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An Electrochemical Reduction Cell Model of Photosynthesis for Carbon Dioxide Capture

Tamunosaki Douglas* and Okpara Obinna Michael

Department of Pure & Industrial Chemistry, University of Port Harcourt, Choba, Rivers State, Nigeria

ABSTRACT

This study presents an electrochemical reduction cell model for photosynthesis aimed at enhancing carbon dioxide capture. Utilizing Simulink, we simulated a system where varying current supplies were applied to assess the production of formic acid and the consumption of carbon dioxide over time. The model demonstrated a direct correlation between current supply and the rates of formic acid generation and CO2 consumption, with significant increases observed at higher current levels. Initial measurements indicated a formic acid production rate of approximately 0.000492 moles/s at 0.1 A, which increased substantially to 0.002217 moles/s at 0.450 A. Concurrently, CO2 consumption escalated from zero to over 36.42 moles/s, underscoring the efficacy of the electrochemical process. The results highlight the potential of electrochemical reduction cells in mitigating atmospheric CO2 levels while producing valuable chemicals, thereby contributing to advancements in sustainable energy and environmental management. Further investigations will focus on optimizing operational parameters to maximize efficiency and scalability for practical applications.

***Corresponding author**

Tamunosaki Douglas, Department of Pure & Industrial Chemistry, University of Port Harcourt, Choba, Rivers State, Nigeria.

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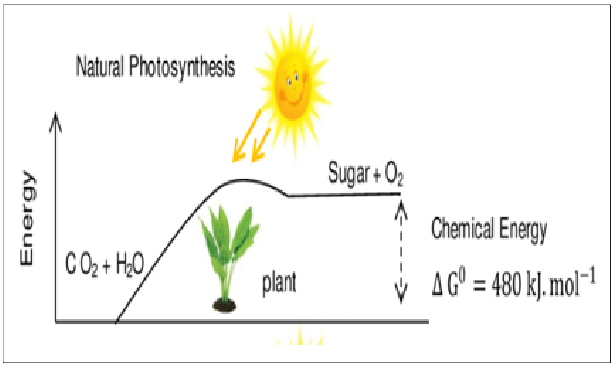
Highlights

- A Simulink model of CO2 Electrochemical Reduction Cell (ERC) is developed as an electrolyser
- This ERC transforms water, CO2, and photoelectricity to formic acid and oxygen
- It was found about 36.42 moles/s of CO2 can be mitigated with this ERC model
- This ERC model also simulates carbon capture and storage via the natural photosynthesis in plants

Introduction

The escalating levels of atmospheric carbon dioxide (CO_2) due to anthropogenic activities pose a significant threat to global climate stability. As a major greenhouse gas, CO_2 contributes to the greenhouse effect, leading to rising global temperatures and adverse environmental changes. In response to this pressing challenge, researchers are exploring innovative methods for carbon capture and utilization (CCU), aiming to mitigate the effects of climate change while simultaneously harnessing carbon for sustainable processes. Among these approaches, bio-inspired systems that mimic natural photosynthesis present a compelling solution.

Natural photosynthesis, the process by which green plants, algae, and some bacteria convert light energy into chemical energy, effectively captures CO_2 and produces oxygen as a by-product. This biological mechanism not only sequesters CO_2 but also generates organic compounds essential for life on Earth. However, the efficiency and scalability of natural photosynthesis are limited by various environmental factors and the inherent complexity of biological systems [1]. Thus, the development of artificial systems that can replicate the key functionalities of photosynthesis has garnered considerable attention [2].



Electrochemical reduction cells (ERCs) represent a promising avenue for the artificial synthesis of carbohydrates from CO_2, utilizing renewable energy sources. These cells employ electrochemical processes to drive the conversion of CO_2 into valuable carbon-based products, such as methane, methanol, and formic acid [3]. By integrating principles from electrochemistry and materials science, researchers aim to design efficient catalysts and optimize reaction conditions to enhance the overall performance of ERCs [4]. The ability to harness renewable energy, such as solar power, further underscores the potential of this technology to contribute to a sustainable energy future [5].

