

Evaluation of energy requirements for chemicals and fuels manufactured via electrochemical reduction of carbon dioxide

Dal Mas, Riccardo; Somoza-Tornos, Ana; Kiss, Anton A.

DOI

[10.1016/B978-0-443-28824-1.50354-9](https://doi.org/10.1016/B978-0-443-28824-1.50354-9)

Publication date

2024

Document Version

Final published version

Published in

Proceedings of the 34th European Symposium on Computer Aided Process Engineering

Citation (APA)

Dal Mas, R., Somoza-Tornos, A., & Kiss, A. A. (2024). Evaluation of energy requirements for chemicals and fuels manufactured via electrochemical reduction of carbon dioxide. In F. Manenti, & G. V. Reklaitis (Eds.), *Proceedings of the 34th European Symposium on Computer Aided Process Engineering: 15th International Symposium on Process Systems Engineering (ESCAPE34/PSE24)* (pp. 2119-2124). (Computer Aided Chemical Engineering; Vol. 53). Elsevier. <https://doi.org/10.1016/B978-0-443-28824-1.50354-9>

Important note

To cite this publication, please use the final published version (if applicable).
Please check the document version above.

Copyright

Other than for strictly personal use, it is not permitted to download, forward or distribute the text or part of it, without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license such as Creative Commons.

Takedown policy

Please contact us and provide details if you believe this document breaches copyrights.
We will remove access to the work immediately and investigate your claim.

Green Open Access added to TU Delft Institutional Repository

'You share, we take care!' - Taverne project

<https://www.openaccess.nl/en/you-share-we-take-care>

Otherwise as indicated in the copyright section: the publisher is the copyright holder of this work and the author uses the Dutch legislation to make this work public.

Evaluation of energy requirements for chemicals and fuels manufactured via electrochemical reduction of carbon dioxide

Riccardo Dal Mas,^a Ana Somoza-Tornos,^a Anton A. Kiss^{a,*}

^a *Department of Chemical Engineering, Delft University of Technology, Van der Maasweg 9, 2629 HZ Delft, Netherlands*

A.A.Kiss@tudelft.nl

Abstract

As the urgency of reducing greenhouse gas emissions increases, the chemical industry is moving towards more sustainable applications, such as substituting fossil feedstock with renewable ones. The development and implementation of novel technologies will entail momentous, system-wide changes to allow for the production of chemicals and fuels. This work aims at providing an overview of the energy requirements for the production of several chemicals by means of electrochemical reduction of CO₂ (ECO2R), in order to aid the decision-making process to select the products on which further research and development efforts should focus.

The results demonstrate that the production of C₁ oxygenated molecules, such as carbon monoxide and methanol, via ECO2R would have significantly lower requirements in terms of renewable energy generation when compared to fully reduced hydrocarbons (methane, ethylene) and ethanol. This would lead to a less demanding implementation of electrochemical CO₂ utilisation technologies, allowing for a more streamlined deployment of ECO2R within existing supply chains.

Keywords: CO₂ electroreduction; CO₂ utilisation; green processing; electrification

1. Introduction

The electrochemical reduction of CO₂ (ECO2R) has emerged in recent years as an interesting path for the production of sustainable chemicals and fuels within the wider scope of de-fossilisation of the chemical industry (i.e. substitution of fossil resources with renewable ones). It also holds the promise of valorising CO₂, thus incentivising its capture, and potentially helping in mitigating greenhouse gas emissions.

Many factors will play a role in determining the development of ECO2R as part of the chemical industry of the future, alongside biomass-based productions, green hydrogen and overall electrification. Parallel to the experimental efforts dedicated to improving the performance of the electrochemical conversion step, high-level (Verma et al. 2016) and detailed techno-economic assessments (Somoza-Tornos et al. 2021) have studied the economic viability of the production of several chemicals through ECO2R. However, the scale of renewable electricity generation required by these processes, once deployed at the industrial level, appears to be a factor often overlooked.

