The optimal is not always the best
Life cycle impacts of near-optimal energy systems

de Tomás-Pascual, Alexander; Pérez-Sánchez, Laura; Sierra-Montoya, Miquel; Lombardi, Francesco; Pfenninger-Lee, Stefan; Campos, Inês; Madrid-López, Cristina

DOI
10.1016/j.apenergy.2025.126487

Publication date
2025

Document Version
Final published version

Published in
Applied Energy

Applied Energy 399 (2025) 126487

Contents lists available at ScienceDirect

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy

The optimal is not always the best: Life cycle impacts of near-optimal energy systems

Alexander de Tomás-Pascual [a,*], Laura À. Pérez-Sánchez [a], Miquel Sierra-Montoya [a], Francesco Lombardi [b], Stefan Pfenninger-Lee [b], Inês Campos [c], Cristina Madrid-López [a,*]

[a] Institut de Ciencia i Tecnologia Ambientals ICTA-UAB, Universitat Autònoma de Barcelona, Bellaterra, Cerdanyola del Vallès 08193, Spain
[b] Faculty of Technology, Policy, and Management, TU Delft, Netherlands
[c] Centre for Ecology, Evolution and Environmental Changes (CE3C), Faculty of Sciences of Lisbon University, Campo Grande, 1749-016 Lisboa, Portugal

HIGHLIGHTS

- We analyze 260 near-optimal energy system designs for Portugal in 2050 using LCA.
- Near-optimal system designs can outperform the cost-optimal one regarding environmental impacts.
- More technological diversity in the energy system can lead to higher environmental impacts.
- System designs emphasizing wind over solar PV and batteries consistently yield lower environmental impacts.

ARTICLE INFO

Keywords:
Energy system optimization models
Life cycle assessment
Energy transition
Environmental impacts
Technological diversity

ABSTRACT

Energy system optimization models (ESOMs) can be used to guide long-term energy transitions but often overlook environmental impacts and the diversity of solutions close to the cost-optimal one. Here, we combine an ESOM using Modelling to Generate Alternatives (MGA) with Life Cycle Assessment (LCA) to evaluate 260 near-optimal and technologically diverse carbon-neutral energy system designs for Portugal in 2050 across five environmental indicators: climate change, land use, water use, ecotoxicity, and materials. Using the Calliope energy modelling framework and ENBIOS for environmental assessment, we find that system designs whose cost is within 10 % of the minimum feasible cost provide up to 50 % lower environmental impacts. Our results reveal a trade-off between technological diversity and environmental performance, showing that while diversity enhances resilience, this may come with a significant increase in environmental drawbacks. Solar photovoltaic and battery technologies dominate the environmental impacts, particularly in water consumption and critical material use. This study shows that traditional cost-optimal energy system designs may not be environmentally optimal. Exploring near-optimal alternatives reveals lower-impact solutions and supports more inclusive planning for energy transitions.

1. Introduction

Energy system optimization models (ESOMs) are widespread tools to inform policymaking [1]. They do so by finding the system design or planning strategy that enables achieving a given policy target, such as carbon neutrality, at the minimum cost. In order to optimize the energy system design, ESOMs use projected assumptions on system cost and renewable resource availability, energy demands, network topology, and various technical constraints [2].

Despite their value for decision-making, ESOMs have two key limitations. First, ESOMs equate the “cheapest” solution (techno-economically optimized) with the “best” solution. By doing so, they ignore the fact that slightly more “expensive” but different alternatives may offer advantages such as better political agreement, transition speed, or public opinion [2–8]. Second, ESOMs often lack transparency and robust handling of structural and parametric uncertainties [9]. While methods like stochastic programming mitigate parametric uncertainty (related to the input data), structural uncertainty-arising from the difference between the model and the real world- has gained attention in recent years.

* Corresponding authors.
E-mail addresses: cristina.madrid@uab.cat, alexander.detomas@uab.cat (C. Madrid-López).

https://doi.org/10.1016/j.apenergy.2025.126487
Received 16 January 2025; Received in revised form 4 June 2025; Accepted 15 July 2025
Available online 25 July 2025

As a perfect example of a "wicked problem" [10], the energy transition is ambiguous and constrained by the interdependencies between technological, societal, and environmental factors. This complexity amplifies the uncertainties in modelling, especially when key social and environmental aspects are overlooked. A narrow focus on technological or economic goals can result in overly optimistic, unrealistic transition pathways, ignoring constraints like resource limits or social resistance. Excluding these factors risks creating inefficient, inequitable solutions that can lead to unforeseen challenges and impractical, disruptive outcomes [11].

The Modelling to Generate Alternatives (MGA) method [12], first applied to energy system models by DeCarolis [13], addresses part of this structural uncertainty by searching the feasible, near-optimal region of the energy system design space for alternative configurations that may account for "unmodelled" objective. This method acknowledges that achieving a perfect representation of real-world behaviour is unattainable and that practically viable solutions may not align with the modelled cost-optimum nor with the "Pareto-optimal" solutions reflecting a handful of explicit objectives. The near-optimal region of solutions in MGA provides a regional and technological diversity of configurations, making it possible to generate debate with stakeholders with different interests and visions, and evaluation of dimensions that are difficult to insert in an optimization function. This methodological exploration of near-optimal solution spaces for enhanced multi-criteria performance finds parallels in diverse fields, such as the use of meta-heuristic approaches to explore energy-efficient and demand-responsive production scheduling in manufacturing systems under time-of-use electricity pricing [14]. The MGA approach has been mostly used to design electricity supply systems [2,4,13,15–19]. In some cases, it has also addressed the whole energy system [20–22]. This approach has sometimes addressed direct greenhouse gas and particulate matter emissions [4,16]. However, an MGA analysis has not yet been used to assess a wide array of environmental impacts.

Resilience theory offers one approach to understanding a system's ability to cope with changing circumstances and disruptions [23]. Although the concept of resilience can be broad and somewhat ambiguous, in the context of energy systems, it is closely associated with diversity and interconnectedness [24]. Several studies have analysed how diversity contributes to resilience in energy matters [25–27]. However, while the positive link between diversity and resilience is well established [25], the potential trade-offs between resilience and environmental impacts remain underexplored.

In light of global challenges such as climate change and geopolitical instability, building resilient energy systems is increasingly critical. A diverse array of electricity production sources can help mitigate risks and ensure continuity under disruptive conditions. For example, Mühlemeier et al. [25], demonstrated this concept by quantifying the diversity and connectivity of energy systems to assess the resilience of the transition to an energy system based on renewable sources. Yet, despite the recognized benefits of diversity for resilience, its environmental implications are still not understood. On the other hand, while the positive relationship between energy system diversity and resilience is well-established, there remains a significant gap in our understanding of the environmental implications of highly diversified energy systems.

This study contributes to closing the gap between energy system optimization models based on the Modelling to Generate Alternatives (MGA) and broad-spectrum environmental impact assessment. We present the environmental analysis of a techno-economically defined option space of 261 different energy transition configurations in Portugal for 2050. This methodological integration serves a dual purpose. First, it highlights the benefits of presenting policymakers with a range of energy transition alternatives, which can be evaluated based on criteria that go beyond what is accounted for by the original ESOM. This enables better-informed and flexible decision-making. Second, specific to our LCA assessment, it helps policymakers better understand environmental impact trade-offs, facilitating that sustainability considerations are integrated into long-term planning.

To achieve this, we link two open-source frameworks: Calliope, an energy system modelling framework, and the Environmental and Bioeconomic System Analysis (ENBIOS) tool, an analytical tool that integrates Life Cycle Assessment (LCA) with the Multi-Scale Integrated Analysis of Societal and Ecosystem Metabolism (MuSIASEM) framework. These tools allow us to address three research questions: (1) How do the environmental impacts of a single-solution optimization compare to the impacts of a range of alternatives produced by an MGA method? (2) In what ways do environmental impact trade-offs shift with variations in the technological mix? (3) What is the relationship between technological diversity in electricity production and environmental impacts?

By addressing these questions, this study not only contributes to answering the calls for closing the sustainability gap in energy system modelling but also contributes to generating insights into the understanding of the complex interplay between system diversity, technological choices, and environmental outcomes.

