

Supplementary Information

Study of the NaOH(s)-CO₂(g) reaction creating value for industry. Green natrite production, energy, and its potential in different sustainable scenarios.

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Figure S1. (a) XPS spectra for γ -Na₂CO₃ obtained by chemical transformation with solid-based NaOH technology for CO₂ capture. (b) C1s, (c) Na1s and (d) O1s spectral region in high-resolution XPS spectra. Minoritarian peaks: a1: CKLL; a2: OKLL; a3: NaKLL1; a4: NaKLL; a5: Si2s; a6: Si2p; a7: Na2s; a8: O2s – Na2p.

Figure S2. (a) Thermogram TGA-DSC corresponding to γ -Na₂CO₃ obtained by chemical transformation with solid-based NaOH technology for CO₂ capture. (b) ATR-FTIR spectrum from γ -Na₂CO₃ (natrite) into of 4000 to 400 cm⁻¹, and ampliation between 1100 to 1060 cm⁻¹ region. (c) ²³Na and ¹³C MAS-NMR spectra from γ -Na₂CO₃ (natrite).

Figure S3. Sustainable model with natrites sold, NaOH regeneration and average carbon footprint.

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Table S1. Average DFTB values

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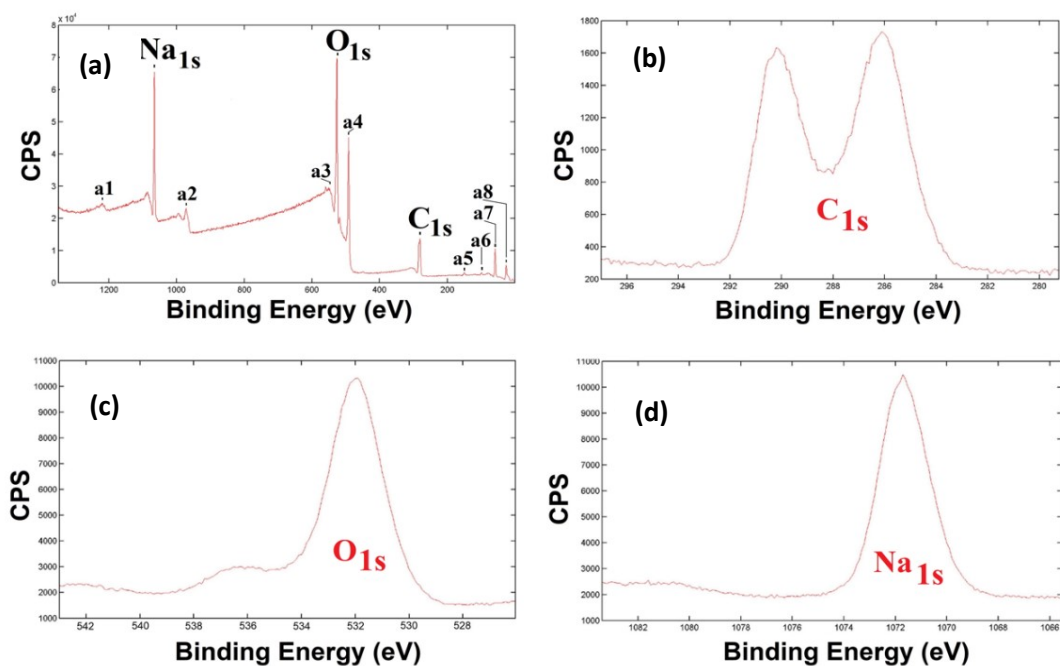


