CHIST-ERA-19

SEEDS Project

Deliverable 2.2

Socio-environmental metabolic pattern and associated impacts of energy system scenarios

(V.2.1)

February 2024

Document history

Version	Publication Date	Change
1.0	June 2022	Initial version
2.0	February 2024	Revision to include results from the two rounds of spores for the participatory processes, which include not only electricity but the whole energy system (electricity, heat, conversions, storage) in Portugal. ENBIOS has been updated and improved: - Changes in conversions (section 6.2) - Addition of inventories related to hydrogen (section 6.3) - Double counting
2.1	Feb 2024	Update of coauthors

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Executive Summary

Environmental parameters play a relevant role in determining sustainable energy systems but are often overlooked in energy system optimization models. This omission can lead to misleading decision-making processes.

The SEEDS project focuses on creating feasible and environmentally sustainable energy scenarios, using Portugal as a case study. By integrating energy system optimization, participatory feedback, and comprehensive environmental analysis, SEEDS aims to develop achievable pathways to a more sustainable future.

The technologically and regionally diverse energy configuration scenarios were obtained through Calliope. Calliope is an energy modelling framework that focuses on flexibility, temporal and regional resolution. In this project, it used economic costs to find a diversity of near-optimal solutions. The first set included 260 different alternatives, while the second set (with 270 alternatives) was obtained after a participatory process which enhanced the production of specific configurations according to the stakeholder preferences.

The work presented in this deliverable consists of the estimation of life cycle impacts of these sets of scenarios. Within the LIVEN group at ICTA-UAB, we are actively working on ENBIOS, a python-based framework that combines Life Cycle Assessment (LCA) with Multi-Scale Integrated Analysis of Societal and Ecosystem Metabolism (MuSIASEM). This integrated approach offers a holistic understanding of the socioenvironmental implications associated with different energy transition configurations with a hierarchical structure.

To characterise the technologies compassed by the Calliope model, we conducted an analysis using ENBIOS 2.1.12 and data from ecoinvent 3.9.1. We analysed the results for the following impact metrics: Global Warming Potential (GWP), Agricultural Land Occupation (LOP), Water Consumption Potential (WCP), Freshwater Eutrophication Potential (FEP) and Surplus Ore Potential (SOP). The analysis was performed for two sets of results.

Spore 0 is used as a benchmark, which represents the cost-optimized configuration. The first round of 260 spores shows that spore 0 is centrally located in the distribution of impacts for GWP. Most configurations show lower impacts for LOP and WCP, whereas FEP and SOP place spore 0 in the lower section of the distribution. Results suggest that solar technologies and batteries have a significant contribution to the general impact of the configuration.

The second round of spores, produced after a participatory process, presents statistically similar distributions in all categories except for the surplus ore potential, which presents a narrower distribution with lower impacts. The two rounds of energy configuration scenarios in Portugal provide a diversity of impacts in different dimensions that can allow public debate on location and technology preferences for energy transitions.

1 Introduction

Environmental parameters are key in the definition of sustainable energy systems yet excluded from most energy system optimization models (Martin et al., 2023). Still, decision-making may be misleading without considering them (Süsser et al., 2022).

SEEDS is a project that focuses on creating environmentally sustainable and economically feasible energy scenarios for countries undergoing an energy transition. Through this approach, SEEDS seeks to create achievable pathways for Portugal's energy sector, used as a case study, to transition towards a more sustainable future.

This project integrates various approaches, including an optimization of the energy system, derived from the Calliope modelling framework, participatory feedback from the local population, and an environmental analysis that seeks to go beyond carbon emissions. The inclusion of stakeholders is important in different stages: the choice of indicators, the first round of preferences via Webapp from which Calliope will be adapted to make a more adapted second round of results. All these results and process were discussed in a final workshop.

In this report, we describe the methods and results of the Environmental Impact Assessment for energy scenarios in Portugal.

