# Supplementary material for **Evaluating the Sustainability of Electrochemical $CO_2$ Capture Technology through LCA and LCC: A Winery Industry Application**

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An emerging alternative to amine scrubbing is the use of electrochemically produced sodium hydroxide to fix $CO_2$ as carbonate. The mechanism of this process is based on the fact that in a wet alkaline medium, $CO_2$ is physically absorbed and instantly reacts with NaOH according to the reaction pathways presented in equations 1-3 [7].

$$CO_{2(aq)} + H_2O \overset{K_1}{\rightleftharpoons} H_2CO_3 \quad (1)$$

$$H_2CO_3 + OH^- \overset{K_2}{\rightleftharpoons} HCO_3^- + H_2O \quad (2)$$

$$HCO_3^- + OH^- \overset{K_3}{\rightleftharpoons} CO_3^{2-} + H_2O \quad (3)$$

In a highly alkaline medium (excess NaOH), reaction 3 is carried out immediately after reaction 2, resulting in the formation of sodium carbonate as the product. However, for prolonged capture, NaOH becomes limiting, and the reverse of reaction 3 sets in, producing sodium bicarbonate as the product.

The EDEN technology is designed to operate in both electrolysis and fuel-cell modes. The electrolysis reactions involve anodic oxidation of water to oxygen (Equation (4)) and oxidation of chloride ions to chlorine gas (Equation (5)). Chlorine may undergo chemical disproportionation to hypochlorous acid (Equation (7)) after dissolving in water (Equation (6)), which can then dissociate into hypochlorite ions (Equation (6)). The cathode reduces water to hydrogen and hydroxide ions (Equation (9)). Also, chlorine generated at the anode can be reduced at the cathode due to crossover, potentially competing with water reduction and producing chloride ions [9].

$$H_2O \rightarrow 0.5\, O_2 + 2H^+ + + 2e^- \quad (4)$$

$$2Cl^- \rightarrow Cl_2(g) + 2e^- \quad (5)$$

$$Cl_2(g) \rightarrow Cl_2(aq) \quad (6)$$

$$Cl_2(aq) + H_2O \rightarrow HClO + HCl \quad (7)$$

$$HClO \rightarrow H^+ + ClO^- \quad (8)$$

$$2H_2O + 2Na^+ + 2e^- \rightarrow H_2 + 2\, NaOH \quad (9)$$

Table S1: Material selection for each scenario studied.