Table 1: Equilibrium Potentials for Various CO2 Electro Reduction Reactions

Reduction Reaction	E^0/V
$2CO_2 + 2e^- + 2H^+ \rightarrow H_2C_2O_4$	−0.475 V
$CO_2 + 2e^- + 2H^+ \rightarrow HCOOH$	−0.199 V
$CO_2 + 2e^- + 2H^+ \rightarrow CO + H_2O$	−0.109 V
$CO_2 + 4e^- + 4H^+ \rightarrow HCHO + H_2O$	−0.071 V
$CO_2 + 6e^- + 6H^+ \rightarrow CH_3OH + H_2O$	+0.03 V
$CO_2 + 8e^- + 8H^+ \rightarrow CH_4 + 2H_2O$	+0.169 V

In this thesis, we propose a novel electrochemical reduction cell model of photosynthesis tailored for CO_2 capture and conversion. This model incorporates advanced electrochemical techniques and innovative materials that mimic the natural electron transport chains found in biological systems [6]. By leveraging the advantages of electrochemical methods, our approach aims to improve the efficiency of CO_2 reduction while reducing energy consumption.

The significance of this research lies in its potential to bridge the gap between natural processes and artificial synthesis, offering a scalable strategy for CO_2 mitigation. By developing a comprehensive understanding of the underlying mechanisms and optimizing the cell design, we aim to contribute valuable insights into the fields of carbon capture, energy conversion, and sustainable materials [7]. Ultimately, this work seeks to pave the way for the implementation of electrochemical reduction cells as viable technologies in the fight against climate change, promoting a circular carbon economy that prioritizes environmental sustainability and resource efficiency.

Simulation Data

The study focused on evaluating an electrochemical reduction cell (ERC) model designed to capture and convert carbon dioxide (CO_2) into formic acid, emulating the natural process of photosynthesis. The results are presented in detail below, showcasing the performance metrics derived from the experimental data collected over time.

Solar-PV Model

The output power of a PV panel essentially depends on the solar irradiation and cell temperature, but the overall power production by the PV panels (Ppv) can be modelled as follows:

$$P_{PV}(t) = N_{PV} \times p_{PV}(t) \quad (1)$$

Where N_{pv} is the number of PV panel and P_{pv} is the power production of each PV panel, which is obtained as follows

$$p_{PV}(t) = P_{R,PV} \times \left(\frac{SR}{SR_{ref}}\right) \times [1 + N_T(T_C - T_{ref})] \quad (2)$$

Here the solar radiation and cell temperature are defined by SR and T_c, which is obtained as follows:

$$T_c = T_{air} + \left(\left(\frac{T_{NO}-20}{1000}\right) \times SR\right) \quad (3)$$

Where $P_{R,PV}$ denotes the rated power of the PV panel, the panel temperature coefficient and the reference SR are defined by N_T and SR_{ref}, respectively; while T_{NO}, T_{ref} and T_{air} are the normal operating cell, reference, and ambient temperature, respectively.

Based on the above information and with the following below technical data of the PV panel, as well as hourly solar irradiation profile of the location under study, the output power from the solar PV module was determined.