The many products which synthesis has been demonstrated via low temperature electrolysis of CO₂ (in scope for this work, while the high temperature process is not as it only allows for the production of carbon monoxide) will place different requirements in terms of electricity generation. The integration of chemical and electricity

productions will have effects on the economics and environmental performance of the processes, assessed at a high level studying two different scenarios based on carbon intensity of the grid electricity and electricity price. Emphasis is placed on comparing the scale of the renewable power plants that would fulfil the demand for the production of selected chemicals and fuels, comparing the currently demonstrated performance with the forecasted one, before assessing the primary energy input required for the production of the latter and comparing it to their specific energy.

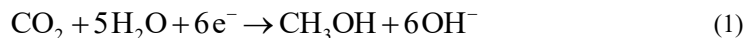
2. Problem statement

In the perspective of a future process industry, in which a number of possible sustainable routes will be available and will go alongside one another, decisions will be made on what the best technologies to substitute current supply chains are, taking into account the scale at which these currently operate. The production of the chemicals and fuels will place requirements of different magnitude on the overall production system, once scaled up to industrial level.

To aid these decisions, a fundamental analysis of the different products has been carried out, evaluating the energy requirement for their production via ECO2R and checking how much CO₂ can be converted and considering the different scales at which each product is typically manufactured.

3. Methodology

The analyses have been based on fundamental calculations for each product, assumed to be manufactured in a plant of 100 kt/y capacity. The stoichiometry of the cathodic semi-reaction (Zhang et al. 2018) is used to calculate the electric current i . For the example of methanol, assuming alkaline environment, the reaction can be written as:



and based on the desired production rate of methanol the current is calculated as:

$$i = \dot{n}_e \cdot F, \quad (2)$$

where $\dot{n}_e$ is the rate at which electrons are transferred and F is Faraday constant.

Combining this with the voltage V applied to the electrochemical cell, the total power requirement P has been calculated as:

$$P = i \cdot V \quad (3)$$

The products analysed, with their respective market price, are carbon monoxide (600 \$/t), formic acid (740 \$/t), methanol (600 \$/t), methane (180 \$/t), ethanol (1000 \$/t) and ethylene (1300 \$/t). These products are the ones to which the greatest attention has been dedicated in the ECO2R literature. The electrolytic cell performance data can be found in Huang et al. 2021, while the carbon footprint of electricity data are obtained from Gabrielli et al. 2023. As the goal of the analysis is the comparison of products and the evaluation of the energy requirements for the electrolysis process, Faradaic efficiencies have been considered 100% for each product and separation processes have not been included in the scope.

The energy consumption of separation processes derives from literature (Strojny et al. 2023 for CO₂ capture; Muñoz et al. 2015 for methane/CO₂; Shahandeh et al. 2015 for methanol/water; Kunnakorn et al. 2013 for ethanol/water).

4. Results and discussion

Figure 1 and Figure 2 display the effect of carbon emissions intensity and electricity price on a gross margin model for different products and on a gross CO₂ emissions mitigation through ECO2R potential. It appears clearly that the current conditions (carbon footprint of the grid of 0.45 kg CO₂/kWh and electricity price of 0.18 \$/kWh) and cell performance would not allow for a profitable nor environmentally friendly production of any chemical by means of these technologies, while for the conditions considered in the 2050 scenario (0.01 kg CO₂/kWh, 0.03 \$/kWh) all products would allow for CO₂ emissions mitigation, albeit at different gross margin levels. Methanol, ethanol and methane do not appear to be profitable even taking into account future, forecasted cell performance and low electricity price. On one hand, this analysis demonstrates the importance of a low-carbon energy system to power ECO2R, as the CO₂ emissions from the electricity generation alone would vastly offset the carbon fixed in the products. On the other hand, it is evident that the profitability at industrial scale could only be achieved under very favourable conditions and not for all the chemicals and fuels considered.

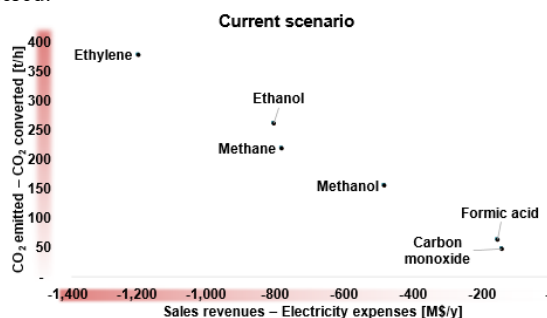


Figure 1: Gross margin and gross CO₂ emissions reduction for different products in the current scenario (0.45 kg CO₂/kWh, 0.18 \$/kWh).