2 Methodology - ENBIOS setup

In the SEEDS project, we develop the environmental and biophysical systems assessment tool ENBIOS (Madrid-López et al., 2022). ENBIOS is a Python-based tool that incorporates both Life Cycle Assessment (LCA) and Multi-Scale Integrated Analysis of Societal and Ecosystem Metabolism (MuSIASEM) methodologies. Within SEEDS, ENBIOS has been adapted to be used as a MuSIASEM checker (D2.1).

Figure 2 shows a general workflow of the ENBIOS setup. The first step of the ENBIOS setup is to add the configuration of the energy system, which are the system results of Calliope (spores, relaxed cost-optimization results). With this information, we create both the structure and quantitative relations of the MuSIASEM dendrogram within ENBIOS. The lower levels of the dendrogram are the energy supply technologies. The structure of the MuSIASEM dendrogram and their internal organization in ENBIOS can be consulted in section 2.2.

The MuSIASEM perspective is complemented with a life cycle perspective: from raw material extraction to manufacturing, installation, and operation. For each energy technology, ENBIOS includes inventory data and calculates its impacts.

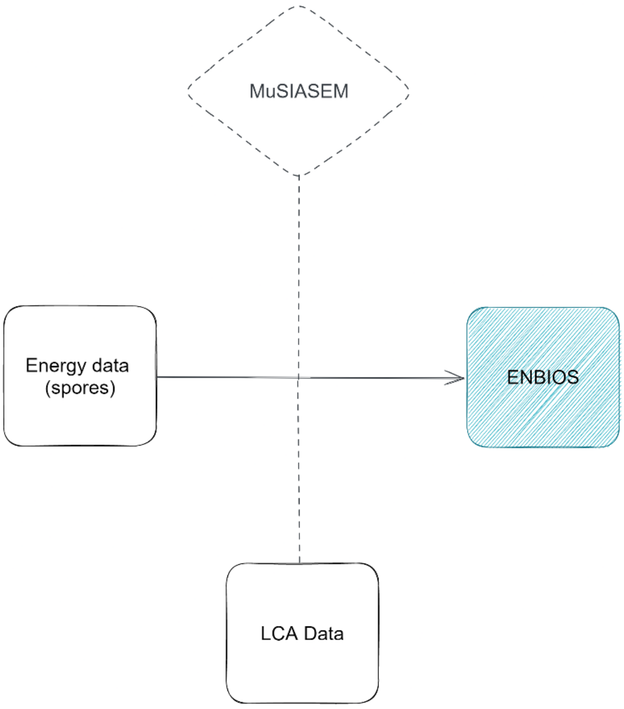

***Figure 1**: General workflow*

2.1 Scope and data

We used ENBIOS version 2.1.12 (Madrid-López et al. 2023) to quantify the environmental impacts of 261 and 271 energy configurations, named *spores*. These spores were near-optimal solutions calculated with the Calliope energy modelling framework (Pfenninger, 2017) within the SEEDS project. We also used life cycle inventory data from Ecoinvent 3.9.1. cut-off (Wernet et al., 2016).

The geographical resolution of the data is divided into two major regions, Portugal's north, and south (*PRT 1 & 2*). The north groups Norte and Centro, while the south groups Lisboa, Alentejo, and Algarve. Each region is split into different subregions for addressing regional variability of wind and PV production. Regional distribution has not been included in this deliverable but is relevant in modelling terms and could be analysed as further work.

Regarding the scope of the energy system, we consider energy extraction, transformation, and storage. We do neither consider transmission nor end-use. The temporal scope is year 2050, for which all Calliope SPORES are defined.

2.2 MuSIASEM settings

2.2.1 Dendrogram or system structure

The MuSIASEM *dendrogram* is a hierarchical representation of the relations within the system. This classification guides the upscaling component of the ENBIOS assessment, from the life cycle impacts of each technology to the full impacts of the energy system.

The relations between the levels can be guided by many parameters and in SEEDS are guided by *capacity* and *generation*.

The structure of the dendrogram is unique for the whole project, but the quantitative relations or shares between levels change with the SPORE.

Figure 2 shows the dendrogram used in SEEDS where functional and structural processes are represented. It is a way to express if a process is a structure that can be located in space and which has a connection with the ecosystem (wind turbine) or if it is a more general activity performed by the society to maintain itself (producing electricity). Level n-3 shows structural processes, which are indeed LCA-based activities, as explained below.