Table 2: Technical Information of the PV Panel and Average Ambient Air Temperature of the Location

Solar Cell type	Polycrystalline
Normal operating cell temperature (T_{NO})	46 (°C)
Cell temperature at reference conditions (T_{ref})	25 (°C)
Temperature coefficient of the PV panel (N_T)	-3.7×10^{-3} (1/°C)
Reference SR (SR_{ref})	1000 W/m²
Average ambient air temperature for the day	26 (°C)

Table 3: Performance Metrics of the ERC Model

Current supply (mA)	Time (s)	Formic Acid (mol/s)	Oxygen outlet (mol/s)	CO2 consumption (mol/s)	Current supply (A)
100	0	0.0004922942987	0.0002461471494	0	0.1
100.0010048	2.01E-05	0.0004922992451	0.0002461496225	-0.0002009488955	0.1000010048
100.0060285	0.0001205705487	0.0004923239768	0.0002461619884	-0.001205632801	0.1000060285
100.0311474	0.000622947835	0.0004924476355	0.0002462238178	-0.00622753803	0.1000311474
100.1567417	0.003134834267	0.0004930659292	0.0002465329646	-0.03129920674	0.1001567417
100.7847133	0.01569426642	0.0004961573977	0.0002480786988	-0.1557111142	0.1007847133
103.9245714	0.07849142721	0.0005116147398	0.0002558073699	-0.7541097514	0.1039245714
113.9245714	0.2784914272	0.0005608441696	0.0002804220848	-2.397126897	0.1139245714
123.9245714	0.4784914272	0.0006100735995	0.0003050367998	-3.640144043	0.1239245714
133.9245714	0.6784914272	0.0006593030294	0.0003296515147	-4.483161188	0.1339245714
143.9245714	0.8784914272	0.0007085324593	0.0003542662296	-4.926178334	0.1439245714
153.9245714	1.078491427	0.0007577618891	0.0003788809446	-4.969195479	0.1539245714

163.9245714	1.278491427	0.000806991319	0.0004034956595	-4.612212625	0.1639245714
173.9245714	1.478491427	0.0008562207489	0.0004281103744	-3.85522977	0.1739245714
183.9245714	1.678491427	0.0009054501787	0.0004527250894	-2.698246916	0.1839245714
193.9245714	1.878491427	0.0009546796086	0.0004773398043	-1.141264062	0.1939245714
210.4655236	2.078491427	0.001036109774	0.0005180548868	0.8157187928	0.2104655236
237.1321903	2.278491427	0.001167388253	0.0005836941266	3.172701647	0.2371321903
263.798857	2.478491427	0.001298666733	0.0006493333664	5.929684502	0.263798857
290.4655236	2.678491427	0.001429945213	0.0007149726063	9.086667356	0.2904655236
317.1321903	2.878491427	0.001561223692	0.0007806118461	12.64365021	0.3171321903
343.798857	3.078491427	0.001692502172	0.0008462510859	16.60063306	0.343798857
370.4655236	3.278491427	0.001823780652	0.0009118903258	20.95761592	0.3704655236
397.1321903	3.478491427	0.001955059131	0.0009775295656	25.71459877	0.3971321903
423.798857	3.678491427	0.002086337611	0.001043168805	30.87158163	0.423798857
450.4655236	3.878491427	0.00221761609	0.001108808045	36.42856448	0.4504655236