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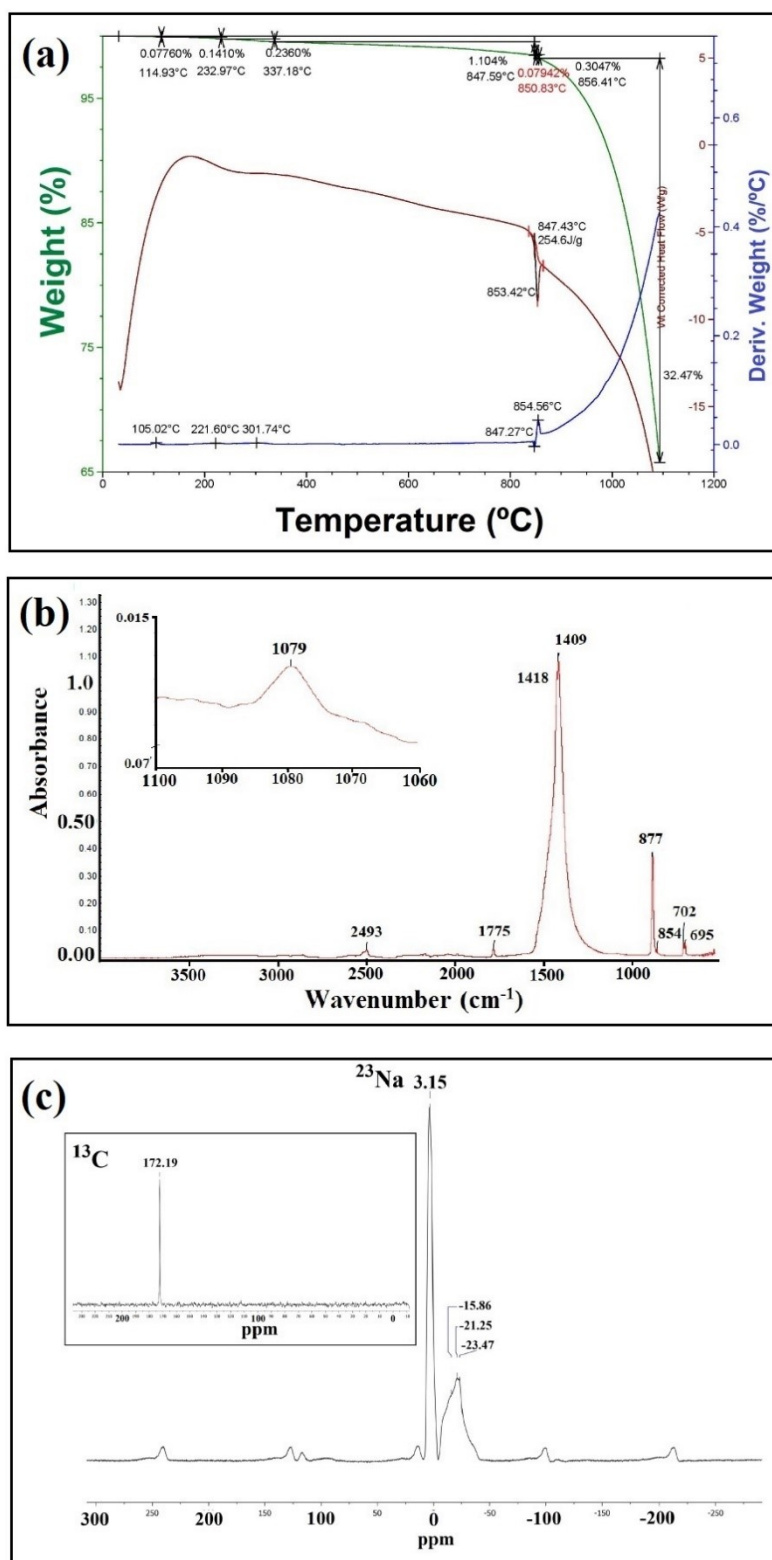