| **FU = 1 g $CO_2$ Captured** | | | Unit | Material Quantity | Material Quantity per FU | Scenarios | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Module | Component | Material Selected in SimaPro | | | | 1 | 2 | 3 | 4 | 5 |
| | | **Materials (Manufacturing + Processing)** | | | | | | | | |
| Electrolyzer | Cathode | Titanium, {GLO} market for titanium \| Cut-off, U | g | 6.159 | 3.33E-04 | ✓ | ✓ | ✓ | ✓ | X |
| | Anode electrode, Cell C | Titanium, {GLO} market for titanium \| Cut-off, U | g | 1.547 | 8.35E-05 | ✓ | X | ✓ | X | X |
| | | Carbon black, {GLO} market for carbon black \| Cut-off, U | g | 0.042 | 2.27E-06 | | | | | |
| | | Rhodium, {GLO} market for rhodium \| Cut-off, U, **for Ruthenium catalyst** | g | 0.007 | 3.82E-07 | | | | | |
| | | Platinum, {GLO} market for platinum \| Cut-off, U, **for Platinum (catalyst)** | g | 0.006 | 3.38E-07 | | | | | |
| | | Tetrafluoroethylene, {GLO} market for tetrafluoroethylene \| Cut-off, U | g | 0.003 | 1.73E-07 | | | | | |
| | Anode electrode, Cell B | Titanium, {GLO} market for titanium \| Cut-off, U, **for Titanium Sheet** | g | 10.613 | 5.73E-04 | X | ✓ | X | ✓ | X |
| | | Rhodium, {GLO} market for rhodium \| Cut-off, U, **for Ruthenium catalyst** | g | 0.064 | 3.46E-06 | | | | | |
| | | Platinum, {GLO} market for platinum \| Cut-off, U, **for Platinum (catalyst)** | g | 0.043 | 2.30E-06 | | | | | |
| | | Titanium, {GLO} market for titanium \| Cut-off, U, **for Titanium (catalyst** | g | 0.427 | 2.30E-05 | | | | | |
| | Membrane (Nafion) | Tetrafluoroethylene, {GLO} market for tetrafluoroethylene \| Cut-off, U | g | 1.676 | 9.05E-05 | ✓ | ✓ | ✓ | ✓ | X |
| | | Sulfuric acid, {RER} market for sulfuric acid \| Cut-off, U | g | 0.419 | 2.26E-05 | | | | | |
| | Gasket | Silicone product, {RER} market for silicone product \| Cut-off, U | g | 38.426 | 2.08E-03 | ✓ | ✓ | ✓ | ✓ | X |
| | Screws support | Steel, stainless 304, {RNA} quarto plate | g | 91.176 | 4.92E-03 | ✓ | ✓ | ✓ | ✓ | X |
| | Screws | Polyethylene terephthalate, {GLO} market for polyethylene terephthalate, granulate, bottle grade \| Cut-off, U | g | 25.176 | 1.36E-03 | ✓ | ✓ | ✓ | ✓ | X |
| | End and Bipolar | Methyl methacrylate, {RER} market for methyl methacrylate \| Cut-off, U | g | 143.210 | 7.73E-03 | ✓ | ✓ | ✓ | ✓ | ✓ |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | Plates | Methyl methacrylate, {RER} market for methyl methacrylate \| Cut-off, U | g | 48.251 | 2.61E-03 | | | | | |
| Storage and Connections | Pipes | Silicone product, {RER} market for silicone product \| Cut-off, U | g | 91.1 | 4.92E-03 | ✓ | ✓ | ✓ | ✓ | (x1) ✓ |
| | Tanks (2) | Methyl methacrylate, {RER} market for methyl methacrylate \| Cut-off, U | g | 469.389 | 5.07E-03 | | | | | |