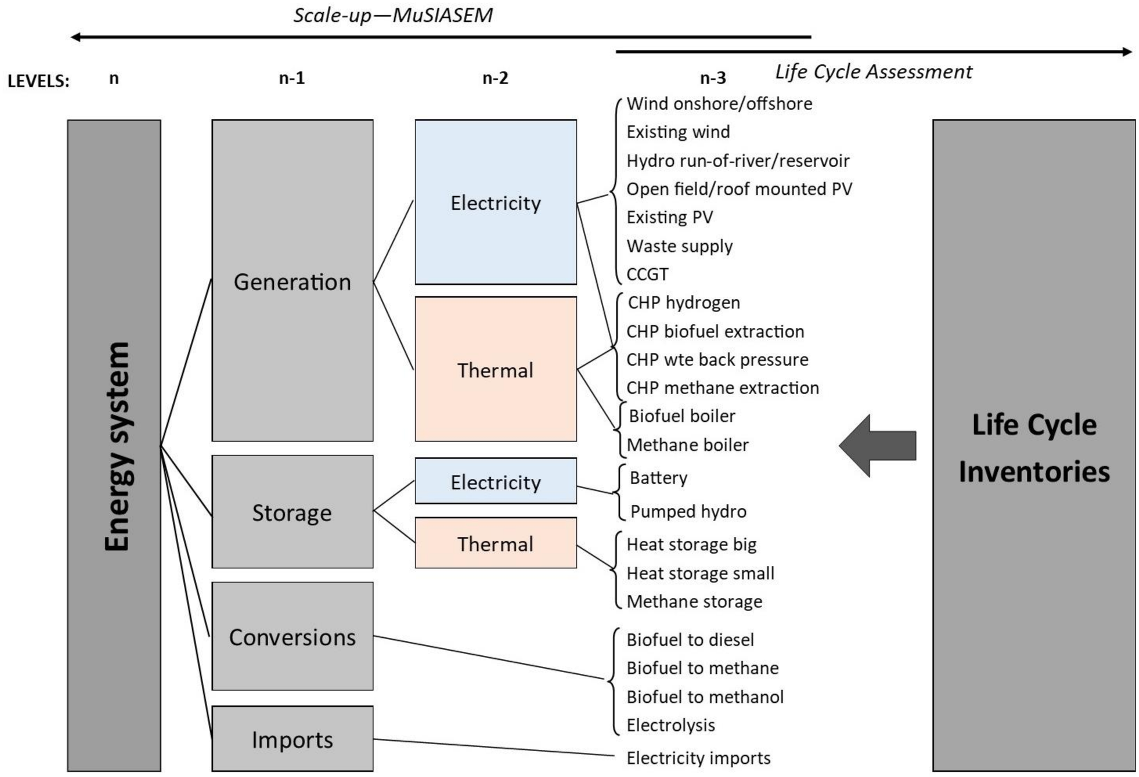

Figure 2 *Dendrogram of the energy system under analysis, showing the hierarchical representation at different levels. The level n-3 is linked to Life Cycle Inventories.*

2.3 Softlink with Calliope

In SEEDS, we construct our dendrogram at the lowest level considering the energy transformation technologies in the Calliope output files. The *"flow out sum"* provides a part of the required information. However, certain categories in this file belong to the End-Uses, and as a result, they have been excluded from our analysis. Also, Calliope represents the entanglement of the energy system. Some of these processes provide energy carriers to other processes of storage or further transformation (Figure 3).

