Universitat Autònoma de Barcelona

Sustainable-by-design energy systems for the energy transition

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MEng thesis

MÀSTER EN ENGINYERIA BIOLÒGICA I AMBIENTAL

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I. Research group

This research project was conducted within the LIVENlab research line, which is part of the Sostenipra Research Group at the Institute of Environmental Science and Technology, Autonomous University of Barcelona (ICTA-UAB). The primary objective of the LIVENlab is to develop an environmental assessment tool that enhances decision-making in selecting the energy technological mix that will return a more sustainable scenario than the current energy plan.

More specifically, this study aligns with the ongoing efforts of the SEEDS project, where we aim to incorporate human elements into the design of energy transition scenarios. This involves the modelling of technical, economic, and environmental parameters, with Portugal as the primary case study. The project consists of a consortium of four European institutions; Centre for Ecology, Evolution and Environmental Changes at FCiências.ID / Universidade de Lisboa; The HCI group at Tallinna Ülikool (Tallinn University); and the Climate Policy research group at ETH Zürich in cooperation with the Department of Engineering Systems and Services at TU Delft. This project has been funded by the European Coordinated Research on Long-term Challenges in Information and Communication Sciences & Technology CHIST-ERA grant CHIST-ERA-19-CES-004, the Swiss National Science Foundation grant number 195537, the Fundação para a Ciência e Tecnologia (FCT) grant number CHIST-ERA/0005/2019, the Spanish Agencia Estatal de Investigación with grant PCI2020-120710-2, and the Estonian Research Council grant number 4-8/20/26.

II. Cover Letter

Dear Editorial Board**,**

Herewith, we would like to submit our innovative article on the relevance of the environmental assessment of energy system models entitled "Sustainable by design energy systems for the energy transition".

Significance of this article: This study contributes to closing the gap of the lack of sustainability parameters in energy system optimization models. Unlike previous studies that predominantly focus on analyzing singular optimal solutions, our research endeavours to bridge this gap by exploring a comprehensive option space encompassing multiple suboptimal energy transition pathways. Limiting the scope to a few configurations neglects the potential alternatives that may yield lower environmental impacts and higher social acceptance.

We present the environmental evaluation of 261 energy transition configurations for the year 2050 in Portugal by combining Life Cycle Assessment (LCA) and Multi-Scale Integrated Analysis of Societal and Ecosystem Metabolism (MuSIASEM) frameworks. We go beyond the mere quantification, differentiating the attributes that render a configuration either low-impact or high-impact in comparison with others. By doing so, our research not only enhances our understanding of the environmental impacts but also sheds light on the specific characteristics that contribute to the relative sustainability of energy system configurations.

Moreover, our study enables the identification of lower-impact alternatives, providing a decision-making option space for stakeholders based on their preferences. Conducted within the SEEDS project, this research recognizes the diversity of energy transition pathways and their environmental impacts, offering decision-makers valuable insights to navigate toward sustainable solutions that harmonize environmental preservation with societal needs.

Our findings are particularly relevant for energy modelers, academics in the field of industrial ecology and energy modelling, NGOs, consulters, and **policymakers.**

The novelty of this work lies in the environmental analysis of a wide range of suboptimal energy transition configurations. It is the first work that compares traditional energy system methods with *modelling to generate alternatives* approaches in terms of environmental impacts.

This work is important as it addresses the deficiency in current sustainability parameters within energy system optimization models. By exploring a diverse range of energy transition pathways, including suboptimal options, it unveils alternatives often overlooked in previous studies focused on singular optimal solutions. This approach not only enhances our understanding of environmental impacts but also provides decision-makers with valuable insights to navigate toward sustainable solutions that balance environmental preservation and societal needs, a key consideration for future energy planning and policy development.

We believe that **Applied Energy is a good match for this research** due to its focus on interdisciplinary research in energy applications. The journal's commitment to innovative approaches aligns with our exploration of diverse energy transition pathways.

The manuscript has been spelled-checked by the author and the supervisor. We are available to review at least three new submissions for Applied Energy within the next year.

Thank you for considering our submission,

Kind regards,

Alexander de Tomás Pascual and Cristina Madrid López

III. Highlights

- **Research highlights 1:** We combined Energy System Optimization Models with Life Cycle Assessment (LCA) and Multi-Scale Integrated Analysis of Societal and Ecosystem Metabolism (MuSIASEM) frameworks generating 261 energy transition configurations for the year 2050 in Portugal**.**
- **Research highlights 2:** Conventional energy system optimization techniques are able to produce low environmental impact configurations compared to other alternatives.
- **Research highlights 3:** Configurations emphasizing higher thermal storage and thermal generation tend to pose greater environmental harm.
- **Research highlights 4:** We find no apparent trade-offs in environmental impacts when viewed from the broad lens of an energy system perspective, whereas we can observe them at disaggregated levels.

1 Introduction

Policymakers recognized the need for long-term energy planning during the ‘70s oil crisis, which led to the development of energy policy as a field [1]. The development of linear programming following the end of World War II allowed for the deployment of the first energy system models (ESM) [2] which were concerned with several purposes, such as better energy supply system design given a level of demand forecast, better understanding of the present and future demand-supply interactions, among many others [3].

While energy systems models were initially focused on energy security and costs, climate change policy has emerged as a powerful factor driving many studies, with a focus on pathways to achieve significant reductions in greenhouse gas emissions [4,5]. According to the Intergovernmental Panel on Climate Change (IPCC) [6], renewable energy must supply 70-85% of the world’s electricity by 2050 to limit global warming to 1.5ºC. The swift to a low-carbon energy system is necessary in order to reduce the impacts of climate change on energy systems. However, this transition is far more complex than replacing fossil energy with renewable energy [7]; it is defined as a wicked problem because the achievement of these objectives may result in a cascade of new, unforeseen, and unwanted challenges [8]. This is so, in part, because the definition of energy policy objectives highly relies on energy modelling with energy models which usually obviate social and environmental parameters. Not only this omission risks the suitability of the models, but it may also result in erratic or impractical energy transition strategies [9].

The combination of Life Cycle Assessment (LCA) and ESM can provide solutions to handle trans-disciplinary issues such as energy transition [10]. Previous research has attempted to combine models of energy systems with life cycle assessments. However, as noted by Junne et al. [11] most of these studies have covered a limited number of technologies or have narrow sectoral boundaries. Only a few have broken down environmental impacts into operation and construction[12–14], and none, except for the authors mentioned, have adjusted the global background electricity mix. To the best of our knowledge, all these previous studies have relied on non-open-source frameworks, either the energy or the environmental models, and none of them include uncertainty analysis.

Additionally, it is important to note that current research tends to only examine a limited range of scenarios. This could obscure other solutions that could satisfy the needs of multiple stakeholders involved in transitioning to renewable energy systems [15]. The application of energy models that generate multiple feasible alternatives allows energy modelers to better support decision-making processes [16]. Moreover, the open examination of a wide range of alternatives along with a holistic approach to the environmental consequences beyond carbon emissions could improve decision-making and social acceptance of decarbonisation policies.

Meanwhile, the scientific community has been experiencing an atmosphere of declining trust in the public sphere. These dangers for science become most evident when models are used as policy tools [17] (e.g., consider, for instance, the criticism and skepticism towards climate change or epidemiological models). Black box models do not perform well in this context; they cannot be verified, discussed, or challenged [18]. Hence, transparency criteria must be adopted to allow third parties to replicate the results. In this context, open-source, sensitivity auditing, uncertainty analysis, and communication play a distinguishing role.

This study contributes to closing the gap of the lack of sustainability parameters in energy system optimization models based on the *Modeling to Generate Alternatives* (MGA) approach. We do so by calculating and assessing an *option space* of suboptimal energy transition pathways instead of a unique optimal solution. Besides, we acknowledge the challenge of choosing "the best" scenario in an option space for a decision with high stakes and high uncertainty. We combine two open-source tools (Calliope and ENBIOS) to analyze the environmental impact of 261 energy transition configurations for the 2050 energy transition scenario in Portugal.