This work has been carried out in the context of the project CHIST-ERA project SEEDS (Stakeholder-Based Environmentally-Sustainable and Economically Doable Scenarios for the Energy Transition) [28], which aimed to integrate stakeholders co-design, energy modelling, and environmental assessment.

2. Methods

To address the research questions outlined in Section 1 (linking system diversity, technological choices, and environmental outcomes), we integrate two computational frameworks: Calliope for energy system modelling (Section 2.2) and ENBIOS for environmental impact assessment (Section 2.3). We demonstrate this approach through Portugal's 2050 energy transition (Section 2.1).

2.1. Case study

We assess the environmental performance of a techno-economically defined option space of 261 different energy transition configurations in Portugal for 2050. Portugal has set highly ambitious goals in its National Energy and Climate Plan. These goals include reducing greenhouse gas emissions in 45–55 % by 2030 (compared to the baseline year of 2005), with 80 % of its electricity production sustained by renewable sources, and a reduction of 65 % in energy dependency. Its decarbonisation policies will entail significant investments in solar, wind, offshore wind, and green hydrogen technologies. Despite these ambitious goals, Portugal is highly vulnerable to climate change impacts and environmental degradation [29]. The country is equally financially constrained in the European context [30], with wide-ranging energy poverty problems [31]. Portugal, thus, offers a good case study to leverage trade-offs between technological choices, socioeconomic challenges, and environmental concerns.

Part of the parameters considered in energy modelling were fine-tuned according to the narrative assessment completed within the SEEDS project [32]. The narratives were identified using interviews, focus groups, workshops, and Delphi surveys. We identified two main groups of narratives within Portuguese policy and regulatory frameworks. The mainstream narrative reflects the fossil-fuel-based socio-technical paradigm, emphasizing centralized renewable systems, top-down governance, economic growth, and new energy exports. In contrast, the alternative narrative focused on energy democracy and decentralized governance, promoting socio-technical innovations like energy communities, citizen-led investments, and peer-to-peer exchanges.

2.2. Energy system model and Modelling to Generate Alternatives

We developed multiple energy transition configurations using the

Calliope framework, an open-source tool that allows building energy system models while keeping user-friendly characteristics [33]. The framework is based on linear programming algorithms while also accepting mixed-integer optimization, helping to design energy systems in which renewables play a prominent role. Calliope's key features include handling high spatial and temporal resolution and easily running on high-performance computing systems. Moreover, Calliope provides an in-built MGA functionality based on the highly customizable SPORES MGA algorithm (see Section 2.2.1). The basics of the Portuguese model are covered below (see Section 2.2.2).

2.2.1. The SPORES MGA approach

Energy system optimization models typically identify a system configuration to reach a target with the minimum cost [9]. Nevertheless, focusing on a single solution may hide feasible but perhaps radically different alternatives [13]. Similarly, generating a set of Pareto-optimal solutions with multi-objective optimisation may be insufficient, given the countless objectives that matter in the real world [12]. This is particularly notable for an energy transition issue involving many heterogeneous stakeholders across scales. Accordingly, the popularity of modelling to generate alternatives (MGA) approaches has increased dramatically in this field in the last few years [34]. Among the many MGA methods tailored to energy system optimization, SPORES - or Spatially Explicit Practically Optimal Results [35] - is designed particularly to target both spatial and technological diversity within the generated system configuration options while also allowing for a good degree of parallelisation and efficient computation. Here, we apply SPORES to Portugal as a case study, generating over 261 different energy transition configurations for the year 2050.

More precisely, the 261 solutions (which we also call "SPORES", as the method that generates them) are obtained based on the workflow depicted in Fig. 1, which builds on recent work from our author team [22] and leverages SPORES capacity to use different MGA objectives in parallel to explore the option space efficiently and effectively. In a nutshell, the cost-optimal solution is identified as the starting point. Then, SPORES search for new feasible solutions that diversify the technologies deployed and are compared to the previous solution(s).

Mathematically, this results from incrementally assigning penalties, or weights, to spatially explicit capacity investment decision variables that featured prominently in previous solutions. As highlighted in Fig. 1, many runs expand the above search by using a multi-MGA-objective formulation, which combines the search for spatially and technologically distinct solutions with the intensification of specific system features, for instance, the high or low deployment of a given technology. We call "intensification" the push for a given feature to be either at its minimum or maximum feasible value. As shown in previous work [36] the use of "intensification" objectives ensures that we capture extreme technological boundaries of the solution space and otherwise hard-to-discover system configuration options. In all runs, we force the generated near-optimal solutions to be within 10 % of the cost of the least-cost feasible solution. This relaxation is in line with previous studies [18,21,35] and within the range of the relaxations deemed realistic by studies that look into empirical evidence for willingness to pay for features of interest in system design [37].

In practice, we generate a total of 80 SPORES in four parallel batches using the default single-MGA-objective (Eq. 1, b = 0) applied to the decision variables of four different energy sectors: power ($n = 50$ SPORES), heating, mobility and synthetic fuels ($n = 10$ per sector). Then, we generate up to 180 SPORES across multi-MGA-objective batches (Eq. 1, b ≠ 0) that alternatively maximize (n = 10) or minimize (n = 10) each of the following nine critical technology assets: wind onshore, wind offshore, wind overall, open-field solar PV, roof-mounted solar PV, biofuels, battery storage, electrolysis and transmission capacity. This leads to a total of 260 (80 + 180) different system SPORES, or 261 when including the cost-optimal solution used as the starting point.

The SPORES optimisation problem can be formulated as in **Eq.1**.

$$\min Y = a\cdot\sum_j\sum_i w_{ij}x_{ij}^{cap} \pm b\cdot\sum_j x_{ij}^{cap}$$

$$\text{s.t.} \, \text{cost}_n \leq (1+s)\cdot\text{cost}_0$$

$$\boldsymbol{Ax} \leq \boldsymbol{b}.$$

$$x \geq 0 \tag{1}$$

where *i* and *j* indicate the *i-th* technology category and the *j-th* location in the model; *xcap_ij* is the capacity investment decision variable for the *ij-th* location-technology pair; and *xcap_(i)j* is the capacity decision variable associated with a technology that we may want to intensify in the resulting technology mix. Wij is the weight assigned to the capacity investment decision variable *ij-th* location-technology pair. The weight is assigned incrementally at each iteration, penalising those decisions that have already been explored, as described in prior work [22]. The *a* and *b* coefficients are the weights associated with the different components of the objective function: when *b* has a positive sign, we minimize the "intensified" technology; when *b* has a negative sign, we maximize it. If *b* is null, the formulation collapses into the default case with a single objective (Fig. 1)). *A*, and *b*, are a matrix and a vector of coefficients

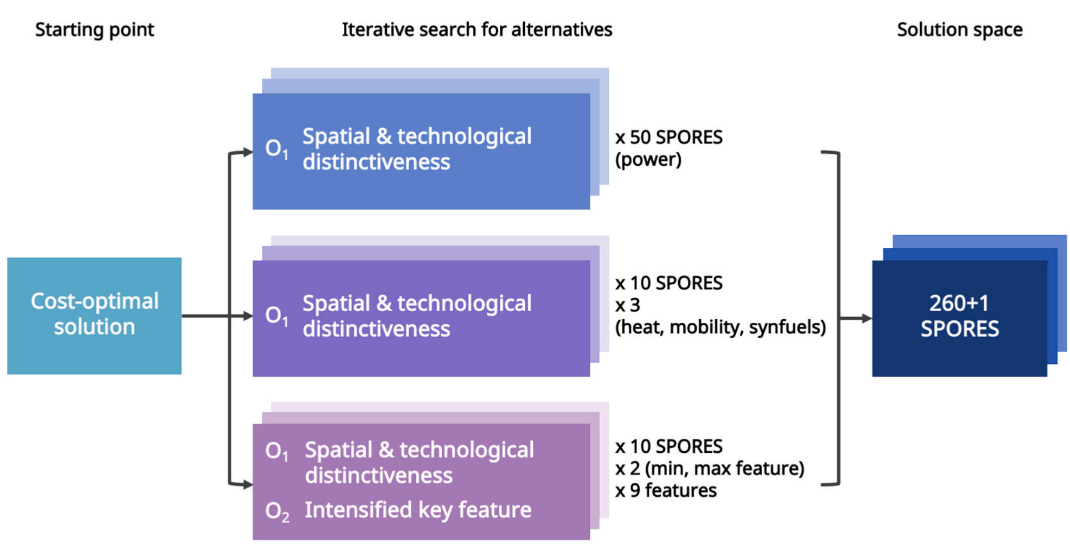

Fig. 1. Conceptual representation of the SPORES workflow we adopt in this study.

representing the physical constraints of the problem, while x is the vector of decision variables; $cost\_n$ is the total annualised system cost, which is bound to remain within a marginal relaxation of the optimal cost *(cost0)*; and s is the accepted cost relaxation, also known as cost slack.

