Systems & Control Transactions

Research Article - Peer Reviewed Conference Proceeding
ESCAPE 35 - European Symposium on Computer Aided Process Engineering
Ghent, Belgium. 6-9 July 2025
Jan F.M. Van Impe, Grégoire Léonard, Satyajeet S. Bhonsale,
Monika E. Polańska, Filip Logist (Eds.)

PSE PRESS

Multiscale analysis through the use of biomass residues and CO_2 towards energetic security at country scale via methane production

Guillermo Galán[a], Manuel Taifouris[a], Mariano Martín[a]*, and Ignacio E. Grossmann[b]

[a] University of Salamanca, Department of Chemical Engineering, Salamanca, Salamanca, SPAIN
[b] Carnegie Mellon University, Department of Chemical Engineering, Pittsburgh, PA, U.S.A.
* Corresponding Author: mariano.m3@usal.es.

ABSTRACT

The growing demand for sustainable energy has driven research into renewable methane production to reduce greenhouse gas emissions and reliance on fossil fuels. Promising feedstocks include lignocellulosic dry residues, wet waste, and captured CO_2, converted via gasification, anaerobic digestion, and synthetic processes with renewable hydrogen. This study uses a multiscale approach to compare these sources, incorporating a techno-economic evaluation to identify key performance indicators (KPI) for facilities and renewable energy sources. A facility location problem (FLP) determines plant locations and production capacities, considering material availability and transportation costs. The analysis focuses on the decentralised use of wastes and CO_2 from point and diluted sources across Spain, employing an MILP model to optimise waste and CO_2 utilisation alongside solar and wind energy systems. Results highlight lignocellulosic dry waste and CO_2 captured with MEA from point sources as the most promising options. Sensitivity analysis predicts methane prices between 13.028 €/MWh and 47.216 €/MWh through 2050, requiring substantial investment for full methane self-sufficiency. With carbon taxes, the price could drop to 10.735 €/MWh by 2050, competitive with current natural gas prices.

Keywords: DAC, electrolysis, green hydrogen, synthetic natural gas, strategic CO_2 and biomass waste valorisation, methane production and distribution

1. INTRODUCTION

Industrial and transportation growth has increased atmospheric CO_2 levels from 300 ppm in the late 19th century to 425 ppm in 2024, contributing to a 1°C global temperature rise [1]. The 2015 Paris Agreement aims to limit warming to 1.5°C, reducing emissions by 55% by 2030 and achieving net zero by 2050 [2].

Meeting these targets requires transitioning to decarbonised energy systems, especially in the energy and chemical sectors. Geopolitical disruptions, mainly the Ukraine conflict, highlight Europe's energy vulnerabilities, emphasising the need for self-reliant solutions. Synthetic methane production offers a promising route to energy resilience and reduced fossil fuel dependence. The CO_2 capture methods include biomass growth, which absorbs CO_2 naturally and engineered systems that capture emissions from industrial sources and the atmosphere. Biomass can be used to produce bioethanol, DME, methanol [3], and biodiesel, but challenges such as land, water, and fertiliser limit its scalability. Dry wastes such as lignocellulosic raw material are used via gasification to produce synthetic biomethane. Manure, municipal solid waste (MSW), and sludge are processed via anaerobic digestion to produce biogas and biomethane [4], though logistics and environmental issues reduce efficiency, leading to landfill or incineration. Carbon capture, utilisation, and storage (CCUS) technologies are crucial for meeting climate targets by capturing CO_2 from industrial sources for storage or conversion. Methods such as physisorption and amine-based chemisorption face challenges in capturing ambient CO_2 due to high energy demands. Direct air capture (DAC) technologies, such as alkaline solutions and BPMED, show promise, especially when combined with renewable hydrogen to produce methanol or synthetic methane [5].

Current research often addresses processes separately from biomass supply chain optimisation, MSW-to-liquid-fuel, and biogas and CO_2 utilisation, but few integrate waste, biomass, and CO_2 for synthetic methane production [6]. This study fills this gap by offering a multiscale framework to enhance energy security, using an extended Facility Location Problem (FLP) is formulated as a Mixed-Integer Linear Programming (MILP) across 356 Spanish shires to optimise waste utilisation into methane, integrating various feedstocks and technologies for sustainable energy independence.

