Sustainability analysis of different ethylene production routes

1 Introduction

Ethylene is a widely used commodity chemical with a global market value of 161.1 billion USD [1]. As a primary component in most plastics, ethylene is economically valuable. The main process route employed in its production is steam-cracking of hydrocarbons such as naptha and ethane. There exist alternative routes to ethylene production. One such route is bio-ethylene production from dehydration of bioethanol. The bioethanol is commonly derived from biomass feedstock such as sugarbeet, sugarcane and molasses [2].

An alternative novel route to ethylene production is an electrocatalytic one which involves the reduction of high purity carbon dioxide [3].

The bio-ethanol dehydration and electrochemical CO_2 catalytic reduction processes are both potential viable alternative means by which ethylene can be produced on a mass scale.

The main aim of this report is to conduct Life Cycle Analyses (LCAs) for ethylene production via the dehydration of bioethanol derived from sugarcane, and the electrocatalytic reduction of CO_2. Both processes were assumed to occur in production plants located in the United States of America. Estimates of the CO_2 emissions and power, as well as land use requirements for each process are compared, using the functional unit (FU) of 1 ton of ethylene produced. The results of the analyses are also compared using sustainability metrics commonly employed in LCA.

2 Methodology for electrochemical CO_2 reduction process

An efficient model for the electrochemical reduction of CO_2 to ethylene employs a porous CuO catalyst and involves use of high purity CO_2. The electrolyser unit of the model consists of an anode where O_2 is produced and a cathode where ethylene is produced **[4]**.

A production rate of 100 t day^{-1} of ethylene was assumed for a production plant employing the technology mentioned in the model. This technology is not commercially available yet. The production plant was assumed to operate for 350 days per year with an overall lifetime of 20 years **[5]**.

The amount of power required for the specified ethylene production rate was estimated at 107.2 MW using parameter values for the electrolyser unit shown in Table 1. These values are based on a model developed to simulate the electrocatalytic reduction process, using engineering approximations. An ethylene yield of 86 % was assumed **[5]**.

Table 1: Parameter values employed in estimating the power requirement of the electrolyser unit to deliver 100 t day^{-1} of ethylene at an assumed ethylene yield of 86 % **[5]**.

Ethylene production / t day^{-1}	100
Ethylene selectivity (Faradaic Efficiency) / %	90
Ethylene conversion / %	95
Ethylene yield / %	86
Operating time / days per year	350
Plant lifetime / years	20
Current density / A cm^{-2}	0.3
Electrolyser area / m^2	17690

Cell voltage / V	2
Power requirement / MW	107.2

The major contributor to the overall power requirement for ethylene production was assumed to be the electrolyser unit. The CO_2 adsorption unit was neglected since, its power requirement was found to be orders of magnitude lower. The power was converted to 25.7 kWh of electricity requirement per kg of ethylene produced using the specified ethylene production rate of 100 tonnes day^{-1}. The electricity supply was assumed to be met by Coal (19.8 %), Natural Gas (41.4 %), Nuclear (20.2 %), Solar (2.3 %), Wind (8.6 %) and Hydro Power (7.5 %) in proportions analogous to the share of each energy type of the US energy mix **[6]**.

Conversion factors obtained from US government sources were employed to estimate the amount of land required per kWh of electricity produced by each energy type of the US energy mix **[7].** Using these conversion factors, the amount of land in m^2 per kWh of electricity generated was estimated at 165.6. The ethylene production rate of 100 tonnes day^{-1} and 25.7 kWh of electricity requirement per kg of ethylene produced were used to arrive at a land requirement in km^2 per ton of ethylene produced of 4.26.

The greenhouse gas emissions of the electrocatalytic reduction of CO_2 to ethylene were assumed to be dominated by the power requirement of the electrolyser unit. A value of 0.429 kg of CO_2 equivalent ($CO_{2\ (eq)}$) per kWh of electricity produced was used to estimate the green house gas emissions of the process **[8]**. Using the 25.7 kWh of electricity requirement per kg of ethylene, the greenhouse gas emissions of the process were estimated at 11 tonnes of $CO_{2\ (eq)}$ per ton of ethylene produced.

Figure 1 depicts a flow diagram of the processes involved in the production of ethylene via electrocatalytic CO_2 reduction. The system boundary employed is encompassed by the dashed black line shown in Figure 1. A gate-to-gate analysis was employed.