Thus, we provide a better comprehension of the multiple trade-offs for near-optimal energy transition configurations that will translate into higher social acceptance and lower environmental damage. Most notably, we address the absence of prior research that analyses a substantial number of alternative scenarios and the methodological challenges inherent to the high-dimensional option space of alternatives.

With this work, we answer the following research questions: i) How do the environmental impacts of the unique energy pathway of singular-solution optimization models compare to the impacts of an array of alternatives from a multi-solution optimization model?; ii) What are the defining attributes that classify an energy pathway from an option space as sustainable? And iii) What are the trade-offs between different environmental impacts?

2 Materials & Methods

2.1 Energy System Model for Scenarios Development

Energy systems are defined as the process chain (or a subset of it) from the extraction of primary energy to the use of final energy to supply services and goods [19,20]. We refer to energy systems models as the mathematical representation of the behavior of energy systems and are used to study possible various energy-related problems[21].

Calliope is an open-source tool that allows building energy system models while keeping user-friendly characteristics [22]. It is based on linear programming algorithms while also accepting mixed-integer optimization, helping to develop energy systems in which renewable energy plays a distinct role. Calliope's key features include the ability to handle high spatial and temporal resolution and easily run on high-performance computing systems[22].

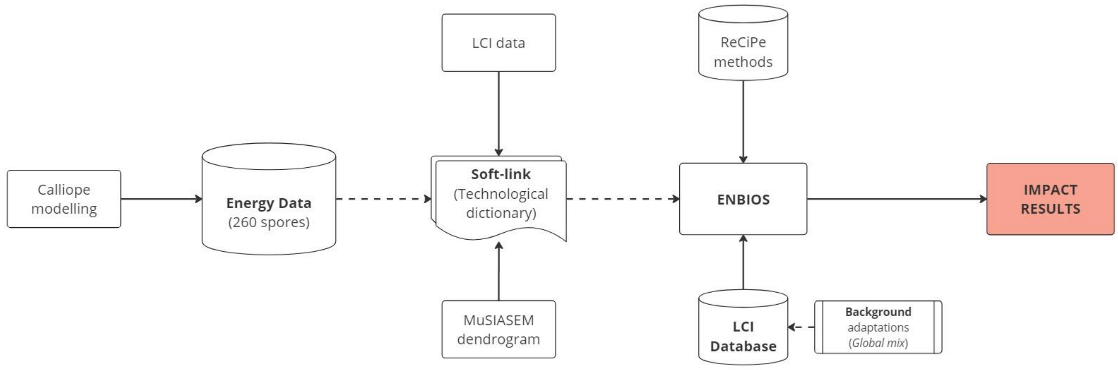
Energy system optimization models identify the system configuration to reach a target with the minimum cost [19]. Nevertheless, focusing on a single optimal solution may hide feasible but perhaps radically different alternatives [15]. This fact becomes notable when considering the different stakeholders involved in the energy transition. In that regard, SPORES [23] appears as an extension of the modelling to generate alternatives (MGA) method. This approach generates multiple energy system configurations with high shares of renewable generation using high spatial and temporal resolution.

The SPORES approach has been applied for Portugal as a case-study, generating over 261 different energy transition configurations by the year 2050. In this work, we use the output of this modelling carried out in the SEEDS project [24] .

2.2 Environmental modeling with ENBIOS

We used ENBIOS (Environmental and Bioeconomic System Analysis) [25] version 2.1.12 to analyze the environmental impacts of over 261 energy transition configurations in Portugal. ENBIOS is a Python-based tool that integrates both Life Cycle Assessment (LCA) and Multi-Scale Integrated Analysis of Societal and Ecosystem Metabolism (MuSIASEM) methodologies. A general description of the methodology is shown in Fig [**1**].

Figure 1: *Methodology summary*



2.3 LCA settings

This study has been conducted following the ISO standards 14040/14044 [26] for LCA studies.

2.3.1 Goal and scope

The objective of this study is to evaluate the environmental impacts across various categories associated with different energy transition configurations as outlined by Calliope. The *functional unit* for this analysis is specified as the energy production for each technology identified within every scenario, a similar approach such as Blanco et al. [27]. In other words, rather than calculating the environmental impacts of a product, it is defined as the satisfaction of the energy demand (composition) of every different pathway included in the energy modelling.

In terms of the scope, the energy modeling divides Portugal into two regions: North and South. Each region is further divided into multiple subregions. Because of the lack of regionalized data, we kept the analysis at the national level. Therefore, the results are presented at a national level rather than at a regional level. We have a yearly resolution, and the time scope is year 2050.

The foreground system comprises the technologies present in the energy modeling data, including electricity and thermal generation technologies, storage, electricity imports, and processes that convert energy carriers (such as biofuel to methanol). To link the energy data with the LCA data, a "*technology mapping*" was carried out. This involved connecting each technology to an LCI dataset using a *soft-link* approach. An external module, specific for the soft-linking between Calliope and ENBIOS has been developed [28] .

The energy modeling framework generated several output files, containing information about the energy production mix, installed capacity, and import dependencies, among others. The data used in this study was sourced from the "*flow out sum*" file, which contains information on the energy mix of each spore. The file corresponds to the net energy requirements (NER), and it's expressed in TWh. To connect with the inventory data, unit conversions were required. For more information regarding the conversions, check out the supplementary materials 8.2.

2.3.2 Life cycle inventory

The Life Cycle Inventory (LCI) data used in this study was obtained from the ecoinvent 3.9.1 cutoff database [29]. The region of Portugal was selected as activity location wherever possible for the activities. In cases where that was not available, the closest region was chosen as a proxy. Inventories for green hydrogen production were extracted from the literature because they were either not available on ecoinvent or did not represent the technology under study accurately. Finally, for the case of hydrogen turbines, where no inventories were available, a normal natural gas turbine from ecoinvent was selected and modified as a proxy. A list of the mapping, sources and modifications can be found in the supplementary materials.

The sectors and technologies included range from electricity and thermal *generation* technologies, electricity and thermal *storage*, *carrier conversion* technologies, and *imports* of electricity.

2.3.3 Prospective inventory modification

The global markets for electricity were adapted using 2050 projections in order to consider future background changes in the electricity markets. The background processes were modified by changing the market for electricity activities. The data for this modification is based on a 2ºC increase scenario in 2050, provided by Teske et al. [30] and processed by Junne et al [11]. This data defines an electricity mix for different world regions. To summarize, we have identified all the countries that have one or multiple markets for electricity and matched each of them with the different regions set in the projection. Then, we updated every market with the values defined in the corresponding region and made some corrections to match different ecoinvent versions. The code is available in our GitHub repository (https://github.com/LIVENlab/Sparks.git) to ensure transparency and replicability. This modification is applied only once to the entire database.