2. METHODOLOGY

This work evaluates renewable resources and biowastes, such as lignocellulosic waste, manure, MSW, sludge, and captured CO_2, to reduce fossil fuel dependence. It optimises waste treatment, CO_2 capture, hydrogen electrolysis, and methane production, relying on decentralised utilisation powered by PV and wind energy [6].

2.1. Process level analysis

This section depicts technologies for waste management, CO_2 capture, and methane conversion, focusing on waste recovery, gasification, digestion, hydrogen production, and renewable energy harvesting.

2.1.1. Waste treatment technologies

Gasification: This process converts lignocellulosic waste into syngas for biomethane production using an indirect gasifier-combustor. H_2S is removed with ZnO, and methanation produces biomethane, refined by PSA to reduce CO_2 to 2% [7].

Anaerobic digestion: This technology processes high-water-content biowaste to produce biogas, upgrading it to biomethane with H_2S, CO_2, NH_3, and H_2O removal [7].

2.1.2. CO_2 capture technologies

Point sources: CO_2 is captured using aqueous amine solutions (MEA) at 25-30°C and partial pressures over 0.05 bar, achieving 90-95% removal at 0.1 bar, with a 20% MEA concentration.

Diluted sources: CO_2 is captured from the air via DAC technology. Fans pass air through KOH-based solutions, where KOH converts CO_2 into HCO_3^- and CO_3^{2-} ions. KOH is regenerated with $Ca(OH)_2$, producing $CaCO_3$, which is dried and calcinated with biogas to regenerate $Ca(OH)_2$[6].

2.1.3. Electrolytic hydrogen production

Green hydrogen is produced via water electrolysis using solar or wind power, and purified by condensation, deoxygenation, and zeolite dehydration.

2.1.4. Energy harvesting

Wind energy: A GE 1.5sle turbine with a nominal power of 1,500 kW is considered. Installation costs in 2022 are 1,600 €/kW, and operating costs are 0.026 €/kWh. CO_2 emissions are 0.012 $kgCO_2$/kWhe.

Solar energy: PV panels generate power, with each 4 m² panel producing 1 kW peak (kWp) at 25% efficiency (η_{PV}). The total panel surface reaches up to 7 m² due to installation needs. In 2022 costs are 1,050 €/kWp and 0.042 €/kWh, with CO_2 emissions of 0.048 $kgCO_2$/kWhe.

2.1.5. Methane synthesis

e-Methane is produced from CO_2 via methanation using renewable hydrogen and captured CO_2 at 1-30 bar and 140°C-350°C. Synthetic biomethane is obtained from syngas methanation, while biomethane comes from biogas upgrading. Purification achieves over 95% methane purity.

2.2. Process technologies surrogate modelling and process scale-up

The formulation of the FLP requires surrogate input-output models for the waste processing technologies, including manure, 63-368 kt/year, MSW, 20-53 kt/year, and lignocellulosic biomass, 10-820 kt/year, with corresponding CAPEX and OPEX. Up to 50 designs are modelled, yielding 0.012, 0.070, and 0.285 $kg_{Biomethane}$/kg [7].

The CO_2 capture modelling includes yields, energy requirements, and linearised CAPEX and OPEX for MEA and conventional DAC systems. CAPEX and OPEX follows Sinnott's methodology, excluding waste disposal. Auxiliary costs (steam, water, energy) are based on mass and energy balances. CAPEX includes equipment sizing for compressors, heat exchangers, filters, and cyclones.

2.3.1. Description of resources

The extended FLP model includes CO_2 capture, biomass availability, and processing methods across 356 Spanish shires, limiting surface use by up to 2%. It prioritizes PV panels for renewable power. Gasification processes dry lignocellulosic biomass, while wet wastes require anaerobic digestion. CO_2 emissions, measured in kt_{CO_2}/year, include industrial, agricultural, livestock, and transport sources using MEA and DAC systems. Solar and wind availability are based on annual averages of solar irradiance, and wind velocity.

2.3.2. Formulation of the FLP problem

Each shire is defined by its capital city's latitude and longitude, evaluating CO_2 capture, sun and wind availability, and shire area for PV panels, considering:

1. Biowaste, CO_2 captured from point and diluted sources using MEA solutions and DAC technology, solar radiation and wind velocity data, and land availability to

build infrastructures.