2.2.2. The Portuguese Calliope model

The Calliope-Portugal model is derived from the existing Sector-Coupled Euro-Calliope model, which encompasses all European countries' energy sectors (electricity, heat, transport, and industry). [21]. In the version of Calliope-Portugal used in this paper [22], we increased the spatial granularity of wind and solar resources by adopting the finer-resolution data for Portugal available from the Euro-Calliope model [5]. The model forces supply to meet the demand using energy technologies that have no direct emissions or whose emissions can be compensated by capture. This results in a system based on renewables, sustainable biofuels, and green hydrogen and synthetic derivatives fuels. We split Portugal into two macro-nodes, North and South. These are connected via electricity transmission lines. We considered the network's constraints and the Sector-Coupled Euro-Calliope's expansion potential. Within each of the macro-nodes, the model can deploy renewable power capacity in many sub-regions (18 in total), corresponding to the country's administrative regions, with different land availability and capacity factors.

We replaced other European countries with a stylised representation of the import and export of electricity and hydrogen at a fixed price. The price reflects the historical average electricity price for trade with neighbouring Spain. The price per kWh for hydrogen is calculated assuming a market price of 1.5 EUR/kg for green hydrogen in 2050 and 33.3 kWh/kg as the lower heating value.

We set the weather year to 2016, having identified it as a "typical" year among those available from the Euro-Calliope dataset. For additional model assumptions and their rationale, we refer the readers to the publication that first introduced the Sector-Coupled Euro-Calliope model [21]. The Calliope-Portugal model files are publicly available on Zenodo [38] as part of a prior publication from the SEEDS project [22].

2.3. Environmental modelling with ENBIOS

ENBIOS (Environmental and Bioeconomic System Analysis) [39] is an analytical framework and Python-based tool for the environmental assessment of energy transition scenarios. It integrates Life Cycle Assessment (LCA) –using the Brightway2 [40] LCA framework– and the Multi-Scale Integrated Analysis of Societal and Ecosystem Metabolism (MuSIASEM). In this work, we have further developed the connection between Calliope and ENBIOS 2.1.12 to model the environmental impacts.

This section summarizes the ENBIOS methodology, as depicted in Fig. 2. For an extensive explanation, see the Supplementary information.

2.3.1. LCA settings

The functional unit is the satisfaction of one year of energy demand, keeping the analysis at the national level due to the lack of regionalized life cycle inventory (LCI) data. In LCA jargon, the foreground system includes all modelled technologies, such as energy generation, storage, imports and conversions (e.g., biofuel to methanol). A "technology mapping"linked the energy model to LCA data using Sparks [41], a module developed for soft-linking ESOM and ENBIOS.

LCI data was sourced from the ecoinvent 3.9.1 cutoff database [42], considering Portugal as the primary location for activities whenever possible. Hydrogen-related inventories were sourced and adapted from the literature. The supplementary materials (section 0) provide a full breakdown of all data sources, assumptions, and modifications.

We incorporated 2050 projections into the background system to account for future technological developments and updated global electricity markets based on these projections. [43]. Electricity markets are aligned with regional projections from a 2 °C scenario as described by Junne et al. [44]. However, we did not modify individual technology parameters (e.g., efficiency, material intensity). We aim to demonstrate the benefits of coupling MGA with LCA to explore option spaces rather than to calculate absolute environmental impacts. Double-counting impacts were avoided by modifying the LCI database to remove downstream connections as proposed by Volkart et al. [45].

We used the life cycle impact assessment methodology ReCiPe midpoint 2016 v1.03 with a hierarchical (mid-term) perspective [46]. From this method, we selected the following impact categories: climate change (*global warming potential*), land use (*agricultural land occupation*), water use (*water consumption potential*), ecotoxicity (*freshwater eutrophication potential*) as they are covered in the literature as the most important impacts of energy transition technologies.

2.3.2. Upscaling and trade-offs with MuSIASEM

The soft-linking approach was complemented by a bottom-up characterization of the energy system using the MuSIASEM framework. Fig. 3 shows the MuSIASEM dendrogram, a hierarchical energy system representation covering the aggregation distribution at different analytical levels. We used the dendrogram to connect two specific levels: n (energy system level) and n-3 (technological level). The information from the n-3 level is the one soft-linked to the LCA modelling in ENBIOS.

To examine the trade-offs between environmental impacts, we applied linear regression coefficients to assess the relationship between indicators. In this case, the analysis specifically concentrates on the relationship between the dendrogram levels n (energy system) and n-3 (specific technologies). This differentiation allows us to compare the most aggregated view of the energy system (n) with a more detailed breakdown (n-3). With this link, we assessed how the system's

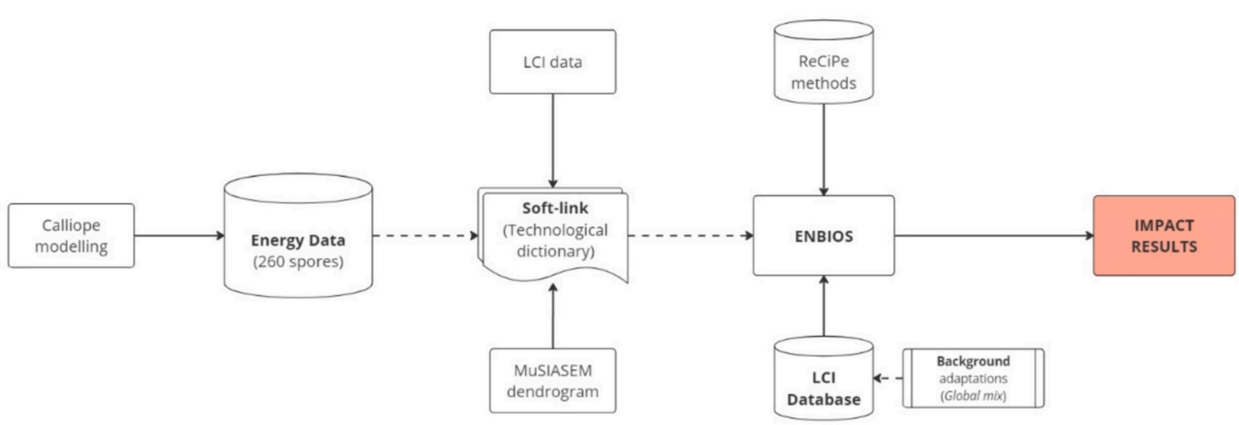

Fig. 2. Summary of the structure of the analysis with ENBIOS.