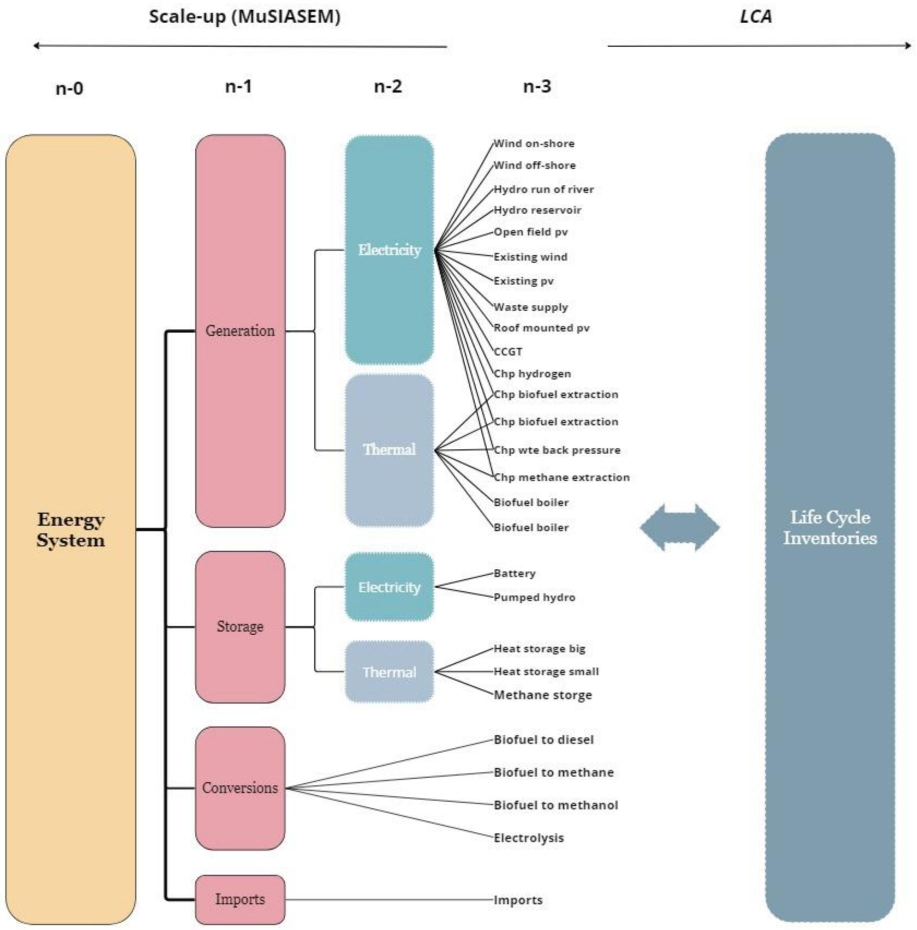
2.3.4 Life cycle impact assessment (LCIA)

As for the life cycle impact assessment, we use ReCiPe midpoint indicators 2016 v1.03 [31], covering different impact categories: climate change (global warming potential), ecotoxicity (*freshwater ecotoxicity potential and marine ecotoxicity potential*), land use (*agricultural land occupation*), water use (*water consumption potential*), particulate matter formation (*particulate matter formation potential*) and material resources (*surplus ore potential*). Additionally, we incorporate natural resources (*biotic resources*) from Ecological Scarcity 2021 [32]. The ReCiPe methods were applied from a hierarchical perspective, which is situated between the short-term focus of individualism and the more cautious, egalitarian approach.

2.4 Upscaling with MuSIASEM

The soft-linking approach was complemented by a *bottom-up* characterization of the energy system coming from the MuSIASEM framework. Fig [2] shows the *dendrogram*, a hierarchical representation of the energy system that can be useful for the comparison of different scenarios at different levels. This information is softlinked to the LCA modelling. The energy system is divided into generation, storage, conversions, and imports. The first two categories are further divided into electricity (mechanical energy) and thermal technologies.

Figure 2: *Integrating the representations of MuSIASEM and LCA*



2.5 Analysis of model, results, and uncertainty

In this work, we analyzed the uncertainty propagation by using the most common approach: the Monte Carlo method [33]. While this method is effective, it requires a significant amount of computational effort. Typically, the method needs between 1,000-10,000 iterations to achieve convergence [33] and it is difficult to calculate the precise number of iterations required. Still, we opted for Monte Carlo simulations as it is a well-accepted and robust method. We performed 500 iterations in one spore selected randomly from the set of results. The results are presented in a distribution plot in Fig [**10**].

We also conducted a study to analyze the relationship between inputs (energy data) and outputs (environmental impacts). Specifically, we examined the technologies that are associated with a particular environmental impact by observing the correlation between the input (amount of a particular technology) and the output (environmental impact). We used linear regression coefficients and Spearman correlations. These analyses were conducted using the NumPy[34] and SciPy[35] packages in Python.

All the impacts are presented in ranges between 0 and 1, with 0 being the lowest value of the array and 1 being the highest to allow the comparison between different indicators with different units. This approach provides a consistent framework for evaluating different statistics, while keeping numbers interpretable, which is practical for policymakers.

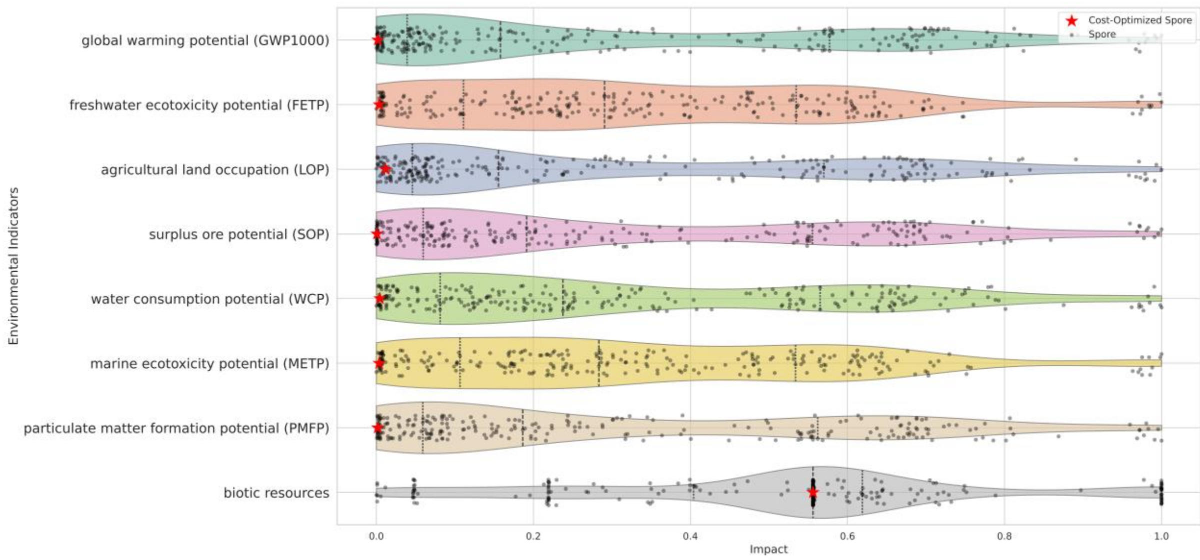
Additionally, we applied K-Means to cluster the different spores [36] and was examined through the Silhouette coefficient. Then, a Random Forest Regressor algorithm [36] was applied to the input dataset and the clusters obtained, with the goal of predicting to which group of impact belongs based on the energy composition. It was trained by partitioning the dataset into 70% training and 30% testing. Finaly, feature importance values were extracted to provide insights into the contribution of various inputs to observed environmental impacts.

3 Results

3.1 General distribution of results

We calculated the environmental impacts of 261 different energy transition configurations in Portugal for the year 2050. Firstly, at the first level (*n*, *Energy system*) and as shown in Fig [**3**] we can observe a tendence of accumulation of pathways in the lower sections of the distribution (area between 0 and 0.4) except for biotic resources. This fact, also remarked by the median lines on the violins, indicates that most configurations tend to a lower impact. On the other hand, Fig [**3**] also indicates the position of the spore *"0"* within the distribution. This spore is the initial result generated by Calliope and all subsequent spores are produced based on this output. Essentially, it is the *minimum* cost solution, and it matches the outcome that a conventional cost-optimization modelling would produce. It can be observed that this "*cost-optimized"* spore is one of the configurations with the lowest overall environmental impact in the set of results, except, again, for the biotic resources indicator. Excluding the uncertainties and epistemological limitations discussed in further sections, our findings suggest that configurations relying solely on monetary and demand parameters are able to align with environmental parameters, at least when compared to other configurations based on cost relaxation (spores).

