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Long-term stochastic modelling and economic assessment of a centralised CCU network☆

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HIGHLIGHTS

- Country-wide implications of deploying centralised CCU were stochastically evaluated.
- Cost of CO2 abatement (10th–90th percentile) is between 800 and 1121 €/tonne CO2.
- The rate of installation of electrolysers is the most important driver for costs.
- Portugal's energy system does not achieve 0 natural gas imports by 2050 without CCU.

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ABSTRACT

An Energy System Model (ESM) was developed to evaluate, under uncertainty, the net present value (NPV) and Greenhouse Gas (GHG) Emission abatement potential of centralised e-methane production in Portugal between 2030 and 2070. It is the first article to adopt a stochastic, simulation-based approach rather than an optimisation approach to study the effects of Carbon Capture and Utilisation (CCU) networks within ESM.

The model, called "Long-term Uncertainty Stochastic Outlook" (LUSO) was developed using a top-down approach in the Low Emissions Analysis Platform (LEAP) software. The electricity, industrial, transport, residential, and services sectors were modelled simultaneously, with hourly-resolved load curves of 192 time slices. Fourteen variables were varied stochastically across 1300 runs. The sensitivity of NPV and GHG Emission Abatement results to the fourteen variables was analysed using both tornado charts and multivariable linear regression.

Results show that centralised e-methane production in Portugal is not economically viable and would yield limited emission-reduction benefits if current historical trends in key macroeconomic variables are maintained. The NPV (at a 4% discount rate), cumulative GHG emissions avoided, and NPV/CO_2 avoided (10th to 90th percentile ranges) vary, respectively, between −60 to −46 B€, 46 to 69 Mt. CO_2 eq, and from 800 to 1121 €/tonne CO_2.

Future work should add technical depth, using recursive calculations to better represent macroeconomic variables like GDP and its link to energy demand. It could also develop dynamic models of electric mobility and utility-scale storage, examining how their evolving demand and supply patterns interact with future electricity grids.

1. Introduction

The energy transition is essential to keeping global average temperatures within the 1.5 °C to 2 °C range above pre-industrial levels. However, uncertainty remains regarding both the relative effectiveness of the technological pathways and the appropriate timing for their implementation to achieve this goal. Although it is broadly acknowledged that clean energy investments must expand by approximately 1%

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of global GDP annually through 2030 [1], the optimal distribution of such capital across the various existing decarbonization vectors remains indeterminate.

One of the current potential decarbonisation vectors is the carbon capture and utilisation (CCU) technology. CCU uses hydrogen in combination with carbon dioxide captured from industrial point sources, biogas upgrading plants or directly from the atmosphere to produce, for example, a relevant product such as e-methane. *E*-methane can mitigate a large share of natural-gas-derived CO_2 emissions by enabling the substitution of fossil natural gas without changes to end-user or transport infrastructure. In 2021, these emissions amounted to 11 Mt. CO_2 in Portugal, making CCU a likely essential decarbonization pathway until 2050 in the view of policymakers [1].

Our previous analysis found that a centralised e-methane network with a production of 9.3 TWh would require annual subsidies of €3.4 billion between 2030 and 2055 to achieve breakeven with a 95% probability [2].This occurs during simultaneous optimization of both cost and environmental impacts associated with e-methane production. This substantial subsidy results from the significant gap between the current cost of e-methane (0.20–0.31 €/kWh) and that of fossil methane (0.06 €/kWh) [2]. The difference is primarily driven by the high cost of hydrogen, which accounts for roughly 90% of the total cost of producing e-methane via CCU [2]. The previously modelled CCU network was optimized, but a macroeconomic, top-down perspective on its inclusion in the Portuguese energy system remains unresolved. The beforementioned high subsidy requirement could be justified if the current decarbonization trajectory falls short of meeting the goals of the Paris Agreement and achieving carbon neutrality by 2050. It would also be justified if the cost of CO_2 abatement through alternative technologies or vectors exceeds the subsidy required to produce e-methane via CCU. These questions can only be meaningfully addressed through a comprehensive analysis of how the CCU network interacts with and integrates across other economic sectors. This is because the activity sectors that depend on natural gas—and, by extension, on the e-methane that would replace it—follow their own decarbonization pathways. These factors must be considered to fully assess the viability of investing in e-methane through CCU.

Decarbonisation via CCU can be analysed using Energy System Models (ESMs). ESM are closed systems, mathematically formulated, that balance the interactions among energy consumption, production, and transformation across several economic sectors as a function of multidimensional variables related to technology, the economy, policy, and climate [3]. These models are typically developed over time horizons spanning from 20 to 50 years [4] and are designed to orchestrate multiple pathways that facilitate systemic transformations in societal energy production and consumption. Their results aim at informing policy-makers on the requirements to achieve climatic goals and their implications [5] and have been used in regional energy planning in the European Union. For example, they are at the foundation of Portugal's National Energy and Climate Plan, which outlines the necessary steps to achieve energy transition goals over the next 10 years [6].

Examples of ESM applications in CCU are presented in Table S-1. Their analysis reveals that ESMs are typically implemented in a deterministic manner, relying on single long-term projections of key parameters to inform their energy planning decisions [7]. Uncertainty in these forecasts is usually handled through scenario analysis, where “what-if” narratives are explored to analyse long-term policies [8] [9] [10] [11] [12] [13] [14] [15] [16]. Such an approach cannot fully anticipate actual developments in energy systems and is too limited to capture the full range of possible model outcomes. An example of such a limitation is demonstrated by a US EIA study, which found industry final energy demand ranging from −40 to 31% when performing deterministic forecasts [7]. This is because the study failed to accurately account for the evolution of demand, market price dynamics, and consumer responses to the technical landscape across end-use activity sectors.

Secondly, ESM are generally modelled as optimisation problems, where, for instance, the objective function is set as the minimisation of total energy costs [9] [10] [11] [13] [14] [15] or emissions [17], or a combination of these by taking into account the maximization of profits by energy producers [8]. An emission mitigation target is usually imposed as a model constraint (for example, carbon neutrality or 95% emission reductions by 2050) [8] [12] [16]). This forces the ESM to converge on a future state of the energy system that meets those requirements, despite potential incompatibility with stakeholder expectations [4]. Finally, optimisation makes the models extremely sensitive to user-input parameters and/or constraints, leading to results that vary significantly across similar case studies. For example, Bardon et al. (2025) highlighted that results from ESM models by different authors for projected GHG emissions in the global aviation industry in 2050 ranged from 60 to 3391 Mt. CO_2 Eq. [17], due to different user assumptions and ESM modelling frameworks.

The third aspect concerns the difficulty of accounting for all aspects of the energy system and their relationships with society in a mathematical model, including market failures, unpredictable consumer behaviour, modelling/measurement errors, and even rebound effects. All this compromises the ability of any single ESM to predict the future state of the energy system [18] [19]. This underscores the importance of adequately incorporating uncertainty into the ESM to support robust policy planning [4] [18]. To address this, probabilistic projections are an option because they combine predictive thinking with in-depth uncertainty assessment and thus can provide greater accuracy than deterministic methods [19]. Nevertheless, only about one-third of ESM studies in recent years accounted for uncertainty [3], and none focused on CCU.

The existing national ESM, used for example for estimating the potential of CCU for decarbonisation in Portugal, as documented by Portugal's National Energy and Climate Plan and by the Portuguese Energy and Geology Directorate (Direção Geologia e Geologia) [6] [1] evidence the aspects mentioned before on the trends for the existing energy models. The ESM outcomes shown in the National Energy and Climate Plan (model so-called TIMES-PT) are deterministic results of cost-optimisation of the Portuguese energy system under two scenarios. Conversely, the study by the Directorate that developed the model JANUS, presents results for a deterministic, non-optimized scenario (CN50) which reflects the Directorate's agreed-upon vision of how the energy system should operate to meet legal decarbonisation targets while satisfying energy demand. These two approaches offer an opportunity to demonstrate the benefits of an alternative ESM approach for modelling the potential benefits of CCU.

To address current literature gaps, this work develops an exploratory stochastic simulation-based energy system model spanning 2022–2070 to produce e-methane via CCU by capturing CO_2 from industrial sources. No optimisation is performed. The results determine whether the net present value (NPV) and CO_2 emission avoidance associated with the hypothetical existence of a centralised e-methane production plant in Portugal are beneficial compared to its exclusion from the Portuguese energy decarbonisation strategy. Results will inform policymakers by providing probabilistic cost estimates of CO_2 abatement through CCU technology and insights into its absolute emission-reduction potential, thereby supporting decision-making amid uncertainty. The work's novelty lies in the stochastic assessment of centralised CCU deployment within a LEAP-based Energy System Model, having Portugal as a case study. To do so, different combinations of key macroeconomic and demographic variables likely to influence the outcomes of the ESM will be simulated together. By doing so, it is possible to capture all possible developments in the future national energy system under uncertainty and, in the end, inform on the likelihood of the economic feasibility of such an investment. Furthermore, the stochastic projections of these key variables (e.g., macroeconomic, technical, market-related, including, for instance, projected vehicle sales) are performed based on their recent trends and evolution.

This article is structured as follows: Section 2 describes the

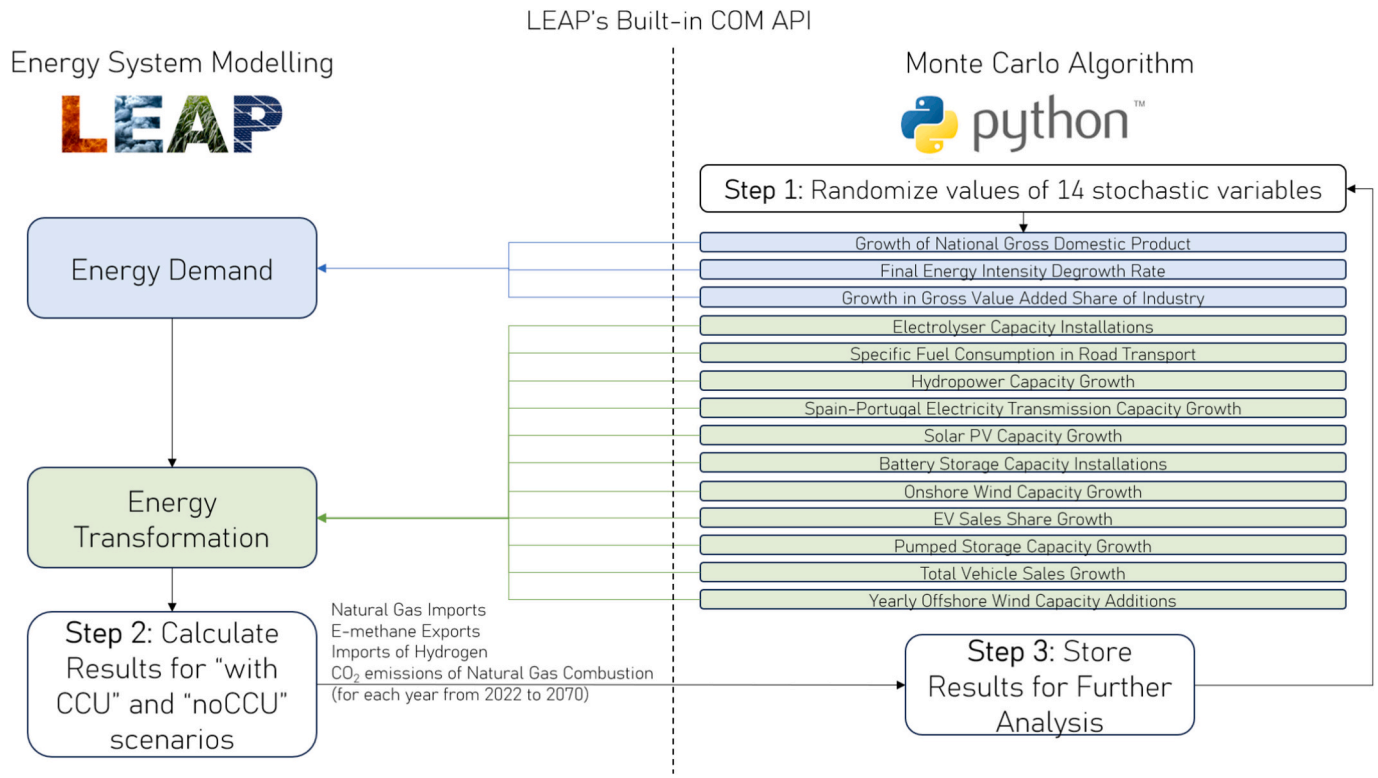


Fig. 1. Interaction between the ESM and the Monte Carlo algorithm developed in Python.

methodology, where the LEAP is used to model the national energy system and the modelled stochastic ESM with and without the CCU network used to produce e-methane. Section 3 presents results and discussion. It shows and compares the results obtained with those from the existing national reference ESM. This section discusses the implications of the results for a wide audience (e.g., scientists and policy-makers), overviews the viability of the CCU network and at the end identifies the limitations of the work. Finally, Section 4 draws the conclusions and provides recommendations for future work.

