

## Understanding the Factors Influencing Carbon Dioxide Dilution in an Aluminum Electrolysis Cell

Mohammadreza Basohbatnovinzad<sup>1</sup>, Lukas Dion<sup>2</sup>, Kadiata Ba<sup>3</sup>, Simon-Olivier Tremblay<sup>4</sup>, Sébastien Guérard<sup>5</sup> and Jean-François Bilodeau<sup>6</sup>

1. PhD Student

2. Professor University, Director

3. Professor University, Co-Director

4. Research Professionnal

Université du Québec à Chicoutimi, CURAL-GRIPS, Saguenay, Canada

5. Research Scientist, R&D

6. Principal Advisor, R&D

Rio Tinto – Arvida Research and Development Centre, Saguenay, Canada

Corresponding author: [mbasohbatn@etu.uqac.ca](mailto:mbasohbatn@etu.uqac.ca)

<https://doi.org/10.71659/icsoba2024-al034>

### Abstract

The Hall-Héroult process is widely employed worldwide to produce aluminum. Inherently, this process also generates significant emissions of carbon dioxide, a greenhouse gas as a by-product of the reaction. As the bubbles formed during the electrolysis escape from the electrolysis cells, they induce the generation of a gas flow underneath the anodes, which are expelled due to the buoyancy forces of the melt. The rate of the gas flow generated, and the incident gas concentration of the output gas will be dependent on numerous different factors. In this work, a numerical model was developed to replicate the chemical reactions in the vicinity of an anode assembly leading to the generation of carbon monoxide and carbon dioxide. The output gases are then routed to the gas exhaust with fluctuating concentrations due to changes in the conditions, which may result in variations in the amount of carbon dioxide and carbon monoxide being produced under steady state. Hence, the purpose of the experimental plan is to simulate the operations of a specific number of different situations so as to illustrate the extent of the operational conditions that can be expected in the industry in the future. In order to accomplish this purpose, the numerical model was developed using ANSYS Fluent and a validation process was developed to confirm the accuracy of the model. During the investigations, various conditions were meticulously examined, analyzed and evaluated, including the pressure at the gas exhaust point, the air entering the electrolysis process, the effect of current efficiency, the amount of current flowing through the cell, the height of the channel, the anode size and other factors, in order to comprehensively understand the effect of these factors on the concentration of gas within the cell.

**Keywords:** Hall-Héroult process, Chemical reactions, ANSYS Fluent, Gas concentration, Current efficiency.

### 1. Introduction

Aluminum is a metal widely used in a variety of applications, including transportation and construction, due to its unique properties [1]. Canada is one of the major producers and exporters of aluminum. In 2020, Canada produced approximately 3.2 million tonnes of aluminum, with 90 % of this production taking place in Quebec [2]. Various strategies, such as increasing energy and material efficiency and incorporating renewable energy sources, have been implemented to reduce the environmental impact of aluminum production. While progress has been made, there is still a long way to go in achieving sustainable aluminum production. The industry must focus on working towards a low-carbon future that balances environmental concerns with economic growth [3].

This project will provide important information regarding the potential CO<sub>2</sub> concentration that can be achieved in an electrolysis cell while also describing the gas properties in terms of chemistry and temperature. This information will help define the applicability of different potential solutions for subsequent CO<sub>2</sub> capture. The level of greenhouse gases in the atmosphere has rapidly risen since the aluminum industrial revolution. The principal gases associated with climate change are carbon dioxide and carbon monoxide. Carbon dioxide is considered the main greenhouse gas due to the significant amount of emissions released into the atmosphere [4]. The aluminum industry is responsible for significant carbon dioxide emissions, as it is the main gas emitted from the electrolysis cells due to the raw materials (petroleum coke and coal tar pitch) used in anode production. The intensity of these gas emissions depends on a multitude of factors such as the current efficiency ( $\epsilon$ ), cell amperage (I), the electrolysis cell structure, and the anode conditions, namely its ability to withstand O<sub>2</sub> and CO<sub>2</sub> oxidation. Efforts are being made on different levels to reduce GHG emissions, and this study investigates the behavior affecting CO<sub>2</sub> concentration specifically [5]. In this research, a three-dimensional model was created and solved using a numerical method employing a finite difference algorithm within the Ansys/Fluent software. The main objective is to investigate the distribution of gas pressure and CO<sub>2</sub> concentration in the space volume above the crust, under steady-state conditions for a specific set of operating conditions. The proposition of a pathway for potential CO<sub>2</sub> reduction is directly aligned with the main goals of this project. Using the numerical simulations developed, it will be possible to recommend alternative scenarios in which the dilution rate of carbon dioxide can be reduced while limiting the impact on fugitive emissions. The primary indicators examined for validation of the model encompass gas output velocity and concentrations, which are compared with industrial data obtained from previously documented sources in the literature. Additionally, gas collection efficiency is examined in relation to the structure of the gas gathering system and the operation of the electrolytic cell.