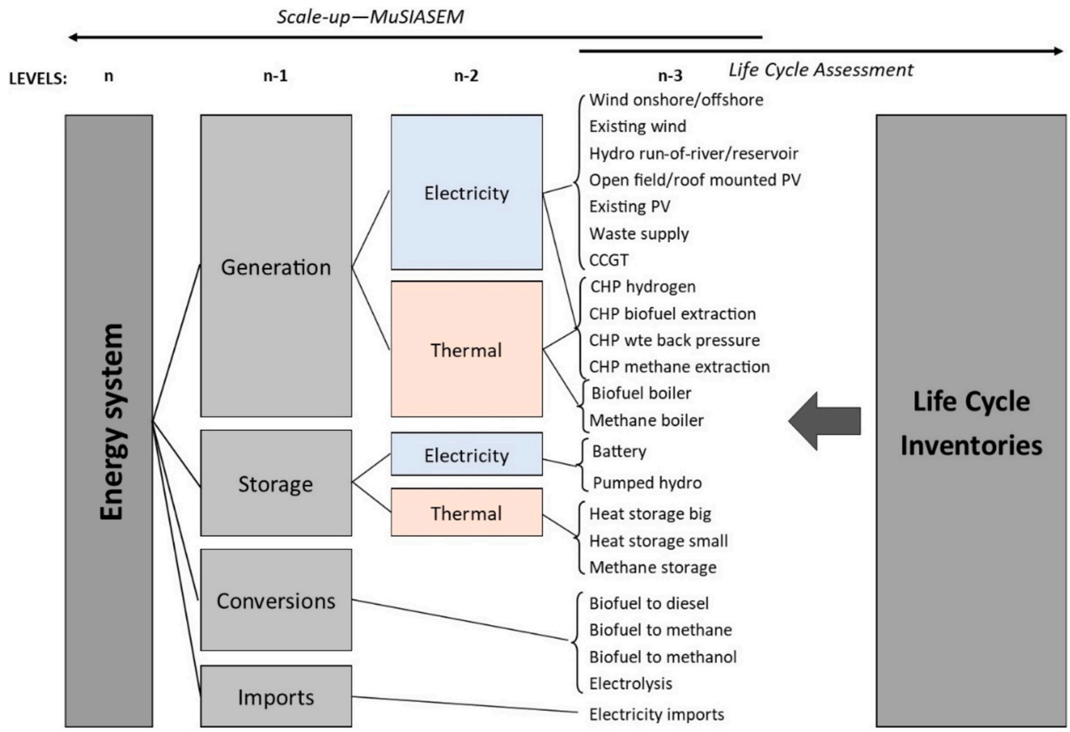

Fig. 3. Dendrogram of the energy system under analysis, showing the hierarchical representation at different levels. The level n-3 is linked to Life Cycle Inventories.

environmental impacts change with increasing granularity.

Additionally, we used Spearman-Rank correlations, a non-parametric measure of rank correlation, to examine the influence of different technologies or dendrogram levels on the total environmental impact. Spearman's method is particularly useful for detecting monotonic relationships between variables without assuming linearity [47]. This approach allows us to understand how the various components contribute to the overall environmental impact of the energy system.

We explored the influence of the diversity of energy production and the environmental impacts. To this end, we used the Gini-Simpson index [48] as a measure of diversity (**Eq. 2**) and compared the configurations with the top and bottom 5 % diversity values.

$$D = 1 - \sum_{i=1}^{S} p_i^2 \tag{2}$$

where p is the proportion of electricity produced by technology i in a given configuration, and S is the total number of technologies.

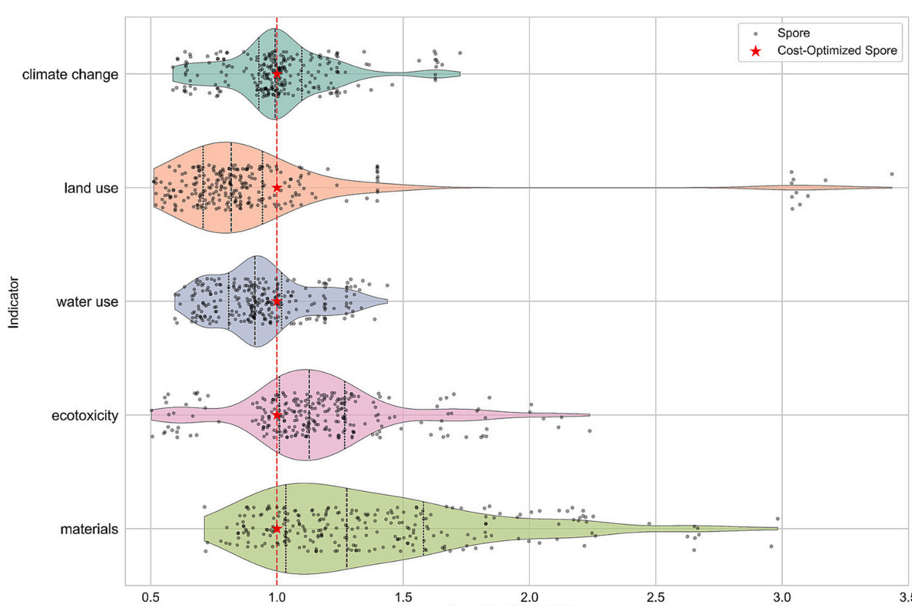

Fig. 4. Environmental impacts of the different energy configurations, normalized according to the cost-optimized configuration at the energy system level (n). The vertical red line highlights the optimized configuration's position across different indicators. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

3. Results

3.1. *Breaking the single cost solution: Environmental trade-offs in the option space*

The Calliope-Portugal model returned one option space of 260 alternative energy transition configurations. We then compared the environmental impacts of the single cost-optimal solution with the results of the option space. Our results indicate that the single optimal solution (cost-optimized spore) is not the configuration with lower environmental impacts within the option space generated by the model, as illustrated in Fig. 4. Compared to the option space, the cost-optimized solution leads to higher impact values for land use (over Quartile 3, >Q3) and water consumption (≈Q3), a median value for global climate change, and lower impact values for ecotoxicity (Q1) and material use (<Q1).

3.2. *How impacts vary with the technology mix: Relevance of wind, solar, and batteries*

To evaluate the SPORES outcomes, we analyze trade-offs between impacts and technologies. To this end, we first looked for correlations among the environmental impacts at the energy system level (n). Our analysis revealed no significant trade-offs across the various environmental impacts (see **Fig. S4**).

We investigated the main drivers of the environmental impacts for the whole energy system (n) and the different energy system technologies (TWh) (n-3) using Spearman rank correlations Fig. 5. We observed two significant positive correlations: batteries with material use ($\rho = 0.9$) and open PV panels with water use ($\rho = 0.89$). These results indicate that increasing the energy production of these technologies generally leads to higher impact configurations for these indicators. Also, we found that wind onshore negatively correlates with the different environmental impacts (Fig. 5).

To determine the causes and explanations behind this result, we looked at the correlations in the energy configuration definitions of the different spores. We found that open-field PV and wind onshore electricity production are negatively correlated ($r = -0.64$), as shown in **Fig. S3**. A significant deployment of one technology generally implies a low existence of the other. In the same direction, a negative correlation exists between wind onshore and batteries($r = -0.63$). Therefore, the Spearman correlation indicates a negative correlation of wind onshore, as the more wind onshore installed, the less solar PV and batteries, which translates into a lower overall impact configuration.

Further results support this statement: the configurations with the maximum amount of wind and minimum solar technologies perform better (in environmental impacts) than those with a high amount of solar and minimum wind (Fig. 6). Additionally, Fig. 6 shows that configurations with maximum battery deployment perform poorly across all studied indicators.

When analysing Fig. 6, two factors are crucial: total demand and efficiency. Environmental impact scales linearly with demand, meaning technologies with higher demand in specific configurations lead to greater impacts. In contrast, efficiency modulates these outcomes by producing lower environmental impacts per unit of energy output. **Fig. S6** presents the relative normalized impact values of various technologies per unit of energy produced. Wind and solar technologies demonstrate lower impact values than other energy sources, whereas batteries show considerably higher impact intensities. This observation is further supported by **Fig. S5**, which shows that solar and wind technologies exhibit higher impacts due to their large-scale deployment, despite their lower impact values per unit of energy.

On the other hand, batteries have a significantly higher impact intensity per unit of energy produced (flow out in this case), reflecting their lower life-cycle efficiency. This is a noteworthy consideration given the limited availability of battery systems across the various configurations compared to wind and solar technologies (**Fig. S5**). It is important to note that wind and solar technologies have a lower impact than other technologies, but solar tends to return higher impacts than wind turbines. For example, solar technologies have a climate change impact 4 times higher than wind turbines and can occupy up to 20 times more land (**Table S3**).

Finally, contribution analysis reveals that silicon (multi-Si) production is the dominant factor driving the water use on solar panels, accounting for 93 % of the impact). In contrast, the surplus ore potential of batteries is primarily influenced by the production of lithium hydroxide (41 %) and NCA hydroxide (cathode, 20 %).