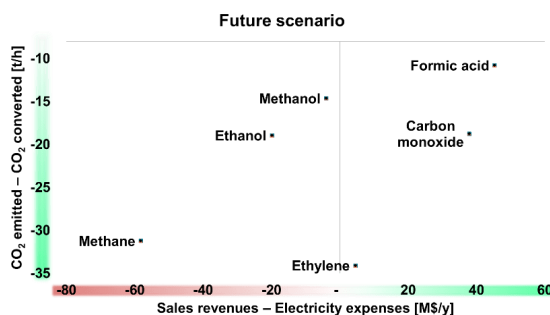


Figure 2: Gross margin and gross CO₂ emissions reduction for different products in the 2050 scenario (0.01 kg CO₂/kWh, 0.03 \$/kWh).

Figure 3 shows the overview of the requirements in terms of number of electrolyzers and renewable power generation installation (either offshore wind turbines, assuming a capacity factor of 50%, or PV farm area) for the production of different chemicals, evaluated on the same production basis of 100 kt/y. As these products have different market sizes and supply chains, the additional context of the conventional plant capacity is added, together with an indication of how much CO₂ is converted to each product.

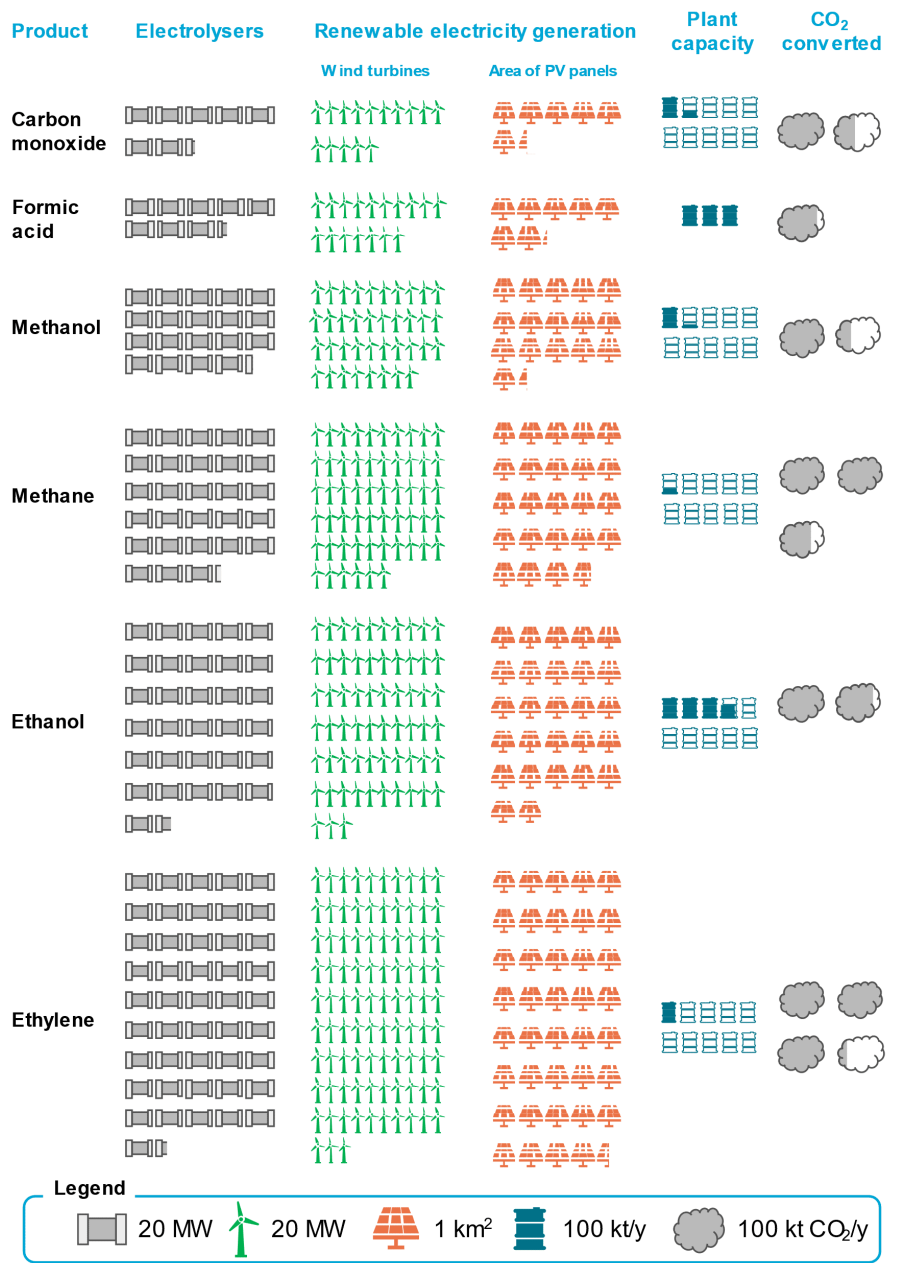


Figure 3: Overview for different products of ECO2R of: electrolysers; renewable power generation given by either number of offshore wind turbines or area of PV panels in the Netherlands; comparison of plant capacity with representative conventional plant size; CO₂ converted. The common production basis for each product is 100 kt/y. Biomethane and bioethanol plants are used for the plant capacity comparison for methane and ethanol, respectively.

Table 1: Summary of results for most relevant products of ECO2R for different scenarios (C: current performance; F: future performance). Electrolyser size: 20 MW; Wind turbine size 20 MW (currently at the prototype level for offshore installations), 50% capacity factor; PV performance in the Netherlands; conventional plants for methane and ethanol are taken for biomethane and bioethanol productions, respectively.

Product	Electrolysers		Renewable power generation				Capacity	CO ₂ converted [kt/y]
			Wind turbines		Area of PV [km ²]			
	C	F	C	F	C	F		
