Numerical Modelling of Voltage Drop due to Anode Bubbles

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Abstract

The formation, travelling, coalescence, and detachment of CO_2 bubbles have an important impact on the anode-cathode distance (ACD) voltage drop, both in its magnitude as well as in its fluctuation frequency and amplitude. The study and understanding of the bubble flow can help in developing anode geometry solutions to minimize the bubble induced voltage drop, contributing to reduce the cell specific energy consumption.

With the increase of computational power, it is now possible to study the bath bubble flow under the anodes in more detail. Individual transient bubble structures can be followed along their paths including growth, coalescence, and detachment from the anode surface. The mesh size is the limit on the minimum diameter of a bubble to be individually represented and described in the model. This type of model requires also small timesteps in order to represent the complex behaviour of the fluids in the ACD space. The voltage drop in the bath is calculated by solving the electric equations coupled with the multiphase bath/bubble flow, where the presence of the gaseous phase resistance results in perturbations in local current density.

In this work, the bubble flow under the anode is studied for a variety of geometric configurations: flat anodes, inclined anodes, anodes with slots including different types and number of slots. The results show that the bubble behaviour is very sensitive to the geometric features of the anodes. Consequently, the results also show that the bubble layer voltage drop is also strongly influenced by the anode geometry, inclination, slot type and number.

Keywords: Bubble flow, Anode slots, Bubble layer resistance, Bath voltage drop, Coalescence and break up.

1. Introduction

Since the beginning of the industrial Hall-Héroult process, the bubble formation at the anode surface plays an important role in the aluminium electrolysis. These bubbles are a mix of mainly CO_2 (typical 80 % - 90 %) with CO and other minor contributions produced in the dissociation of alumina combined with carbon consumption of the anode inside the cryolite [1]. In modern cells, anodes and cathodes are disposed horizontally; the gases are formed at the anode bottom surface to which a bubble layer attaches due to buoyancy. Since the industrial electrolysis is a continuous process, the small formed bubbles grow, coalesce to a critical limit, and then break up toward the sides of the anodes, giving space for newly formed gases and maintaining a time averaged constant gas flow during the process. Fortin et al. [2] described the bubble flow behaviour by constructing a physical model. In 2006, another physical model was presented; the behaviour of bath flow was described with the help of PIV measurements [3].

The bubble layer inside the electrolyte impacts the process in two main aspects:

- Bath flow pattern: The bubble coalescence, travelling, and break-up drags the bath under the anodes creating the so called “bath induced flow”. Previous studies [4, 5] have demonstrated that this effect is the dominant driving force in the bath velocity field inside

the cell, outweighing the contributions from the metal drag and MHD forces. The bath movement features are of paramount importance in the dissolution and transport of alumina as well as in the homogenization of bath temperature by energy transport.

- Extra electric resistance in ACD (anode-cathode distance): Because of the gases' high electrical resistivity, the bubble distribution in the ACD layer affects the electrical current paths, and as a result, the voltage drop is increased if compared to a pure liquid bath. Understanding the behaviour of bubbles can help to create anodic design innovations that could potentially reduce the electrolysis cell voltage drop and the specific energy consumption.

2. Numerical Modelling of Bath/Bubble Flow

Some studies on bath flow numerical modelling can be found in the literature. Previous works [4] [6] attempted to reproduce the PIV measured flow by using a steady state multiphase flow technique (Eulerian-Eulerian flow). These studies contributed to the understanding of the time-averaged flow behaviour inside the bath. Usually, it was found that strong bath recirculations are formed inside the side channels and the central channels. These recirculations are important for bath mixing, and the alumina transport can be studied with such an approach.

However, the real bath/bubble flow presents a strong transient component within the bubble layer region due to the process cycle of bubble formation, growth, and break-up. A simulation of the ACD voltage drop is highly dependent on the local transient distribution of the gas. A predictive model must be able to define individual bubbles along with the growth, coalescence, and break up processes, in order to define the current path variations over time. A mesoscale model is presented in [7, 8] where small scale bubbles are treated with diffusion equations, and medium/large scale bubbles are treated as individual entities.

In the present work, the bubble generation, travelling, coalescence, and break-up is modelled by direct transient simulation. It means that the small-scale nucleation of bubbles observed in the model is dependent on the mesh resolution. In the models presented here, scales larger than ~1-1.5 mm are possible to be individually described. This is a great advance compared with the large-scale bulk model (averaged steady state) presented in earlier works which were developed for other purposes, such as alumina transport and energy transport studies. The full transient model is then capable of predicting the local influence of bubble evolution on the electric currents and bath voltage drop overtime. The mesh must be as refined as possible in the critical bubbles' region, that is, at the anode bottom and sides. Small timesteps are required, in the order of 0.01 s or even smaller, depending on the desired detail of the flow pattern calculation. This results in computationally heavy transient models requiring days of calculation even on a last generation multi-core computer. With this approach, some relevant studies can be performed, for example: the influence of anode geometry on the bath voltage drop, the impact of slots on bubbles and voltage drop. Depth, thickness, number, and position of slots can be studied and optimized.

In the numerical modelling presented here, the anode gas pore saturation is considered the main transport mechanism of the formed gas before bubble nucleation. In 2018, Poncsák and Kiss [9] published experimental work describing this process where the anode bottom becomes saturated with gas during electrolysis, preventing bath diffusion through the pores. The generated gas first saturates the electrode pores making it possible for the gas to travel through the pores, and then it starts to nucleate bubbles at anode surface irregularities. This process makes the CO_2 production at the surface nearly uniform regardless of the local electrical current concentrations caused by bubble travel. Therefore, the model boundary conditions must reflect this assumption.

Predicting the ACD voltage drop with bubbles has been a challenge in the history of electrolysis cell modelling. To the best of the authors' knowledge, this article presents the first accurate simulation of bubbles (and ACD) transient voltage drop in a three-dimensional realistic immersed anode geometry, capable to assess and quantify the impact of geometric modifications such as anode slots.

The model can be used as a tool for optimizing the anode shape, the design and number of slots. This impacts the cell specific energy consumption due to the reduction of bath voltage drop and potentially improving current efficiency. Improving the gas removal efficiency also reduces voltage fluctuations, possibly reducing the probability of anode effect occurrence.

6. References

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