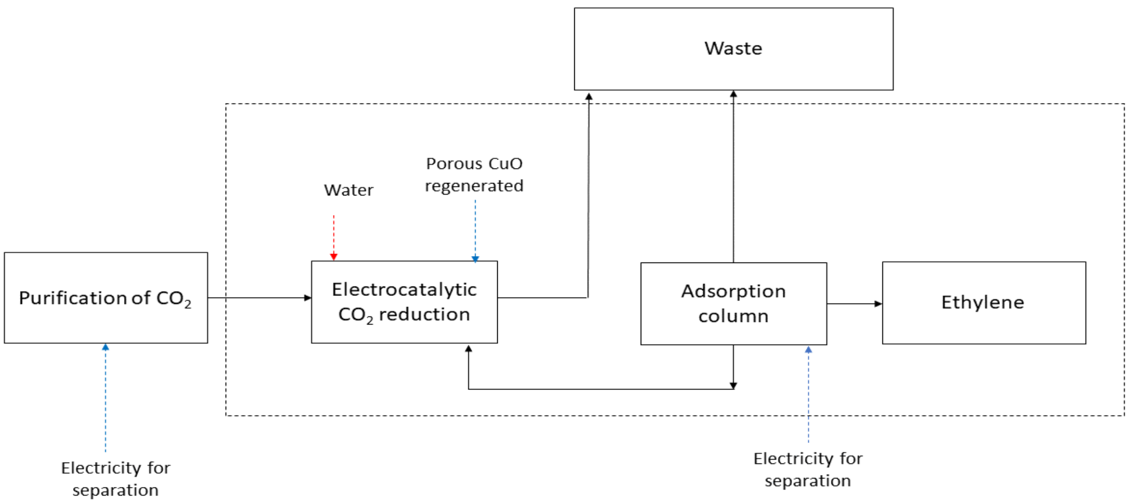

Figure 1: Schematic of flow diagram of processes involved in the production of ethylene via electrocatalytic CO_2 reduction.

Integration of the electrocatalytic CO_2 reduction was excluded from the system boundary to allow better comparisons with the bioethanol dehydration process to be made.

3 Methodology for sugarcane to bio-ethylene production process

Unlike the gate-to-gate approach employed for the electrocatalytic reduction process, a cradle-to-gate approach was employed for the bio-ethylene production process. Figure 2 depicts a flow chart of the processes involved in the production of bio-ethylene from sugarcane sourced from Brazil.

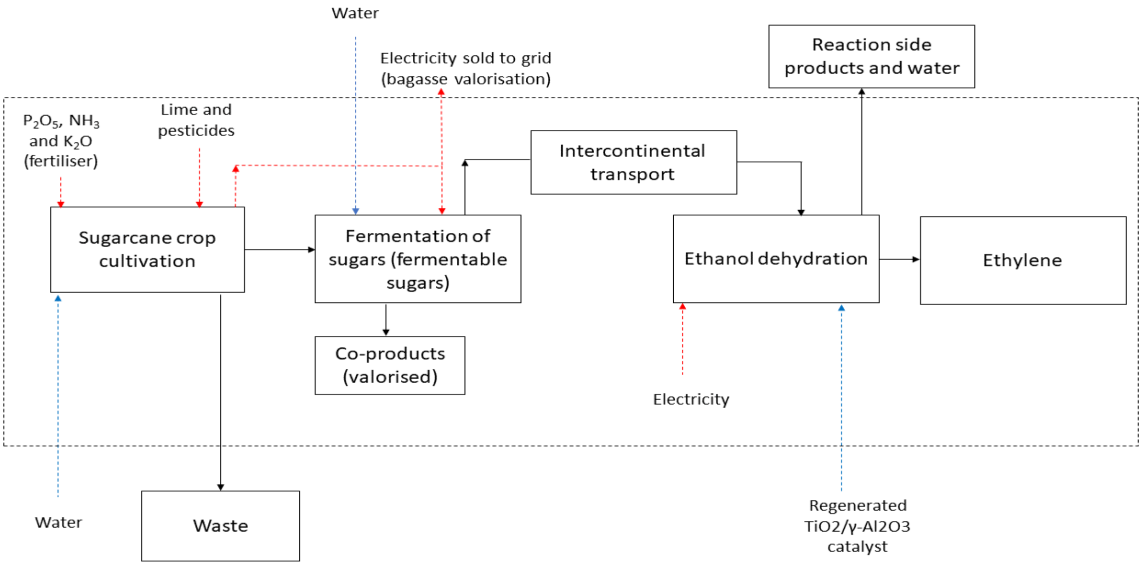

Figure 2: Schematic of flow chart of processes involved in the production of bio-ethylene from sugarcane. The dashed black line represents the system boundary employed.

An ethylene from bioethanol yield of 71 % was assumed for a production plant operating for 280 days per year with a lifetime of 20 years. The ethylene flowrate was estimated at 4.2 tonnes h^{-1} and the required bioethanol flowrate was estimated at 9.6 tonnes h^{-1}. As a result, the ratio of ton of bioethanol per ton of ethylene was estimated at 2.1, for a γ-alumina catalyst system **[9, 10]**.

