VirtualBatteryFoam: A Multi-physics Numerical Solver to Simulate the Aluminium Electrolysis Process

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Abstract

Aluminium electrolysis is a very complex process consisting of various phenomena occurring in a highly coupled manner. A thorough understanding of the process is essential to enhance the cell efficiency and to reduce the production costs. Additionally, the shift towards renewable sources of energy demands for process and design flexibility. To realize the aforementioned goals, a detailed study of the process and the cell design is essential. Hence, in the present work, a numerical solver called "VirtualBatteryFoam" is developed in OpenFOAM® which can perform 3D cell simulations with fully solved physical phenomena. The solver consists of various models to capture magnetohydrodynamic and thermoelectric fields, electrochemistry with mass transfer, gas bubble dynamics and solidification process, capturing the evolution of ledge. In the first part, the numerical approach taken to develop the models is introduced. In the next part, verification of the various physical phenomena occurring in a typical cell including the long wave instability (sloshing), ledge formation and effect of gas layer formation on the electric field are presented.

Keywords: Aluminium electrolysis, numerical model, magnetohydrodynamics, thermoelectric field, OpenFOAM®.

1. Introduction

Aluminium production is a complex multi-scale, multi-physics process with a high degree of coupled non-linear dynamics. The process for production of aluminium is called Hall–Héroult process, which is named after its inventors who independently of each other developed and patented the electrolytic process in 1886. In this process, alumina (Al_2O_3) is dissolved in electrolytic bath mainly comprising of liquid cryolite (Na_3AlF_6) along with aluminium fluoride (AlF_3), calcium fluoride (CaF_2) and many other additives in small quantities, which is then subjected to a high electric current. The supplied electrical energy reduces the aluminium oxide to aluminium. The industrial process is carried out with prebaked carbon anodes, which is oxidized in parallel. The primary chemical reaction in its most simplistic form can be written as follows:

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

A part of the dissolved aluminium reacts back with the CO_2 to produce Al_2O_3, thereby reducing the efficiency of the process. The back reaction can be written as:

$$2Al + 3CO_2 = Al_2O_3 + 3CO \quad (2)$$

Current efficiency, i.e., the ratio of actual amount of aluminium produced to the theoretical amount, is calculated with the help of the Faraday's law. The current efficiency in a typical aluminium cell ranges between 90 – 96 % [1, 2]. The gas (CO_2, CO) bubbles produced during the reduction process accumulate under the anode by coalescence, thereby influencing the local current density and the cell electrical resistance. The accumulated bigger bubbles pass in the bath and rise around the anode by displacing the bath at the ends and the sides. This release of gas bubbles creates circulation in the bath region resulting in the disturbance of the bath-aluminium interface.

High electric current in the range of 150 - 600 kA is supplied to a typical aluminium cell in the industry. At each cell, a voltage of 4 - 4.5 V occurs which can be attributed to decomposition potential, cathodic and anodic over-voltages, ohmic voltage drop in the cell and the external circuitry [1, 2]. A typical aluminium smelter has 100 – 450 electrolytic cells arranged in side-to-side or end-to-end configuration. Such huge electric currents create a strong magnetic field, generating Lorentz forces on the moving liquid metal and electrolytic bath inside the aluminium cell. Depending on the design of the external circuitry, distribution of the current density in the pot and the velocity field of the liquid metal itself, the Lorentz forces can stabilize the bath-metal interface or may sometimes lead to an unstable condition. The instability of the interface in extreme cases results in a short circuit when the liquid aluminium comes in contact with the anode surface. Additionally, the bubble dynamics influence the bath-aluminium interface and thereby affect the magnitude and orientation of the Lorentz forces in the cell. Hence it is vital to understand the magnetohydrodynamic (MHD) instabilities arising due to various cell parameters, so that the critical operating conditions of the cell can be established.

The high currents supplied to the cell generate huge amount of ohmic heat or popularly known as Joule heat. Typically, around 50 % of the supplied energy is lost as heat to the surroundings [1, 2]. The heat generated inside the pot facilitates the reactions to take place, as it maintains the required thermal environment. But a steep temperate gradient exists from the inside of the pot to the external surroundings. This temperature gradient leads to solidification of the molten cryolite around the internal linings of the cell. The solidified cryolite is called the ledge which protects the cell from the aggressive molten cryolite. The position of the ledge is dependent on various parameters like the applied current, the velocity field inside the cell and the composition of the electrolyte among many others. The ledge profile influences the cell chemistry and the cell hydrodynamics as well. The cell chemistry is influenced through the change in composition of the bath which in turn influences various physical properties of the bath. The ledge position affects the distribution of the electrical current density which in turn influences the Lorentz forces, thereby the velocity field and cell stability.

As evidently seen from the above discussions, all the phenomena in the aluminium reduction cell are strongly coupled with each other and a slight disturbance to any of the cell parameters can either lead to cell instability or the cell dynamics can stabilize itself. A numerical model capturing the main physical phenomena should help us understand the complex process. Through a systematic understanding of the underlying physics, process flexibility and increase in cell efficiency can be realised. The focus of the present work is to develop models to capture the distribution of temperature, electric current density, velocity field, gas bubble dynamics, aluminium production and MHD phenomena. This is realised through step-by-step development of various mathematical models to capture the complex physical process occurring in the cell. The goal of the project is to develop a single solver with all the mathematical models as shown in Figure 1.

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