2. Methodology

This section outlines the development of the Energy System Model (ESM). This model, built using the LEAP software, is called Long-term Uncertainty Stochastic Outlook, or LUSO for short. The methodology section describes the use of LEAP to build the model structure (Section 2.1.), defines system boundaries (Section 2.2.), time resolution, and sector coverage, and presents the stochastic variables and equations applied (Section 2.3.). It also explains how energy demand and transformation processes are modelled (Sections 2.4. and 2.5.), and concludes with the method used to estimate Net Present Value (NPV) to assess the profitability of investing in a centralised CCU unit (Section 2.6.).

2.1. The LEAP software and the ESM structure

LEAP is a software tool for modelling energy systems that enables the estimation of pollutants from a wide range of energy and non-energy sources. It is a scenario-based software designed for medium- to long-term modelling, featuring an annual calculation time step with hourly temporal resolution [20]. This makes it well-suited for modelling renewable electricity generation and its relationship to sector-specific energy "load curves", which represent the share of total electricity consumption in each hour, enabling separation between night and day and between peak-to-peak power consumption [21]. It has been used by the Portuguese Energy and Geology Directorate to develop, for example, the National Hydrogen Strategy [22]. The present work uses the LEAP software version 2024.4.0.8 [23].

To perform stochastic energy system modelling in LEAP, it was necessary to develop a Python Monte Carlo script and integrate it with LEAP's built-in Component Object Model (COM) application programming interface (API). Fig. 1 shows the interaction between the ESM and the Monte Carlo algorithm, implemented in Python within the LEAP software.

The script performs multiple iterations of a repetitive task. In step 1, the script randomises the values of stochastic variables according to predefined distributions for each variable. These are then uploaded to LEAP to carry on the simulation. In step 2 and for each iteration, two simulations are performed – one where a centralised CCU is deployed ("with CCU"), and one where it is not ("no CCU"). In step 3, the simulation allows the calculation of the values needed to estimate the Net Present Value (NPV) and CO_2 abatement cost of CCU. These values include net imports of natural gas and hydrogen, exports of e-methane, and CO_2 emissions from natural gas combustion. The latter results from the built-in emission factors in LEAP withdrawn from the IPCC 6th Assessment Report [24]. The results obtained for a total of 1300 iterations were saved for further analysis.

2.2. ESM system boundaries

The ESM scope covers continental Portugal. It subdivides each year into 192 time slices (4 seasons, 2-day types – weekday and weekend, and 24 h each). Results are calculated and output at an annual timestep, spanning 2022 through 2070. The latter year represents the typical maximum time horizon used in a study—approximately 50 years into the future [14]. In addition, one objective of this work is to assess the potential benefits of synthetic methane production beyond the project's economic lifetime (25 years after 2030). Extending the analysis to 2070 ensures that the potential long-term benefits of the CCU network may

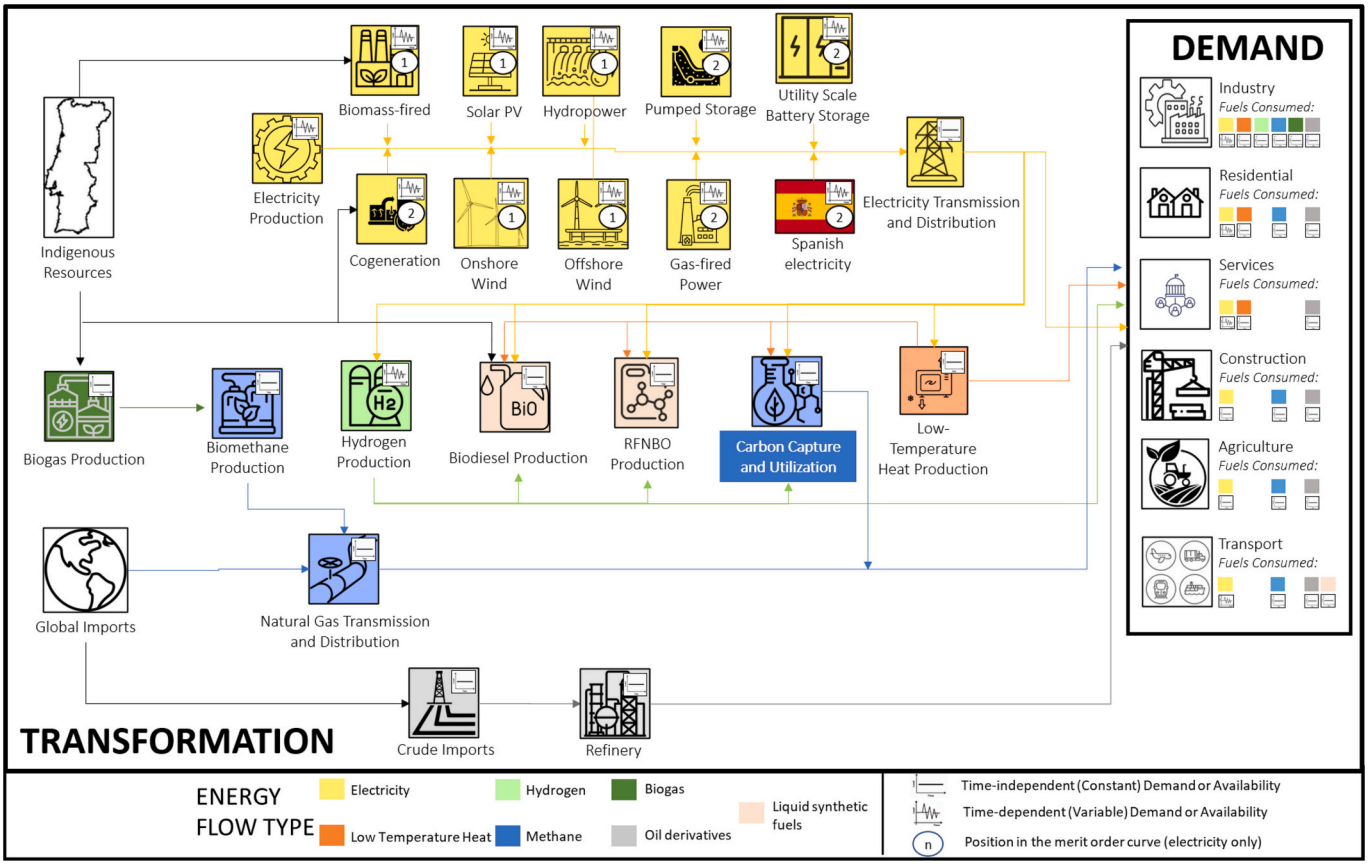


Fig. 2. System boundaries of the ESM. Details on each energy demand and transformation module are in Tables S-2 to S-6. For simplicity, the existing energy flows of natural gas from transmission and distribution to cogeneration and gas-fired power blocks are omitted, as well as the RFNBO and Biodiesel energy flows to the demand sector.

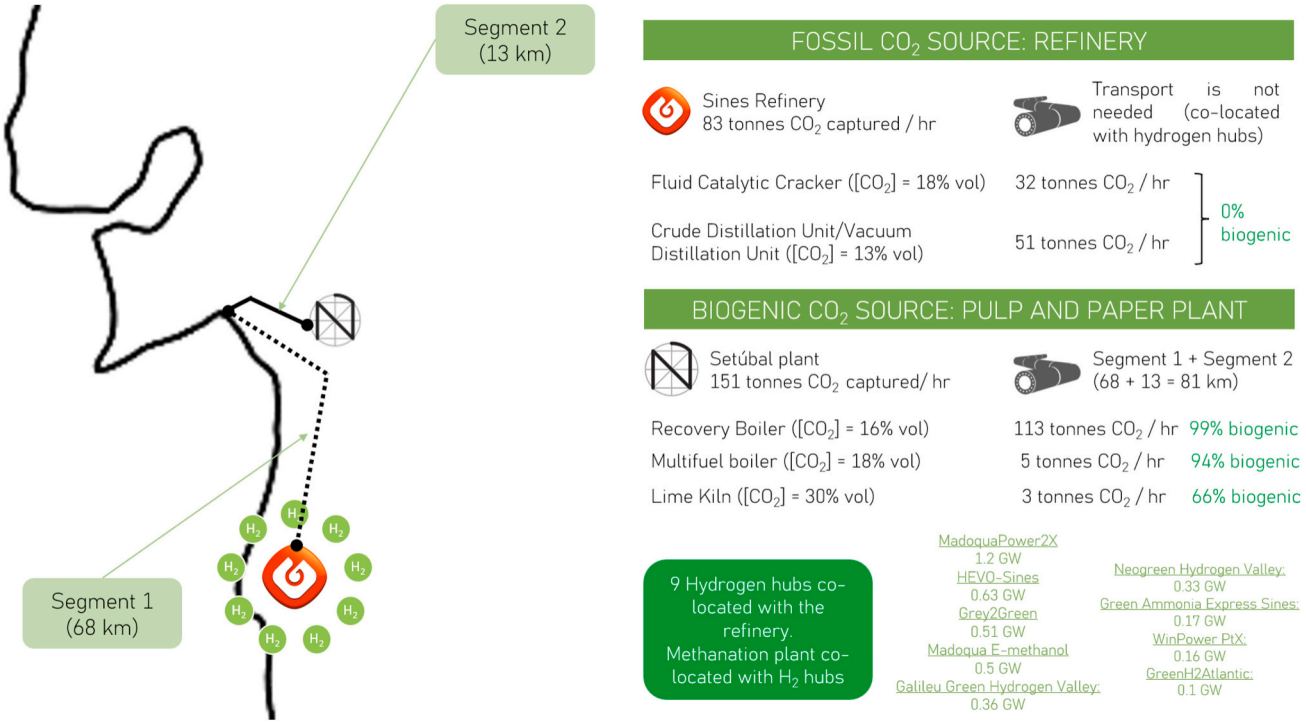


Fig. 3. Schematic of the CCU network in this work, result of a combined optimisation of costs and environmental impacts of e-methane, developed in previous work [2].

Table 1
Minimum, central and maximum values for the variables used in the stochastic analysis. Statistical distributions were assumed to be triangular for all cases except for annual offshore wind capacity.

Stochastic variable	Activity sectors affected	Minimum	Central	Maximum	Limit	Observations
Electrolyser Capacity Multiplier, $ECI_{multiplier}$, used to calculate electrolyser capacity in each year.	Energy Transformation[a]	0.08 (assumes that only 4% of the announced projects will be installed on their announced dates)	1 (assumes that 52% of the announced projects are installed (average between 4 and 100%)	1.92 (assumes that 100% of announced projects in Portugal will be installed on their announced dates)	N/A	Assumption for "Maximum" case - IEA Hydrogen Project Database [26] and public media announcements. Assumption for "Minimum" case: percentage of projects with FID or under construction today, 4% [27].
Final Energy Intensity Degrowth Rate (%/year), $FEI_{degrowth}$	Energy Demand[b]	−2.25%/year (trend 2000–2022)	−2.79%/year (trend 2015–2022)	−3.58%/year (trend 2019–2022)	N/A	Odysse-Mure data for aggregate Portuguese industry since 2000 until 2022 [28]
Growth in GVA Share of Industry (%/year), GVA_{growth}	Energy Demand[c]	−0.13%/year	0.06%/year	0.32%/year	N/A	Linear growth rates that match with the expectations in the Nacional roadmap for carbon neutrality for the GVA share of industry in 2050 [29]
Specific Fuel Consumption of Road Transport (MJ/100 km), SFC_{road}	Energy Demand	−20% of central values.	Weighted average fuel economy by power-train type.	+20% of central values	N/A	Fuel consumption based on the weighted average of the most sold vehicles in Portugal by brand and power-train type according to data from INE [30]. Parametric variation of ±20% adopted based on recommendations by Moret et al. [7].
Hydropower Capacity Growth (%/year), HPC_{growth}	Energy Transformation[d]	0.01%/year (trend 2018–2020)	1.89%/year (trend 2016–2018)	3.21%/year (trend 2018–2022)	9 GW	Monthly installed capacity data from Portuguese Transmission System Operator REN between 2015 and 2022 [31]
Spain-Portugal Electricity Transmission capacity growth (%/year), ETC_{growth}	Energy Transformation[e]	2.67%/year (trend 2016–2018)	4.36%/year (trend 2020–2022)	8.30%/year (trend 2010–2018)	N/A	Yearly data reported by ERSE for maximum interconnection capacity available for importing purposes between 2007 and 2022 [32].
Solar PV capacity growth (%/year), PVC_{growth}	Energy Transformation[f]	14.9%/year (trend 2016–2019)	25.9%/year (trend 2018–2022)	36.8%/year (trend 2021–2022)	77 GW	Monthly installed capacity data from Portuguese Transmission System Operator REN [31] between 2015 and 2022. Technical implementation limit from LNEG's "go-to areas" report [33].
GDP growth multiplier, used to calculate GDP in each year, GDP_{mult}	Energy Demand[g]	−0.4	0	0.7	N/A	Central GDP growth trajectory equal to LEAP's built-in IPCC SSP3 trajectory, the one which deviates the least from projections assumed by previous work by the National Energy and Climate Plan, the Directorate of Energy and Geology or the Roadmap for Carbon Neutrality.
Battery storage capacity installations (MW/year), BSC_{yearly}	Energy Transformation[h]	85 MW/year	141 MW/year	184 MW/year	N/A	The "central" case assumes the timely commissioning of the announced utility-scale battery storage projects and the calculated growth rate between 2025 and 2030 (Alcoutim BESS, BigBATT, Sol de Évora BESS, Graça do Divor BESS, Pego Cluster Storage, and PRR-awarded projects) [34] [35] [36] [37]. Minimum and Maximum growths calculated using a [−40%;+30%] range.
Onshore Wind Capacity Growth (%/year), ONW_{growth}	Energy Transformation[i]	0.84%/year (trend 2016–2019)	1.04%/year (trend 2019–2022)	1.47%/year (trend 2015–2022)	10.4 GW	Monthly installed capacity data from Portuguese Transmission System Operator REN [31] between 2015 and 2022. Technical implementation limit from the National Energy and Climate Plan [6].
EV sales share growth (%/year), EV_{growth}	Energy Transformation[j]	14.3%/year (trend 2020–2021)	27.4%/year (trend 2021–2022)	47.2%/year (trend 2016–2019)	100%	Historical values obtained from the crossing of data for total vehicles sold [38] and EV + PHEV sales [39] between 2012 and 2022.
Pumped Storage Capacity Growth (%/year), PSC_{growth}	Energy Transformation[k]	3.33%/year (trend 2016–2019)	5.53%/year (trend 2020–2022)	10.6%/year (trend 2015–2022)	3.9 GW	Monthly installed capacity data from Portuguese Transmission System Operator REN [31] between 2015 and 2022. Ceiling of 3.9 GW determined using the same ratio between maximum