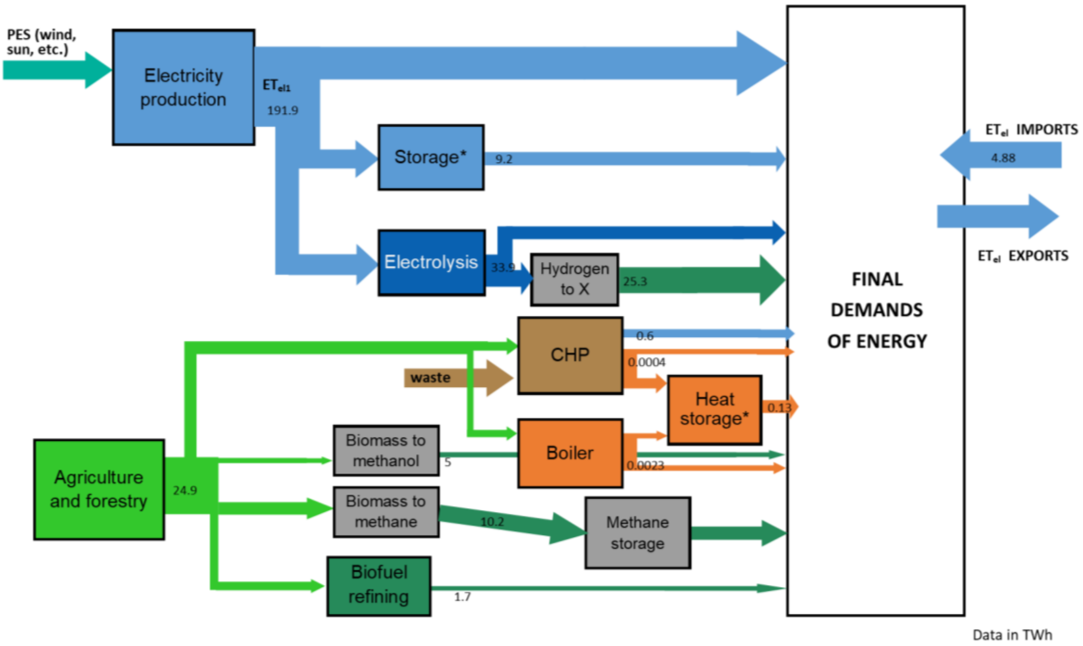

***Figure 3**: Non-exhaustive energy flows in Calliope, with energy values of spore 0 (first round of results) in TWh. Light blue arrows refer to electricity, dark blue to hydrogen, orange to heat, light green to biomass, dark green to diesel and kerosene.*

We have to take this into account when assigning these Calliope results to Life Cycle Inventories in order to avoid double accounting. For example, Calliope provides the outputs of electricity production in wind, solar and hydro. However, some of this electricity will go into electrolyzers for hydrogen production. If we assign the value of electricity production as a Functional Unit (FU) and the output of hydrogen production as another FU, we are counting twice the impacts due to electricity for hydrogen production (in its own chain and then in the electricity) (Figure 4). To address this, we have followed two different strategies: (i) we have eliminated the exchange related to the potential double-counted intermediate energy carriers, such as in the case of electrolysis and (ii) we have selected relevant categories (e.g., biofuel supply is not included as it is taking part of the LC of CHP, biofuel refining, biomass to methane, etc.).

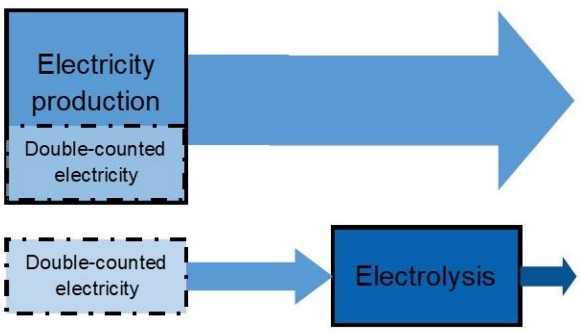

***Figure 4**: Potential double counting in impact assessment of electricity and hydrogen production, where the impacts of electricity could be accounted in the two chains*

In the case of storage technologies, the logic is different since their reference flows are related to the capacity (power, volume, kg of batteries) and not to the stored energy. Calliope provides results in TWh, and we had to make assumptions to link those to capacities, making assumptions on lifetime, and the energy stored in a year (see section 6.2 on conversions). Since these LCI from ecoinvent refer to the production of the batteries, they do not have any exchanges related to the energy they store and therefore there is no double counting.