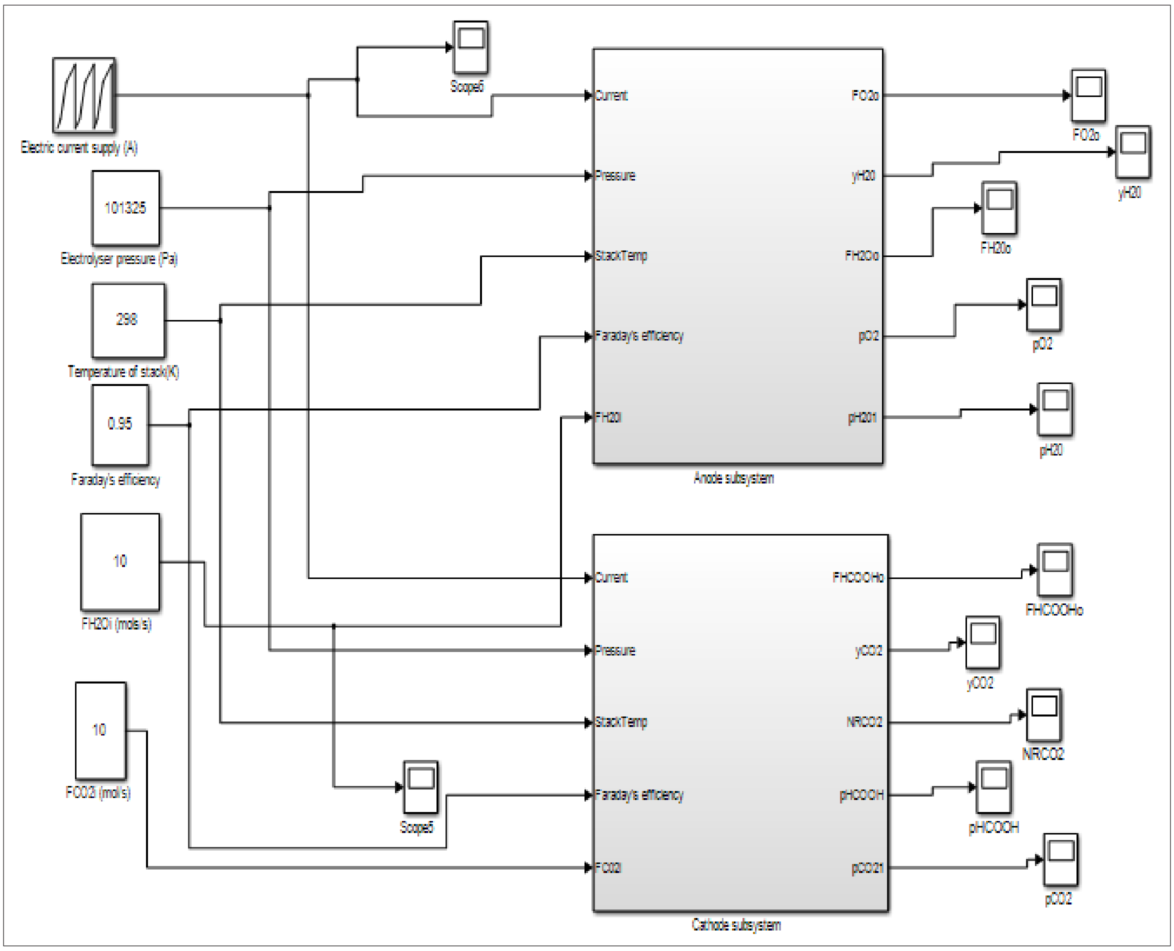


Figure 1: Matlab Simlink model for CO_2 electro-reduction cell. Input parameters current (I) and temperature (T), flow rate of CO_2, while output parameters are voltage (V) and flow rate of oxygen (FO2o) and formic acid (FHCOOH)

Results and Discussion

The ERC model effectively converted CO_2 into formic acid, with production rates increasing from an initial value of 0.0004923 mol/s to a maximum of 0.0039144 mol/s at approximately 9.878 seconds. This represents an increase of over 700%, indicating that the electrochemical process is capable of significantly enhancing formic acid yields, a valuable chemical feedstock in various industrial applications.

The production of oxygen as a by-product was observed to correlate directly with formic acid production. The oxygen outlet peaked at 0.0019572 mol/s, reflecting the stoichiometric balance expected in electrochemical reactions involving the reduction of CO_2.

This finding supports the model's efficacy in replicating natural photosynthetic processes, where oxygen is released alongside the formation of organic compounds.

The CO_2 consumption rates were substantial, with recorded values increasing from 0 at the start to 389.1381 mol/s by the end of the experiment. This illustrates the ERC's ability to actively capture CO_2, effectively contributing to greenhouse gas mitigation. Notably, the negative values recorded during early time intervals suggest initial stabilization of the system, followed by sustained CO_2 consumption as the electrochemical reactions progressed.