(*continued on next page*)

Table 1 (*continued*)

Stochastic variable	Activity sectors affected	Minimum	Central	Maximum	Limit	Observations
Vehicle Sales Growth (%/year), VS_{growth}	Energy Transformation[l]	3.21%/year (trend 2020–2022)	4.87%/year (trend 2012–2022)	13.6% (trend 2012–2018)	N/A	and existing capacity in 2022 for regular hydropower capacity. Historical values obtained for total vehicles sold between 2012 and 2022 [38].
Yearly Offshore Wind Capacity Additions (MW/year), $OFFW_{growth}$	Energy Transformation[m]	320	–	360	9.4 GW	Assuming between 200 and 400 MW of offshore wind installed in 2025, and a subsequent growth rate that enables reaching 2 GW by 2030 as per the first offshore wind auction to occur in Portugal. Maximum limit value is determined by the Portuguese plan for offshore wind energy published in 2025 [40].

Below are listed the intermediate variables used to estimates the stochastic results.

[a] $ECI_{year\ i} = ECI_{year\ i_{central}} \times ECI_{multiplier}$

[b] $FEI_{industry,i} = FEI_{year\ i-1} \times \left(1 + FEI_{degrowth}\right)^{year_i - year_{i-1}}$

[c] $GVA_{industry_i} = GVA_{industry_{2022}} \times \left(1 + GVA_{growth} \times \left(year_i - 2022\right)\right)$

[d] $HPC_{year\ i} = HPC_{year\ 2022} \times \left(1 + HPC_{growth} \times \left(year_i - 2022\right)\right)$

[e] $ETC_{year\ i} = ETC_{year\ 2022} \times \left(1 + ETC_{growth} \times \left(year_i - 2022\right)\right)$

[f] $PVC_{year\ i} = PVC_{year\ 2022} \times \left(1 + PVC_{growth} \times \left(year_i - 2022\right)\right)$

[g] $GDP_{year\ i} = GDP_{year\ i-1} + \left(GDP_{year\ i_{SSP3}} - GDP_{year\ i-1_{SSP3}}\right) \times \left(1 + GDP_{mult.}\right)$

[h] $BSC_{capacity_{year\ i}} = BSC_{capacity_{2025}} + \left(BSC_{yearly} \times \left(year_i - 2025\right)\right)$

[i] $ONW_{capacity_{year\ i}} = ONW_{capacity_{year\ 2022}} \times \left(1 + ONW_{growth} \times \left(year_i - 2022\right)\right)$

[j] $EV\ Sales\ Share\ of\ New\ Vehicles: EV_{share_{year\ i}} = \dfrac{EV_{share_{year\ i-1}}}{1 - EV_{growth}}$

[k] $PSC_{capacity_{year\ i}} = PSC_{capacity_{2022}} + \left(PSC_{yearly} \times \left(year_i - 2022\right)\right)$

[l] $VS_{total_{year\ i}} = VS_{total_{year\ 2022}} \times \left(1 + VS_{growth} \times \left(year_i - 2022\right)\right)$

[m] $OFFW_{capacity_{year\ i}} = OFFW_{capacity_{year\ 2025}} \times \left(1 + OFFW_{growth} \times \left(year_i - 2025\right)\right)$

not be underestimated.

The model works by stepwise calculation of energy demand and transformation. At each time step, it first calculates energy demand, which is a function of user-inputted demographic and macroeconomic data. The energy transformation side then responds to those energy demands, including the transformation of energy forms into others (for example, conversion of fossil fuels to electricity) and the extraction of natural resources (e.g. biomass) required to produce other forms of energy, such as electricity. Pollutant emissions are estimated based on the direct emissions from the combustion of fossil fuels to meet those energy demands.

The ESM developed in this work captures energy demand and transformation across several activity sectors. The sectors include industry (disaggregated by sub-sector), residential, services, construction, agriculture, and transport (including light passenger vehicle, aviation, and national and international maritime transport). The sectors captured by energy transformation are biogas production, electricity production, hydrogen production, low-temperature heat production, renewable fuel of non-biological origin (RFNBO) production, oil refining, biodiesel production, biomethane production, synthetic methane production, and transmission of electricity and natural gas. Fig. 2 shows the system boundaries of the ESM developed in this study and Fig. 3 shows the outline of the CCU network considered in this study, optimized in previous work [2].

The exclusions are listed next. The national autonomous islands are excluded. On the demand side, heavy and commercial passenger vehicles were excluded due to limited information on vehicle sales by powertrain, age, fuel economy, and mileage. Although representing about 23% of total transport sector demand [23], this segment is not expected to significantly change results because it is not expected to compete with the CCU network for electricity. Current trends indicate that the adoption of battery-electric vehicles, particularly fuel-cell vehicles, remains very limited. Instead, a gradual replacement of internal combustion engines with hybrid vehicles is expected. This could, however, change radically if a net-zero trajectory policy is radically adopted from 2030 onwards [25]. On the transformation side, no constraints were added to the availability of bio-based natural resources, as their quantification lies beyond the scope of this study. These are considered to remain identical in both scenarios (with and without CCU networks). This assumption will also not affect the CCU network. It only influences the share of bio-based resources imported when compared to those produced domestically.

To estimate the net emissions of CO_2 from natural gas mixed with e-methane, combustion emissions were calculated in the model by subtracting a share of the total emissions proportional to the share of e-methane in circulation within the transmission network. For simplification purposes, no leakage of methane was assumed in the pipelines. This does not affect the results significantly as leaks will be the same with and without CCU, and because the characterization factor for biogenic methane is very similar to fossil methane (27.9 vs 29.8 kg CO_2 eq/kg CH_4).

The subsequent sections present the stochastic analysis and explain how their variables are used to calculate both energy demand and its transformation throughout the system. Later, the remaining equations used to calculate energy demand and transformation are described.

2.3. Stochastic analysis

In each iteration of the Monte Carlo algorithm, the stochastic variables were varied. These exogenous variables act as independent inputs to the model and are not influenced by other variables within the system. The central, minimum, and maximum values of these variables are shown in Table 1. As LEAP does not inherently support stochastic modelling of its key decision variables, we incorporated a stochastic

framework by defining intermediate dependent variables derived from the stochastic inputs. Some auxiliary parameters are used in the formulas for these dependent variables, whose values are listed in Table S-2. Figs. S-1 to S-13 show the historical variation for these dependent variables and their projections until 2070. Specific Fuel Consumption of Road Transport (SFC_{road}) is an exception and is assumed to be constant over the time analysed. This is due to a lack of better information on future perspectives for fuel consumption.

Triangular distributions were assumed for all independent variables (as in Table 1). This is because triangular distributions provide a practical compromise between representing uncertainty and avoiding unsupported statistical assumptions. These distributions require a plausible lower bound, upper bound, and most likely value that can be supported by the existing evidence. This is not new and has been adopted by other ESM studies [41] [42] [43] [44] [45]. For example, Escribano et al. [41] provides a particularly relevant case for emerging hydrogen deployment, such as the hydrogen deployment modelled in the present work. Future 2030 hydrogen production was represented by a triangular distribution, in which the lower bound corresponded to current operational capacity, the mode incorporated operational capacity together with projects at the feasibility, FID, or construction stages, and the upper bound additionally accounted for potential deployment.

2.4. Energy demand

In this work, the total final energy demand in each sector was calculated using the equations identified in Table 2. The subscripts *"i"* refer to year, *"j"* refers to iteration, "*k*" refers to vehicle type and "*l*" to vehicle age.

$$
\begin{cases}
\boldsymbol{GDP_{mult} > 0} \begin{cases} Share_{H_2 j,i} = Share_{H_2 central,i} \times \left(1 - \dfrac{GDP_{mult,j}}{GDP_{mult,max}}\right) \\ Share_{NGj,i} = Share_{NG,central,i} \times \left(1 + \dfrac{GDP_{mult,j}}{GDP_{mult,max}}\right) \end{cases} \\
\boldsymbol{GDP_{mult} < 0} \begin{cases} Hard-to-abate\ sector \begin{cases} Share_{H_2 j,i} = Share_{H_2 central,i} \times \left(1 + \left(10\%^{*} \dfrac{GDP_{mult,j}}{GDP_{mult,min}}\right)\right) \\ Share_{NGj,i} = Share_{NG,central,i} \times \left(1 - \left(10\%^{*} \dfrac{GDP_{mult,j}}{GDP_{mult,min}}\right)\right) \end{cases} \\ Not\ hard-to-abate\ sector \begin{cases} Share_{electricityj,i} = Share_{ectricity,central,i} \times \left(1 + \left(10\%^{*} \dfrac{GDP_{mult,j}}{GDP_{mult,min}}\right)\right) \\ Share_{NGj,i} = Share_{NG,central,i} \times \left(1 - \left(10\%^{*} \dfrac{GDP_{mult,j}}{GDP_{mult,min}}\right)\right) \end{cases} \end{cases}
\end{cases}
$$

Some energy demands remain constant throughout the year, while others fluctuate. The demands of the industrial, residential, services, and electric mobility sectors were defined with hourly resolution. The load curves for residential and electric mobility sectors were modelled based on data from Portugal [46] [47]. The load curves for industry and services were based on French data, respectively, for "manufacturing processes" and "offices", due to the lack of Portuguese data [48]. As shown in Fig. S-14, for example, the energy demand curve for a 24 h period during an autumn weekday, covering the period from 2022 to 2070, is shown using the central case values for all activity sectors. The load curves represent energy demand for 2022 (no CCU) and for 2030–2070 (with CCU).

The total energy demand is also split by each fuel type (as outlined in Fig. 2, includes, electricity, low temperature heat, hydrogen, methane, biogas, oil derivatives, and liquid synthetic fuels). For the "central case," the share of each fuel can be consulted in Tables S-4 (for the industrial, residential, services, construction, agriculture, and fisheries sectors) and S-5 (for the transportation sector). This is done for the analysis period (2022–2070). All these shares are kept constant across all iterations except for electricity, natural gas and hydrogen in "non-cogeneration" processes. For both scenarios, they were modelled in each iteration "j" for each year "i" as a function of the GDP_{mult}[1] by using the equations described below. It is assumed that $GDP_{mult} = 0$ for the central case to be aligned with Central GDP growth trajectory equal to LEAP's built-in IPCC SSP3 trajectory. This is the trajectory that deviates the least from projections assumed by the National Energy and Climate Plan, The Directorate of Energy and Geology Report, or the Roadmap for Carbon Neutrality Report (as indicated in Table 1).

When GDP_{mult} is different than 0, the shares of electricity and hydrogen were adjusted consistently with variations in the natural gas share to sum up 100%. When the proportion of natural gas in the mix decreased (or increased), the corresponding deficit (or surplus) was proportionally compensated by electricity and/or hydrogen, depending on the activity sector. This approach ensures internal consistency among energy carriers while avoiding over- or under-estimation of total final energy demand. The substitution between natural gas, electricity, and hydrogen was defined by specific sectoral rules, reflecting the expected technological and infrastructural feasibility of each energy carrier for each respective end-use sector.

The reason for this is that the share of natural gas in the final energy consumption of Portuguese industry is strictly related to the GDP growth, as observed by the strong and positive correlation ($R^2 = 0.97$) between historical GDP values and the share of natural gas in the final

[1] GDP_{mult} is an independent stochastic variable (see Table 1), ranging between −0.7 and 0.4. It represents the difference between GDP growth for an iteration "j" and the value estimated for the central case. Positive GDP_{mult} values means growths larger than the central case. Negative values represent smaller growths than the central case. The respective GDP growth trajectories as a function of GDP_{mult} (shown in Figure S-7) are calculated using the equation described in alinea g from footnotes of Table 1.

Table 2
Estimation of the total energy demand (E_{demand}) per activity sector modelled.

