the ledge thickness decrease was 21.3 % lower, while the superheat increase was reduced by 33.8 %. However, the bath temperature rise was increased by 25.0 %. On the other hand, at the end of the solidification period, the ledge thickness increase was 25.6 % lower, while the reduction in superheat was 38.3 % lower despite a 17.1 % higher reduction in bath temperature. At the end of the melting and solidification periods, AlF_3 concentration changed by -12.5 % and +10.6 %, respectively, compared to the case with constant bath chemistry. The Python submodel paves the way for future enhancements of the full model by leveraging Python features unavailable in the commercial finite-element software.

Keywords: Transient thermoelectric model, Finite-element method (FEM), Bath chemistry, Mass transfer, Aluminium reduction cell.

1. Introduction

Aluminium is a metal with interesting thermo-mechanical properties – a good heat dissipator with a high mechanical strength-to-density ratio – that makes it suitable for use in many applications.

This metal is still being produced in the industry from its oxide through the conventional Hall-Héroult process in aluminium electrolysis cells (AEC) [1]:

$$2Al_2O_3 + 3C = 4Al + 3CO_2 \quad (1)$$

Alumina, a reactant in this process, is regularly fed to these cells where it dissolves in a cryolite-based electrolyte (Bath). Normal baths would mainly consist of cryolite (Na_3AlF_6), aluminium fluoride (AlF_3), calcium fluoride (CaF_2), and alumina (Al_2O_3) [2]. As the temperature in the vicinity of the side walls of the cell falls below the liquidus temperature of the bath, it freezes thus forming a solid called "the ledge". This ledge shields the cell lining from both physical and chemical degradation caused by the electrolytic bath and the liquid aluminium beneath it [3]. Thus, it is of utmost importance to ensure the existence of this layer and control its thickness [4] as failing to do so would result in a shortened cell life, which in turn would lead to unnecessary expenditure and increased residual materials [5]. This is especially important when the heat balance of the cell shifts, for instance, due to a power modulation. However, given the harsh conditions prevailing within electrolysis cells, measuring the evolving thickness and shape of the ledge using sensors immersed in the molten bath is extremely challenging if not altogether impractical [6]. To overcome this shortcoming, thermoelectric models of the AEC are widely used to predict the thermoelectric state of the cells and the ledge profile [3].

LeBreux et al. [6] introduced an online estimation tool to predict the evolving ledge profile in AECs by integrating thermal measurements with numerical simulations of the cell. Their results demonstrated that the tool could provide continuous and automated estimates of the ledge profile with an accuracy of ±2 cm, without the need for intrusive measurements or manual intervention by operators. Wong et al. [7] investigated the feasibility of power modulation and the resulting cell response using a spatially discretized dynamic material and energy balance model grounded in the principles of the thermodynamic laws. The results indicated that while a temporary change in power prevents the ledge from immediately returning to its original thickness, it gradually recovers over time. Moreover, repeated power modulation at relatively high frequencies may cause the average ledge thickness (during each consecutive melting and solidification phases) to converge to a constant value only after multiple cycles. Zhang et al. [8] developed a transient, strongly coupled thermoelectric model to investigate the dynamic behaviour of temperature distribution and heat dissipation in AECs under increased current conditions. Their results indicated that a current increase of up to 10 % over 2 hours caused minimal variation in the ledge profile. While the heat dissipation rate in the upper part of the cell (including the anode rod, steel stubs, and cover) changed, the percentage of change was lower than that of the other parts.

Allard et al. [9] developed an improved finite-element thermoelectric model of an AEC by measuring anode cover material (ACM) and anode crust profiles and their thermal conductivity and emissivity. Their model was also capable of predicting the cavity shape by utilizing a radiosity module coupled with an iterative method. Results indicated that increasing the ACM thickness decreases top heat losses and increases side heat dissipation while bottom losses stay unchanged leading to side ledge shrinkage and melting of the anode crust. In another study, Allard et al. [10] developed a new modelling approach to account for the displacements of solid bodies, e.g., anode, and moving boundaries, e.g., bath/ledge and crust/cavity interface, in finite element models which was demonstrated in a transient thermoelectric model of an AEC submitted to an increase in operating voltage. The simulation revealed that the anode cover deteriorates, and the side ledge thickness decreases in such a situation. It should be noted that the top heat dissipation remained higher (+1.4 % of the total dissipation), due to the ACM transformation into anode crust during the voltage increase, even after the operating voltage had been restored to its nominal value.

Lalancette et al. [5] proposed a new approach for online thermal diagnosis and process control, involving the development of a novel 2D model derived from an existing 3D slice model. Testing

6. References

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