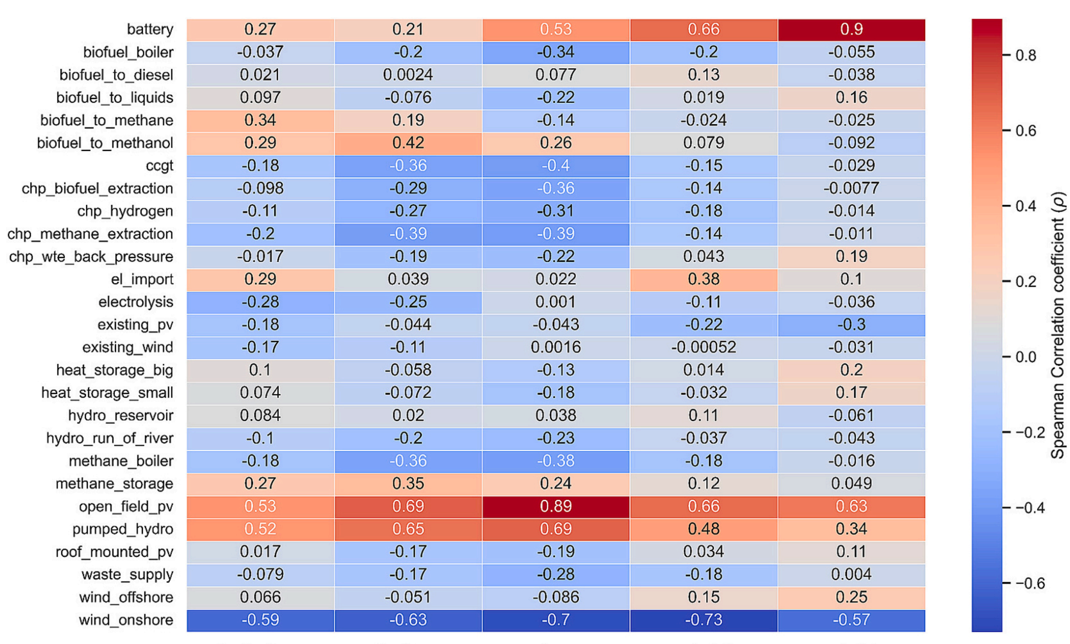

Fig. 5. Spearman correlation values.

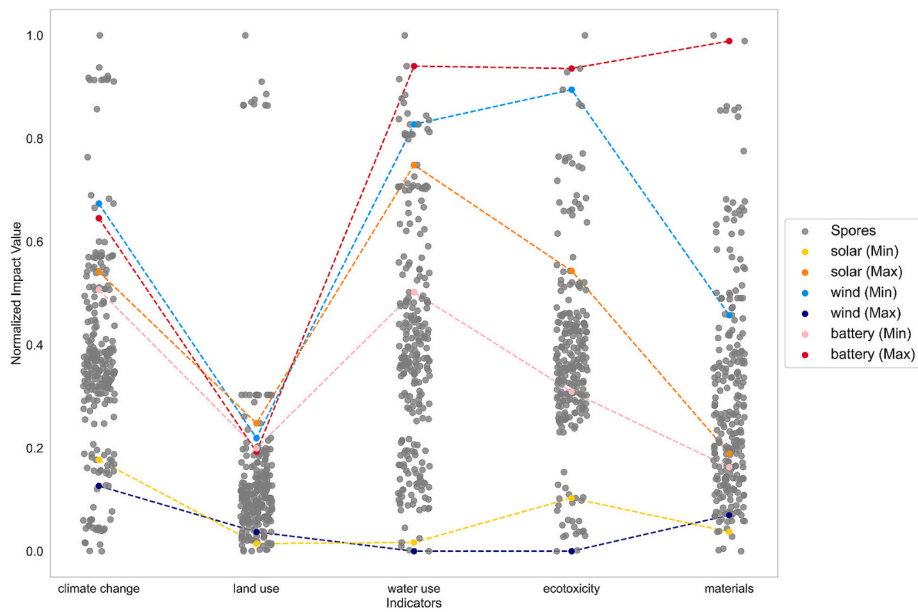

Fig. 6. Environmental impacts of the different spores. To compare different units, results have been normalized between 0 (min impact) and 1 (max impact). Lines show different energy configurations with minimum (*Min*) and maximum (*Max*) production of wind, solar, and battery technologies.

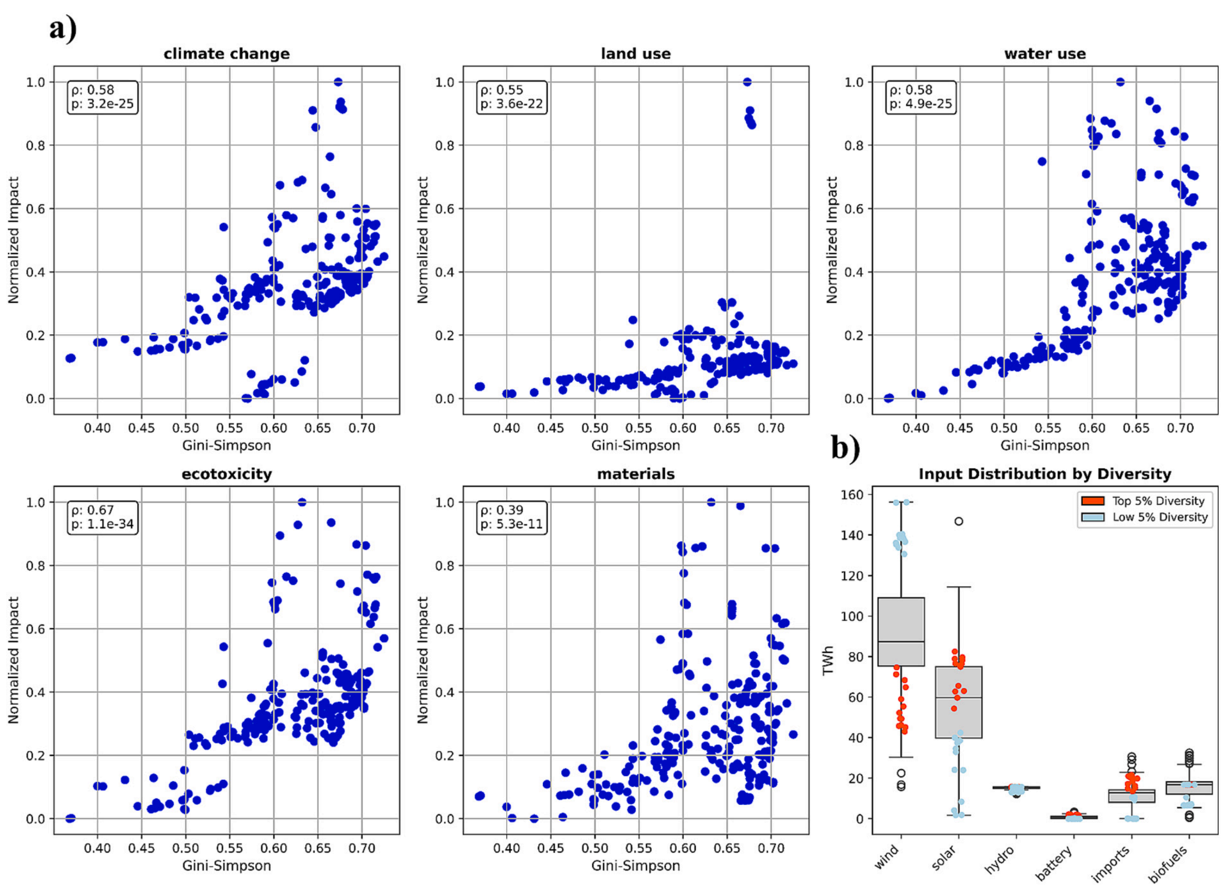

Fig. 7. a) Normalized environmental impacts of SPORES (blue) plotted against the Gini-Simpson diversity index. Spearman rank correlation coefficient (ρ) and corresponding *p*-value (p) are reported. Environmental impacts are normalized to a scale from 0 (minimum impact) to 1 (maximum impact) for comparability across indicators. **b)** Contribution of each technology group to electricity production in selected SPORES (TWh). The five SPORES with the highest and lowest diversity (top and bottom 5 %) are highlighted. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

3.3. Higher technological diversity correlates with increased environmental impacts in energy configurations

We examined the trade-off between the diversity of electricity production technologies and the environmental impacts. As depicted in Fig. 7, our findings suggest a positive trend: energy system configurations characterized by greater technological diversity exhibit higher environmental impacts. This positive relationship is statistically significant ($p < 0.01$), and the strength ranges from moderate ($\rho = 0.39$) in the case of materials to strong ($\rho = 0.67$) for ecotoxicity.