Sectors	Equation	
Industry	$E_{demand\,i} = GDP_i \times \frac{GVA_{2022}}{GDP_{2022}} \times GVA_{industry\,i} \times GVA_{subsector\ (\%)\,i} \times FEI_{subsector\,i}$	[1]
Residences	$E_{demand\,i} = E_{demand\,per\ dwelling} \times N_{dwellings} \times \frac{GDP_{simulation\ j\,i}}{GDP_{year\ i_{SSP3}}} \times \frac{GVA_{2022}}{GDP_{2022}} - \left(E_{demand\,per\ dwelling} \times N_{dwellings} \times \left(\frac{GDP_{simulation\ j\,i}}{GDP_{central\,i}} - 1\right) \times Elasticity_{residential}\right)$	[2]
Services	$E_{demand\,i} = E_{demand\,central.i} \times \frac{GDP_{simulation\ j\,i}}{GDP_{central\,i}} \times \frac{GVA_{2022}}{GDP_{2022}} - \left(E_{demand\,central.i} \times \left(\frac{GDP_{simulation\ j\,i}}{GDP_{central\,i}} - 1\right) \times Elasticity_{services}\right)$	[3]
Road transport	$E_{demand_i} = \sum_{vehicle\ type_k} \sum_{vehicle\ age_m} \left(N_{vehicles\,k,i,m} \times Fuel_{economy_{k,i,m}} \times Mileage_i\right)$	[4]
Construction	$E_{demand\,i} = GDP_i \times \frac{GVA_{2022}}{GDP_{2022}} \times GVA_{construction.i} \times FEI_{construction\,i}$	[5]
Agriculture	$E_{demand\,i} = GDP_i \times \frac{GVA_{2022}}{GDP_{2022}} \times GVA_{agriculture.i} \times FEI_{agriculture_i}$	[6]

energy consumption in the industry sectors (as shown in Table S-3). This is because higher energy costs, such as those associated with the transition from fossil fuels to hydrogen, may reduce economic productivity by increasing production costs. These costs are, in general, passed to consumers, eroding purchasing power and slowing overall GDP growth [49].

When GDP_{mult} is positive (i.e., the GDP grows more than the "central" case), the share of hydrogen in the final energy mix of each activity sector is reduced by the same amount, and the share of natural gas increases. Notably, when GDP_{mult} is negative (i.e., GDP growth is lower than in the "central" case), the calculations differ between hard-to-abate and non-hard-to-abate sectors. Hard-to-abate sectors are defined as those in which more than 50% of heat demand occurs at temperatures exceeding 500 °C [50]. Our approach assumes that in cases where $GDP_{mult} < 0$, only hard-to-abate sectors can increase the share of hydrogen in final energy demand above the central case. The not hard to abate sectors increase the share of electricity instead. This assumption is because, in sectors that are not hard to abate, electrification is typically more cost-effective and readily available than hydrogen-based energy. Heat pumps are both more efficient and economic, avoid heat losses from combustion exhaust, and transfer heat, much like refrigerators or air conditioners, rather than generating it from energy inputs [42]. In the present work the potential adoption of either hydrogen or electrification for situations where $GDP_{mult} < 0$ was arbitrarily capped at 10% above the levels for the 'central' case. This is because projected energy mixes for the national industrial energy transition, as provided by the national energy authority, are already considered optimistic given the current deployment of hydrogen in Portugal. For example, its projections estimate that hydrogen will account for 12% of the cement sector's energy mix by 2040, whereas currently no hydrogen is used in the industry [51].

Other variables showing a strong correlation coefficient (R above 0.95 or below −0.95, include: EV sales, energy intensity of industry, GDP, hydropower installed power capacity, onshore wind capacity, pumped storage capacity, share of natural gas used in industry, installed solar power, and electric transmission capacity. These were still modelled as independent from each other due to the following:

- **The EV sales either with the installed capacity of solar power ($R = 0.97$) or the electrical transmission capacity between Spain and Portugal ($R = 0.96$).**

These relations were disregarded due to the difficulty in determining whether solar power capacity or transmission capacity influences EV sales the most. The literature suggests that residential solar installations reduce marginal charging costs, thereby spurring EV adoption [52], and that grid reliability, supported by transmission capacity, mitigates consumer hesitancy [53]. However, it is unclear which mechanism is the primary driver in the Portuguese context or has the larger impact on adoption rates. Furthermore, EV sales reach 100% by 2031 (see Fig. S-10), even under the Minimum EV uptake trajectory, and therefore, model results would not change significantly by adding these correlations.

- **Hydropower Installed Capacity and Pumped Storage Capacity ($R = 1.00$).**

This is because the existing hydropower capacity in Portugal is close to its technical limit (8.2 GW vs 9 GW), and it would not make sense to model Pumped Storage Capacity deployment as a function of conventional hydropower deployment. Pumped storage continues to be installed despite a net zero growth in conventional hydropower capacity in similar regions in Western Europe and does not require natural river basins or conventional hydro potential to occur [54].

Finally, though onshore wind capacity and final energy intensity of industry demonstrate a strong negative correlation (−0.96), they were still modelled independently as there is no evidence to reject spurious correlation between them.

Noteworthily, in addition to the parameters listed in Table S-2, the modelling of energy demand from the transportation sector required consideration of the vintage stock profile and vehicle survival probability. The analysis considered the distribution of vehicles by age in Portugal, along with the age-dependent probability that a vehicle remains in operation each year. Portugal-specific vehicle profiles for ICE vehicles and survival probability were taken from the literature [55]. The stock profile for electric and plug-in hybrid vehicles was calculated based on the sales and stocks of electric vehicles between 2011 and 2022 [56] (see Figs. S-15 and S-16).

2.5. Energy transformation

Energy transformation is governed by user-defined conditions and constraints. Details on how energy transformation is modelled in LEAP can be found in the LEAP user manuals [47] [48].

Table S-6 presents the parameters used to model energy transformation and describes the assumptions for the processes involved in producing each fuel. The electricity production curve for the 24-h autumn weekday is shown for the central case (from 2022 to 2070) in Fig. S-17, including dispatch for each electricity production technology (e.g., solar PV, wind).

Model results for the 2022 "central" case were compared with observed energy demand and transformation in that year across all activity sectors and fuels to verify model calibration, with particular focus on electricity production. This is due to its central role in the Portuguese energy system (as seen in Fig. 2). A comparison between the electricity production in 2022, as reported in Portugal's national energy balances [49], and the electricity consumption predicted by the ESM, shows a deviation of 2% (204 PJ versus 209 PJ) (as seen in Fig. S-18). Hourly

Table 3
Percentiles of the results of NPV, GHG Emission Abatement and NPV/CO_2 avoided, as well as the revenues and expenses of the numerator in eq. 7, necessary for the calculation of the NPV.

Results and details used to calculate NPV (eq. 7)	P10 (10th percentile)	P25 (25th percentile)	P50 (Median)	P75 (75th percentile)	P90 (90th percentile)	Average value
NPV (B€)	−46	−49	−54	−58	−60	−54
GHG Emissions Avoided (Mt CO_2 eq)	69	64	57	51	46	57
NPV/CO_2 Avoided (€/tonne CO_2)*	800	853	931	1026	1121	949
Revenues and expenses (M€/year)	P10	P25	P50	P75	P90	Average
Avoided Natural Gas Imports ($CS_{av.NGimports}$)	412	362	293	169	73	265
Revenues of Exports – *E*-methane ($R_{exp,e\text{-}methane}$)	0	0	0	0	0	2
Cost of Imports – H_2 ($E_{importsH2}$)	−18	−415	−820	−1089	−1304	−757
Lost Fiscal Revenues (VAT) ($E_{lost\ fiscal\ revenue}$)	−18	−41	−72	−88	−100	−64
Lost Fiscal Revenues (ETS) ($E_{lost\ fiscal\ revenue}$)	−51	−167	−307	−415	−513	−298

* Expresses the percentile of the distribution of the 1300 values calculated in each iteration by dividing the NPV by the GHG abatement in each iteration.

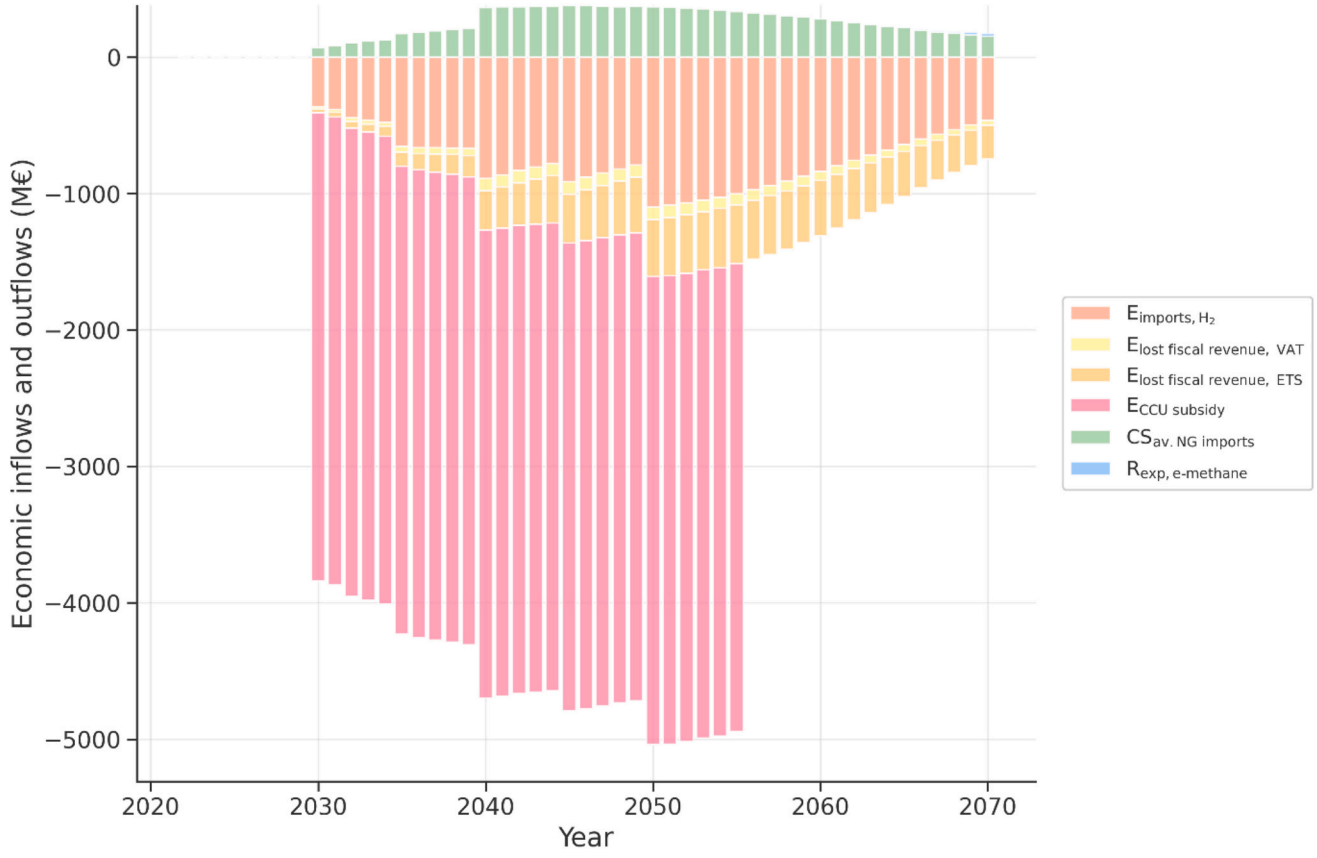


Fig. 4. Averaged annual revenues and expenses by component used in Eq. 7.

deviations for each technology, tested using data from REN (Portuguese Transmission System Operator) [31], are typically between ±1GW (P25-P75 range) but may deviate as much as ±4 GW, with the largest deviations observed for hydropower, wind, natural gas-fired generation, and energy imports from Spain (Fig. S-19). It is then possible to conclude that our model results fall within the expected deviation, as indicated by the 2022 results for energy demand and transformation. The values for final energy demand by fuel range from 18 PJ for diesel, which represents approximately 8% of total diesel demand (Fig. S-20). Natural gas shows a deviation of 9 PJ (or 9%), resulting mostly from the industrial sector demand (slightly less than 6 PJ), of which the highest deviation is in the chemistry and plastics sector (about 2 PJ) (see Fig. S-21).

2.6. Estimation of the net present value (NPV)

Net Present Value (NPV) represents the difference between the cash flows (i.e., revenues and expenses) over a given period, based on a specified discount rate. Projects with positive NPV are profitable, while those with a negative NPV are not financially sound.