2. Surrogate models using first principles such as mass and energy balances, thermodynamic equilibrium and correlations based on predicting yield, production, and costs for CO_2 capture, renewable energy, biomass gasification, anaerobic digestion, hydrogen production, and methane synthesis, estimating performance and costs, such as CAPEX and OPEX, based on the last processes facility capacities.

3. Network modelling for biomass, CO_2, and hydrogen transportation between production sites and processing installations, optimising the use of decentralised resources to reduce transportation costs.

4. An objective function to maximise CO_2 usage within the budget, minimising network costs. The objective is to maximise the CO_2 captured within the assigned budget, focusing on minimising network costs through the integration of transportation, processing, and renewable energy generation.

Key variables include selecting biomass and CO_2 sources, facility capacities, and locations for CO_2 capture, hydrogen, and renewable energy production.

2.3.3. Resolution method and limitations

The resolution method optimises resource integration and cost efficiency, starting with a process-level analysis of waste treatment, CO_2 capture, hydrogen production, and energy generation. This is expanded into a multiscale framework that integrates different levels of analysis: a process-level evaluation, which assesses technologies and costs; a resource availability analysis, which considers the spatial distribution of biomass, waste, and CO_2 sources; and a country-level optimisation scale, which determines the optimal locations for facilities based on economic and geographic constraints. The FLP is formulated as an MILP model to optimise facility locations and costs, ensuring decentralised production and strategic energy security. Limitations include data availability, uncertainties in technology performance, and external factors like legislative changes, which may impact technology deployment and require further investigation.

3. CASE STUDY

3.1. General settings, constraints, and assumptions of the case study

The FLP optimisation model is formulated analysing 356 Spanish shires. It considers 29,900 kt/year of dry waste, 121,400 kt/year of manure, 9,500 kt/year of MSW, 3,400 kt/year of sludge, and CO_2 emissions from human activities, totalling 93,327 kt_{CO_2}/year and 102,250 kt_{CO2}/year, from point and diluted sources. Renewable energy data is sourced from Sun and Wind Atlas. The MILP considers a 10,195 M€ MITECO budget, 23,911 equations, and 91,192 variables, and is solved using CPLEX.

3.2. Working data, parameters, variables, and evolution over the time horizon

The study analyses waste availability in 2022, 2030, and 2050, with Spain's population of 50–60 million stabilising waste generation through improved consumption, ensuring consistent synthetic biomethane and biogas production. CO_2 availability is based on 2022 data, assuming constant emissions despite policy cuts. By 2050, CAPEX for PV panels drops from 1,050 to 297.8 €/kWp, and wind turbines from 1,600 to 1,138.7 €/kW. OPEX falls for PV from 0.042 to 0.009 €/kWh and wind turbines from 0.026 to 0.013 €/kWh. Synthetic methane production integrates CO_2 capture, water use, H_2 and O_2 generation, while carbon taxes rise to 180 €/t_{CO_2}.

4. RESULTS AND DISCUSSION

This section analyses decentralised methane production from lignocellulosic waste, manure, MSW, and CO_2, focusing on costs in MITECO's 2020–2050 budgets. It assesses CAPEX and OPEX, a sensitivity analysis on infrastructure, prices, and carbon tax credits, as well as limitations like data gaps and legislative uncertainty.

4.1. Analysis of current state: Year 2022

4.1.1. Use of the different waste materials, CO_2 capture, and use

Without a carbon tax, synthetic bio-methane and bio-methane are produced using 26,702 kt/year of lignocellulosic dry biomass, 83,070 kt/year of manure, and 7,775 kt/year of MSW. Waste treatment needs 11,174 M€ as investment and 5,341 M€/year in operating costs. The optimal scenario prioritises lignocellulosic dry waste for its high yield, especially in river-adjacent regions like the Duero, Ebro, and Guadalquivir (Figure 1a). Manure and MSW contribute 2,750 kt/year and 1,790 kt/year of biomethane, respectively. Shires where manure is used are shown in Figure 1b, but sludge is excluded due to its moisture content [7]. CO_2 capture reaches 5,858 kt/year, below previous estimates of 10,000–12,500 kt/year [6]. MEA solutions, chosen for low costs, are used in northern Spain and the Balearic Islands. Carbon taxes phase out manure and MSW, cutting costs by over 50%.