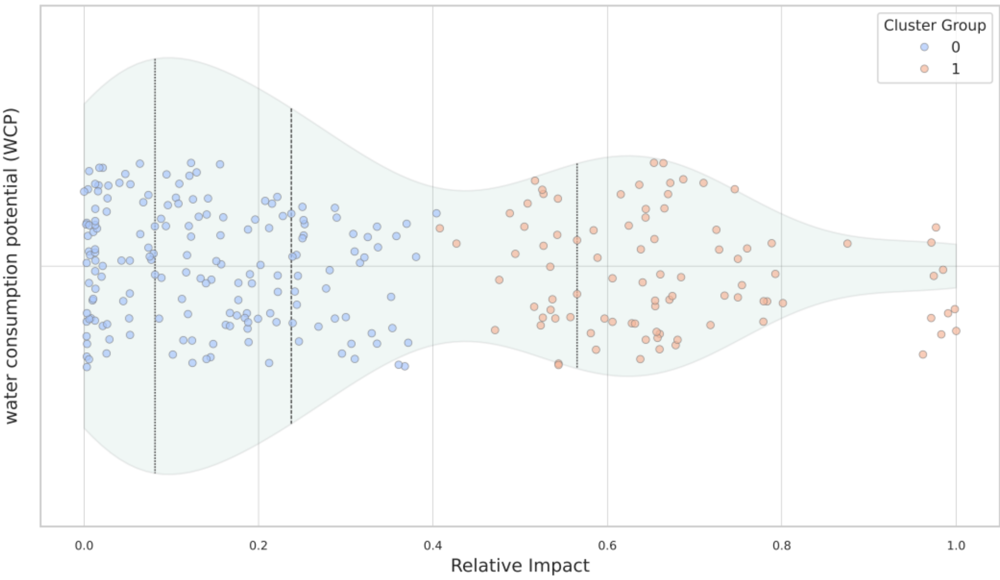
Figure 3: *Distribution of the Environmental impacts of 261 pathways. Normalized between 0-1 by the smallest and highest value*.



The different spores were clustered according to the relative impact in the different categories using K-means. The biotic resources indicator was excluded from this analysis due to its different distribution, as shown in Fig [**3**], which would eventually result in a disturbance in the clustering process. As a result, the spores were successfully clustered into two different groups, which can be regarded as "*low-impact spores*" (group 0) or "*high-impact spores*" (group 1) and resulting in

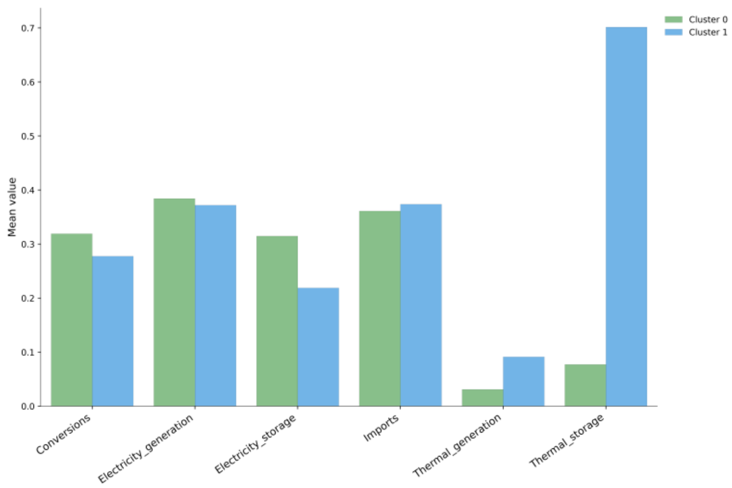
171 and 90 spores respectively. The clusters obtained a global Silhouette coefficient of 0.71, indicating a good differentiation between the groups. An example of the grouping is shown in Fig [**4**].

Figure 4: *Example of clustering. Water consumption results for the whole energy system (n)*



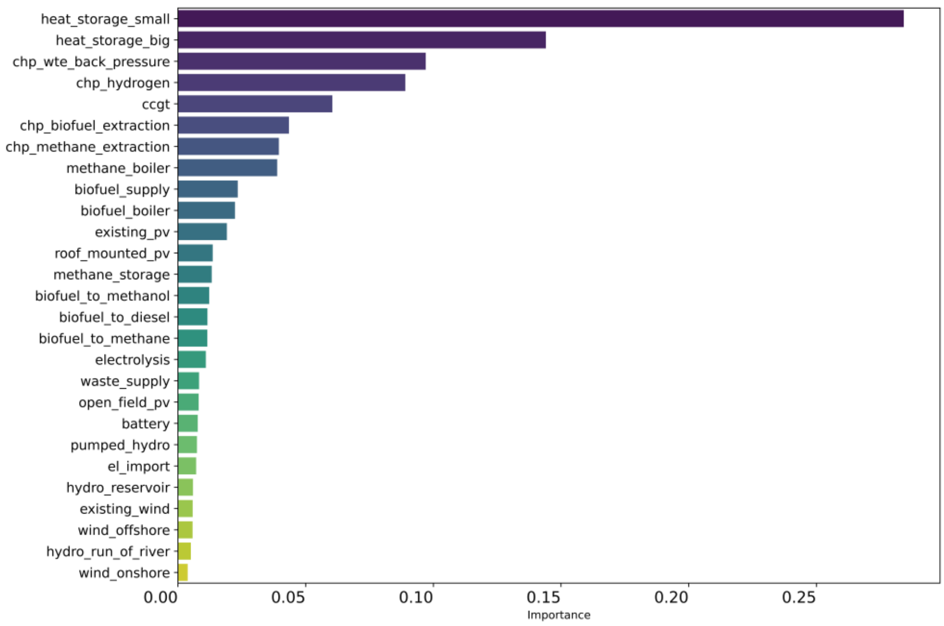
We investigated the factors in the input (energy data) that may be responsible for the differentiation between high-impact spores and low-impact. Initially, we found no significant differences in the energy composition between groups 0 and 1 when looking at the *n-1* level (generation, storage, conversions, and imports). However, significant differences emerged when analyzing the n-2 level. According to the *p-values* of the mean differences as depicted in Fig [**5**], high-impact spores tend to have a larger amount of thermal storage and produce more heat, while lower-impact spores tend to have more electricity storage.

Figure 5: *Mean differences between energy input clusters. p-values: 0.03, 0.67, <0.01, 0.58, <0.01, <0.01 respectively*



Upon closer inspection of the system, we conducted an analysis at the n-3 level. This involved employing a random forest regressor to predict the assignment of spores to either cluster 0 or 1 based on their mix configuration. The dataset was partitioned into 70% training and 30% testing set, resulting in a 100% accuracy score in predictive performance. Then, we computed the feature importance, and the result is presented in Fig [**6**]. Heat storage technologies have a high influence on the predictive capabilities of the model, followed by combined heat and power technologies.