The cash flows for each Monte Carlo iteration are calculated by the differences between the “with CCU” and “no CCU” scenarios. The only difference between the two scenarios is the inclusion of the CCU network in the e-methane transformation module. In the “no CCU” scenario, e-methane is exclusively produced from the CO_2 captured in biogas upgrading plants, while “with CCU” includes also the e-methane produced in the centralised CCU network. This work assumes that the

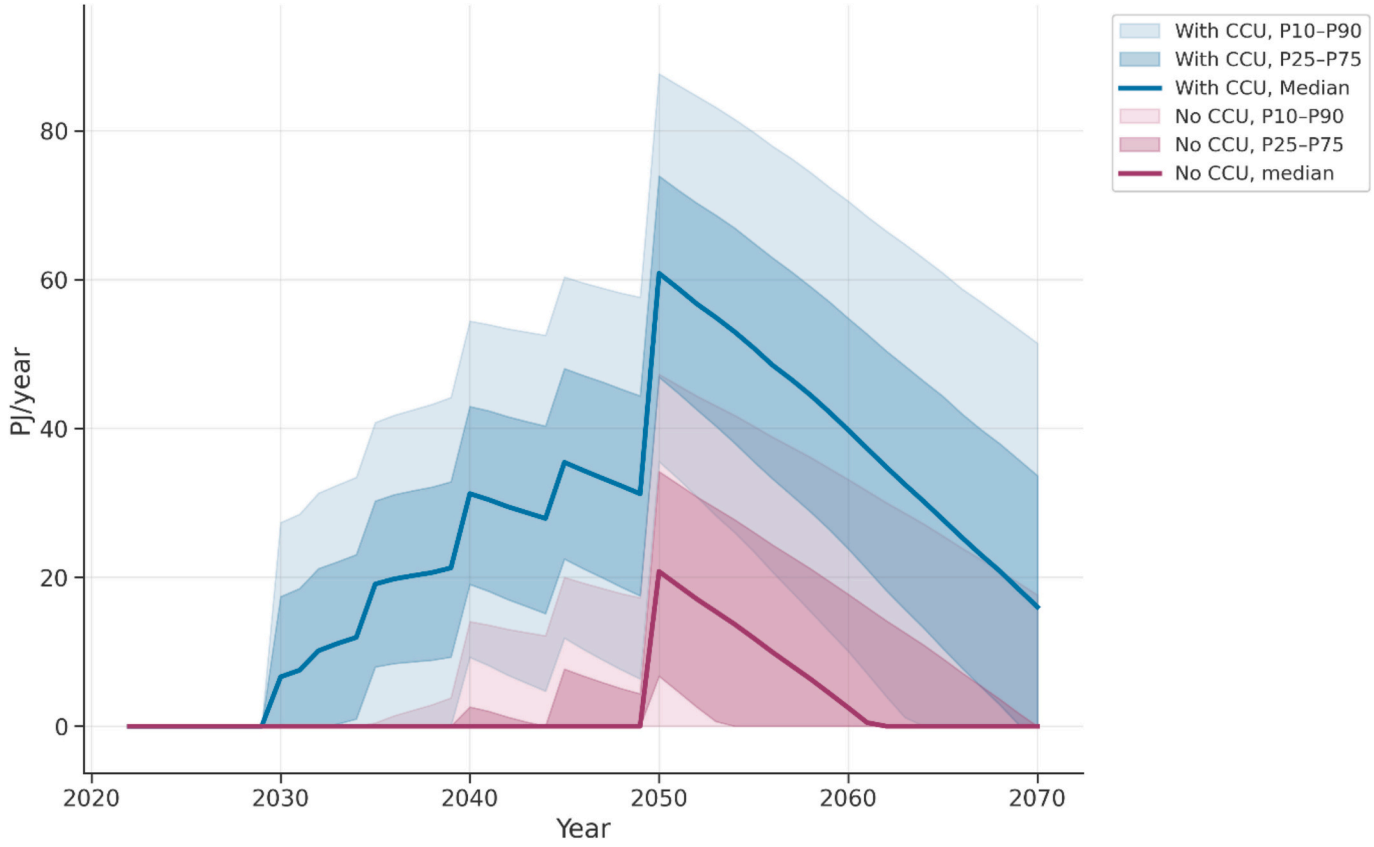


Fig. 5. Estimated national imports of hydrogen for the scenarios with the centralised CCU network (With CCU, blue) and without it (No CCU, mauve). National estimates from the work of the National Energy and Climate Plan and the Portuguese Directorate for Energy and Geology are not plotted in this chart. This is because hydrogen supply consistently exceeds demand in these publications. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

government is the subsidiser of the CCU network in this Build-Own-Operate-Transfer (BOOT) business model. A discount rate of 4% ("i") was assumed, in line with Portuguese cost-benefit and cost-effectiveness analyses carried out for the public sector [57]. Eq. 7 is used for calculating NPV, including all revenues and expenses.

$$NPV = \sum_{t=2022}^{t=2070} \frac{CS_{av.NG\ imports} + R_{exp.e-methane} - E_{imports\ H_2} - E_{lost\ fiscal\ revenue} - E_{CCU\ subsidy}}{(1+i)^t} \quad (7)$$

Cost Savings correspond to the cost savings associated with the avoided fossil natural gas imports ($CS_{av.NGimports}$). Revenues correspond to the exports of e-methane when supply exceeds demand ($R_{exp,e\text{-}methane}$). The expenses correspond to additional imports of hydrogen due to insufficient supply ($E_{importsH2}$), the lost fiscal revenue ($E_{lost\ fiscal\ revenue}$), including the value added tax (VAT) and Emission Trading System taxes (ETS),[2] and the CCU subsidy ($E_{CCU\ subsidy}$) attributed by the national government to assure profitability of the CCU network. The $E_{CCU\ subsidy}$ was determined in a previous paper [2] and corresponds to the 95th percentile of the gap between the break-even costs of e-methane and those of fossil natural gas, necessary to allocate low capital and revenue security costs to all elements of the CCU value chain. This is coherent with a levelised cost of e-methane of 0.43 €/kWh, calculated for a period of 25 years and a discount rate of 4.5%. This cost is derived from a CO_2 capture cost of 141 €/tonne CO_2, a cost of CO_2 transport of 37 €/tonne and a cost of H_2 production of 11 €/kg, the latter corresponding to 96% of the total costs of e-methane. Of these, around 70% of the total cost corresponds to investment costs and cost of capital, split roughly 50/50 between the electrolysers and the renewable power plants which provide them with green electricity [2].

This subsidy is attributed for the 25 years of the project's economic lifetime (from the year of installation, 2030, until 2055), but is null afterwards, because the ownership of the CCU network is transferred to the state after that year.

The costs of natural gas and hydrogen, as well as the ETS price, were modelled stochastically over time based on the ranges of existing forecasts for these variables from the IEA [50], Frieden et al. [51], and historical trends [58] (see Fig. S-22).

3. Results and discussion

Section 3 presents the analysis results. Section 3.1 reports the

[2] The BOOT model assumes that e-methane is exempted from these taxes. Thus, implementing the CCU network would cause these tax revenues to disappear.

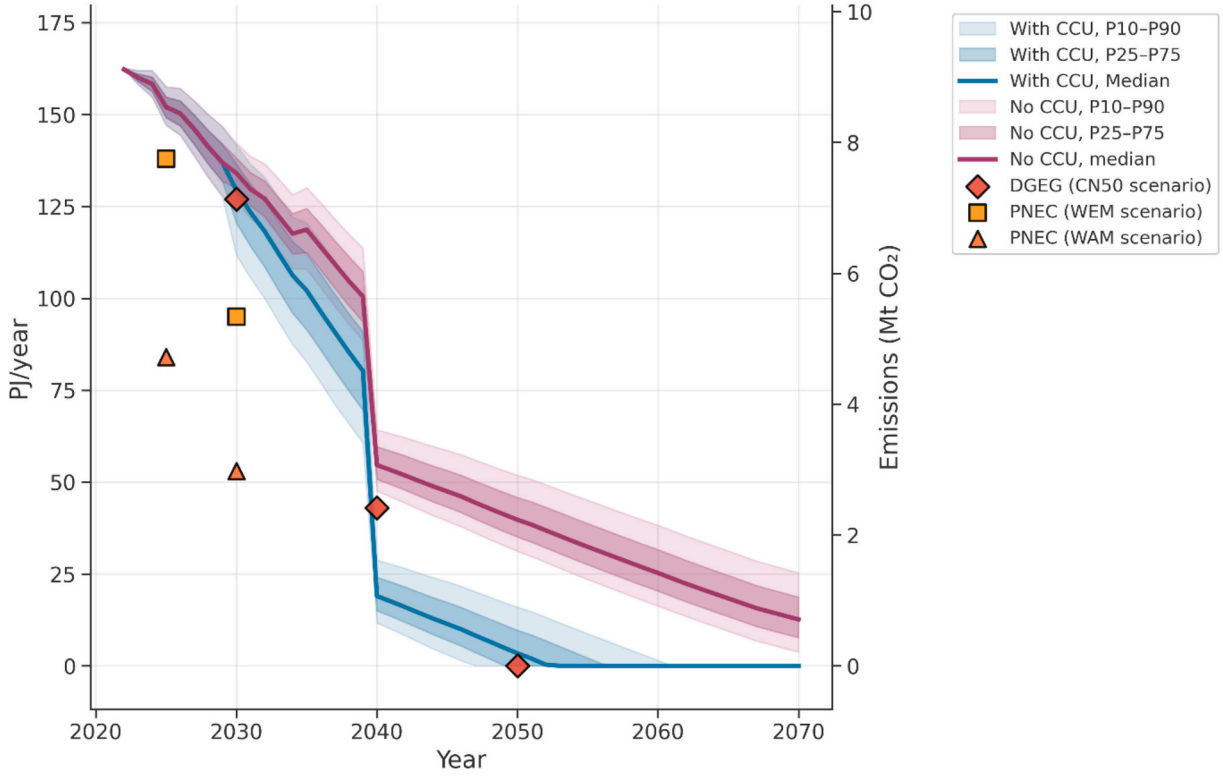


Fig. 6. Imports of Natural Gas to Portugal in scenarios comprehending the centralised CCU network ("With CCU", blue) and scenarios without it ("No CCU", mauve). Included are also the values of natural gas imports from the ESM of the Portuguese Directorate of Energy and Geology (DGEG) and estimates of natural gas imports in the latest National Energy and Climate Plan (PNEC) with Existing Measures (WEM) and With Additional Measures (WAM), to be read on the y-axis (PJ/year). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

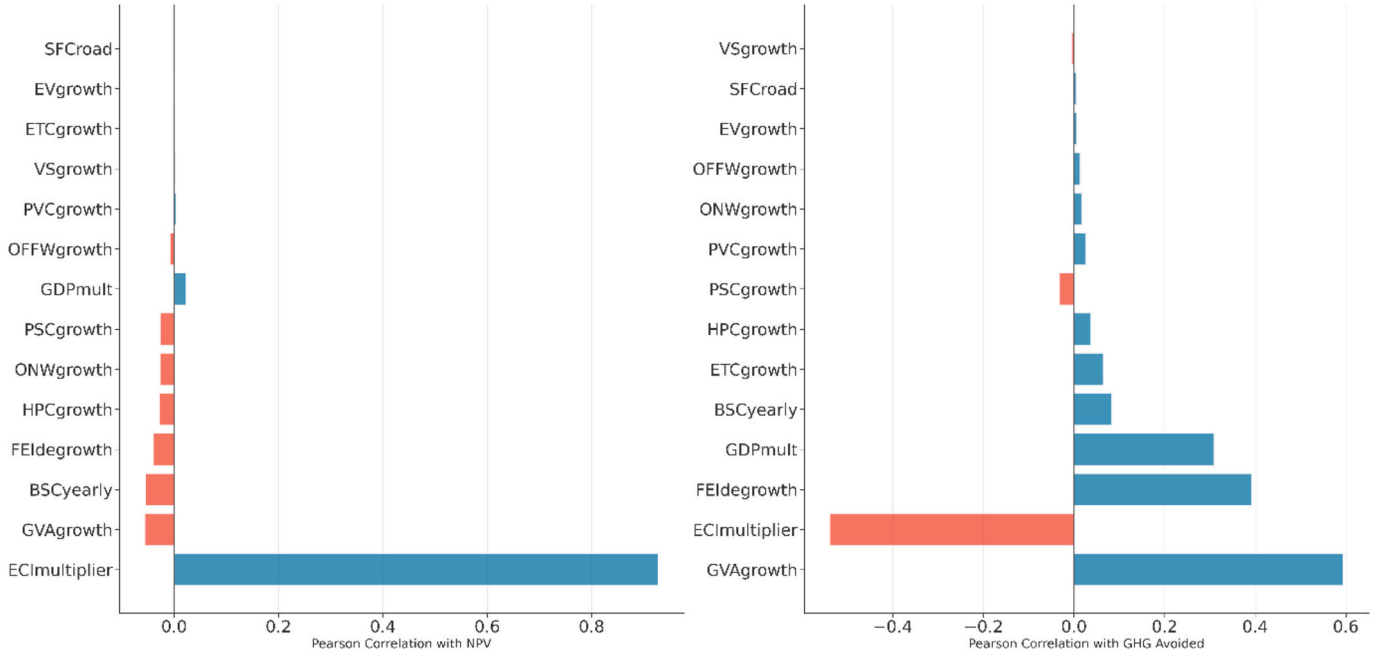


Fig. 7. Pearson's correlation of NPV (left) and GHG emissions avoided (right) to each one of the stochastic variables used in the energy system model.