CO	7.4	4.6	15	9	6.3	3.9	14%	157.1
HCOOH	8.4	6.0	17	12	7.1	5.1	287%	95.7
CH ₃ OH	19.2	12.9	38	26	16.3	11.0	12%	137.5
CH ₄	28.1	15.9	56	32	23.9	13.5	3%	275.0
CH ₃ CH ₂ OH	31.7	25.0	63	50	27.0	21.2	37%	191.3
C ₂ H ₄	46.4	26.1	93	52	39.4	22.2	10%	314.3

A distinction can be drawn between the first three products (carbon monoxide, formic acid and methanol) and the last three, as a product such as ethylene requires extremely large amounts of energy even for small capacity as compared to classic steam crackers, whereas formic acid can be produced at scale with relatively contained installations.

These results are further corroborated by the data in Table 1, which includes a comparison of the current (C) and future (F) performance. The forecast improvement in the performance is likely to be significant for some products, such as methane and ethylene, while for ethanol the development is going to be lower. In all cases, the energy usages are very significant, as can be seen by the tens of wind turbines necessary for the production of ethylene, even at relatively small scale. C₁ oxygenated molecules, on the other hand, appear to be more scalable, even though when extrapolating at the actual industrial scale the energy demand is still extremely high (a methanol plant of 2500 t/d would require ~220 wind turbines of 20 MW with 50% capacity factor).

Special attention can be given to ECO2R fuels, which might play a role in the defossilisation of hard to abate sectors such as aviation and transportation. Figure 4 shows how the energy input to produce fuels – considering the capture of CO₂, the electrolysis (current performance) and the separation – is about 3-7 times higher than the specific energy content of the fuel itself.