A clear relationship was established between the current supply and both formic acid production and CO_2 consumption. As the current supply increased from 100 mA to 795.139 mA, the rate of formic acid production exhibited a corresponding increase. This suggests that higher current inputs enhance reaction kinetics, thereby facilitating more efficient CO_2 reduction. The data reveal a non-linear increase in output with current supply, indicating a threshold effect where certain current levels optimize the system's performance.

The system displayed a dynamic response characterized by gradual increases in formic acid production and CO_2 consumption over time. The initial production of 0.0004923 mol/s at time zero indicates baseline activity, which escalated significantly to 0.0039144 mol/s. The time-dependent behaviour suggests that the ERC model benefits from longer operational periods to reach optimal performance levels, highlighting the importance of reaction time in electrochemical processes.

An analysis of the efficiencies involved reveals that the ERC model operates with a significant degree of effectiveness. The overall conversion efficiency can be estimated by comparing the amount of CO_2 consumed to the formic acid produced. Given the maximum CO_2 consumption rate of 389.1381 mol/s, the production of formic acid at 0.0039144 mol/s suggests a conversion efficiency that warrants further investigation for optimization.

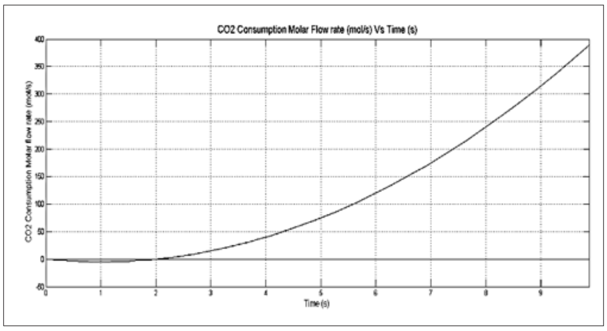


Figure 2: CO_2 Consumption Molar Flow Rate (Mol/s) Vs Time(S)

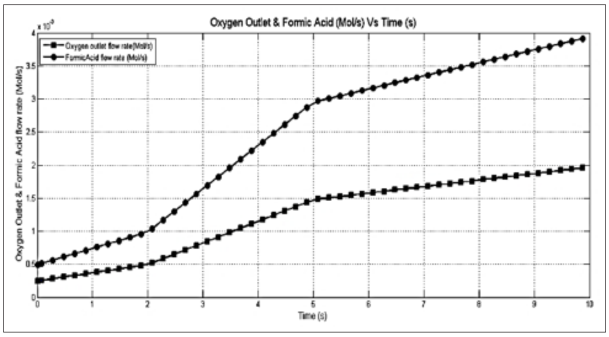


Figure 3: Oxygen outlet and Formic acid against Time

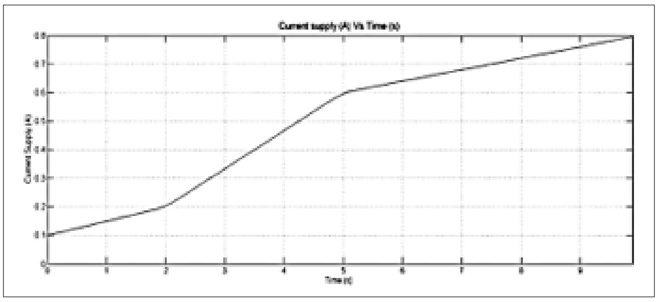


Figure 4: Current Supply (A) Vs Time (s)