4.1.2. Production of renewable energy

The system requires 147 km² of PV panels, approximately 2% of Spain's available area, and 2,465 wind turbines. Combined, investment and operating costs reach up to 28,020 M€ and 2,430 M€/year, generating 7.3 GW, over 6% of Spain's 2022 electricity output. PV panels are prevalent in southeastern Spain, with wind turbines in coastal and mountainous regions (Figures 1e and 1f). With

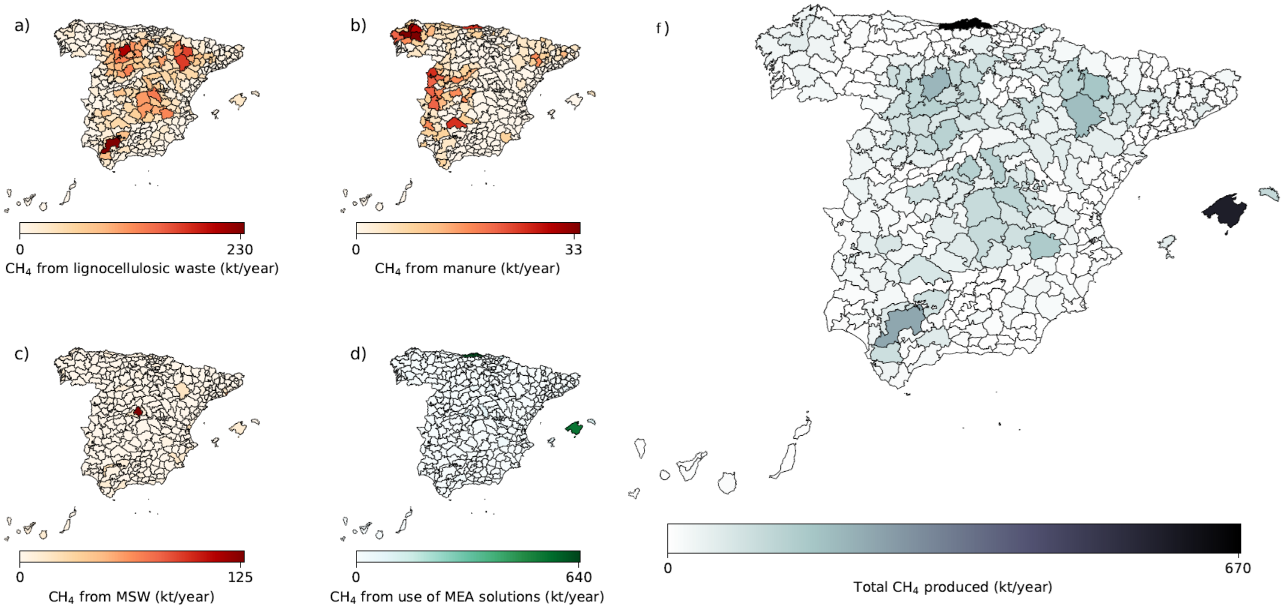

Figure 1. Distribution of lignocellulosic dry waste (a), manure (b), MSW (c), sludge (d), and methane production (f) by shires in Spain in 2022, without carbon tax.

a carbon tax, synthetic methane demand doubles the PV panel area to 290 km², representing an increase of almost 100%, while turbine numbers remain stable. Costs rise to 49,355 M€ and 4,282 M€/year, with energy output growing to 12.4 GW. PV panel deployment expands, but turbine locations remain unchanged.

4.1.3. Methane production

Synthetic methane production requires 3 kg_{CO_2}/kg_{CH_4} and 0.41 kg_{H_2}/kg_{CH_4} [6]. Without carbon taxes, Spain produces 11,104 kt/year of renewable methane, covering nearly 46% of national consumption in 2022 [7]. Synthetic biomethane comes mainly from lignocellulosic waste, 7,610 kt/year. Investment and operating costs are 14,440 M€ and 5,900 M€/year. Hydrogen needs are 805 kt_{H_2}/year, costing 3,202 M€ and 304 M€/year. With a carbon tax, lignocellulosic waste generates 7,610 kt/year of biomethane, 31.5% of consumption, and synthetic methane rises to 3,300 kt/year, with total methane production reaching 10,910 kt/year and costs dropping to 11,989 M€ and 3,284 M€/year.