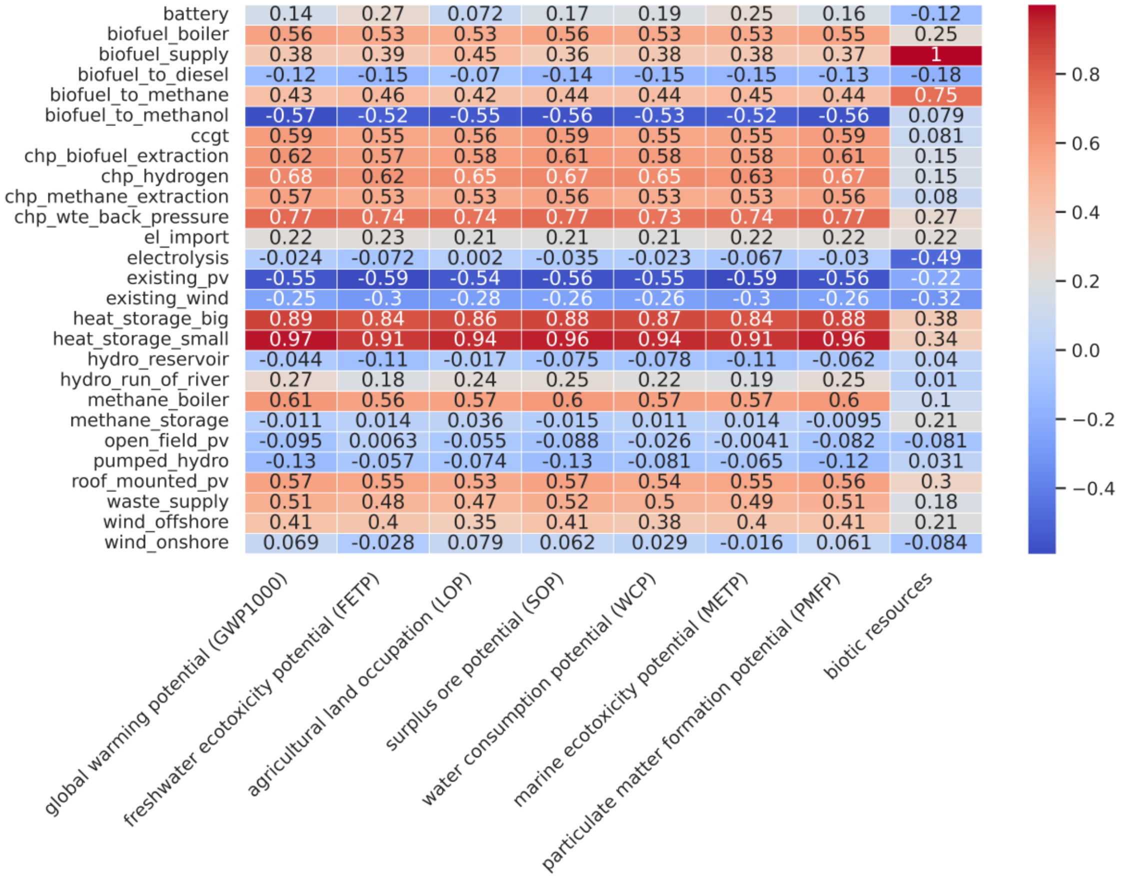
Figure 6: *Feature importance of Random Forest Regressor*



These results align with the observation made on level 2: thermal technologies play a decisive role on the overall impact of the configuration. This idea is further supported by the Spearman correlation values between energy inputs (n-3 level) and the general impacts in each category, which is shown in Fig [**7**]. Additionally, Fig [**7**] indicate a strong correlation between biofuel supply and the biotic resources indicator. This result explains the almost "discrete" distribution observed in Fig [**3**], which may follow the demand of biofuel supply defined in the spores.

However, it is important to approach the negative values presented in the analysis with caution. The strength of Spearman correlation lies in its ability to handle non-linear relations. This attribute proves valuable in our context, where we are linking individual inputs to the overall impact generated by the collection of technologies. Consequently, a negative relationship becomes implausible from a Life Cycle Assessment standpoint. It should be noted that the Spearman correlation may not fully capture the dynamics of other components when assessing individual technologies. Global Sensitivity Analysis techniques would provide a more nuanced perspective, offering insights into the interplay of factors influencing the outcomes.

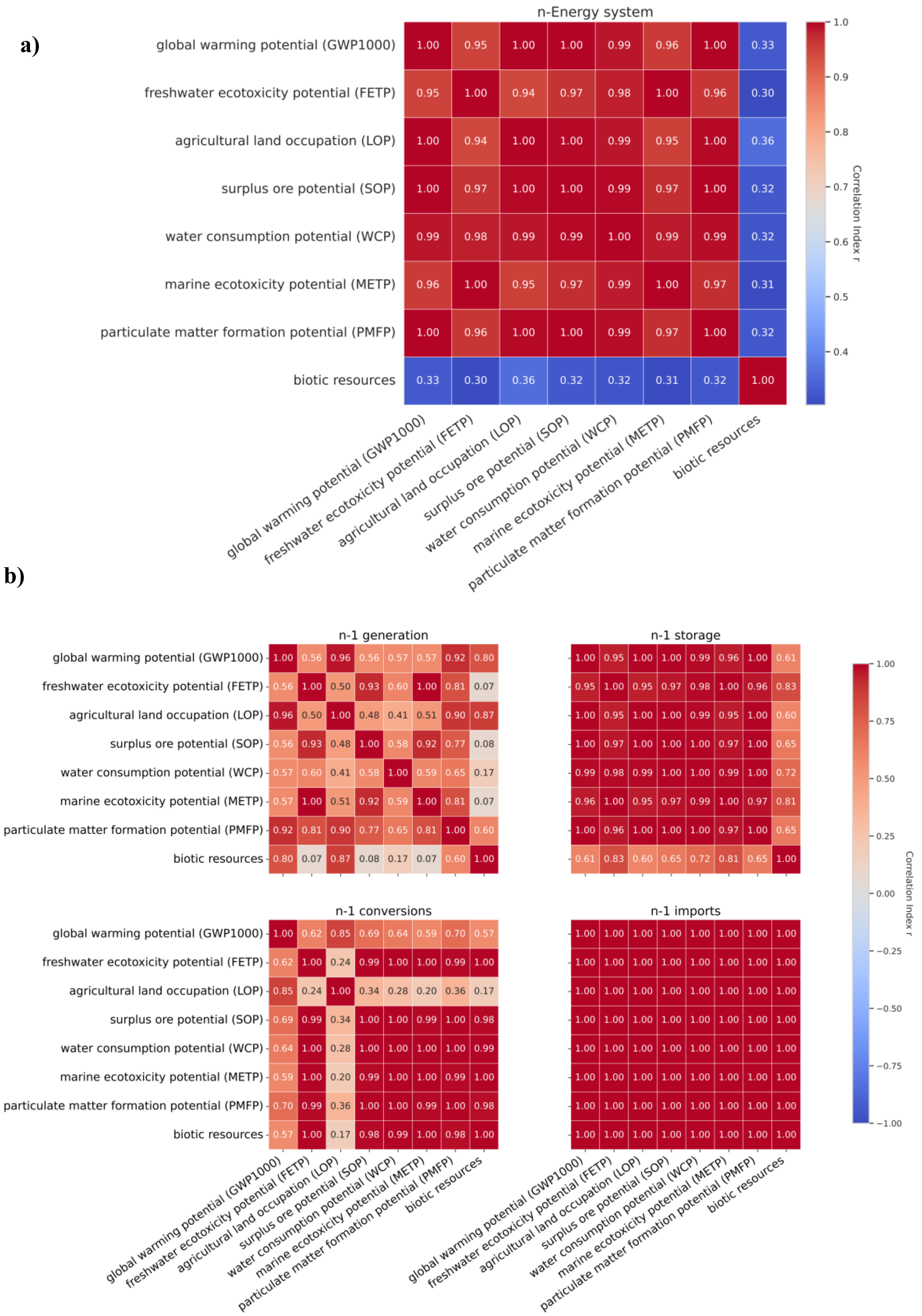
Figure 7: *Spearman correlation values between impact categories (n) and input technology (TWh)*



3.2 Trade-offs and selection of spores

We then examined whether there are trade-offs between the different environmental impacts. The findings indicate a strong correlation between most impact categories, apart from the biotic resources category (Fig [**8, a**]). This suggests that if one energy configuration has a significant impact on certain categories, it is highly probable that all other categories will have the same level of impact as well. Thus, the results reject the notion of multiple trade-offs between environmental impacts when examining multiple alternatives, at least when viewed from an energy system perspective (n).

Figure 8: *Correlation coefficients (r) between impact categories at the energy system (n) (a) and n-1 levels (b).*



Nevertheless, as we delve into deeper layers of the system, this notion becomes less clear. It is the case for *generation* and *conversions* categories, where this correlation diminishes, and potentially allowing for trade-offs in the design and selection of this levels (Fig [**7 b**]). The observed absolute correlation for the *imports* can be attributed to the fact that the level comprises only one activity, as illustrated in Fig [**2**].