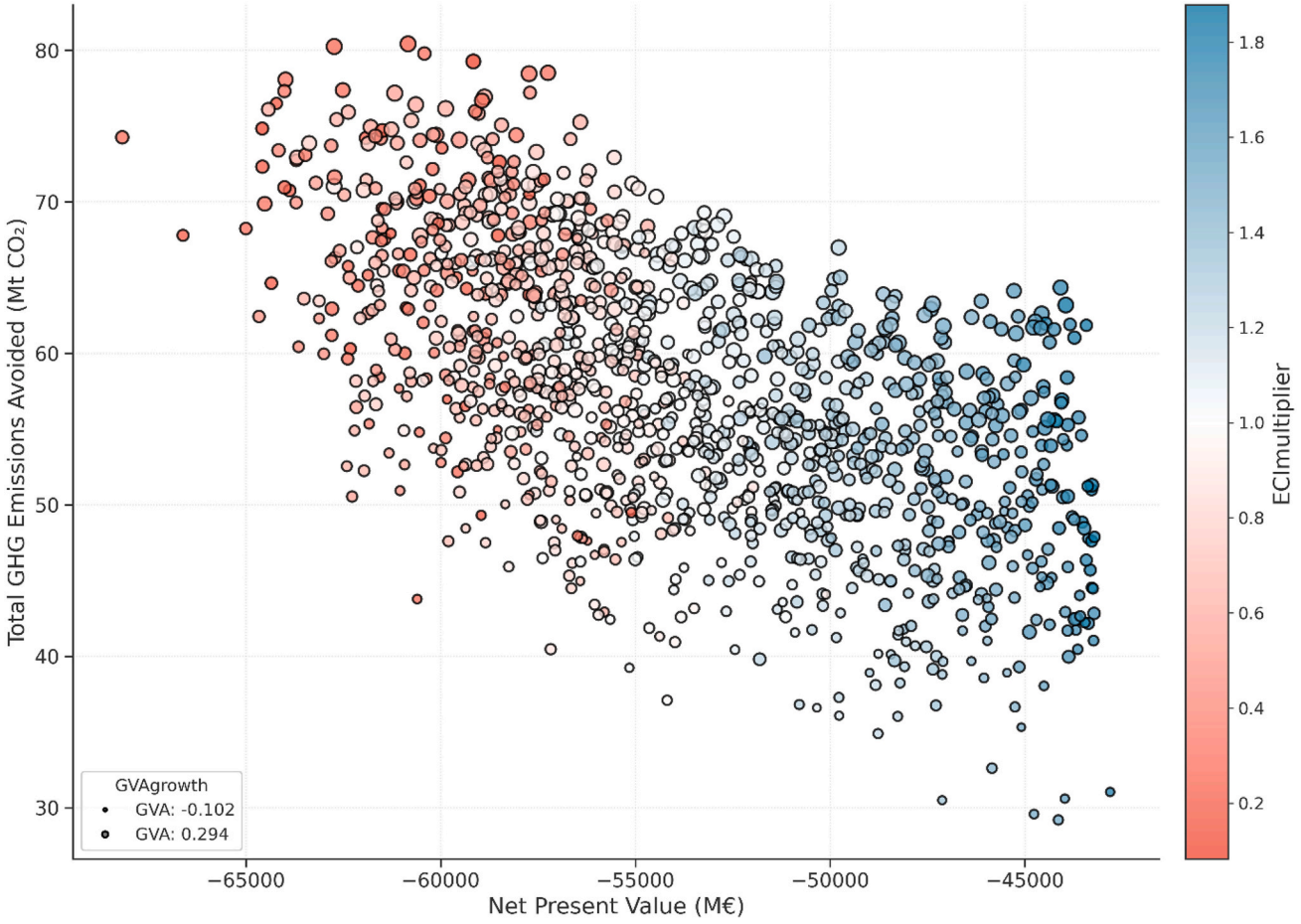


Fig. 8. Relation between NPV and GHG emission avoided as a function of the $ECI_{multiplier}$, and the GVA_{growth}.

Table 4
Multi-variable linear regression of GHG Emission avoided and NPV as a function of the most statistically significant variables of the stochastic ESM.

GHG Emission Avoidance ($R^2_{adjusted} = 0.96$, $\beta_0 = 99$, Standard Deviation = 8.94)						
Coefficients	**Independent Variable**	**Standardised Value of the Coefficient**	***p*-value**	**VIF**	**Confidence Intervals**	**Results obtained when all variables are constant and this variable is increased by one standard deviation:**
β_1	GVA_{growth}	5.63	<0.001	1.8	[5.54,5.72)	GHG emissions avoided increase between 5.5 and 5.7 Mt. CO_2 eq.
β_2	$FEI_{degrowth}$	3.65	<0.001	51	[3.56,3.75]	N/A (VIF > 10)
β_3	GDP_{mult}	3.17	<0.001	1	[3.07,3.26]	GHG emissions avoided increase between 3.1 and 3.3 Mt. CO_2 eq.
β_4	ETC_{growth}	0.55	<0.001	18	[0.46,0.65]	
β_5	BSC_{growth}	0.15	0.001	37	[0.06,0.25]	N/A (VIF > 10)
β_6	PVC_{growth}	0.13	0.004	29	[0.04,0.23]	
β_7	$ECI_{multiplier}$	−5.22	<0.001	8	[−5.31,-5.12]	GHG emissions avoided decrease between 5.1 and 5.3 Mt. CO_2 eq.
NPV (R^2 adjusted = 0.92, $\beta_0 = -69{,}000$, Standard Deviation = 5.3)						
Coefficients	**Independent Variable**	**Standardised Value of the Coefficient**	**p-value**	**VIF**	**Confidence Intervals**	**Results obtained when all variables are constant and this variable is increased by one standard deviation:**
β_1	GVA_{growth}	−478	<0.001	2	[−580,-377]	NPV decreases between 377 and 580 M€
β_2	$FEI_{degrowth}$	−292	<0.001	8	[−393,-191]	NPV decreases between 191 and 393 M€
β_3	$ECI_{multiplier}$	4912	<0.001	8	[4811,5013]	NPV increases between 4.8 and 5.0 B€

statistical outcomes of the stochastic analysis, including distributions for NPV, GHG emissions avoided, and key cost and revenue components, as well as the main cash flow drivers distinguishing the "No CCU" and "With CCU" scenarios. Section 3.2 examines the sensitivity of NPV and emissions avoided to input variables, highlighting the most influential factors. Section 3.3 assesses the statistical significance of these variables through multivariable regression. Section 3.4 compares the study's results with other Portuguese energy system analyses to provide context. Finally, Sections 3.5 and 3.6 discuss the broader implications of the findings and outline the study's main limitations.

3.1. Results for NPV and GHG mitigation

Table 3 shows the NPV and GHG Emissions avoided results for over 1300 iterations of the stochastic model. The Table shows the 10th, 25th, 50th, 75th and 90th percentile (P10, P25, P50, P75 and P90), as well as the average for all 1300 iterations for these results. Revenue and expenses (eq. 7) are also presented. The CCU subsidy is 3400 M€/year across all iterations.

The CCU network applied within the Portuguese Energy model shows an median NPV of −54 B€ (ranging from −60 to −46 B€) and avoids the emissions of 57 Mt. CO_2 eq (ranging from 46 to 69 Mt. CO_2

eq). The median NPV/CO_2 Avoided is 931 €/tonne CO_2 and ranges from 800 to 1121 €/tonne. Even in the best-performing economic scenarios (P10), the NPV is negative (−46 B€). This is because the annual CCU subsidy is substantially higher than the revenues (3400 M€/year vs 412 M€/year at its best). The largest contributor to the network's negative net balance is the required import of hydrogen, with a median of −820 M€/year. The hydrogen import is needed because the electrolyser capacity is insufficient to meet the demand of all activity sectors.

3.1.1. NPV results

Fig. 4 presents the details of the annual-averaged values for each revenue and expense over time. These correspond to parameters used in the numerator of eq. 7, and they do not account for the annual discount rates, "*i*", from the same equation. From 2055 onwards, CCU subsidies are no longer available due to the end of the project's economic lifetime and the consequent transfer of ownership from the original operators to the state.

Fig. 4 shows that the net balance between revenues and expenses is always negative. Expenses are, on average, 17 times higher than the revenues (4519 vs 267 M€/year). The largest cash flow share in each year is contributed by CCU subsidies (75% of the overall cash flow), Hydrogen imports (17%), and Lost Fiscal Revenues (7%).

Expenses grow between 2030 and 2055, as CCU subsidies and the cost of hydrogen imports outweigh the revenues from avoided natural gas imports. From 2055 onwards, the CCU ownership is transferred to the state. Although expenses decline between 2055 and 2070, the overall economic balance remains negative, as hydrogen import costs and lost fiscal revenues do largely exceed the savings from avoided natural gas imports.

Expenses do not rise steadily between 2040 and 2055. They increase only in 2045 and 2050, and decline in the other years within the period. In 2045 and 2050, an incremental hydrogen demand is required to produce Renewable Fuel of Non-Biological Origin (RFNBO). This demand stems from the need to fulfil the country's quotas for synthetic jet fuel in national and international aviation fuel demand, set to be 15% of total jet fuel demand by 2045 and 35% by 2050 [59] (as shown in Table S-6). Fig. 5 shows the difference in hydrogen imports between the cases with and without the CCU network. The peaks in hydrogen demand are visible. Hydrogen imports fall between 2040 and 2044 and again between 2045 and 2049 because the annual addition of electrolyser capacity boosts domestic hydrogen production, reducing the volume that needs to be imported.

For the values above 0, we can say that in at least 50% of the runs it is necessary to import hydrogen after 2050. The median trajectory for the "no CCU" case in Fig. 4 (represented by the mauve line) indicates that hydrogen imports are required in over 50% of the model's assessed iterations after 2050, even without a CCU network. This shows that the current and expected national installed capacity for hydrogen supply will be insufficient to meet either the future hydrogen demands required for the hypothetical centralised national CCU network or the forecasted national consumption (as revealed by the "No CCU" case) within the evaluated period.

3.1.2. GHG emissions avoided

The GHG abatement potential is proportional to the reduction in natural gas imports. This is because only the direct combustion emissions are accounted for in the calculation of GHG avoided. Fig. 6 shows the differences in natural gas imports in the "With CCU" and "No CCU" scenarios, as well as the abated GHG emissions.

The red diamond shapes in the figure represent estimates of natural gas imports to the country from the most recent report from Portugal's Energy and Geology Directorate [1], which are outputs of the CN50 scenario. The CN50 scenario delineates the necessary trajectory for the Portuguese energy system (based, among others, on installed capacities of renewable energy plants) to achieve carbon-neutrality targets. Squares and triangles represent estimates of natural gas imports from the latest National Energy and Climate Plan, based on both deterministic scenarios, namely, With Existing Measures (WEM) and With Additional Measures (WAM) [6]. These two scenarios have a similar scope to the estimated by the National Energy Directorate (CN50), as they delineate the necessary trajectory to achieve national carbon neutrality by mid-century. While both the WEM and WAM scenarios are cost-optimized trajectories of the Portuguese economy towards carbon neutrality, they differ in two aspects. The WAM targets carbon neutrality in 2045 rather than 2050, and it accounts for additional demands from future industrial projects, which are disregarded in WEM.

The installation of the CCU network (in 2030) immediately reduces the country's imports of fossil natural gas upon its entry into operation. However, there is a notable difference in avoided imports between 2030 and 2040, and thereafter (2040–2070). The CCU network implies that its operational electricity demand, together with the pre-existing national electricity demand, exceeds the nationally installed renewable power capacity, leading the country to rely more on gas-fired electricity generation between 2030 and 2040 than in the "no CCU" case. As a result, the "with CCU" scenario achieves lower avoided greenhouse gas emissions in the period between 2030 and 2040 compared to the 2040–2070 period as observed by comparing the difference between the blue and mauve shaded lines.

After 2040, combined-cycle power plants are phased out as mandated by national law. The country relies on energy imports from Spain to meet its demand. That explains the widening gap in natural gas imports between "With CCU" and "No CCU" after 2040, as well as the higher revenues from avoided natural gas imports (as in Fig. 4). It is important to note that only with the "With CCU" scenario is possible to reach zero fossil natural gas imports (and related GHG emissions) between mid-2040s and 2060 (10th and 90th percentile of the iterations, respectively). This is because hard-to-abate sectors continue to use fossil natural gas in the "No CCU" scenarios until 2070.

3.2. Correlation between the stochastic variables, NPV, and GHG emissions avoided

The sensitivity of NPV and avoided GHG emissions to each stochastic variable is evaluated. Fig. 7 indicates that the $ECI_{multiplier}$ and $GVA_{growth\ (\%)}$ show the strongest correlation with variations in NPV and avoided GHG emissions, suggesting that the model is particularly sensitive to

Table 5
Amounts of CO_2 captured annually from point sources and DAC. Point Sources in this study includes the CO_2 captured in the CCU network and the CO_2 captured in biogas plants for upgrading to biomethane. Sources: PNEC [6] and DGEG [1].