4.1.4. Evolution of self-sufficiency methane percentage, and methane prices

In 2022, methane self-sufficiency without carbon taxes is 30.7%, with lignocellulosic waste contributing 25% of the budget. MEA solutions raise self-sufficiency to 42.9% at 300%, with full self-sufficiency needing 410.4% and methane prices reaching 124.69 €/MWh. With a carbon tax, CO_2 capture accelerates, favouring MEA. Lignocellulosic waste provides 31.5% self-sufficiency at 15% of the budget, while MSW replaces manure at 125%, adding 2.1%. Full self-sufficiency requires four times the budget, reducing methane prices to 100.35 €/MWh. By 2030 and 2050, MEA and DAC reduce prices and self-sufficiency.

4.1.5. Environmental impact of energy generation: CO_2 emissions, minerals required, and water use

Among renewable sources, PV panels emit 2,325 kt_{CO_2}/year and wind turbines 188 kt_{CO_2}/year, contributing 1.19% and 0.10% to Spain's 2022 CO_2 emissions. PV panels are preferred for cost-effectiveness, requiring 55,759 t of minerals, accounting Cu, Ni, Mn, Cr, Mo, Zn, Rare Earths, Si. Mineral extraction emits 321 kt_{CO_2} for PV and 86 kt_{CO_2} for wind, totalling 2,646 kt_{CO_2}. Water usage is $1.6 \cdot 10^7$ m³/year for PV, $6.7 \cdot 10^5$ m³/year for wind turbines, and $7.3 \cdot 10^6$ m³/year for hydrogen production. A carbon tax boosts PV panel deployment, increasing emissions from mineral extraction and resource demands. Mineral needs rise to 90,077 t of minerals. The CO_2 emissions reach 5,051 kt_{CO2} for PV and 273 kt_{CO2} for wind turbines. Water use is up to $3.06 \cdot 10^7$ m³/year for PV.

4.2. Analysis of the future status: Years 2030 and 2050

4.2.1. Use of the different waste materials, CO_2 capture, and its use

By 2030, lignocellulosic dry waste will produce 25,292 kt/year of synthetic biomethane, a 5.28% decrease from 2022 due to lower technology costs and improved efficiency (Figure 2a). Investment and operating costs will drop to 5,604 M€ and 1,826 M€/year, a reduction of 49.84% and 65.81%, excluding manure and MSW (Figures 2b, 2c). Point sources will emit 29,378 kt_{CO_2}/year, increasing by 400% with lower costs and efficiency gains (Figure 2d). Spain's carbon tax of 150 €/t_{CO_2} will reduce lignocellulosic waste use to 20,328 kt/year, lowering costs to 3,688 M€ and 1,130 M€/year, while MEA solutions capture 32,231 kt_{CO_2}/year (Figure 2d).By 2050, lignocellulosic waste use will drop to 24,052 kt/year, with costs at 5,044 M€ and 1,591 M€/year. With a 180 €/t_{CO_2} tax, waste use will fall to 2,719 kt/year, and MEA will capture 42,258 kt_{CO_2}/year (Figure 2d).

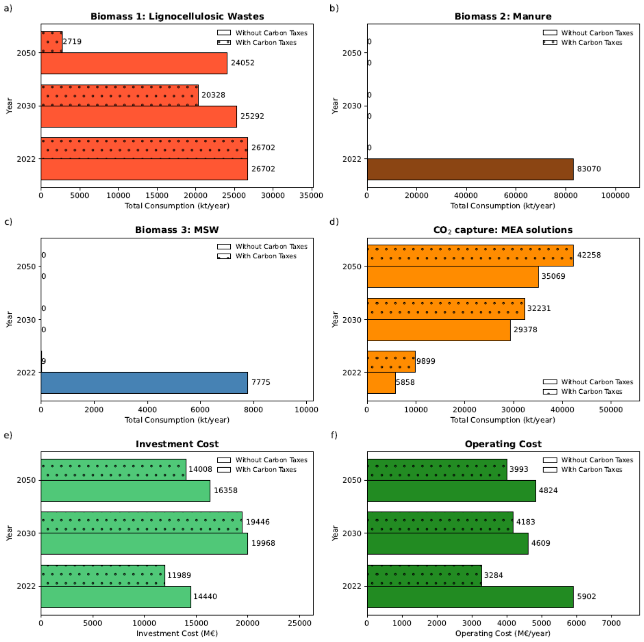

Figure 2. se of Lignocellulosic dry waste (a), manure (b), MSW (c), MEA CO_2 capture (d), total investment (e) and total operating costs (f) for 100% methane self-sufficiency, without and with carbon taxes, 2022, 2030, 2050.