## 2. Literature Review

Many authors have studied the exhaust gas gathering efficiency and CO<sub>2</sub> capture simulation of aluminum electrolysis cells using numerical simulations and Computational Fluid Dynamics software. The Hall-Héroult process, while essential for aluminum production, emits a significant amount of CO<sub>2</sub> into the atmosphere. To address this issue and reduce CO<sub>2</sub> emissions from aluminum production, it is crucial to develop technologies for capturing and storing the CO<sub>2</sub> emitted during the process [6]. Simulation models are created using software like Aspen Plus and Aspen Hysys to evaluate CO<sub>2</sub> capture in aluminum production. In Aspen Hysys, a closed-loop model is used to simulate the CO<sub>2</sub> capture process, which is vital for addressing climate change concerns. These models allow for the analysis of different CO<sub>2</sub> concentrations and capture rates [7]. This research has provided valuable information on potential CO<sub>2</sub> concentrations achievable in electrolysis cells, as well as describe gas properties in terms of chemistry and temperature to define the applicability of potential CO<sub>2</sub> capture solutions. The proposal of a pathway for potential CO<sub>2</sub> reduction aligns directly with the main goals of this project. The aim of this investigation is to evaluate the potential for CO<sub>2</sub> capture from aluminum production by looking at conditions where the CO<sub>2</sub> concentration would be higher than 4 vol% [8].

CFD software is used to implement simulations of a 400 kA aluminum cell. Cell gas collection systems are studied, and the multi-physics field model for the aluminum electrolysis gas gathering system is established. The main conclusions are as follows: The cell has two short sides, called the tap end and the duct end. opening the tapping end side hooding panels has a greater impact on exhaust gas flow than opening the duct end side hooding panels. Due to this, the average flow rate in the two ducts declines and affects the exhaust gas flow rate, indicating that opening the cell hooding panels has little effect, and maintains gas stability under the hood of the electrolysis

range of cell conditions that could favor a reduced CO<sub>2</sub> dilution rate while limiting the risk of fugitive emissions.

Finally, this work also highlighted that the base case operational scenario is likely much stronger than needed to prevent fugitive emissions under idealistic hooding conditions. While the real operations scenarios need to be taken into consideration, along with expected cell operations that will influence the opening of the hoods and tapping door. A periodic modulation of the exhaust pressure quickly appears as a suitable potential solution that could increase the CO<sub>2</sub> concentration in specific local regions of the electrolysis cell.

Future developments using this model will require thorough experimental in-situ validations in order to provide even more precise investigations regarding concrete or futuristic solutions to reduce the dilution rate of the carbon dioxide while mitigating the potential harm coming from fugitive emissions.

## 6. Acknowledgements

The authors express their gratitude to Rio Tinto for their technical collaboration, the financial support and the permission to publish these results. The authors would also like to thank the Natural Sciences and Engineering Research Council of Canada (NSERC) and the Regroupement Aluminium (REGAL) for their financial support.

## 7. References

1. André Charette, Yasar S. Koçaefe, and Duygu Koçaefe, Le carbone dans l'industrie de l'aluminium, 2012 Les presses de l'aluminium.
2. Richard McDonough, Aluminum Industry in Canada, *Aluminum International Today*, November-December 2022, 33-37.
3. Olivier Jos, Peters Jeroen, and Greet Maenhout, *Trends in global CO<sub>2</sub> emissions*, 2012 report, European Commission, PBL Netherlands Environmental Assessment Agency.
4. Udara S. P. R. Arachchige, Dinesh Kawan, and Morten C. Melaaen, Simulation of carbon dioxide capture for aluminum production process, *International Journal of Modeling and Optimization*, 2014, 43-50.
5. Philippe Ouzilleau, Aimen E. Gheribi, and Patrice Chartrand, Prediction of CO<sub>2</sub>/CO formation from the (primary) anode process in aluminum electrolysis using an electro thermodynamic model (for coke crystallites), *Electrochimica Acta*, 2018, 916-929.
6. Mengzhi Guo et al., A highly efficient and stable composite of polyacrylate and metal-organic framework prepared by interface engineering for direct air capture, *ACS Appl. Mater. Interfaces* 2021, 13, 18, 21775–21785.
7. Sithara Dayarathna et al., Simulation of CO<sub>2</sub> capture from an aluminum production plant, *WIT Transactions on Ecology and the Environment*, 2014, 729-739.
8. Annete Mathisen et al., Investigation into optimal CO<sub>2</sub> concentration for CO<sub>2</sub> capture from aluminum production, *Energy Procedia*, Volume 37, 2013, 7168-7175.
9. Hongliang Zhang et al., Numerical Simulation Study on Gas Collecting System of 400 kA Grade Aluminum Electrolytic Cell, *Light Metals* 2018, 573-586.
10. LI Xue-jiao et al, Numerical Simulation Study on Gas Gathering Structure of Aluminum Reduction Cell, *Journal of Northeastern University (Natural Science)*, 2022, 43 pages.
11. Odd Edgar Bjarno, and Geir Wedde, A device and a method of cleaning an effluent gas from an aluminum production electrolytic cell, Canadian Patent Application CA 2 827 357C, Publication date 2012/08/23.
12. *ANSYS FLUENT Theory Guide*, ANSYS 2011, 794 pages.
13. P. Fellner et al., *Aluminum Electrolysis: Fundamentals of the Hall-Héroult Process*, Beuth Verlag GmbH, 2011.

14. Asbjorn Solheim, and amuel Senanu, Recycling of the flue gas from aluminum electrolysis cells, *Light Metals* 2020, 803-810.
15. Thor Anders Aarhaug, and Arne Petter Ratvik, Aluminum primary production off-gas composition and emissions, *JOM*, February 2019, Vol. 71, 2966-2977, <https://doi.org/10.1007/s11837-019-03370-6>.
16. Kai Grjotheim, and Halvor Kvande, *Introduction to Aluminum Electrolysis*, Aluminum-Verlag 1993, Düsseldorf, Germany, 260 pages.