As mentioned above, *Transmission* and *Demand* have not been considered. While transmission is occasionally included in LCI data, a thorough decomposition of each inventory is necessary to study it. Demand lies out of the scope of this study and the current capabilities of ENBIOS. Some energy technologies could not be included in the system due to the lack of LCI, listed in Table 1.

Table 1: *Calliope categories not included in ENBIOS environmental assessment. Biofuel supply has been excluded to avoid double counting issues.*

Demand	Energy system
• Electric heater • Electric hob • Gas hob • Light transport EV • Light transport ICE • Heavy transport EV • Heavy transport ICE	• Dac • H_2 imports and exports • Hydrogen storage • Hydrogen to liquids • Hydrogen to methane • Hydrogen to methanol • Heat pumps • Biofuel supply

2.4 LCA settings

ENBIOS calculates a set of indicators of environmental impact for each of the processes in the dendrogram, starting with the structural processes at the lower level. The link between the technologies in the calliope scenarios and the inventory data is presented in Annex 1. In SEEDS, inventory data is taken from Ecoinvent 3.9.1 cut-off (Wernet et al., 2016). To connect each technology with an LCA inventory, unit conversions were needed. Data on generation from Calliope is expressed in TWh whereas some inventories are expressed in other units. The detailed conversion factors for each technology are detailed in Appendix 6.2.

Global electricity markets were adapted according to 2050 projections in order to consider future changes in the background. The data for this modification is based on a 2ºC increase scenario provided by Teske (2019) and processed by Junne et al. (2020). To summarize, we have identified all the countries that have one or multiple markets for electricity (high voltage) 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.

2.4.1 Impact Assessment Methods

The impact assessment methods used in this study were sourced from *ReCiPe midpoint H 2016 v1.03* (Huijbregts et al., 2017) and the impact categories: Global Warming Potential (GWP100), Agricultural Land Occupation (LOP), Surplus Ore Potential (SOP), Water Consumption Potential (WCP) and Freshwater eutrophication potential (FEP).

***Table 2:** ReCiPe Impact categories* (Huijbregts et al., 2017) *used in SEEDS*

Impact category	*Indicator*	*Unit*	*Charachterization factor*	*Abbr (official)*
Land Use	occupation and time-integrated land transformation	m^2 x yr annual cropland-eq	agricultural land occupation	LOP
Water Use	increase of water consumed	m^3 water-eq consumed	water consumption potential	WCP
Mineral Resource scarcity	ore grade decrease	kg Cu-eq	surplus ore potential	SOP
Climate change	Infrared radiative forcing increase	kg CO_2-eq to air	global warming potential	GWP
Freshwater Eutrophication	phosphorus increase in freshwater	Kg P-eq to fresh water	freshwater eutrophication potential	FEP

3 Results and discussion

3.1 First round of spores

3.1.1 Level n – energy system.

Figure 5 shows the environmental impacts of the first round of spores. Results have been normalized to simplify the visualization and harmonize the different units and scales. We use the spore number 0 as a reference since it is the cost-optimal one with a classical optimization method. This is the single result that many energy models would provide. Starting with the Global Warming Potential (GWP), spore 0 occupies the centre of the distribution, with about 50% of energy configurations with less impact and 50% with more impact. As for the other indicators, we can divide them into two classes according to the position of spore 0 in the distribution: (i) the majority of configurations show a lower impact than spore 0, as in agricultural land occupation and water consumption potential) and (ii) spore 0 has lower impacts than most of the near-optimal scenarios, as for freshwater eutrophication potential and surplus ore potential.