		2030			2040			2050		
		Values in Mt			Values in Mt			Values in Mt		
		Point Sources	DAC	Total	Point Sources	DAC	Total	Point Sources	DAC	Total
PNEC	WEM (With Existing Measures)	0	–	0	0.2	–	0.2	–	–	
	WAM (With Additional Measures)	0.1	–	0.1	3.9	–	3.9	–	–	
DGEG	CN50	1.0	–	1.0	3.5	1.7	5.2	7.8	5.0	13
This study	With CCU, "central"	1.8	0.1	1.9	2.2	0.8	3.0	2.2	2.4	4.6
	No CCU, "central"	<0.1	0.1	0.1	0.4	0.8	1.2	0.4	2.4	2.8

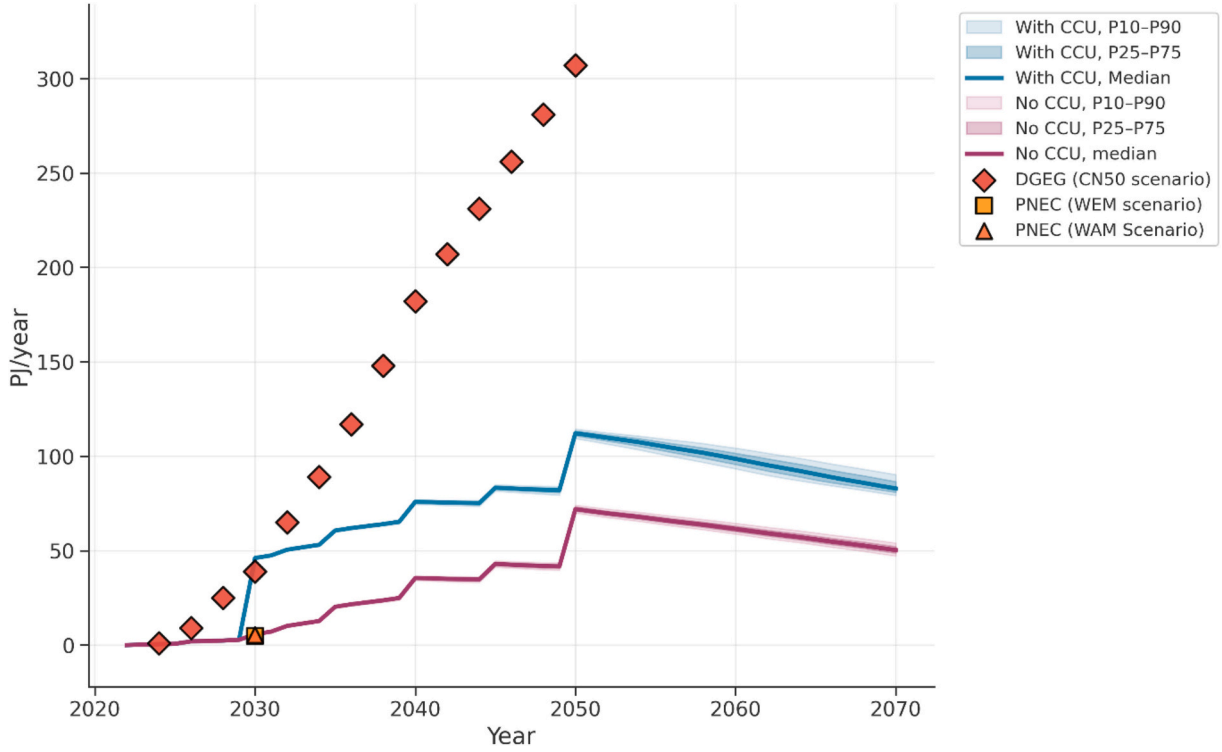


Fig. 9. Hydrogen production requirements in Portugal in this study but also set by models from PNEC and DGEG. DGEG results include also the exports of hydrogen. The observed spread in hydrogen demand is small because the demand for hydrogen depends on the energy mix of each activity sector, in which hydrogen is a small component compared to the other energy vectors. Therefore, the demand does not vary significantly between iterations.

these two variables.

To deepen the analysis, the NPV and avoided GHG emissions were plotted as functions of the two influential variables: electrolyser capacity and the share of industry GVA. Fig. 8 shows the results for the 1300 runs of the analysis. NPV and avoided GHG emissions tend to be inversely proportional.

A larger $ECI_{multiplier}$ (blue) is associated with higher NPV values but relatively lower avoided GHG emissions. This occurs because higher electrolyser capacities, as expected, reduce the need for hydrogen imports (thereby lowering costs and increasing NPV). However, this effect is offset by increased generation from natural gas–fired power plants in Portugal between 2030 and 2040, which raises GHG emissions. Consequently, avoided emissions are lower compared to scenarios where hydrogen is imported, as the burden of electricity generation is shifted to the countries producing the hydrogen.

Lower $GVA_{growth\ (\%)}$ (smaller bubbles), reflecting reduced industrial activity in the country, is associated with less avoided GHG emissions. This is because energy demand in industry (and, consequently, natural gas demand and GHG emissions) is proportional to the GVA. Inversely, higher $GVA_{growth(\%)}$ results in more emissions avoided, particularly after 2060, when all fossil natural gas imports cease in the "With CCU" scenario but continue in the "No CCU" scenario.

3.3. Statistical significance of the stochastic variables

Statistical significance allows to determine quantitatively how a change in one standard deviation of a variable can affect the results for NPV and avoided GHG emissions. This complements the analysis in Section 3.2 by identifying which variables have the largest impact on the results and quantifying how a one-standard-deviation change in each variable affects the outcomes.

The multivariable linear regressions for NPV and avoided GHG emissions yielded R^2 values of 0.87 and 0.96, respectively. Table 4 shows the coefficients, *p*-values, variance inflation factor (VIF), confidence interval, and interpretation of the coefficients for each independent variable. These regressions correspond to the best-performing multivariable regression specification, obtained through backward stepwise elimination starting from the full model. Predictors were sequentially removed based on statistical insignificance ($p > 0.05$), and model performance was evaluated using adjusted R^2 and 5-fold cross-validated R^2. Variance inflation factors (VIF) were computed to control for multicollinearity.

Only seven of the fourteen variables are statistically significant in predicting the GHG emissions avoided. Among the seven variables, only GVA_{growth}, GDP_{mult} and $ECI_{multiplier}$ show a VIF below 10. This suggests that even if the other variables help predict avoided GHG emissions, their coefficients should be interpreted with caution. This is because variables with VIFs above 10 indicate a high likelihood of multicollinearity, which can inflate their significance in predicting outcomes due to correlations with other predictors. In sum, the findings allow to conclude that GVA_{growth}, $FEI_{degrowth}$, GDP_{mult}, and $ECI_{multiplier}$ are the most significant and meaningful variables for predicting the overall performance of the ESM with CCU compared to without CCU.

3.4. Results comparison with national reference documents

Our results are difficult to compare with those from national estimates from ESM developed in the context of the modelling from the National Energy and Climate Plan's (PNEC) [6] and the Portuguese Energy and Geology Directorate (DGEG) [1]. Due to the lack of available public data, it is not possible to robustly replicate the assumptions and modelling procedures of these two models. The PNEC estimates are based on the TIMES-PT ESM, an optimisation model different from LEAP [17], and on DGEG's model (JANUS), programmed in LEAP. The results of this work project the range of possible future outcomes for the energy system based on historical trends, whereas existing national models outline the behaviour the energy

system must adopt to achieve policy-imposed targets. The growth or degrowth of key variables in this work was projected based on the range of existing historical trends. The model from DGEG simulated Portugal's ESM in "backcasting mode". This is to say that the scenario design begins with public policy targets (such as renewable energy shares, GHG emission ceilings, and energy efficiency obligations) and only permits a pre-defined set of technological value chains to operate [1].

Despite the models' differences, it is possible to compare three aspects, namely, 1) the amount of CO_2 captured for CCU purposes and its origin; 2) the imports of natural gas to Portugal, and 3) the total domestic hydrogen production. As PNEC and DGEG assume that no hydrogen imports would be required, no comparison is possible for this aspect. Renewable electricity capacity growth was not compared, as it serves as an input to our model rather than an output, unlike within the modelling from PNEC and DGEG. However, this aspect will be briefly discussed in the subsection on natural gas imports.

3.4.1. Carbon dioxide captured for CCU purposes

Table 5 allows comparison of CO_2 captured from point sources (industry and biogas plants) and Direct Air Capture (DAC) for 2030, 2040, and 2050.

For 2030, the amount of CO_2 captured in the central "With CCU" scenario is much larger than in the DGEG and PNEC WAM scenarios. The "No CCU" scenario aligns with the PNEC estimates for 2030 (0–0.1 Mt. CO_2/year). For 2040, the amount of CO_2 captured in our study (1.2–3.0 Mt. CO_2 eq/year), is within the range of PNEC (0.2–3.9 Mt. CO_2/year), but considerably below the estimates of DGEG of 5.2 Mt. CO_2/year (42–77% less in 2040 for the "With CCU" and "No CCU" cases, respectively). The difference in CO_2 captured between our study and that of DGEG is even higher in 2050 (7.8 Mt. CO_2/year), 64 and78% higher in 2050 when compared to the "With CCU" and "No CCU" cases, respectively.

The reason for the discrepancy in total CO_2 captured between our work and DGEG is not entirely clear, but two factors seem likely. First, the CO_2 capture capacity for synthetic fuel production is much higher in DGEG CN50 scenario for 2040 and 2050. The DGEG scenario estimates a production of CO_2-based e-fuels (e-methane, jet fuel, and methanol) of 18, 67, and 113 PJ/year for, respectively, 2030, 2040, and 2050. Our estimate is 36, 53, and 75 PJ/year for the same period. The smaller synthetic fuel production capacity in our work is based on the assumption that only the imposed quota of RFNBO for aviation would be produced. By contrast DGEG estimates that Portugal could also produce RFNBO for export. Second, in DGEG's model, an additional 2.3 Mt. CO_2/year is captured in 2050 and sent for geological sequestration. The present study assumes no geological storage capacity. No support however can explain the discrepancies in total CO_2 captured between PNEC and this study. This is due to the absence of clear evidence regarding the CO_2 capture capacities assumed in the TIMES-PT model.

3.4.2. Natural gas imports to the country

In this study, the estimates for natural gas imports are more closely aligned with those of DGEG than with those of PNEC (as seen in Fig. 6, Section 3.1.2.). Overall, the "No CCU" scenario shows higher natural gas demand and does not reach zero until 2070. This means that the current trajectories of de-fossilisation are not progressing fast enough to match the ambitions set by the optimized TIMES-PT or the JANUS models [1] [6]. Therefore, if Portugal's developments align with the "No CCU" scenario, natural gas imports are estimated to continue past 2070, despite the government's ambitions of net zero in 2050. Consequently, only the "With CCU" scenario provides a sufficiently robust decarbonisation pathway to reduce fossil natural gas imports to zero between 2047 and 2060 (corresponding to the 10th and 90th percentiles of the iterations, respectively).

National estimates project lower natural gas imports for the period 2022–2030 than those obtained in this study. Both sets of estimates assume the possibility of installing 21 GW of solar and 10 GW of onshore wind capacity by 2030, which could substantially reduce reliance on natural gas–fired electricity generation. This reflects differing assumptions regarding the pace of renewable electricity capacity expansion. Given that a significant share of current natural gas consumption is used for electricity production (approximately 46% in 2022) [60], these assumptions are particularly influential. By contrast, in this study, even the most ambitious growth trajectory results in only 7.5 GW of solar and 6.0 GW of onshore wind capacity installed by 2030.

3.4.3. Hydrogen production requirements

Total hydrogen production requirements in Portugal are shown in Fig. 9 for both our model results and those of DGEG and PNEC.

The total hydrogen production requirements are similar in the "No CCU" case and the PNEC scenarios for 2030, whereas DGEG assumes accelerated growth in demand until 2050, causing a significant disparity when compared to the estimates of this study. As a result, hydrogen demand by 2050 is expected to be three times the "With CCU" case. This is because DGEG ambitious in estimating significant additional demands of hydrogen for jet fuel production (66 PJ/year), hydrogen supplied to power plants (41 PJ/year), renewable methane production (36 PJ/year), hydrogen exports (24 PJ/year), renewable ammonia production (23 PJ/year) and road transport (23 PJ/year). Given the lack of information on the assumptions underlying the modelling of these emergent industries, they were not included in this work. However, this would further support the conclusion that CCU is not an economically viable solution for Portugal, as any additional hydrogen demand would have to be met through imports when domestic electrolyser capacity is insufficient.

3.5. Discussion on the viability of CCU

This section assesses the CCU viability within the national Energy System Model, under the developed probabilistic framework. This work represents an important step towards a more robust assessment of the viability of emerging decarbonization pathways within national energy system models (ESMs). It provides quantitative and statistical information on the economic and environmental trade-offs associated with the implementation of a centralised CCU unit in a nation with severe lags in electrolyser deployment. This study also complements the existing approaches for CCU modelling in ESM, as it enables a better understanding of the risks associated with public investments in new energy vectors. This is done by providing statistical grounds to key investment indicators (e.g. the P10-P90 of the NPV), but also by defining the set of conditions which maximise the benefits of CCU at a national level.