| | | Methyl methacrylate, {RER} market for methyl methacrylate \| Cut-off, U | g | 158.150 | 1.71E-03 | | | | | |
| Compressor | Screws | Steel, stainless 304, {RNA} quarto plate | g | 32.123 | 5.01E-05 | ✓ | ✓ | ✓ | ✓ | ✓ |
| | Pipes | Silicone product, {RER} market for silicone product \| Cut-off, U | g | 14.231 | 3.14E-05 | | | | | |
| | Casing | Polycarbonate, granulate, {GLO} market for\| Cut-off, U | g | 69.721 | 1.23E-04 | | | | | |
| | Electronics | Electronics, for control units, {GLO} market for \| Cut-off, U | g | 215.121 | 3.63E-04 | | | | | |
| Pump(x2) | Screws | Steel, {RNA} stainless 304, quarto plate | g | 29.888 | 4.91E-05 | ✓ | ✓ | ✓ | ✓ | (x1) ✓ |
| | Pipes | Silicone product, {RER} market for silicone product \| Cut-off, U | g | 17.682 | 2.91E-05 | | | | | |
| | Casing | Polycarbonate, granulate, {GLO} market for\| Cut-off, U | g | 68.052 | 1.12E-04 | | | | | |
| | Electronics | Electronics, for control units, {GLO} market for \| Cut-off, U | g | 208.358 | 3.43E-04 | | | | | |
| DC power supply | DC power supply | Steel, chromium steel 18/8 {GLO} market for \| Cut-off, U | g | 332.270 | 5.46E-04 | ✓ | ✓ | ✓ | ✓ | ✓ |
| | | Cable, unspecified {GLO} market for \| Cut-off, U | g | 92.593 | 1.52E-04 | | | | | |
| | | Polyethylene, high-density, granular {GLO} market for \| Cut-off, U | g | 934.053 | 1.54E-03 | | | | | |
| | | Electronics, for control units, {GLO} market for \| Cut-off, U | g | 41.884 | 6.89E-05 | | | | | |
| Absorption Column | Plastic body | Polyethylene terephthalate, {GLO} market for polyethylene terephthalate, granulate, bottle grade \| Cut-off, U | g | 618.48 | 3.67E-03 | X | X | ✓ | ✓ | ✓ |
| | | Ethylene glycol, {RER} market for ethylene glycol \| Cut-off, U | g | 68.72 | 4.08E-04 | | | | | |
| | Sphere glass | Glass tube, borosilicate, {GLO} market for glass tube, borosilicate \| Cut-off, U | g | 2000 | 1.19E-02 | | | | | |
| | Screws | Steel, {RNA} stainless 304, quarto plate | g | 467.5 | 2.78E-03 | | | | | |
| | Gasket | Silicone product, market for silicone product \| Cut-off, U | g | 34.7 | 2.06E-04 | | | | | |
| | | **Operation** | | | | | | | | |
| Feedstock | Electrolyte | Sodium chloride, brine solution, {GLO} market for sodium chloride, brine solution \| Cut-off, U | g | | 24.57 | ✓ | ✓ | ✓ | ✓ | X |
| | Solvent | Neutralising agent, sodium hydroxide-equivalent, {RER} sodium hydroxide to the generic market for neutralising agent \| Cut-off, U | g | | 2.27 | X | X | X | X | ✓ |
| Energy Source | Electricity | Photovoltaic module, building-integrated, for slanted-roof installation {RER}\| photovoltaic module production, building-integrated, for slanted-roof installation \| Cut-off, U | kWh | | 4.74E-03 | ✓ | ✓ | X | X | X |
| | | | | | 7.81E-03 | X | X | ✓ | ✓ | X |
| | | | | | 2.32E-04 | X | X | X | X | ✓ |