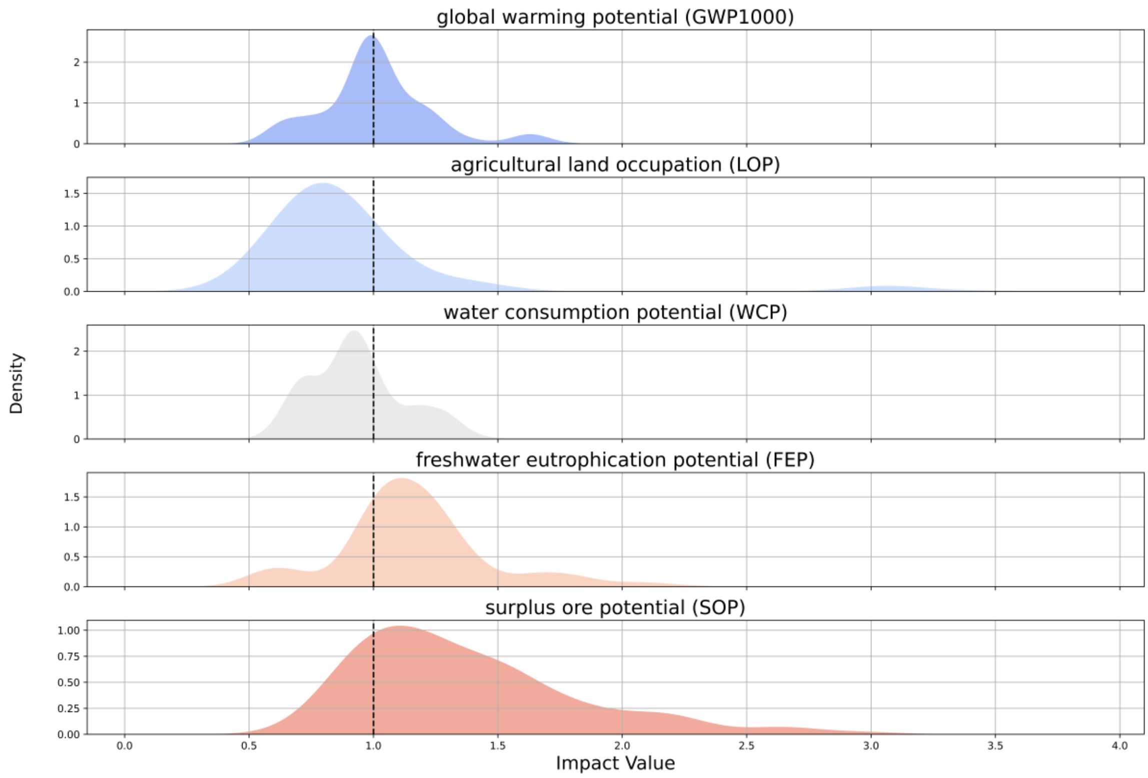

Figure 5: *Environmental impacts of round 1 energy configurations normalized to spore 0 (vertical line)*

On the other hand, the results at the highest level (energy system) don't suggest a strong correlation between impact categories. In fact, as depicted in Figure 6, only agricultural land occupation and global warming potential show insights of correlation (r=0.82), and freshwater eutrophication potential and water consumption potential (r=0.85). That means that, generally, when a configuration has a high impact in one of these categories, it is likely that other mentioned categories are high as well.