Despite the strong correlation between outputs, there is still some room for trade-offs to appear, especially since the energy mix may differ. Table [**1**] displays the top four configurations with the lowest impact for each category. Although these configurations are likely very similar, we observed that a small percentual difference in the energy mix may result in a significant difference in the onsite impacts, and consequently on social acceptance. This amplified effect results from the bigger size of the energy system, which we can better understand due to the upscaling in the analysis. A small percentual change can be traduced a large number new installations for technologies like wind and solar. Table [**1**] illustrates that various SPORES alternatives are viable based on the specific indicator to minimize. To provide a better understanding of the spores' composition, Fig [**10**] shows a comparison of three selected spores from Table [**1**] at the n-2 level, while Fig [**12**] presents the relative input of the entire set of spores at level n-1.

Table 1: *Top 4 spores with the lowest impact for each indicator*

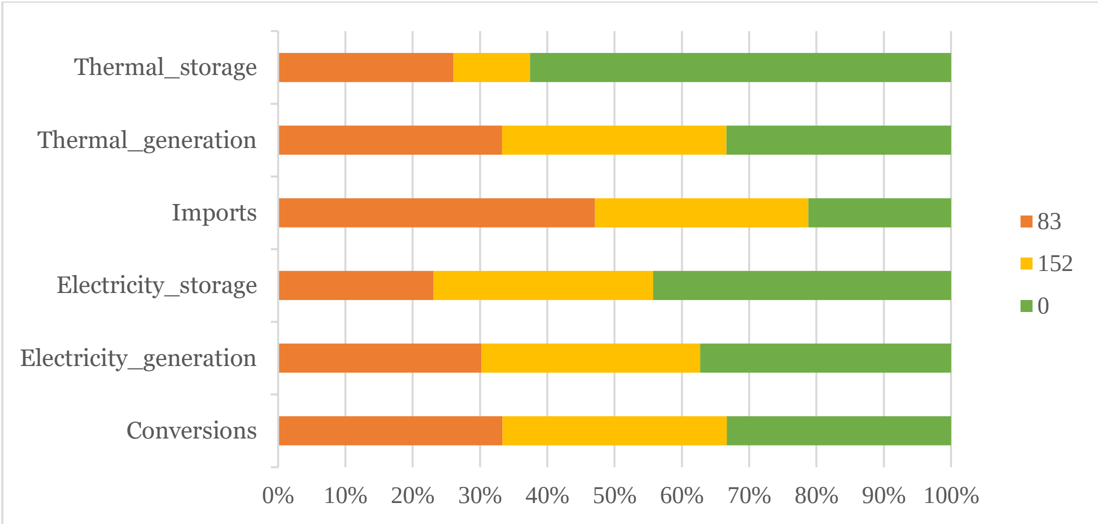
Global Warming Potential	Freshwater Ecotoxicity Potential	Agricultural Land Occupation	Surplus Ore Potential	Water Consumption Potential	Marine Ecotoxicity Potential	Particulate Matter formation	Biotic Resources
83	**83**	191	**83**	**83**	**83**	**83**	51
152	155	192	**152**	**152**	155	**152**	111
155	152	182	155	161	152	155	131
162	**0**	183	162	153	**0**	153	221

Even though a few spores signify themselves by the repeated appearance in the top 4, it will be dangerous to say that these are the best spores. Defining the best energy configuration will also depend on the valuation that different groups would give to the different impacts. For example, Table [**2**] exemplifies that the spore that would be selected for each of the personas based on the possible preferences of *imaginary* stakeholders. Suppose a farmer, *Persona 1*, who is worried about water use and land occupation. In that case, the best configuration for him would be the spore 83. However, for Persona 2, an ecologist worried about water use and the impact on biotic resources, configuration 54 would be more appropriate. Moreover, those who focus on monetary values would choose spore 0, the *cost-optimized* configuration.

Table 2: *Chosen spore based on different preferences.* ***Persona 1****: Agricultural Land Occupation and Water Consumption Potential.* ***Persona 2****: Water Consumption Potential and Biotic Resources.* ***Persona 3****: Freshwater and Marine Ecotoxicity Potential and Biotic resources*.

Persona 1	Persona 2	Persona 3	Best	Best without biotic resources
83	54	191	83	191

Figure 9: *Relative input in n-2 categories. Comparison between spores 83,152 and 0*



3.3 Uncertainty calculations

We performed Monte Carlo simulations to analyse the uncertainty of results. The random spore chosen was number 0, for which 500 iterations were performed. It can be observed that, while some indicators such as marine ecotoxicity potential or surplus ore potential reached convergence, 500 iterations were insufficient for the agricultural land occupation or biotic resources. It is notable that the impact on the water consumption potential has been overestimated. However, the results for the other indicators fall within the range of expectation.

Figure 10: *Monte Carlo simulations. In red, the static value obtained from the single simulation*.

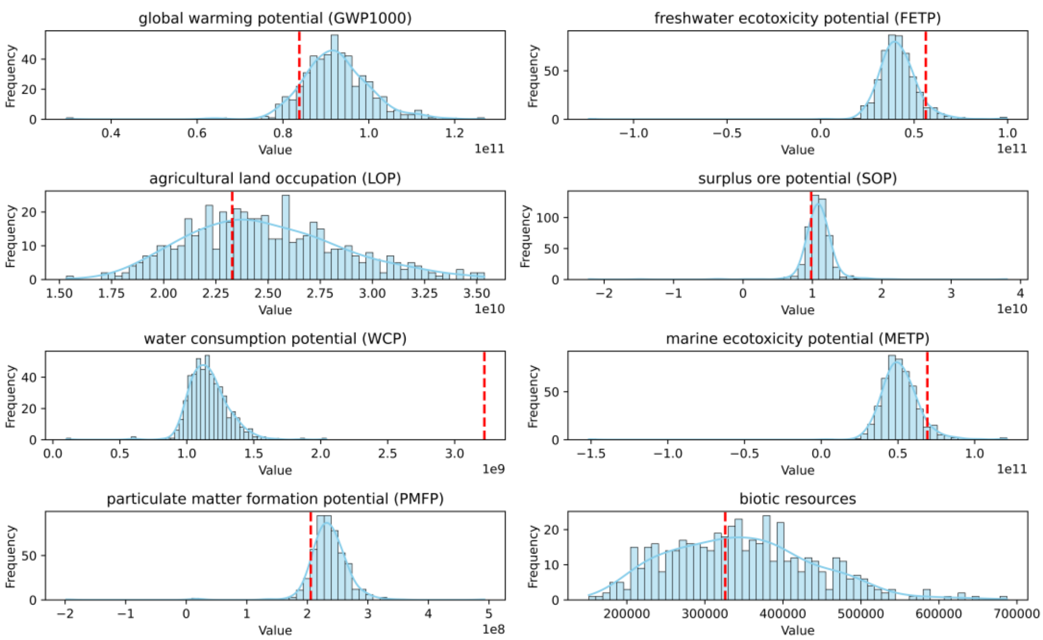


Figure 11: *Relative input values for n-1 levels*

Finally, the high sensitivity of environmental impacts coming from heat storage on the overall can have a second explanation from an uncertainty perspective. Those two technologies are precisely one of the technologies with the lowest technological representativeness between the energy data and the inventory data. This fact combines two types of uncertainty described by Igos et al. [33]: quantity, due to the inherent uncertainty on the input data, and context, due to the decision of the LCA practitioner to select this inventory. As shown in the supplementary materials, thermal storage tanks inventories for thermal storage are hot water storage tanks of 600L and 2000L. Although the structure of the inventory follows a similar approximation to what it's described on [37], the large-scale hot water tanks have a capacity between 500-5000m^3. Thus, as pointed out by Pizzol et al. [38], the effect of economies of scale might reduce considerably the environmental impacts of certain technologies.