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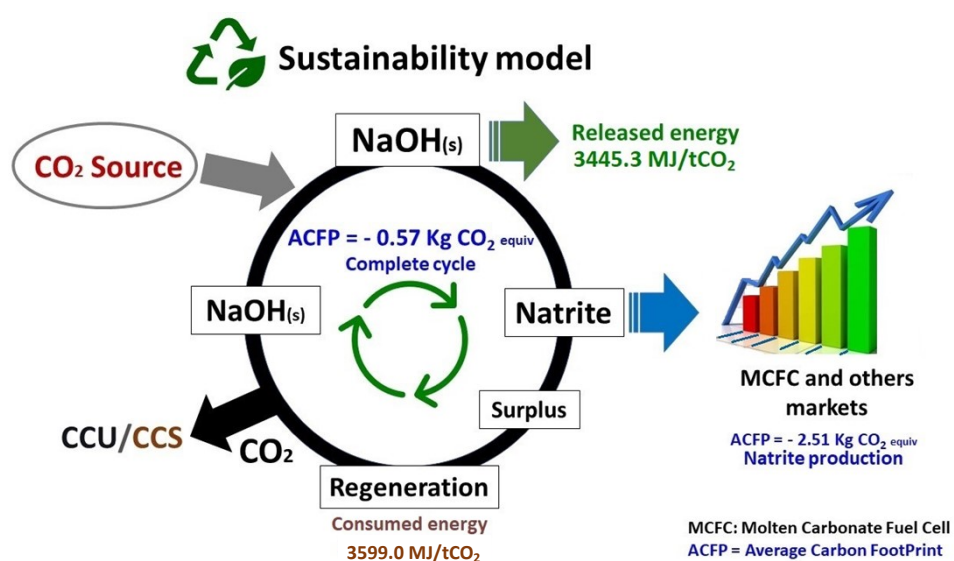


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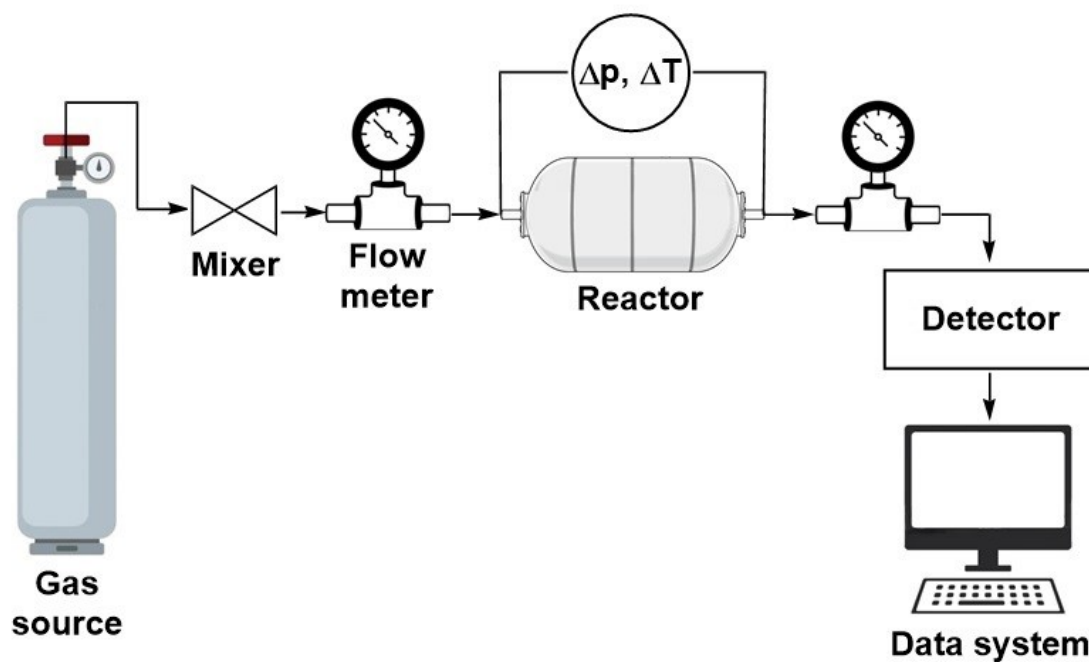


Figure S4. General scheme of the gas analyzing system Horiba-EnviroNics. The overall circuit is operated via the software CO2-REMO