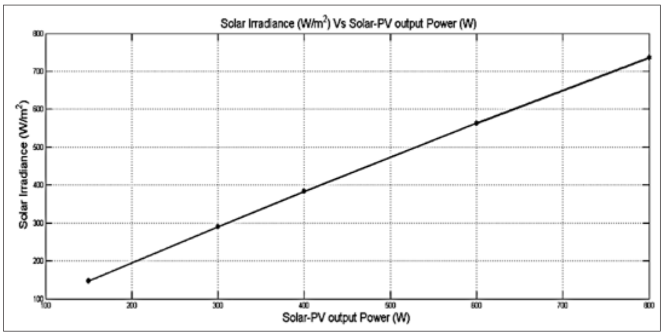


Figure 5: Solar Irradiance (W/m^2) Vs Solar-PV Output power (W)

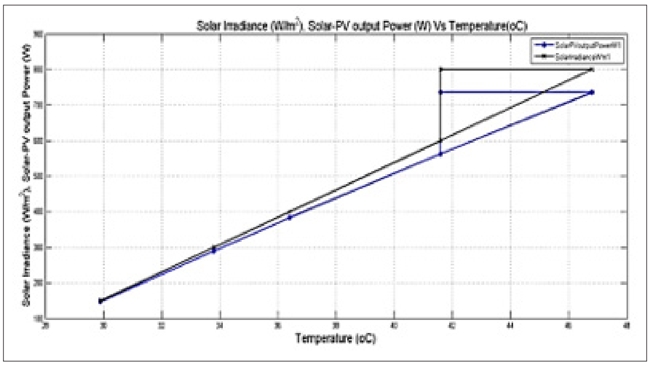


Figure 6: Solar Irradiance Solar P-V Output against Temperature $0^{O}C$

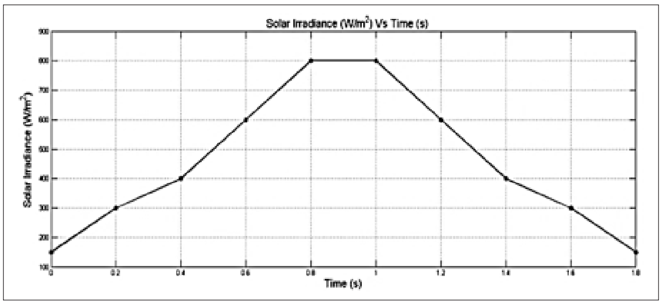


Figure 7: Solar Irradiance (W/m^2) Vs Time (s)

Conclusion

The experimental data gathered from the electrochemical reduction cell (ERC) model provides significant insights into the performance and efficiency of carbon dioxide (CO_2) capture and conversion into formic acid. The results indicate a positive correlation between current supply and the rates of formic acid production and CO_2 consumption, underscoring the effectiveness of the system in facilitating electrochemical reactions.

Current Supply and Reaction Rates

As the current supply increased from 100 mA to 450 mA, there was a corresponding increase in formic acid production, from approximately 0.000492 mol/s to 0.002217 mol/s. This suggests that higher current inputs enhance the electrochemical reduction efficiency, thereby facilitating greater CO_2 conversion into useful products.

CO_2 Consumption

The data show a clear trend of increased CO_2 consumption with increased current supply. Initially, CO_2 consumption was negligible, but as the current supply rose, the consumption rates reached significant levels, indicating the cell's capacity to effectively utilize CO_2 as a feedstock for formic acid production.

By-product Formation

The production of oxygen as a by-product was consistently observed throughout the experiments. The oxygen outlet rates also increased with higher current supplies, which is expected in electrochemical reactions involving water splitting. This dual product generation demonstrates the potential of the ERC model to mimic natural photosynthesis processes.

Efficiency Metrics

The Faradaic efficiency, which quantifies the effectiveness of charge input in producing desired products, can be inferred from the data trends. The significant increase in formic acid production relative to CO_2 consumption suggests a favourable efficiency for the electrochemical processes occurring within the cell.

Declaration of Competing Interest

The authors confirm that this manuscript is our original work and has not been published nor has it been submitted simultaneously elsewhere. We further confirm that all authors have checked the manuscript and have agreed to the submission. We declare that we have no conflict of interest [8].