4 Discussion

4.1 Data Quality

As discussed by several authors (e.g. [11,39]), ecoinvent provides inventory data on various technologies, but it does not cover all sectors and services, making it partial scope. This can have a significant impact on the model, especially for heat storage technologies, where the difference between the inventory data and the expected technology is the largest. Nevertheless, this effect can be reduced through the study of parametric inventories, which could help in transitioning from small-scale inventories to large-scale technologies based on parametric data.

In addition, there are other uncertainties underlying the inventory data. Despite assuming a "business as usual" approach, there is a discrepancy between the modelled technology and the technology that would be used in the future. This effect is notable for the foreground processes, where efficiencies can improve, and in the background, where industrial processes for manufacturing can enhance overall efficiency.

The energy data used as input is subject to several limitations. In short, although the SPORES approach helps to reduce uncertainty related to the model structure [40], it is restricted to the input data used in the model, such as weather, technological data, and narratives. This leads to a form of uncertainty generally known as parametric uncertainty. As a result, the overall uncertainty along the chain of models, which includes Calliope-Enbios is not addressed.

Finally, the linearised approach of LCA cannot catch scale implications of environmental impacts, as the impact scale linearly with the demand of the technology. Therefore, natural variations such as saturation of secondary interactions are not considered in this methodology.

4.2 Methodological limitations

This study does not separate the inventory data into operation and construction. Thus, the amount of impact related to the different life cycle phases remains unknown in our study.

On the other hand, double accounting is a common issue affecting (especially) energy LCA, and it has been discussed by several authors [11,39,41–45]. Although we are aware of this matter, addressing it is not within the scope of this study.

Some technologies and sectors have been excluded due to several reasons. Technologies falling under *transmission* or *demand* categories were excluded due to methodological limitations. Besides, some technologies were excluded due to the lack of life cycle inventories: *hydrogen to liquids, hydrogen to methane, hydrogen to methanol* and *DAC (Direct Air Capture).* Therefore, the scope of the study does not cover all the information coming from Calliope.

As for the results, this study suffers from epistemological limitations. The option space created by the impact of 261 spores divides energy configurations into "*low-impact"* and "*high-impact".* However, it is important to note that this is only in reference to the option space generated, and to truly determine whether the impact is high or low, it should be compared to an external value outside of the option space. This could be the 2024 data, other countries, or other scenarios. We are only seeing a photo of 261 configurations for the year 2050, so it is necessary to think outside the box to fully understand the context. Moreover, the lack of similar studies analysing a wide option space of alternatives limits the comparison and external validation of our results. Nevertheless, the way in which these results are presented are valuable.

Enhancing the sensitivity analysis could be achieved by incorporating Global Sensitivity Analysis techniques. This approach would enable a more comprehensive understanding of the behaviours exhibited by the technologies yielding negative values in the Spearman correlation results. This refinement would contribute to a more insightful interpretation of the model's intricacies and provide valuable insights into the complex interplay of factors influencing the technologies under study.

Finally, the outcomes are influenced by a cluster of uncertainties inherent in the LCA methodology. Particularly, when confronted with substantial demands (TWh), these uncertainties are magnified, leading to pronounced standard deviations in each outcome. Consequently, the significance of these finding lies in the comparison between alternatives rather than the mere presentation of individual results. According to Hamming et al.[46], the aim of computation is to gain insights rather than just numbers. Therefore, simply stating that the global warming potential for configuration 32 is 1.3e8 tons is *not* valuable as uncertainties may affect this result. Stochastic methodologies, such as Monte Carlo, can prove these results to be inaccurate.

5 Conclusions

In this study, we conducted an analysis of the environmental impacts associated with 261 energy transition configurations in Portugal for the year 2050. The option-space derived from these results suggest that energy transition configurations developed under “as usual” modeling, considering economic and energy demand values, are able to exhibit low environmental impacts in comparison with other spores.

Through clustering, we categorized the configurations into “low-impact” and “high-impact”, revealing a notable trend: configurations featuring higher thermal storage and generation tend to pose a greater environmental harm compared to those emphasizing electricity production. However, it is crucial to recognize the epistemological limitations of our study, as it confines the scope to a specific option-space, rendering us “blind” to scenarios and comparisons beyond its boundaries.

Our data strongly indicates that there are no possible trade-offs in environmental impacts from an energy system perspective; a configuration is either harmful or less harmful. Nonetheless, slight variations within the option-space can yield diverse energy configurations, each potentially influencing specific sites of the country differently. The exception lies in the case of “biotic resources”, where the environmental impact depends on the defined amount of “biofuel extraction” in each configuration.

To advance our understanding, future research should address the limitations discussed in this work. Key areas for improvement include the separation of life cycle stages, mitigating double accounting issues, and incorporating external comparisons beyond the confines of the option-space.

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8 Supplementary Materials

8.1 Summary of technologies and inventories

Technologies	*Activity code*	*Location*	*Time-Period*	*Unit*	*Calliope Unit*	*Conversion*
wind_onshore	electricity production, wind, 1-3MW turbine, onshore	PT	2000-2021	kWh	TWh	1.00E+09
wind_offshore	electricity production, wind, 1-3MW turbine, offshore	PT	2000-2021	kWh	TWh	1.00E+09
hydro_run_of_river	electricity production, hydro, run-of-river	PT	1945 - 2021	kWh	TWh	1.00E+09
hydro_reservoir	electricity production, hydro, reservoir, non-alpine region	PT	1945-2021	kWh	TWh	1.00E+09
ccgt	electricity production, natural gas, combined cycle power plant	PT	2000 - 2021	kWh	TWh	1.00E+09
chp_biofuel_extraction	heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014	PT	2010-2021	kWh	TWh	1.00E+09
open_field_pv	electricity production, photovoltaic, 570kWp open ground installation, multi-Si	PT	2008-2021	kWh	TWh	1.00E+09
existing_wind	electricity production, wind, 1-3MW turbine, onshore	PT	2000-2021	kWh	TWh	1.00E+09
existing_pv	electricity production, photovoltaic, 570kWp open ground installation, multi-Si	PT		kWh	TWh	1.00E+09
roof_mounted_pv	electricity production, photovoltaic, 3kWp slanted-roof installation, multi-Si, panel, mounted	PT	2005-2021	kWh	TWh	1.00E+09
chp_wte_back_pressure	electricity, from municipal waste incineration to generic market for electricity, medium voltage	PT	2012-2021	kWh	TWh	1.00E+09
chp_methane_extraction	heat and power co-generation, natural gas, combined cycle power plant, 400MW electrical	PT	2000-2021	kWh	TWh	1.00E+09
waste_supply	electricity, from municipal waste incineration to generic market for electricity, medium voltage	PT	2012-2021	kWh	TWh	1.00E+09
biofuel_supply	market for ethanol, without water, in 99.7% solution state, from fermentation, vehicle grade	CH	2000-2021	kWh	TWh	1.14E+08