**Table S2:** Electricity prices, emission factors, and emissions prices considered (sourced from Ecoinvent database).

| Electricity source | Price, | Emission factor | Emissions price |
|---|---|---|---|

| | €/kWh | (kg $CO_2$/kWh) | (€/t $CO_2$-eq) |
|---|---|---|---|
| Italy grid mix | 0.195 | 0.35 | 65 |
| Chile grid mix | 0.11 | 0.51 | 4.6 |
| Spain grid mix | 0.17 | 0.21 | 65 |
| France grid mix | 0.171 | 0.09 | 65 |
| California grid mix | 0.065 | 0.38 | 40 |
| Spain's solar energy | 0.05 | 0.07 | 65 |
| Spain wind energy | 0.04 | 0.01 | 65 |
| Spain's nuclear energy | 0.1 | 0.01 | 65 |
| Off-grid solar (Spain) | 0.0073 | 0.006 | 65 |

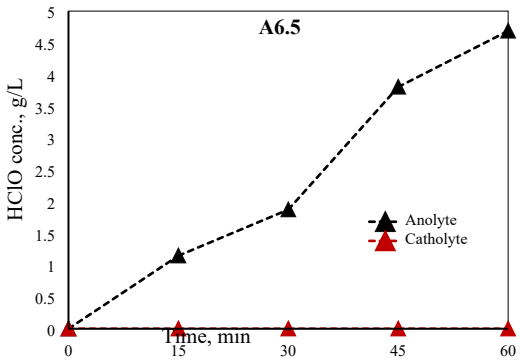


Figure S1. Time course formation of HClO in the catholyte and anolyte

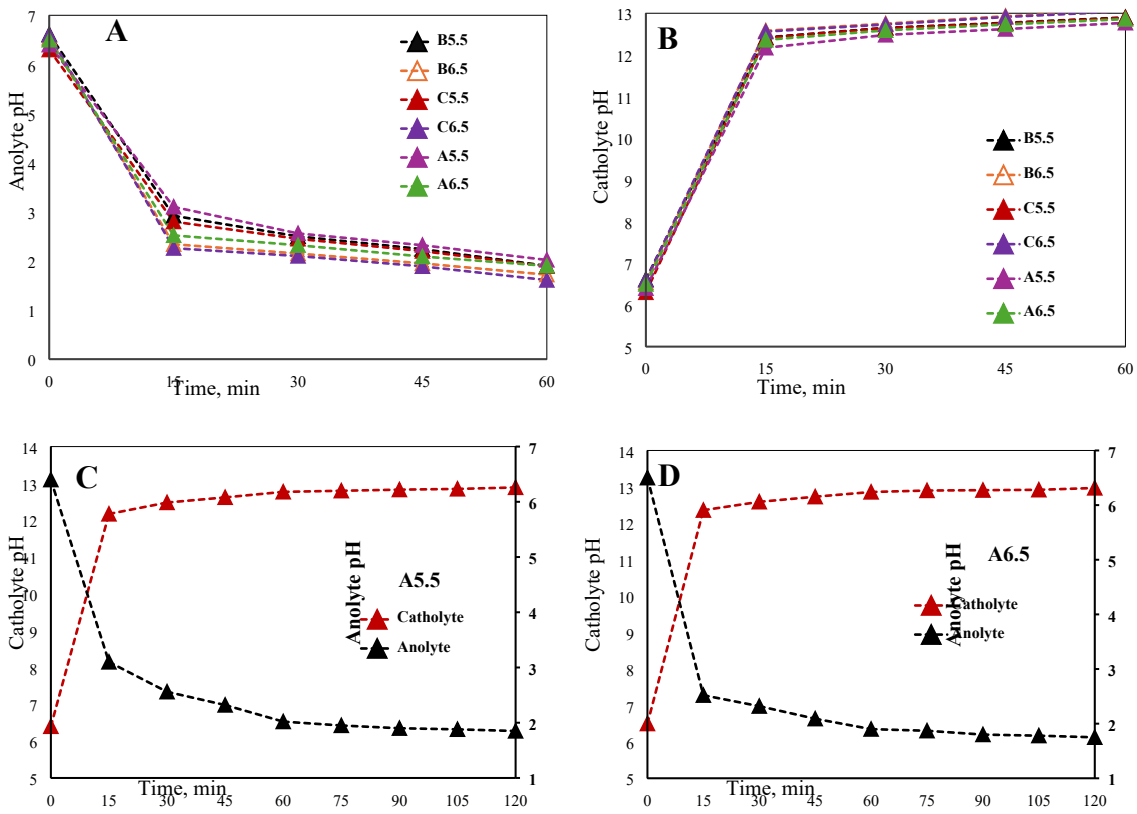


Figure S2. Time course of electrolytes pH trend: (A) anolyte and (B) catholyte for short duration, (C) Catholyte and (D) anolyte for longer duration.

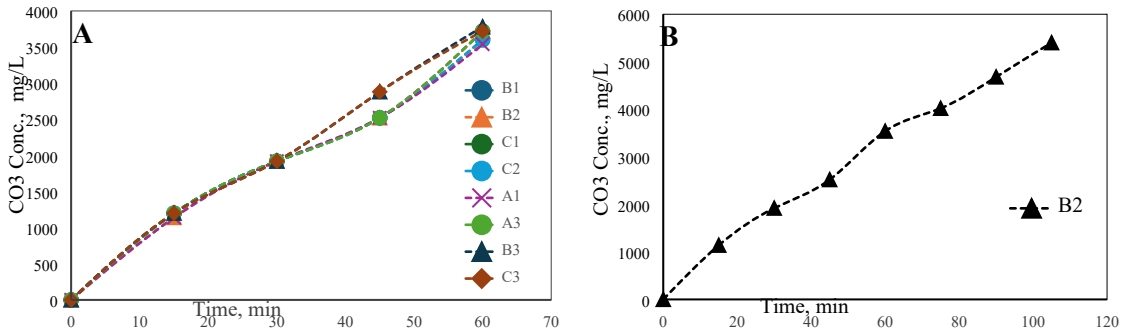


Figure S3. Time course of carbonate formation during electro-absorption of $CO_2$ at 15 mL/min: (A) Comparison of different tested conditions and (B) 120 minutes of $CO_2$ absorption considering conditions of B2.