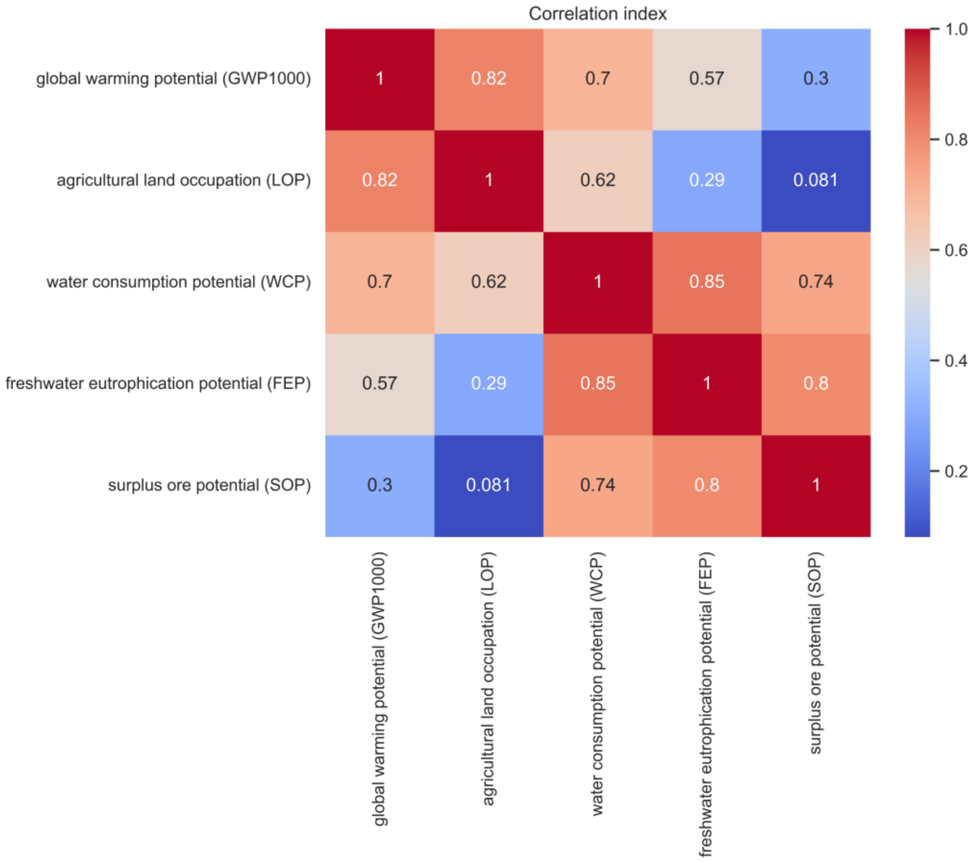

Figure 6: *Correlation index between impact categories at level n. P-values < 0.01*

3.1.2 Level n-3 – energy technologies.

We looked at the relation between different technologies and the total impact of the configuration. We applied Spearman's rank correlations to see the strength and direction of the relation between technological production (TWh) and the impacts at level n (energy system).

Starting with the positive values shown in Figure 7, two values stand out: batteries with surplus ore potential (r=0.9) and open field PV panels with water consumption potential (r=0.89). According to Spearman's correlation assumptions, this indicates that there is a positive (monotonic) relation between these technologies and the indicators. In simpler terms, it means that the more quantity of these technologies is defined in a spore, the more impact it generally generates.

However, caution is needed when interpreting the negative correlations with onshore wind technologies. The presence of these technologies does not necessarily mean a lower impact. Although the impact of wind per unit of energy generated might be slightly lower, as suggested in Figure 8, there is more to it. We need to look at the general distribution of the spore (Figure 9): wind onshore and open field PV are negatively correlated: a significant deployment of one technology generally implies a low availability of the other. Therefore, the Spearman correlation identifies a correlation in the negative direction; "*the more wind onshore there is, the less solar PV, and that generally translates into lower overall impact*". The same expression applies to batteries and wind onshore.