A yield of 0.46 g of bioethanol g of fermentable sugars for the fermentation process was assumed based on information gathered from the literature. A similar process estimates the requirement of 11 tonnes of fermentable sugar per hectare of land per year to deliver the required amount of bioethanol at the specified yield **[11]**. The amount of fermentable sugar and bioethanol yield were used to estimate the tonnes of bioethanol per hectare of land per year required at 5.1. The ratio of 2.1 tonnes of bioethanol per ton of ethylene previously calculated was employed to estimate the amount of land required in km^2 per ton of ethylene produced at 0.05, which is considerably lower that the equivalent value calculated for the electrocatalytic reduction process.

In estimating, the greenhouse gas emissions of bio-ethylene production from Brazilian sugarcane, the dominant contributions were assumed to be those due to agricultural practices to cultivate the sugarcane crops and the highly endothermic dehydration process. Credits were allocated as well, due to electricity production from bagasse residue resulting from sugarcane cultivation and processing. The credits were estimated at 0.24 tonnes of $CO_{2\ (eq)}$ per ton of ethylene produced. This was calculated using results obtained from the literature. The contribution from agricultural practices and that due to the highly endothermic dehydration process were estimated at 1.86 and 3.2 tonnes of $CO_{2\ (eq)}$ per ton of ethylene produced. As a result, the total greenhouse gas emissions were estimated at 4.82 tonnes of $CO_{2\ (eq)}$ per ton of ethylene produced **[12]**.

The mean value of greenhouse gas emissions in tonnes of $CO_{2\ (eq)}$ per ton of ethylene by steam cracking of naptha and ethane was estimated at 3 based on values obtained from the literature **[13]**. This is considerably lower than that calculated for the electrocatalytic reduction of 11 and slightly less than that calculated from the sugarcane to bio-ethylene route.

4 Sustainability metric results and discussion

The sustainability metric estimates mentioned in this section are based on 1 ton of ethylene produced as functional unit. This is because this report does not consider the effects and consequences of scaling up both ethylene production processes. Table 2 depicts the sustainability metric estimates calculated for both process routes.

Table 2: List of estimated sustainability metric values for both ethylene production routes.

Sustainability Metric	Process	
	Sugarcane to bio-ethylene	CO_2 Reduction
Eutrophication potential / tonnes of $PO_{4(eq)}$ per ton of ethylene	0.12	0.15
Acidification potential / tonnes of SO_X (eq) per ton of ethylene	0.03	0.02
Photochemical oxidant potential / tonnes of ethylene$_{(eq)}$ per ton of ethylene	0.07	0.02
Non-renewable energy use per land coverage / GJ per km^2 per ton of ethylene	220	174
Global Warming Potential / tonnes of $CO_{2\ (eq)}$ per ton of ethylene	4.82	11.04
Land use requirement / km^2 per ton of ethylene	0.05	4.26

The values listed in table 2 were estimated based on environmental burdens found in the literature **[14]**. It was not possible to estimate social impact sustainability metrics such as Human Health, due to limited available data. A new metric proposed by several studies in the literature was also evaluated in this report. This metric is defined as Non-Renewable Energy Use per amount of land coverage per functional unit of product generated (ethylene for the purposes of this report). This metric is useful since, there is an increasing scarcity of fertile agricultural land in the world including an increasing need to minimise energy production via non-renewable energy sources **[11]**.

According to Table 2, the sugarcane to bio-ethylene process has similar environmental impacts to the electrocatalytic CO_2 reduction, as far as water and atmospheric pollution are concerned. Their Global Warming Potential, however, differs significantly and so does their land use requirement. The CO_2 reduction process scored the highest in these metrics. This is sensible considering the high-power requirement of the electrolyser. However, the analyses conducted, neglected water requirement for the processes as well as water and energy requirement for catalyst production. Incorporation of these may significantly alter the results.

The quality of the data used to evaluate these metrics is subject to large uncertainties. For example, some studies in the literature quote values based on local conditions and these vary markedly from region to region. For example, a study on ethylene production in Sweden, accounted for bio-ethanol production in Brazil but included contributions based on local Swedish environmental factors **[15]**.

5 Conclusions

Electrocatalytic reduction of CO_2 and bioethanol dehydration offer attractive alternative means by which ethylene can be produced. Each process has its merits and disadvantages; however, more data and more parameters need to be accounted for to better unravel the key similarities and differences between the two processes.

For both processes to become more favourable compared to conventional petrochemical routes, crude oil barrel prices need to increase. Higher carbon taxes may not offer advantages based on the results of this report. Both processes can also become more attractive if oil prices remain at least steady, and raw material prices and electricity prices decrease. In addition, the electrocatalytic reduction route may benefit the most and become even more favourable, despite having not been commercially employed yet, in the scenario that the electricity mix in its location is solely dominated by nuclear power and renewables.

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