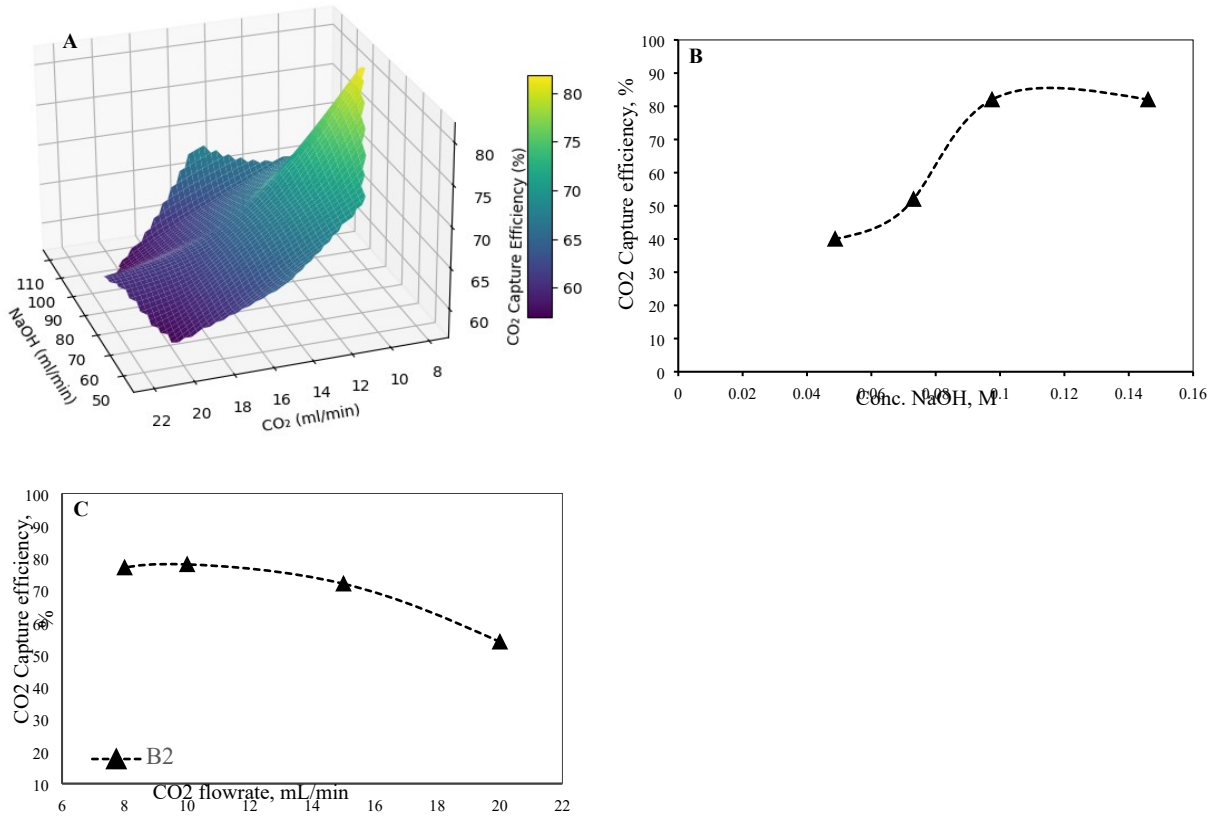


Figure S4: Optimization of studied variables, (A) influence of NaOH flow rate and $CO_2$ flow rate on the capture efficiency in column absorption, (B) influence of NaOH concentration on the capture efficiency in column absorption, (C) influence of $CO_2$ flow rate on the capture efficiency in electro-absorption.

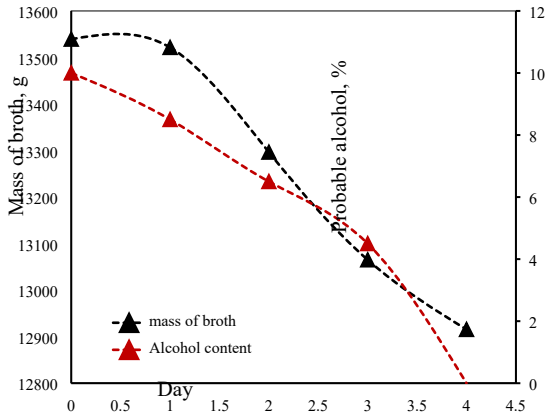


Figure S5. Daily profiles of mass and probable alcohol content of the fermentation broth.