Technologies	Activity code	Location	Time-Period	Unit	Calliope Unit	Conversion
chp_biofuel_extraction	heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014	PT	2010-2021	MJ	TWh	3.60E+09
chp_wte_back_pressure	heat, from municipal waste incineration to generic market for heat district or industrial, other than natural gas	PT	2008-2021	MJ	TWh	3.60E+09
chp_methane_extraction	heat and power co-generation, natural gas, combined cycle power plant, 400MW electrical	PT	2000-2021	MJ	TWh	3.60E+09
biofuel_boiler	heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014	PT	2010-2021	MJ	TWh	3.60E+09
methane_boiler	heat and power co-generation, natural gas, combined cycle power plant, 400MW electrical	PT	2000-2021	MJ	TWh	3.60E+09
battery	market for battery cell, Li-ion	GLO	2011-2021	kg	TWh	6289300000
Heat_storage_big	market for heat storage, 2000l	GLO	2011-2021	unit	TWh	6120000
heat_storage_small	market for hot water tank, 600l	GLO	2011-2021	unit	TWh	20400000
Methane_storage	compressed air energy storage plant construction, 200 MW electrical	RER	2015-2021	unit	TWh	500
pumped_hydro	electricity production, hydro, pumped storage	PT	1945-2021	kWh	TWh	1000000000
el_import	market for electricity, high voltage	ES	2014-2021	kWh	TWh	1000000000
biofuel_to_diesel	market for fatty acid methyl ester	RoW	2011-2021	kg	TWh	133000000
biofuel_to_methane	market for biomethane, high pressure	CH	2000-2021	m3	TWh	23600000
biofuel_to_methanol	market for methanol, from biomass	CH	1995-2021	KG	TWh	159000000
electrolysis	Market for hydrogen production	GLO	2030	kg	TWh	30084235
Chp hydrogen	Chp hydrogen	GLO	NA	kwh	TWh	1000000000

8.2 Unit conversions

8.2.1 Electricity generation

To connect the various technologies and inventories of the dendrogram's "*electricity generation*" level, a conversion between two energy magnitudes is required: Calliope magnitudes, expressed in *TWh,* and the functional of the system, which is in kWh. The conversion can be directly expressed as follows:

$$1\,TWh = 10^9 kWh$$

8.2.1.1 Chp hydrogen

The inventory for chp hydrogen plant was adapted from a conventional chp plant in Portugal. We adapted the input of hydrogen based on the difference in the energy density between natural gas and hydrogen, resulting in 0.649m3 of hydrogen per kWh of production assuming normal conditions. Since the functional unit of hydrogen production activities is in kg and we assumed a 5bar pressure input, it results in 0.054kg of hydrogen referenced to the functional unit of the inventory (1kWh of electricity production).

Finally, the biosphere flows were also adapted. We removed all the biosphere flows except NOx emissions, and water vapor, which was adapted according to stoichiometry relations.

All the code to produce this inventory is open at https://github.com/LIVENlab/Sparks.git

8.2.2 Thermal generation

As of the thermal generation technologies, different conversions have been carried out for those activities expressed in *MJ*, and it can be presented as follows:

$$TWh = 3.6 \cdot 10^9\ MJ$$

The technologies that are under this conversion are the following:

- Chp biofuel extraction
- Chp wte back pressure
- Chp methane extraction
- Biofuel boiler
- Methane boiler

8.2.3 Storage

The storage technologies are modelled from a capacity perspective. Then, we have used the "storage_capacity.csv" data. Only pumped hydro has been modelled using the "flow_out_sum" data. Then, the conversions required are different and case dependent.

8.2.3.1 Batteries

An assumption has been made on top of the inventory used. In *ecoinvent,* the inventory is referenced to the functional unit of 1kg of lithium battery. Thus, a mean energy density of the battery has been assumed to be 240 Wh/kg. Then the conversion used can be expressed as follows:

$$1\,TWh \cdot \frac{10^{12}W}{1TWh} \cdot \frac{1kg\ battery}{240W} = \mathbf{4.5 \cdot 10^{9} kg}$$

8.2.3.2 Heat storage big

In Calliope this technology is described as a “hot water tank 3000L”. In the selected inventory from ecoinvent, the reference unit is a 2m3 hot water tank (unit) and no further description of the capacity of the system is included.

We calculated the storage capacity of the system using energy balances and data from the Danish Energy Agency [47][37] .

Since the energy or capacity of a system can be described as:

$$E(kJ) = Cp \cdot m \cdot \Delta T$$

Where Cp corresponds to the calorific capacity of water at constant pressure (4.2 kJ/kg·ºC), m is the mass of water and ΔT is the difference of temperature between the water and the surroundings, where 90ºC of water and 20ºC of the surroundings have been assumed for the calculations. Then, the capacity of the system is 163.33 kWh per tank. Finally, to fulfil the requirement of supplying 1TWh with this technology:

$$1\,TWh = 6.12 \cdot 10^{6}\ tanks$$

As the data from the inventories are regarded as the impacts of the tank’s manufacture and distribution, it has been modelled as the minimum number of tanks needed to satisfy the requirements of a specific scenario.

8.2.3.3 Heat storage small

In this case, the inventory used is “hot water tank 600L”. The same calculations as before can be done, obtaining the following result:

$$1\ TWh = 2.04 \cdot 10^{7}\ tanks$$

8.2.3.4 Methane storage

The selected process from ecoinvent is "*compressed air energy storage plant construction, 200MW, electrical*", and a unit plant as a reference. Then, to convert it to a Calliope-ENBIOS readable unit, a conversion between the power and the capacity of the system is required. Based on data from the *Danish Energy Agency*[48] [37], a plant of 200MW might be referred as a 2000 MWh plant capacity. Thus

$$1\ TWh = \ 500\ plants$$

8.2.3.5 Pumped hydro

The data used for pumped hydro was sourced from the "flow_out_sum" file. Since the reference unit of the inventory is in kWh, the conversion can be therefore expressed as the electricity generation case, where:

$$1\ TWh = 10^{9} kWh$$

8.2.4 Carrier conversions

This category groups all the technologies which transform or produce energy carriers within the energy system (check figure 3 of the source document) to be used in other processes to produce electricity or heat.

8.2.4.1 Biofuel Supply

The process chosen from ecoinvent is the production of biofuel by means of first-generation stocks; *"market for ethanol, without water, in 99.7% solution state, from fermentation"*. The reference unit is in kg, and consequently a conversion from the reference unit to TWh (energy data) has been applied. In the supplementary materials of ecoinvent include the calorific density of the biofuel, being 31.58 MJ/kg. Hence:

$$1TWh \frac{3.6 \cdot 10^{9} MJ}{1TWh} \frac{1kg\ Bioethanol}{31.58\ MJ} = 113{,}9 \cdot 10^{6} kg$$

8.2.4.2 Biofuel to diesel

The conversion of biofuel to diesel is usually modified by a transesterification process. In ecoinvent, the inventory "market for fatty acids methyl ester" is referenced as 1kg of product. Based on data from Eurostat [47] (Energy Data — 2020 Edition - Products Statistical Books - Eurostat.) , the conversion can be expressed as follows:

$$1TWh\frac{3.6 \cdot 10^9 MJ}{1TWh}\frac{1kg\ Bioethanol}{27MJ} = 113{,}3 \cdot 10^6 kg$$

8.2.4.3 Biofuel to methane

The inventory "market for biomethane, high pressure" is referenced as 1m3 of product, which is compressed at 5bar. Using the law of ideal gases, and assuming a temperature of 298K, the density of the gas is assumed to be 3.31kg /m3. In the supplementary data from ecoinvent, it is reported that the energy density of the gas is 46MJ/kg. Therefore:

$$1TWh\frac{3.6 \cdot 10^9 MJ}{1TWh}\frac{1kg\ CH_4}{46MJ}\frac{1m^3}{3.31kg} = 2.64 \cdot 10^6 m^3$$

8.2.4.4 Biofuel to methanol

The methanol is produced through the gasification of biomass, and the inventory "market for methanol, from biomass" is reported as 1kg of pure methanol. Considering the calorific power of methanol (22.7MJ/kg) [48]:

$$1TWh\frac{3.6 \cdot 10^9 MJ}{1TWh}\frac{1kg\ Bioethanol}{22.7MJ} = 158.59 \cdot 10^6$$

8.2.4.5 Market for hydrogen production

The hydrogen production inventories were extracted from [49,50]. We combined the three main technologies (AWE, SOEC and PEM) into one single activity with 1kg of hydrogen as a functional unit. It receives 0.33kg of each activity mentioned.

Finally, assuming a power density of 120MJ/kg, the final conversion factor results in 30084235 kg/TWh.