Under the assumed business model for CCU implementation at large scale (BOOT business model with a 45-year lifetime), the CCU network delivers net benefits only when a strict set of preconditions is simultaneously fulfilled (as seen in Table 4) and described below.

- **Faster electrolyser capacity deployment:** 7, 8 and 10 GW should be installed by 2030, 2040 and 2050, respectively, to avoid imports leading to higher NPV values.
- **Gradual decline in final energy consumption in Portuguese industry,** associated with increased economic activity and/or changes in final energy intensity. If Portuguese industry's share of the GVA increases on average more than the 50th percentile of historical values (0.06%/year), and/or (less importantly) its final energy intensity decreases less than the 50th percentile of historical values (2.8%/year), CCU would be more advantageous in terms of GHG Emission Avoidance.
- **High Economic Growth**, as measured using the GDP. This occurs because higher GDP levels are associated with increased consumption of low-cost fuels, such as natural gas, resulting in larger avoided emissions between 2050 and 2070, due to CCU deployment. GDP growths higher than the 50th percentile of historical values (1.1, 0.7, 0.5, and 0.4% between 2025 and 2030, 2030–2040, 2040–2050, and 2050–2070, respectively) are good indicators of these conditions.

If these three conditions are not met at the same time, and if current trends for the key variables continue, the most likely (P50) results are: NPV of −54 B€, 57 Mt. CO_2 avoided, and a CO_2 abatement cost of 949 €/tCO_2. As a result, the decision towards decarbonisation should be compared with other investment possibilities before deciding to invest 3.43 B€/year in the CCU network. Despite the high cost of implementing the CCU network, it may still be a viable option if no other cheaper alternatives are found to reduce natural gas emissions by 2050 and meet carbon-neutrality goals (i.e. net-zero CO_2 emissions).

This is particularly relevant considering that the less costly alternative for achieving net-zero emissions is through carbon sequestration in the Land Use, Land Use Change and Forestry Sector, which faces ever increasing risks of carbon reversal in upcoming years. In this sector, about 1.7 to 2.9 Mt. CO_2/year of carbon sinks (P10-P90 range) would be required in the "No CCU" case to achieve zero natural gas-related emissions in 2050 (compared to only 0–0.9 Mt. CO_2 eq/year in the "With CCU" scenario). Even if historical values show this is possible (since 2000, this sink has a median value of −3.6 Mt./CO_2/year), in 2003, 2005, 2016, and 2017, the sector was actually a net emitter of CO_2, due to forest fires (up to 21 Mt. CO_2 in 2017) [61]. Consequently, relying on these carbon emission sinks represents a risky strategy for achieving carbon neutrality, particularly when considering that the probability of wildfires classified as "megafires" (intensities larger than 1000 MW) is expected to occur 2–3.5 times more often compared to the historical period [62]. Therefore, CCU or CCS is likely to serve as a solution through 2050 to deliver the necessary reductions in greenhouse gas emissions.

Another aspect to consider is that CCU is only viable as a direct emissions reduction technology, but not as a life cycle emissions reduction technology. This strategy is designed to reduce CO_2 emissions within Portugal. From a life-cycle perspective, emission reductions within the country's borders may be offset by increases in emissions from fossil-fuel-based electricity generation in other countries. This could occur either in Spain (to meet Portugal's demand for imported electricity) or in the countries that produce the hydrogen imported by Portugal. Therefore, if Portugal adopts a CCU-based decarbonisation strategy, it should also adopt a "consumption-based" decarbonization target, as Sweden does, by extending its national emissions reduction targets to include emissions generated abroad from the production of goods and services consumed in Sweden. [63].

3.6. Work limitations

The limitations of this work are associated with a) the lack of technological detail in building the ESM, b) the use of simplified models to represent pumped storage, grid-scale battery systems, and electric mobility, c) the availability of hydrogen for importation and the uncertainty of electricity importation from Spain and d) the use of triangular distributions for the independent stochastic variables.

The top-down approach used in the modelling lacks the technological detail of bottom-up models such as in the model TIMES-PT. In short, top-down models use macroeconomic data to analyse how the overall macroeconomy and demographics impact energy demand, whereas bottom-up models focus on specific engineering data and technologies to identify the most cost-effective technical solutions to calculate that demand and the cheapest way to fulfil it [64]. The fact that a top-down model was used in this study potentially overlooks the adoption or abandonment of certain technologies as a function of technical and economic variables and how they relate to macroeconomic variables [13] – for example, the effect of evolving electricity prices (as a function of the installed electricity production technologies) in the adoption of electricity-based technologies such as heat pumps. The top-down approach may also overestimate or underestimate the technical potential of direct and indirect electrification across sectors due to the lack of detailed technological representation [8]. For example, industrial clusters may not be able to increase the share of electricity in their final energy demand in areas where electricity grid reinforcements are prohibitively expensive, even if the macroeconomic conditions used as inputs in the top-down model are favourable. Moreover, top-down models may also underestimate the effect that the commissioning of these systems has on the growth of the Portuguese economy, for example, via job creation [4]. Instead of a multivariate relationship among energy demand, GDP, and other system variables, this work uses GDP as the starting point for calculating energy demand. The model's outcomes in each year do not feed back into its calculations, as would occur in more advanced models such as TIMES-PT. The energy demand was calculated in this work as an inelastic relationship with price or climate-change-induced events. This energy-demand modelling also neglects passengers' reactions to higher energy prices, which could be highly relevant levers for reducing demand, creating another feedback loop not considered [16]. Despite these limitations, this study provides a straightforward overview of how a CCU network, grounded in historical trends, could help sharpen the focus on country-level emissions trajectories. Although it could be improved, it provides a rough estimate to alert policymakers to the need for more robust assessments of the role of CCUs in the economy.

Energy storage was also represented in a highly simplified manner. This was done because storage technologies cannot be modelled in LEAP without optimisation. Hydropower pumped storage and centralised battery units were modelled as "dummy electricity generations", i.e., acting as electricity producers when, in fact, they would be discharging electricity produced by other technologies in a previous period. In the model, peak PV production often creates surplus electricity. Without storage, this surplus would be curtailed. By representing batteries and pumped storage as generators, the model effectively assumes that this excess electricity is stored and later discharged to the grid when PV output declines. Therefore, although storage is not modelled explicitly as a charging–discharging process, the approach captures its main system effect - shifting excess PV generation to later periods - and is not expected to materially change the overall result. Despite of that, energy storage capacity is a small fraction of the overall electricity system (as in Fig. 6 and Table 4), and the avoided GHG emissions and NPV show not to be sensitive to these variables. Therefore, we argue that, despite their importance, the simplified mode used for energy storage would not alter the main conclusions of the present study. Electric mobility demand was modelled using two daily load profiles: one for weekdays and one for weekends, based on mobility patterns in the large metropolitan area of Lisbon in 2017 when less than 10% of new vehicles sold each year were electric [53]. No recent information was available to a better estimation on the use of electricity. For example, consumers may prefer to charge at home in the future or charge their vehicles in smart conjunction with electricity grid management in the so-called "Vehicle-to-Grid" regime. However, given the LEAP limitations (modelling without optimisation), this was not performed in this study.

In this work, it was also assumed that hydrogen could be imported from a global market capable of supplying up to 80 PJ/year to Portugal in 2050. If hydrogen is not available for import, synthetic natural gas production would generate no revenue. Under the BOOT model, this would mean that no subsidy would be allocated to the consortium operating the CCU network. It was also assumed that electricity could be imported from Spain up to the full cross-border capacity after 2030. If unavailable, additional electricity, to meet demand, would need to be sourced from natural gas or nuclear power after 2040.

This study also did not consider the potential relocation of industries in response to high energy and ETS prices, nor consumers' preference for cheaper imported goods. These factors could influence total energy demand and the share allocated to electricity or hydrogen [8] [65] [66].

Finally, triangular probability distributions were used to represent uncertainty for parameters where available data were insufficient to reliably define a full empirical probability distribution. Despite that, a defensible minimum and maximum value and a reasonable most-likely value could still be established. However, several variables are highly policy-

dependent and may not follow historical trends over large time horizons adopted in this work. Therefore, future work should include the calibration of the possible evolutions for key independent variables as defined in this work, including their relative likelihood in comparison to each other.

4. Conclusions and future research

This work developed a stochastic energy system model of the Portuguese industrial, residential, transport, and electricity sectors until 2070 and evaluated the Net Present Value (NPV), GHG Emissions Avoided, and Cost of CO_2 abatement of a state-funded commissioning of a centralised Carbon Capture and Utilisation (CCU) network under a Build-Own-Operate-Transfer (BOOT) business model. This was evaluated for 1300 runs varying 14 key input variables. The CCU network was assumed to be commissioned in 2030, capturing 1.8 Mt. CO_2/year and producing 9.3 TWh of methane per year, with an economic lifetime of 25 years, after which the project's ownership is transferred to the state and operated further until 2070. The model was developed with a top-down approach within the Low Emissions Analysis Platform (LEAP) software. Hourly-resolved load and availability curves for 192 time slices were used to estimate energy demand and temporal transformations across the modelled sectors.

Given historical trends in key macroeconomic and technical variables, the commissioning of a centralised CCU network in Portugal is not economically viable and offers limited CO_2 emission-reduction benefits. The NPV (at a 4% discount rate), cumulative GHG emissions avoided and cost of CO_2 abatement (10th to 90th percentile ranges) are, respectively, between −60 to −46 B€, 46 to 69 Mt. CO_2 eq and 800–1121 €/tonne CO_2. This occurs mainly due to two reasons: a) the subsidy attributed to the network's operators between 2030 and 2055 (3.4 B€/year) is much higher than the revenues associated with avoided natural gas imports (up to 412 M€/year, 10th percentile); b) the announced projects for electrolyser capacity in Portugal are unlikely to reach the scale needed to fulfil both the CCU network's demand and the demand of other activity sectors (causing at least 820 M€/year of hydrogen imports in 50% of the scenarios evaluated).

The installed capacity of electrolysers and the growth in Gross Value Added (GVA) share of industry show the strongest correlation with variations in NPV and avoided GHG emissions. Scenario iterations with greater installed capacities of electrolysers have improved NPV because fewer hydrogen imports are needed. However, they are associated with less avoided GHG emissions. This is because in those cases, more natural gas is burnt in power plants to fulfil the country's electrical energy demand, due to the fact that this demand outpaces the installed capacity for the renewable electricity. The growth rate in GVA share of industry was not observed to affect the NPV of CCU significantly, but it does impact avoided GHG emissions. Larger growths in GVA share of industry are associated with higher natural gas demand, and thus, more cumulative CO_2 emissions being avoided in the "With CCU" scenario compared to the "No CCU" scenario.

Only four out of the fourteen variables varied stochastically proved to be statistically significant to predict NPV and GHG emissions avoided. These comprehend, the installed electrolyser capacity growth, the growth in GVA share of industry, the economic growth (GDP) and degrowth rate of final energy intensity. CCU installation has a higher likelihood of reaching 800 €/tonne CO_2 if, it occurs simultaneously the following: Electrolyser Capacity Growth scales up to at least 7 GW in 2030, the GVA share of industry increases more than 0.06%/year, the final energy intensity degrowth is lower than 2.9%/year, and the GDP growth is above 1.1, 0.7, 0.5 and 0.4%/year between 2025 and 2030, 2030–2040, 2040–2050 and 2050–2070.

Centralised CCU for e-methane production may be considered as a viable decarbonization strategy for Portugal if there are no other technologies capable of reducing 1.7 to 2.9 Mt. CO_2eq/year in 2050 with CO_2 abatement costs below 800–1121 €/tonne CO_2. Unless this is proven, CCU should not be considered as a promising solution for the decarbonization of the national energy system in ESM. Unlike cost-optimized ESM from the National Energy and Climate Plan and the Directorate of Energy and Geology, which predict zero imports of hydrogen to fulfil the country's demand during the energy transition, it is shown that prioritising early CCU development before hydrogen infrastructure is in place could lock the country into large-scale hydrogen imports (potentially exceeding 80 PJ by 2050), from uncertain suppliers, thereby worsening energy security and increasing dependency risks.

Future work can cover the limitations previously identified. A broader range of potential outcomes for the Portuguese energy system may be covered (and thus, a more representative distribution of possible results for NPV and GHG emissions avoided) if the following aspects are included in future modelling efforts: a more detailed bottom-up modelling of the ESM, a recursive calculation of GDP and other macroeconomic variables (instead of a unilateral relationship between the two variables), an adequate modelling of energy storage in pumped storage and utility-scale battery systems, an update of electric vehicle charging patterns as well as their potential sector integration with the electricity system via vehicle-to-grid mechanisms and, finally, the adequate modelling of foreign supply of hydrogen and electricity.

Lastly, the re-design of the CCU deployment into a decentralised, modular, small-scale units in hard-to-abate industrial sectors could also be proposed as a future research work to evaluate the potential benefits of such approach when compared to the evaluated centralised deployment.

CRediT authorship contribution statement

Gustavo P. Rangel: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **João F. Moura:** Writing – review & editing, Formal analysis. **Hugo R. Matias:** Writing – review & editing, Supervision, Resources, Conceptualization. **Belmira Neto:** Writing – review & editing, Supervision, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.apenergy.2026.129221.

Data availability

Data will be made available on request.

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