Table S3: Composition of fermentation broth (wine sample) before and after fermentation.

| Sampling Description | pH | °Brix | Total Acidity (g/L) | Malic Acid (g/L) | Lactic Acid (g/L) | Acetic Acid (g/L) | Citric Acid (g/L) | Tartaric Acid (g/L) | Succinic Acid (g/L) | Glycerol (g/L) | Glucose + Fructose (g/L) | Alcohol (% v/v) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Initial sample (unfermented must) | 3.10 | 16.64 | 5.60 | 1.91 | – | – | 3.39 | 1.79 | – | – | 154.00 | 0.30 |

| Sampling Description | pH | °Brix | Total Acidity (g/L) | Malic Acid (g/L) | Lactic Acid (g/L) | Acetic Acid (g/L) | Citric Acid (g/L) | Tartaric Acid (g/L) | Succinic Acid (g/L) | Glycerol (g/L) | Glucose + Fructose (g/L) | Alcohol (% v/v) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Final sample after fermentation | 3.09 | – | 7.40 | 1.66 | 0.16 | – | 3.52 | 1.97 | 0.66 | 5.09 | 0.18 | 8.40 |

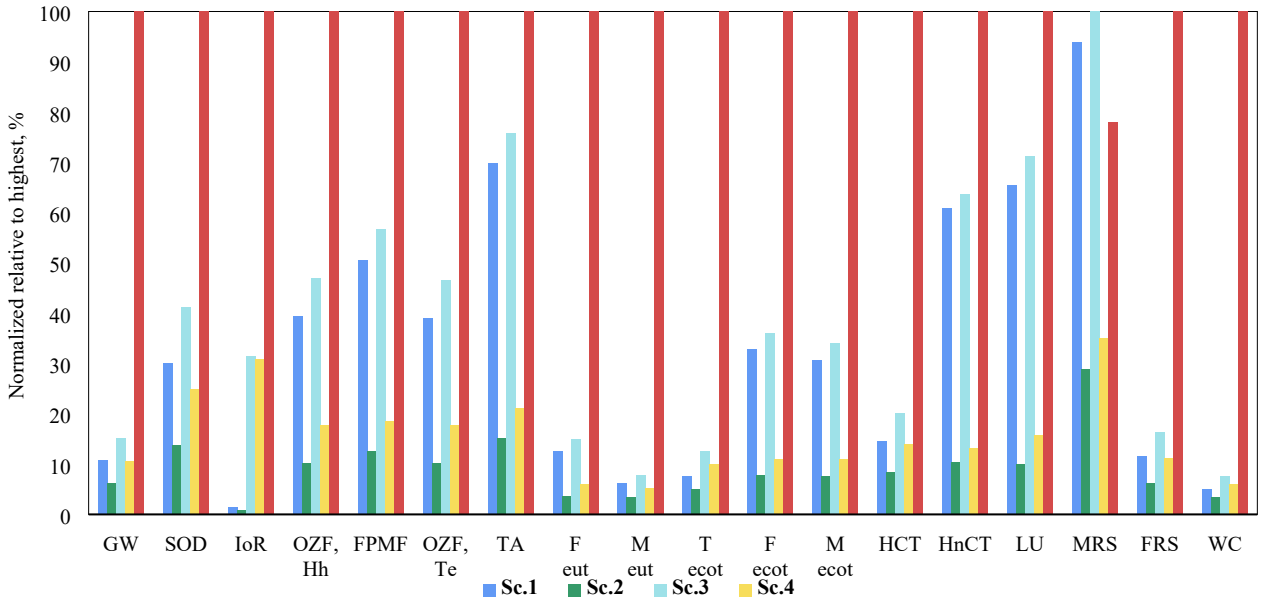


Figure S6. Recipe Midpoint results for the studied $CO_2$ capture scenarios.