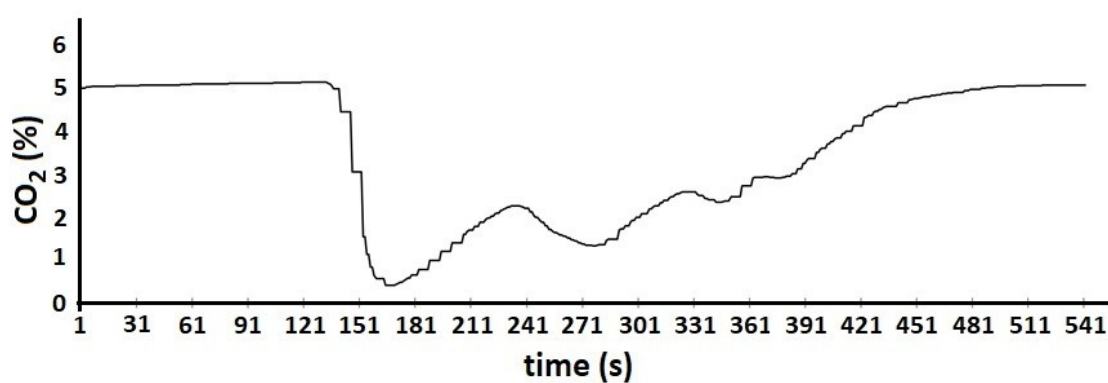


Figure S5. Stages of the study process in each round of capture. Stabilization of the gas source in 5% CO₂ and capture phase until saturation of chemical converter.

Table S1. Average DFTB values.

Parameters	Group 1	Group 2	Group 3
C–O distance (Å)	1.78 ± 0.10	1.79 ± 0.10	1.82 ± 0.12
Na–C distance (Å)	3.44 ± 0.15	3.40 ± 0.14	3.35 ± 0.14
Na–O distance (Å)	2.90 ± 0.14	2.88 ± 0.14	2.87 ± 0.14
CO ₃ ⁻ torsion	0.21 ± 0.19	1.01 ± 0.31	3.90 ± 0.40
Na charge (Mulliken)	$+0.81 \pm 0.13$	$+0.70 \pm 0.10$	$+0.65 \pm 0.10$
Na–CO ₃ ⁻ neighborhood	1.88 ± 0.14	1.85 ± 0.13	1.90 ± 0.15

Table S2. Carbon footprint estimation (kg CO₂ eq.)**S2.1. Na₂CO₃ Commercialization**

Item	Consumption	Carbon footprint unit	Carbon footprint
Avoided CO to atm.	-1.00 kg	1.000	-1.000
Green NaOH	1.25 kg	0.351	0.439
Avoided NaCO ₃	-1.77 kg	0.871	-1.542
Avoided Heat	-3.5 MJ	0.015	-0.050
Total			-2.153

S2.2 NaOH regeneration

Item	Consumption	Carbon footprint unit	Carbon footprint
Avoided CO to atm.	-1.00 kg	1.000	-1.000
Avoided NaOH	-1.25 kg	0.351	-0.439
Electricity	5.0 MJ	0.154	0.770
Heat	20.0 MJ	0.015	0.40
Total			0.269

Table S3. Energy footprint estimation.**S3.1. Na₂CO₃ Commercialization**

Item	Consumption	Energy footprint unit	Energy footprint
Green NaOH	1.25 kg	5.01	6.27
Avoided NaCO ₃	-1.77 kg	9.08	-16.08
Total			-9.81

S3.2 NaOH regeneration

Item	Consumption	Energy footprint unit	Energy footprint
Avoided NaOH	-1.25 kg	5.01	-6.27
Electricity	5.0 MJ	1.25	6.25
Heat	20.0 MJ	0.39	7.80
Total			7.78

Table S4. Operating Cost.

S4.1. Na₂CO₃ Commercialization.

Item	Consumption	Cost per unit (€)	Result Cost (€)
Green NaOH	1.25 kg	0.535	0.438
Avoided NaCO ₃	-1.77 kg	0.368	-0.651
Avoided Heat	3.5 MJ	0.009	-0.025
Total			-0.237

S4.2. NaOH regeneration.

Item	Consumption	Cost per unit (€)	Result Cost (€)
Electricity	3.0 MJ	0.10	0.30
Heat	20.0 MJ	0.009	0.14
Total			0.44