Machine Learning on Electrocatalytic reduction of CO_2 for Preventing Atmospheric Pollution and Producing Valuable Chemicals

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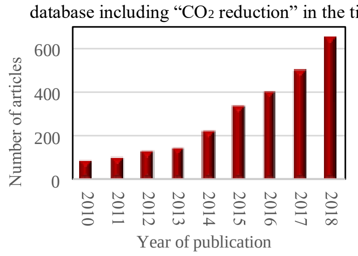
1. Introduction – In most modern industrial processes, massive amounts of flue gases are released to the air because of the combustion of fossil fuels, and these flue gases contain significant amounts of CO_2, which is a greenhouse gas contributing to the global warming. Electrocatalytic reduction is a promising method to eliminate CO_2, providing also the production of valuable chemicals [1]. However, to design an efficient electrochemical cell, there are lots of variables that must be optimized such as the elemental composition of the catalysts in the electrodes, types of membrane and backing layer as well as types of catholyte and anolyte [2]. Because of the concerns related to global warming, the number of articles accumulated on CO_2 reduction increases year by year as shown in Image 1. Hence, the experimental results reported in these articles accumulate exponentially through years and it becomes extremely difficult to review and analyse the results by traditional methods. However, by the help of machine learning based techniques such as exploratory data analysis (i.e. box and whisker plots) and decision trees it is quite possible to extract the hidden patterns, correlations and heuristics from this vast accumulation of experimental results [3]. In this work, recent publications on electrocatalytic reduction of CO_2 were reviewed and a database of 471 experimental results extracted from 34 different articles was constructed. Then, machine learning methods were applied to reveal the conditions leading to higher electroreduction rate and efficiency and product selectivity.

Image 1. Number of articles versus date of publication in the "Web of Science Core Collection" database including "CO_2 reduction" in the title



2. Experimental - Highest rate, highest faradaic efficiency and highest selective product were used as output variables while the elemental composition in cathode catalyst and other operating variables were used as input variables.

3. Results and Discussion - The most obvious results found by the help of the exploratory data analysis is that, using Nafion 212 as the membrane, KOH for catholyte and NaOH for anolyte in the electrolyser decision tree structure classifying the highest selective product is shown in Image 2.

leads to higher faradic efficiencies. The optimal

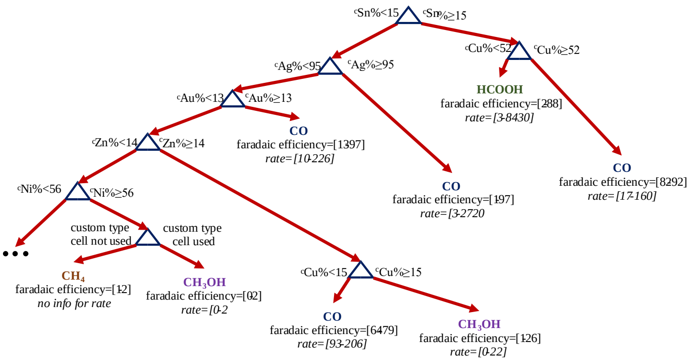


Image 2. Part of a decision tree analysis for the highest selective product, corresponding faradaic efficiencies and rates in $\mu mol/m^2.s$ (training error %7.3, testing error %9.6); [c]refers to cathode

4. Conclusions – The decision tree analysis indicated that there were ten combinations for carbon monoxide production, five combinations providing hydrocarbon production, six combinations leading to formic acid production and two different combinations for methanol production. It was also found that the rates can be put in the order from the highest to lowest as HCOOH, CO, CH_4, C_2H_4 and CH_3OH.

5. References

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