

SUPPORTING INFORMATION

# Shaping the future of methanol production through carbon dioxide utilisation strategies

*Javier Fernández-González, Marta Rumayor\*, Jara Laso, Antonio Domínguez-Ramos,  
Angel Irabien*

University of Cantabria, Department of Chemical and Biomolecular Engineering, Av. Los  
Castros s/n, 39005, Santander, Spain

\* Corresponding author:

Marta Rumayor: University of Cantabria, Department of Chemical and Biomolecular  
Engineering Av. Los Castros s/n, 39005 Santander, Spain;

E-mail: [marta.rumayor@unican.es](mailto:marta.rumayor@unican.es)

Contents:

Number of pages: 2

Number of tables: 2

### Supplementary Note 1 – Process Inventory for direct e-MeOH (CO<sub>2</sub>ER)

Inventory for the CO<sub>2</sub> electrolysis process is given (Table S1). Cathode elements are adapted for MeOH production from a previous work.<sup>1</sup>, assuming CuO<sub>2</sub> as catalyst at a load of 1.8 mg/cm<sup>2</sup>. A proton exchange membrane (Nafion 117) is used. Platinum foil is considered as anodic electrocatalyst. Electrolyzer stack is based on the alkaline design from Zhao et al.<sup>2</sup> Balance of plant uses the inventory from Bareiß et al.<sup>3</sup> Capture of CO<sub>2</sub> is assumed to be performance with amine-based absorption using inventory from Giordano et al.<sup>4</sup> Material and energy needs (water, heat, electricity, minor chemicals) are calculated in the black-box model described in work of the research group.<sup>5-7</sup>

**Table S1.** Simplified inventory to produce MeOH by the CO<sub>2</sub>ER route.

Flow	Scenario		Unit
	SoA	HP	
Inputs			
Anode	4.24 · 10 <sup>-4</sup>	2.23E-05	m <sup>2</sup>
Membrane	6.06 · 10 <sup>-4</sup>	2.79E-05	m <sup>2</sup>
Cathode	4.24 · 10 <sup>-2</sup>	2.23E-05	m <sup>2</sup>
Stack	2.12 · 10 <sup>-4</sup>	1.12E-05	m <sup>2</sup>
Balance of Plant (BoP)	2.12 · 10 <sup>-4</sup>	1.12E-05	m <sup>2</sup>
CO <sub>2</sub> captured	1.63	1.38	kg
Deionized water	3.80	1.80	kg
Electricity	40.6	8.5	kWh
Heat	160.6	20.73	MJ
Outputs			
MeOH	1	1	kg
H <sub>2</sub>	0.19	0.03	kg
O <sub>2</sub>	3.00	0.58	kg
CO <sub>2</sub> to air	0.26	0.18	kg

## Supplementary Note 2 – Process Inventory for H<sub>2</sub>-e-MeOH

Inventory for the H<sub>2</sub>-e-MeOH process is reported in Table S2. Cathode, anode and stack is based on a previous work from Rumayor et al.,<sup>8</sup> BoP and CO<sub>2</sub> capture uses the same as for the CO<sub>2</sub>ER route. CO<sub>2</sub> hydrogenation inventory uses data from Ravikumar et al.,<sup>9</sup>

**Table S2.** Simplified inventory to produce MeOH by the H<sub>2</sub>-CO<sub>2</sub>ER route.

Flow	Value	Unit
Inputs		
Anode	2.23E-05	m <sup>2</sup>
Membrane	2.79E-05	m <sup>2</sup>
Cathode	2.23E-05	m <sup>2</sup>
Stack	1.12E-05	m <sup>2</sup>
Balance of Plant (BoP)	1.12E-05	m <sup>2</sup>
CO <sub>2</sub> captured	1.38	kg
Deionized water	2.1	kg
Electricity	10.86	kWh
Heat	4.6	MJ
Outputs		
MeOH	1	kg
CO <sub>2</sub> to air	0.18	kg

## References

- (1) Rumayor, M.; Dominguez-Ramos, A.; Irabien, A. Environmental and Economic Assessment of the Formic Acid Electrochemical Manufacture Using Carbon Dioxide: Influence of the Electrode Lifetime. *Sustain. Prod. Consum.* **2019**, *18*, 72–82. <https://doi.org/10.1016/j.spc.2018.12.002>.
- (2) Zhao, G.; Kraglund, M. R.; Frandsen, H. L.; Wulff, A. C.; Jensen, S. H.; Chen, M.; Graves, C. R. Life Cycle Assessment of H<sub>2</sub>O Electrolysis Technologies. *Int. J. Hydrog. Energy* **2020**, *45* (43), 23765–23781. <https://doi.org/10.1016/j.ijhydene.2020.05.282>.
- (3) Bareiß, K.; de la Rúa, C.; Möckl, M.; Hamacher, T. Life Cycle Assessment of Hydrogen from Proton Exchange Membrane Water Electrolysis in Future Energy Systems. *Appl. Energy* **2019**, *237* (November 2018), 862–872. <https://doi.org/10.1016/j.apenergy.2019.01.001>.
- (4) Giordano, L.; Roizard, D.; Favre, E. Life Cycle Assessment of Post-Combustion CO<sub>2</sub> Capture: A Comparison between Membrane Separation and Chemical Absorption Processes. *Int. J. Greenh. Gas Control* **2018**, *68*, 146–163. <https://doi.org/10.1016/j.ijggc.2017.11.008>.
- (5) Dominguez-Ramos, A.; Singh, B.; Zhang, X.; Hertwich, E. G. G.; Irabien, A. Global Warming Footprint of the Electrochemical Reduction of Carbon Dioxide to Formate. *J. Clean. Prod.* **2015**, *104*, 148–155. <https://doi.org/10.1016/j.jclepro.2013.11.046>.
- (6) Fernández-González, J.; Rumayor, M.; Domínguez-Ramos, A.; Irabien, Á. CO<sub>2</sub> Electroreduction: Sustainability Analysis of the Renewable Synthetic Natural Gas. *Int. J. Greenh. Gas Control* **2022**, *114*, 103549. <https://doi.org/10.1016/j.ijggc.2021.103549>.
- (7) Rumayor, M.; Dominguez-Ramos, A.; Irabien, A. Formic Acid Manufacture: Carbon Dioxide Utilization Alternatives. *Appl. Sci.* **2018**, *8* (6), 914. <https://doi.org/10.3390/app8060914>.
- (8) Rumayor, M.; Corredor, J.; Rivero, M. J.; Ortiz, I. Prospective Life Cycle Assessment of Hydrogen Production by Waste Photoreforming. *J. Clean. Prod.* **2022**, *336*, 130430. <https://doi.org/10.1016/j.jclepro.2022.130430>.
- (9) Ravikumar, D.; Keoleian, G.; Miller, S. The Environmental Opportunity Cost of Using Renewable Energy for Carbon Capture and Utilization for Methanol Production. *Appl. Energy* **2020**, *279*, 115770. <https://doi.org/10.1016/j.apenergy.2020.115770>.