4.2.2. Production of renewable energy

By 2030, energy production will rely on PV panels across Almería, the Canary Islands, and central regions, covering 1,042 km², up from 147 km² in 2022 (Figure 3a). Investment and operating costs will reach 59,956 M€ and 2,892 M€/year, generating 36.7 GW (Figures 3b–3d). A carbon tax boosts synthetic methane production to 40.2 GW, concerning 2022 levels, at costs of 65,910 M€ and 3,173 M€/year (Figures 3b-3d). By 2050, PV panels will cover 1,511 km², generating 52.8 GW at 64,280 M€ (Figures 3a–3c).

4.2.3. Methane production

By 2030, synthetic biomethane production will focus on gasifying lignocellulosic dry waste and synthesising methane from CO_2 captured via MEA solutions, excluding anaerobic digestion. Output will be 7,208 $kt_{Biomethane}$/year, a 5.29% decrease from 2022. Methane consumption will drop to 18,990 kt_{CH_4}/year [6], with synthetic production rising to 9,793 kt_{CH_4}/year. Costs will total 19,968 M€ and 4,609 M€/year (Figures 2e, 2f). By 2050, lignocellulosic waste use will decrease by 9.93%, producing 6,855 $kt_{Biomethane}$/year. Domestic methane consumption will drop to 13,815 kt_{CH_4}/year [6], while synthetic methane rises to 11,690 kt_{CH_4}/year. Costs will total 16,359 M€ and 4,824 M€/year (Figures 2e, 2f).

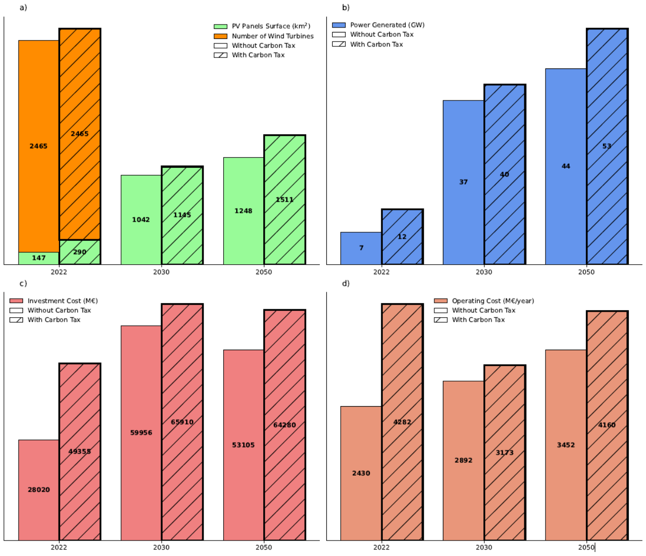

Figure 3. PV panel surface, wind turbines (a), power generation (b), investment (c) and operating costs (d), without and with carbon taxes, 2022, 2030, 2050.

4.2.4. Evolution of self-sufficiency methane percentage, and methane prices

By 2030, lignocellulosic dry waste and MEA solutions will remain key for cost efficiency. Methane prices, excluding carbon tax, will rise to 17.545 €/MWh when employing lignocellulosic dry waste. Once lignocellulosic dry waste is depleted, MEA solutions for CO_2 capture begin to be used until a methane price of 53.547 €/MWh is reached. However, at 100% budget utilisation, the price drops to 43.170 €/MWh. At 300% budget use, lignocellulosic waste will provide 38% of methane self-sufficiency. Carbon taxes will benefit synthetic methane over biomethane, with prices potentially dropping to 23.336 €/MWh. By 2050, advancements will favour MEA solutions. Without a carbon tax, methane will cost 17.545 €/MWh, with MEA solutions at 47.214 €/MWh. At 100% budget utilisation, methane costs 39.577 €/MWh, 40.12% lower than in 2022. Methane self-sufficiency will be achieved with 66.7% of the budget at 35.171 €/MWh, with prices dropping to 12.540 €/MWh at 100% budget use.

