A numerical study of gas production and bubble dynamics in a Hall-Héroult process

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The Hall-Héroult is the major industrial process for aluminium production. It consists of electrochemical redox-reactions inside a crucible of molten electrolyte at circa 960 °C. Pure aluminium is produced at the cathode from alumina (Al2O3) dissolved in molten cryolite, while CO_2 and CO are released at the anode surfaces. The produced gas accumulates under the anode bottom in a thin, insulating layer, that causes additional voltage drops, increasing the power requirement. Therefore, a study of gas generation and bubble dynamics under anode surface and in the crucible is of fundamental importance in an attempt to optimize the process.
In this work, OpenFOAM® v4.1 is used to perform 3D CFD simulations of the Hall-Héroult process. The computational domain consists of an electrolytic cell with two anodes, scaled 1:1. Mass transfer from electrolyte to aluminium, CO_2 and CO are simulated using an Euler-Euler multiphase approach, with a total of 4 fluid components (aluminium, electrolyte, CO_2 and CO). The framework used to perform the simulations is a modified version of the OpenFOAM® solver *reactingMultiphaseEulerFoam*. The current passing through the cell is calculated with the Gauss's law for static electric field. The model used for the mass transfer is the Faraday's law of electrolyis, in which production of reduced or oxidized species is proportional to the amount of current passing through the electrolyte. The numerical model is validated by comparing effects of bubble dynamics on the electric field with experimental measurements available in the literature [1-2]. Results show generation of CO_2 and CO at the anode, aluminium at the cathode and consumption of electrolyte. Mass balance between produced and consumed species is presented. A detailed analysis of additional voltage drop caused by gas production, by anode coverage and by variation of gas layer thickness under the anode surface, for different current densities, is also made.

[1] Zhao et al. (2016). *Anodic Bubble Behavior and Voltage Drop in a Laboratory Transparent Aluminium Electrolytic Cell.* Met.and Mat. Transactions B, 47B,1962-1975.

[2] Zhao et al. (2015). *Observation of anodic Bubble behaviour using Laborarory scale Transparent Aluminium Electrolytic cells.* Light Metals, 801 – 805.