The observed trends align with our previously discussed results and are shaped by the distribution of solar, wind, and battery technologies. Fig. 7 (b) shows the relevance of each technology's electricity production (TWh) in the top and bottom 5 % configurations based on the diversity index. Technologies are grouped into categories (e.g., wind onshore and offshore into 'wind').

The top 5 % most diverse configurations are characterized by low amounts of wind and high proportions of solar, batteries, and imports compared to other alternatives. On the other hand, the bottom 5 % of diverse productions are dominated by extremely high amounts of wind while having low amounts of solar, batteries, imports, and biofuels. Thus, low diversity configurations are mostly dependent on wind technologies, which have lower environmental impacts compared to other alternatives.

4. Discussion and conclusion

In this work we *assess if accepting structural uncertainty in the modelling of energy systems helps us find more sustainable configurations*. To do this, we integrated the MGA approach to energy system optimization using a Calliope-based model and a broad-range environmental assessment completed with the ENBIOS framework. We completed a case study for Portugal using the results of a narrative assessment to identify key energy parameters for modelling.

Our results emphasize that energy system optimization models based on MGA are able to produce a diversity of solutions with a wide range of environmental impacts. This study is the first to integrates modelling to generate alternatives (MGA) for an energy system alongside life-cycle environmental assessment. We found that slightly more costly configurations than the cost-optimal solution can lead to equally feasible configurations with reduced environmental impacts. The impact of cost relaxation (5–10 %) translates into a distribution of environmental impacts, ranging from 50 % less impact to 350 % higher values. These findings add weight to the previous criticism of techno-economic cost-optimized energy system models, which often fail to capture the true costs of energy transitions, as Trutnevyte shows [37]. Relying on single-solution cost-optimized models may not only result in poorly represented real-world systems but also restrict the exploration of equally feasible alternatives that could offer lower environmental impacts and potentially lower public resistance.

This approach makes the relation between technological diversity and impacts more explicit. Our results suggest that configurations with a higher diversity of technologies involved in electricity production tend to produce higher environmental impacts than those focusing on larger shares of wind technology. This result generates a new trade-off, as more diverse energy systems are generally associated with higher resilience [49], highlighting a potential tension in the coordination of energy planning and environmental policy. As highlighted by Jesse et al. [23], the question "*resilience against what*?" becomes particularly relevant. Clarifying the types of risks that resilience strategies aim to address is essential when evaluating whether increased diversity—and its associated impacts—are justified. In the context of energy transitions, where long-term structural changes are being implemented, such trade-offs need careful consideration. Multi-criteria decision analysis and portfolio optimization frameworks can be used in policy-making to systematically weigh the benefits of resilience against environmental costs, enabling the identification of technology mixes that meet both reliability and sustainability targets.

Building on these insights, it is important to consider the role of model structure and data uncertainty in shaping the results. The results are highly influenced by the balance of solar, wind generation technologies, and batteries. In this sense, two additional considerations arise from this: first, results are highly dependent on the model definition and constraints, such as maximum installed capacities allowed, that translate into a more diverse option space for wind and solar capacities (**Fig. S6**).

Second, the uncertainty of the life cycle inventories used also plays a significant role in this sense, most importantly for wind and solar as the main energy producers of the system. Our uncertainty analysis revealed high uncertainty in the results distributions [50]. However, we did not assess the uncertainty of individual inventory datasets, meaning our results strongly depend on the accuracy of the inventory data provided by ecoinvent. We refer to our previous report for a more detailed discussion of uncertainties, including methodological assumptions and data reliability (de Tomás-Pascual et al. [51]). Finally, we acknowledge the limited treatment of biogenic carbon as a result of the environmental modelling approach using the ReCiPe Midpoint H 2016. Specifically, these methods do not account for carbon sequestration resulting from the growth of biogenic components, which could provide a natural offset of some emissions.

Still, regarding specific technologies, our results suggest that solar and battery technologies are the primary contributors to the total environmental impacts. In particular, solar PV panels significantly drive water use, with a contribution analysis identifying multi-crystalline silicon (multi-Si) production as the leading cause. Previous studies, such as Golroudbary, Lundström, & Wilson [52], highlighted the high water and energy demands of multi-Si manufacturing while pointing to potential efficiency improvements and material consumption reductions across the value chain.

Conversely, batteries exhibit a substantial environmental impact per unit of energy compared to other technologies. Particularly, our results showed a strong correlation between battery deployment and the total environmental impacts. Contribution analysis indicates that the production of lithium hydroxide and NCA (nickel-cobalt-aluminium) is a major contributor to this impact. This is primarily due to the relative scarcity of critical materials such as lithium, nickel and cobalt, which increase their environmental footprint. This issue is projected to worsen as greater quantities of raw lithium brine must be extracted to meet the demand for battery-grade lithium [53]. Lithium mining extraction is likely to advance specifically in Portugal, which holds the largest reserves in Europe [54], with at least five major projects under development, although no active mines are currently operational, largely due to environmental concerns and local opposition [55]. Furthermore, emerging technologies like Li-air and Li-S could increase lithium demand in the future. However, the same authors also emphasize the potential benefits of battery reuse and recycling, although significant technical, economic, and safety challenges remain to be addressed [56].

To the best of our knowledge, this study is the first to integrate modelling to generate alternatives (MGA) for an energy system alongside life-cycle environmental assessment. Several authors have previously reported on holistic approaches to the environmental impact of energy systems [44,45,57–59]. However, this study uniquely combines the MGA approach with LCA.

This approach has significant operational applicability. Policymakers can leverage MGA-LCA to develop robust energy strategies that are resilient to future uncertainties, using the generated alternatives to understand the diverse implications of different policy choices. Utilities and regional planners can employ this method to evaluate investment in new energy infrastructure or resource management plans, considering not just economic factors but a comprehensive suite of environmental impacts. Furthermore, the method facilitates stakeholder engagement by providing a clear framework for discussing multiple viable pathways and their environmental consequences, enabling a more inclusive and locally tailored decision-making process.

Specifically, the MGA-LCA method enhances decision-making in several ways. First, it enhances policymaking by addressing structural uncertainties through the MGA approach [60]. This enables policymakers to consider a range of plausible alternatives. Second, it promotes a better-informed approach by incorporating extensive environmental assessment beyond just carbon emissions, such as water usage and resource depletion. Finally, it fosters stakeholder engagement; by presenting multiple preferences, policies can be tailored to meet local needs and values [22]. This participatory potential has been demonstrated in real-world applications such as the decarbonisation planning of Ruhr University Bochum, where MGA was combined with stakeholder input to support more inclusive and practical decision-making [61].

There is still a large potential for further work combining environmental assessment with a large number of energy system configurations to explore trade-offs between energy system designs and their impact systematically. Unlike traditional cost-economic optimization, MGA can produce multiple alternatives that exhibit a wide range of different environmental impacts while also addressing structural uncertainty. This approach allows for the identification of configurations with lower environmental impacts, which could accommodate other factors not considered in this study, such as quicker transition speeds.

Another direction for future work involves incorporating social issues into the analysis, which is critical for a truly multidimensional assessment of sustainability. Social preferences regarding techno-economic issues were integrated by setting constraints for energy modelling, limiting options within the option space. A deeper understanding of what is acceptable in techno-economic terms can better inform the MGA approach to SPORES, leading to increased acceptance of the option space. Moreover, these preferences can shape the definition of indicators to evaluate environmental impact. For instance, we are currently developing acceptance-guided metrics to analyze the socio-ecological impacts of wind power [60], improving their robustness and making them more relevant for decision-making. Finally, another interesting thread of work would be to conduct a similar analysis for social or geopolitical issues, laying the groundwork for a truly holistic assessment of the option spaces.