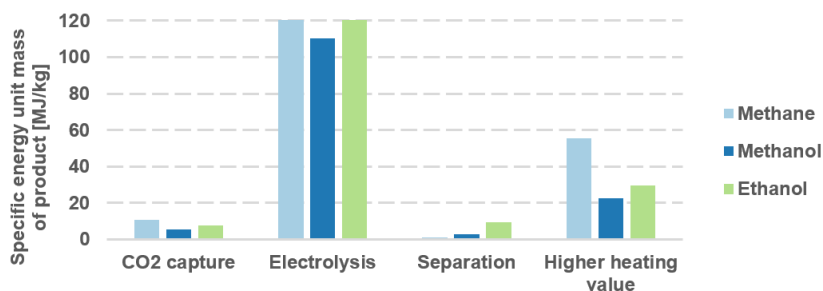


Figure 4: Comparison of energy input for the production of e-fuels via ECO2R and specific energy of the fuel (higher heating value).

Such a holistic view taking into account primary energy consumption is believed to be an important factor in the decision-making process for the selection of the technologies for the production of the fuels of the future.

5. Conclusions

The green electricity demand for the products of low temperature electrolysis has been successfully analysed, highlighting the importance of widely available and cheap renewable power to ensure not only the basic economic viability of the products, but also the possibility of mitigating CO₂ emissions.

Relevant ECO2R products have been compared on a common production basis to demonstrate the vast demand for renewable energy to allow for industrial deployment of these technologies: based on this, it can be concluded that C₁ oxygenated products, namely CO, HCOOH and CH₃OH would offer a better potential for implementation, compared to C₂, such as ethanol and ethylene.

Moreover, e-fuels produced by means of ECO2R, have a specific energy content which is only a fraction of the actual energy required for their production and appear not to be profitable, even when the costs of separation is neglected.

References

- Gabrielli, P., Rosa, L., Gazzani, M., Meys, R., Bardow, A., Mazzotti, M., Sansavini, G., 2023, Net-Zero Emissions Chemical Industry in a World of Limited Resources, *One Earth* 6 (6): 682–704.
- Huang, Z., Grim, R.G., Schaidle, J.A., Tao, L., 2021, The Economic Outlook for Converting CO₂ and Electrons to Molecules, *Energy & Environmental Science* 14 (7): 3664–78.
- Kunnakorn, D., Rirksomboon, T., Siemanond, K., Aungkavattana, P., Kuanchertchoo, N., Chuntanalerg, P., Hemra, K., Kulprathipanja, S., James, R.B., Wongkasemjit, S., 2013, Techno-Economic Comparison of Energy Usage between Azeotropic Distillation and Hybrid System for Water–Ethanol Separation, *Renewable Energy* 51 (March): 310–16.
- Muñoz, R., Meier, L., Diaz, I., Jeison, D., 2015, A Review on the State-of-the-Art of Physical/Chemical and Biological Technologies for Biogas Upgrading, *Reviews in Environmental Science and Bio/Technology* 14 (4): 727–59.
- Shahandeh, H., Jafari, M., Kasiri, N., Ivakpour, J., 2015, Economic Optimization of Heat Pump-Assisted Distillation Columns in Methanol-Water Separation, *Energy* 80 (February): 496–508.
- Somoza-Tornos, A., Guerra, O.J., Crow, A.M., Smith, W.A., Hodge, B.M., 2021, Process Modeling, Techno-Economic Assessment, and Life Cycle Assessment of the Electrochemical Reduction of CO₂: A Review, *iScience* 24 (7): 102813.
- Strojny, M., Gładysz, P., Hanak, D.P., Nowak, W., 2023, Comparative Analysis of CO₂ Capture Technologies Using Amine Absorption and Calcium Looping Integrated with Natural Gas Combined Cycle Power Plant, *Energy* 284 (December): 128599.
- Verma, S., Kim, B., Jhong, H.R., Ma, S., Kenis, P.J.A., 2016, A Gross-Margin Model for Defining Technoeconomic Benchmarks in the Electroreduction of CO₂, *ChemSusChem* 9 (15): 1972–79.
- Zhang, W., Hu, Y., Ma, L., Zhu, G., Wang, Y., Xue, X., Chen, R., Yang, S., Jin, Z., 2018, Progress and Perspective of Electrocatalytic CO₂ Reduction for Renewable Carbonaceous Fuels and Chemicals, *Advanced Science* 5 (1): 1700275.