Appendix

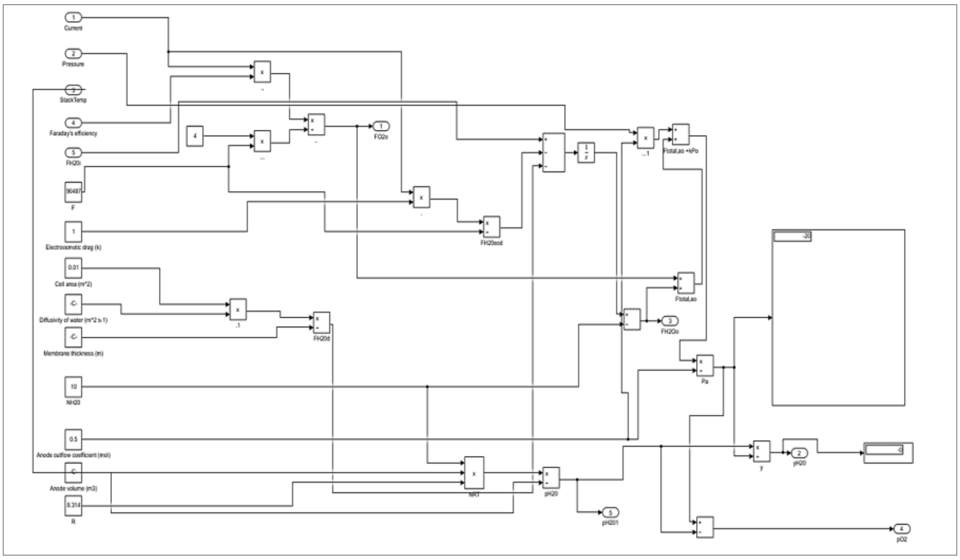


Figure 1: Simulink ERC Anodic Subsystem

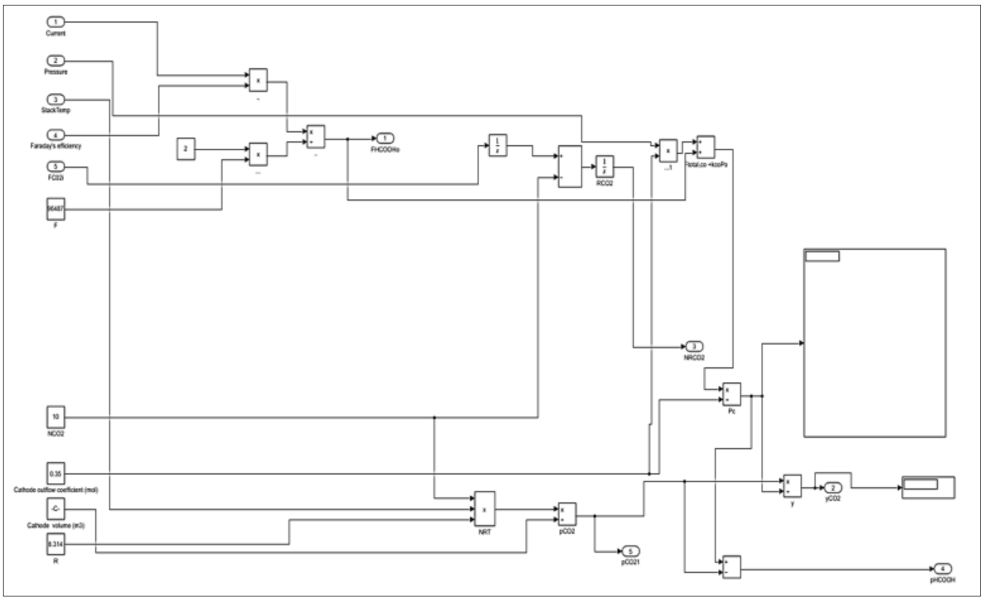


Figure 2: Simulink ERC Cathodic Subsystem

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