CRediT authorship contribution statement

Alexander de Tomás-Pascual: Visualization, Data curation, Writing – original draft, Formal analysis, Writing – review & editing, Investigation, Software, Conceptualization. **Laura À. Pérez-Sánchez:** Supervision, Writing – review & editing, Investigation. **Miquel Sierra-Montoya:** Software, Writing – review & editing. **Francesco Lombardi:** Investigation, Project administration, Writing – review & editing. **Stefan Pfenninger-Lee:** Funding acquisition, Investigation, Writing – review & editing, Conceptualization. **Inês Campos:** Writing – review & editing, Investigation. **Cristina Madrid-López:** Project administration, Supervision, Conceptualization, Writing – review & editing, Funding acquisition, Methodology.

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.

Acknowledgements

This work has been developed as part of the SEEDS project (Stakeholder-Based Environmentally-Sustainable and Economically Doable Scenarios for the Energy Transition) (CHIST-ERA-19-CES-004) funded by the Spanish Research Agency (PCI2020-120710-2), the Swiss National Science Foundation (195537), and the Fundação para a Ciência e Tecnologia (FCT), Portugal (CHIST-ERA/0005/2019). Part of the work was developed during the European Commissions' Horizon 2020 program project SENTINEL (H2020-837089).

It received additional support from the Spanish research Agency with project LIVEN (PID2020-119565RJ-I00), project ETOS (TED2021-132032A-I00), and the Maria de Maeztu Programme for Units of Excellence of the Spanish Ministry of Science and Innovation (ICTA CEX2019-0940-M); the Catalan Government through the SosteniPra group (2021 SGR 00734) and Alexander de Tomás' Joan Oró fellowship (2024FI-100741). It also received funds for Inês Campos' post-doc contract from the Fundação para a Ciência e Tecnologia (2020.01663.CEECIND/CP1605/CT0005).

During the preparation of this work, we used Grammarly to check spelling and improve readability. After using this tool, we reviewed and edited the content as needed. We take full responsibility for the content of the published article.

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.apenergy.2025.126487.

Data availability

Data will be made available on request.

References

[1] Süsser D, Ceglarz A, Gaschnig H, Stavrakas V, Flamos A, Giannakidis G, et al. Model-based policymaking or policy-based modelling? How energy models and energy policy interact. Energy Res Soc Sci 2021;75:101984. https://doi.org/10.1016/j.erss.2021.101984.

[2] Pedersen TT, Victoria M, Rasmussen MG, Andresen GB. Modeling all alternative solutions for highly renewable energy systems. Energy 2021;234:121294. https://doi.org/10.1016/j.energy.2021.121294.

[3] Morgan MG, Henrion M, Small M. Uncertainty: A guide to dealing with uncertainty in quantitative risk and policy analysis. Cambridge University Press; 1990.

[4] Sasse JP, Trutnevyte E. Regional impacts of electricity system transition in Central Europe until 2035. Nat Commun 2020;11:1–14. https://doi.org/10.1038/s41467-020-18812-y.

[5] Tröndle T, Lilliestam J, Marelli S, Pfenninger S. Trade-offs between geographic scale, cost, and infrastructure requirements for fully renewable Electricity in Europe. Joule 2020;4:1929–48. https://doi.org/10.1016/j.joule.2020.07.018.

[6] Victoria M, Zhu K, Brown T, Andresen GB, Greiner M. Early decarbonisation of the European energy system pays off. Nat Commun 2020;11:1–9. https://doi.org/10.1038/s41467-020-20015-4.

[7] Wilson C, Grubler A, Bento N, Healey S, Stercke S de, Zimm C. Granular technologies to accelerate decarbonization: smaller, modular energy technologies have advantages. Science 2020;368:36–9. https://doi.org/10.1126/science.aaz8060.

[8] Xexakis G, Hansmann R, Volken SP, Trutnevyte E. Models on the wrong track: model-based electricity supply scenarios in Switzerland are not aligned with the perspectives of energy experts and the public. Renew Sust Energ Rev 2020;134:110297. https://doi.org/10.1016/j.rser.2020.110297.

[9] Pfenninger S, Hawkes A, Keirstead J. Energy systems modeling for twenty-first century energy challenges. Renew Sust Energ Rev 2014;33:74–86. https://doi.org/10.1016/j.rser.2014.02.003.

[10] Rittel HWJ, Webber MM. Dilemmas in a general theory of planning. Policy Sci 1973;4:155–69.

[11] Süsser D, Martin N, Stavrakas V, Gaschnig H, Talens-Peiró L, Flamos A, et al. Why energy models should integrate social and environmental factors: assessing user needs, omission impacts, and real-word accuracy in the European Union. Energy Res Soc Sci 2022;92:102775. https://doi.org/10.1016/j.erss.2022.102775.

[12] Brill JED. The use of optimization models in public-sector planning. Manag Sci 1979;25:413–22. https://doi.org/10.1287/mnsc.25.5.413.

[13] DeCarolis JF. Using modeling to generate alternatives (MGA) to expand our thinking on energy futures. Energy Econ 2011;33:145–52. https://doi.org/10.1016/j.eneco.2010.05.002.

[14] Wang Y, Li L. Time-of-use based electricity demand response for sustainable manufacturing systems. Energy 2013;63:233–44. https://doi.org/10.1016/j.energy.2013.10.011.

[15] Li FGN, Trutnevyte E. Investment appraisal of cost-optimal and near-optimal pathways for the UK electricity sector transition to 2050. Appl Energy 2017;189:89–109. https://doi.org/10.1016/j.apenergy.2016.12.047.

[16] Sasse J-P, Trutnevyte E. A low-carbon electricity sector in Europe risks sustaining regional inequalities in benefits and vulnerabilities. Nat Commun 2023;14:2205. https://doi.org/10.1038/s41467-023-37946-3.

[17] Sasse J-P, Trutnevyte E. Cost-effective options and regional interdependencies of reaching a low-carbon European electricity system in 2035. Energy 2023;282:128774. https://doi.org/10.1016/j.energy.2023.128774.