4.2.5. Environmental impact of energy generation: CO_2 emissions, minerals required, and water use

By 2030, PV panels will be the main energy source, emitting 6,427 kt_{CO_2}/year, with 2,095 kt_{CO_2} from mineral extraction, accounting for 29% of CO_2 captured by MEA solutions, 29,378 kt_{CO2}/year. Mineral requirements are $2.50 \cdot 10^5$ t, accounting for Cu, Ni, Zn, Si. PV panels use $1.06 \cdot 10^8$ m^3/year of water, 0.19% of Spain's capacity, while hydrogen production uses $3.64 \cdot 10^7$ m^3/year. Carbon taxes increase PV emissions to 7,052 kt_{CO_2}/year, contributing 29% of CO_2 captured by MEA solutions. By 2050, expanding PV panels will raise emissions, mineral demand, and water usage. PV panels emit 3,836 kt_{CO_2}/year, with 2,501 kt_{CO_2} from mineral extraction, totalling 6,337 kt_{CO_2}/year, or 18.07% of CO_2 captured by MEA solutions, 35,069 kt_{CO2}/year. Mineral needs reach $2.98 \cdot 10^5$ t, and water use rises to $1.27 \cdot 10^8$ m^3/year.

5. CONCLUSIONS

This study examines large-scale renewable synthetic methane production from biomass gasification, anaerobic digestion, and CO_2 hydrogenation using green hydrogen. Gasification processes lignocellulosic dry waste, while anaerobic digestion whereas manure, MSW, and sludge, upgrading biogas to biomethane and producing synthetic methane using CO_2 captured from point and diluted sources.

Lignocellulosic dry waste gasification is the most efficient due to its high yield and low moisture content. CO_2 capture from point sources is preferable to DAC, potentially reducing Spain’s industrial emissions by half. A land-use analysis considers decentralised deployment across 356 shires, allocating 2% for PV and wind turbines. By 2050, expanded capacity will ensure energy for CO_2 capture and hydrogen production.

Economic integration of lignocellulosic waste gasification with MEA-based CO_2 capture shows a potential 134.2% natural gas substitution. Investment costs in waste treatment, CO_2 capture, and power generation are projected to decrease, with cumulative costs of 14,008 M€ and 64,000 M€ by 2050.

Synthetic methane production will grow, with emission reductions between 49.8% and 59.6%. The integration of waste treatment, CO_2 capture, and hydrogenation offers a promising path for defossilising the energy sector, requiring strategic investments and policies.

ACKNOWLEDGMENTS

The authors are thankful to the PSEM3 GIR group at USAL and the CAPD at CMU. Fellowship received from the Spanish Government. This work was supported by the Regional Government of Castilla y León (Junta de Castilla y León) and by the Ministry of Science and Innovation MICIN and the European Union NextGenerationEU / PRTR (H2MetAmo project - C17.I01.P01.S21).

REFERENCES

1. NASA, 2024. Carbon Dioxide. Direct measurements, 1958-Present. https://climate.nasa.gov/vital-signs/carbon-dioxide/?intent=121
2. European Commission, 2020. Climate Action. 2030 Climate Target Plan. https://climate.ec.europa.eu/eu-action/european-green-deal/2030-climate-target-plan_en
3. Martín M, Grossmann IE. Optimal simultaneous production of i-butene and ethanol from switchgrass. *Biomass Bioenergy*. 61: 93–103 (2014) https://doi.org/10.1016/J.BIOMBIOE.2013.11.022
4. Sampat AM, Hicks A, Ruiz-Mercado GJ, Zavala VM. Valuing economic impact reductions of nutrient pollution from livestock waste. *Resources, Conservation and Recycling*. 164: 105199 (2021) https://doi.org/10.1016/j.resconrec.2020.105199
5. Gupta S, Li L. The Potential of Machine Learning for Enhancing CO_2 Sequestration, Storage, Transportation, and Utilisation-based Processes: A Brief Perspective. *JOM*. 74: 414–428 (2022). https://doi.org/10.1007/s11837-021-05079-x
6. Galán G, Martín M, Grossmann IE. Multiscale analysis for the utilisation of CO_2 towards the production of chemicals at the country level: Case study of Spain. *J Clean Prod.* 47: 140551 (2024) https://doi.org/10.1016/j.jclepro.2023.140551
7. Taifouris M, Martín M. Towards energy security by promoting circular economy: A holistic approach. *Appl Energy*. 333: 120544 (2023) https://doi.org/10.1016/j.apenergy.2022.120544

© 2025 by the authors. Licensed to PSEcommunity.org and PSE Press. This is an open access article under the creative commons CC-BY-SA licensing terms. Credit must be given to creator and adaptations must be shared under the same terms. See https://creativecommons.org/licenses/by-sa/4.0/