[18] Neumann F, Brown T. The near-optimal feasible space of a renewable power system model. Electr Power Syst Res 2021;190:106690. https://doi.org/10.1016/j.epsr.2020.106690.
[19] Neumann F, Brown T. Broad ranges of investment configurations for renewable power systems, robust to cost uncertainty and near-optimality. iScience 2023;26:106702. https://doi.org/10.1016/j.isci.2023.106702.
[20] Sinha A, Venkatesh A, Jordan K, Wade C, Eshraghi H, de Queiroz AR, et al. Diverse decarbonization pathways under near cost-optimal futures. Nat Commun 2024;15:8165. https://doi.org/10.1038/s41467-024-52433-z.
[21] Pickering B, Lombardi F, Pfenninger S. Diversity of options to eliminate fossil fuels and reach carbon neutrality across the entire European energy system. Joule 2022;6:1253–76. https://doi.org/10.1016/j.joule.2022.05.009.
[22] Lombardi F, Pfenninger S. Human-in-the-loop MGA to generate energy system design options matching stakeholder needs. PLOS Climate 2025;4:e0000560. https://doi.org/10.1371/journal.pclm.0000560.
[23] Jesse B-J, Heinrichs HU, Kuckshinrichs W. Adapting the theory of resilience to energy systems: a review and outlook. Energy Sustain Soc 2019;9:27. https://doi.org/10.1186/s13705-019-0210-7.
[24] Binder CR, Mühlemeier S, Wyss R. An Indicator-based approach for Analyzing the resilience of transitions for energy regions. Part I: theoretical and conceptual considerations. Energies 2017;10:36. https://doi.org/10.3390/en10010036.
[25] Mühlemeier S, Binder CR, Wyss R. "It's an endurance race": an indicator-based resilience analysis of the energy transition in the Allgäu region, Bavaria. GAIA - Ecol Perspect Sci Soc 2017;26:199–206. https://doi.org/10.14512/gaia.26.S1.7.
[26] Kharrazi A, Sato M, Yarime M, Nakayama H, Yu Y, Kraines S. Examining the resilience of national energy systems: measurements of diversity in production-based and consumption-based electricity in the globalization of trade networks. Energy Policy 2015;87:455–64. https://doi.org/10.1016/j.enpol.2015.09.019.
[27] Erker S, Stangl R, Stoeglehner G. Resilience in the light of energy crises – part I: a framework to conceptualise regional energy resilience. J Clean Prod 2017;164:420–33. https://doi.org/10.1016/j.jclepro.2017.06.163.
[28] SEEDS. Project. 2024.
[29] Coelho S, Rafael S, Coutinho M, Monteiro A, Medina J, Figueiredo S, et al. Climate-change adaptation framework for multiple urban areas in northern Portugal. Environ Manag 2020;66:395–406. https://doi.org/10.1007/s00267-020-01313-5.
[30] Sareen S, Shokrgozar S, Neven-Scharnigg R, Girard B, Martin A, Wolf SA. Accountable solar energy transitions in financially constrained. Contexts 2023:141–66. https://doi.org/10.1007/978-3-031-18268-6_6.
[31] Horta A, Gouveia JP, Schmidt L, Sousa JC, Palma P, Simões S. Energy poverty in Portugal: combining vulnerability mapping with household interviews. Energ Build 2019;203:109423. https://doi.org/10.1016/j.enbuild.2019.109423.
[32] Campos I, Brito M, Pfenninger-Lee S, Fazendeiro LM, Luz GP, Lombardi F, et al. Narratives, expectations, and policy criteria for a democratic and socially engaging energy transition. Futures 2024;164:103496. https://doi.org/10.1016/j.futures.2024.103496.
[33] Pfenninger S, Pickering B. Calliope: a multi-scale energy systems modelling framework. J Open Source Software 2018;3:825. https://doi.org/10.21105/JOSS.00825.
[34] Lau M, Patankar N, Jenkins JD. Measuring exploration: evaluation of modelling to generate alternatives methods in capacity expansion models. Environ Res: Energy 2024;1:45004. https://doi.org/10.1088/2753-3751/ad7d10.
[35] Lombardi F, Pickering B, Colombo E, Pfenninger S. Policy decision support for renewables deployment through spatially explicit practically optimal alternatives. Joule 2020;4:2185–207. https://doi.org/10.1016/j.joule.2020.08.002.
[36] Lombardi F, Pickering B, Pfenninger S. What is redundant and what is not? Computational trade-offs in modelling to generate alternatives for energy infrastructure deployment. Appl Energy 2023;339:121002. https://doi.org/10.1016/j.apenergy.2023.121002.
[37] Trutnevyte E. Does cost optimization approximate the real-world energy transition? Energy 2016;106:182–93. https://doi.org/10.1016/j.energy.2016.03.038.
[38] Lombardi F. Calliope-Portugal-HITL-MGA. 2024. https://doi.org/10.5281/zenodo.12784284.
[39] Madrid-Lopez C, Soleymani-Fard R, de Tomás-Pascual A, Sierra M. enbios · PyPI. 2023.
[40] Mutel C. Brightway: an open source framework for life cycle assessment. J Open Source Software 2017;2:236. https://doi.org/10.21105/joss.00236.
[41] de Tomás-Pascual Alexander. SPARKS: A soft linking approach for energy system models and ENBIOS. 2024.
[42] Wernet G, Bauer C, Steubing B, Reinhard J, Moreno-Ruiz E, Weidema B. The ecoinvent database version 3 (part I): overview and methodology. Int J Life Cycle Assess 2016;21:1218–30. https://doi.org/10.1007/s11367-016-1087-8.
[43] Teske S. Achieving the Paris Climate Agreement Goals. Achieving the Paris Climate Agreement Goals: Global and Regional 100% Renewable Energy Scenarios with Non-Energy GHG Pathways for +15C and +2C 2019:491. doi:https://doi.org/10.1007/978-3-030-05843-2.
[44] Junne T, Simon S, Buchgeister J, Saiger M, Baumann M, Haase M, et al. Environmental sustainability assessment of multi-sectoral energy transformation pathways: methodological approach and case study for Germany. Sustainability 2020;12:8225. https://doi.org/10.3390/SU12198225.
[45] Volkart K, Mutel CL, Panos E. Integrating life cycle assessment and energy system modelling: methodology and application to the world energy scenarios. Sustain Prod Consumpt 2018;16:121–33. https://doi.org/10.1016/j.spc.2018.07.001.
[46] Huijbregts MAJ, Steinmann ZJN, Elshout PMF, Stam G, Verones F, Vieira M, et al. ReCiPe2016: a harmonised life cycle impact assessment method at midpoint and endpoint level. Int J Life Cycle Assess 2017;22:138–47. https://doi.org/10.1007/S11367-016-1246-Y/TABLES/2.
[47] Ali K, Al-Hameed A. Spearman's correlation coefficient in statistical analysis. Int J Nonlinear Anal Appl 2022;13:3249–55. https://doi.org/10.22075/IJNAA.2022.6079.
[48] Magurran AE. Ecological diversity and its measurement ecological diversity and its measurement. 1988. https://doi.org/10.1007/978-94-015-7358-0.
[49] Jasiūnas J, Lund PD, Mikkola J. Energy system resilience – a review. Renew Sust Energ Rev 2021;150:111476. https://doi.org/10.1016/j.rser.2021.111476.
[50] de Tomás-Pascual A, Madrid-López C, Villalba G, Soleymani-Fard R, Pérez Sánchez LÀ. Quantification of uncertainty associated with each scenario across multiple dimensions. Deliverable 2.3. Zenodo. 2024. https://doi.org/10.5281/zenodo.11174566.
[51] de Tomás-Pascual A, Madrid-López C, Villalba G, Soleymani-Fard R, Sánchez LÀP. Quantification of uncertainty associated with each scenario across multiple dimensions. 2024. https://doi.org/10.5281/zenodo.11174566.
[52] Golroudbary SR, Lundström M, Wilson BP. Analogical environmental cost assessment of silicon flows used in solar panels by the US and China. Sci Rep 2024;14(1):1–12. https://doi.org/10.1038/s41598-024-60270-9.
[53] Chordia M, Wickerts S, Nordelöf A, Arvidsson R. Life cycle environmental impacts of current and future battery-grade lithium supply from brine and spodumene. Resour Conserv Recycl 2022;187:106634. https://doi.org/10.1016/j.resconrec.2022.106634.
[54] Chaves C, Pereira E, Ferreira P, Dias AG. Concerns about lithium extraction: a review and application for Portugal. Extractive Ind Soc 2021;8:100928. https://doi.org/10.1016/j.exis.2021.100928.
[55] Araújo E, Bento S, Silva M. Politicizing the future: on lithium exploration in Portugal. Eur J Futures Res 2022;10:1–11. https://doi.org/10.1186/s40309-022-00209-3.
[56] Olivetti EA, Ceder G, Gaustad GG, Fu X. Lithium-ion battery supply chain considerations: analysis of potential bottlenecks in critical metals. Joule 2017;1:229–43. https://doi.org/10.1016/j.joule.2017.08.019.
[57] Hertwich EG, Gibon T, Bouman EA, Arvesen A, Suh S, Heath GA, et al. Integrated life-cycle assessment of electricity-supply scenarios confirms global environmental benefit of low-carbon technologies. Proc Natl Acad Sci USA 2015;112:6277–82. https://doi.org/10.1073/pnas.1312753111.
[58] Pehl M, Arvesen A, Humpenöder F, Popp A, Hertwich EG, Luderer G. Understanding future emissions from low-carbon power systems by integration of life-cycle assessment and integrated energy modelling. Nat Energy 2017;2(12):939–45. https://doi.org/10.1038/s41560-017-0032-9.
[59] Rauner S, Budzinski M. Holistic energy system modeling combining multi-objective optimization and life cycle assessment. Environ Res Lett 2017;12:124005. https://doi.org/10.1088/1748-9326/aa914d.
[60] Price J, Keppo I. Modelling to generate alternatives: a technique to explore uncertainty in energy-environment-economy models. Appl Energy 2017;195:356–69. https://doi.org/10.1016/j.apenergy.2017.03.065.
[61] Esser K, Finke J, Bertsch V, Löschel A. Participatory modelling to generate alternatives to support decision-makers with near-optimal decarbonisation options. Appl Energy 2025;395:126184. https://doi.org/10.1016/j.apenergy.2025.126184.