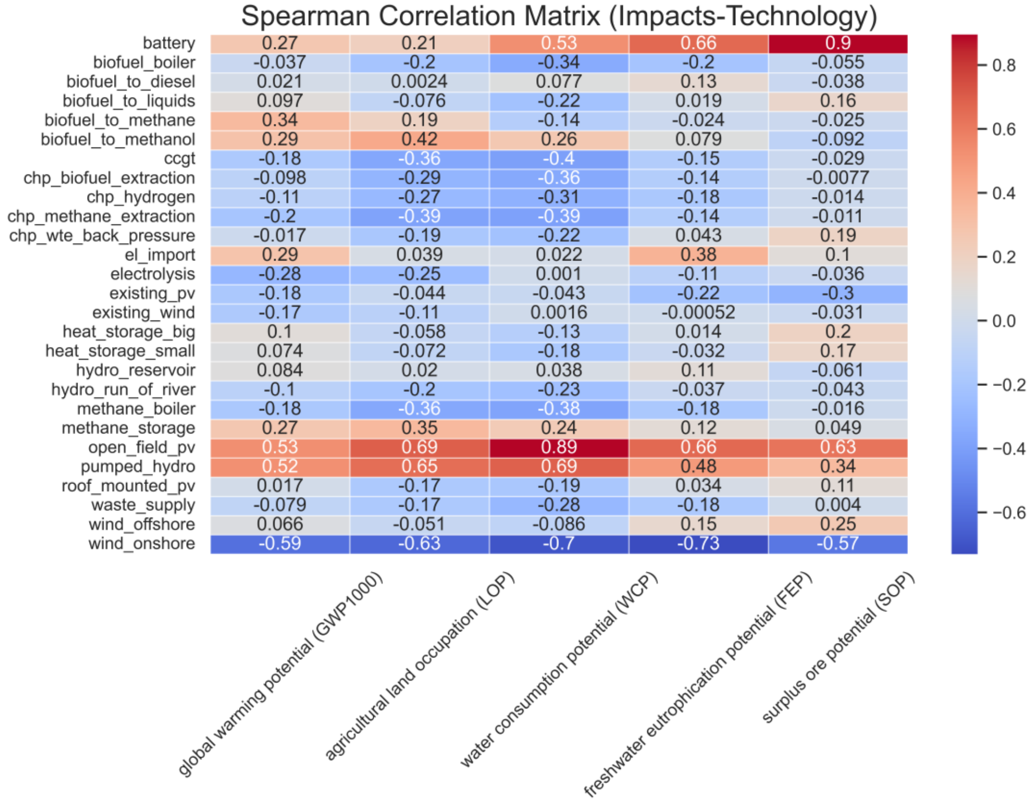

Figure 7: *Spearman correlation matrix of technologies at level n-3 to impacts at level n-1 for round 1*

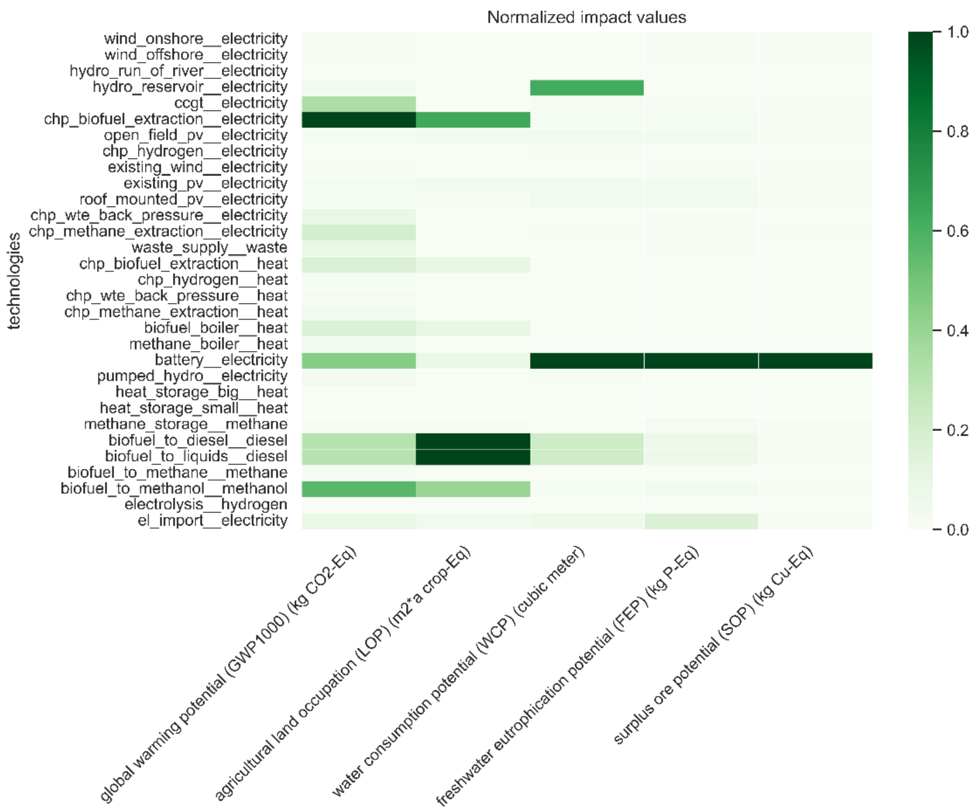

Figure 8: *Impact per TWh normalized between 0 (min) and 1 (max)*

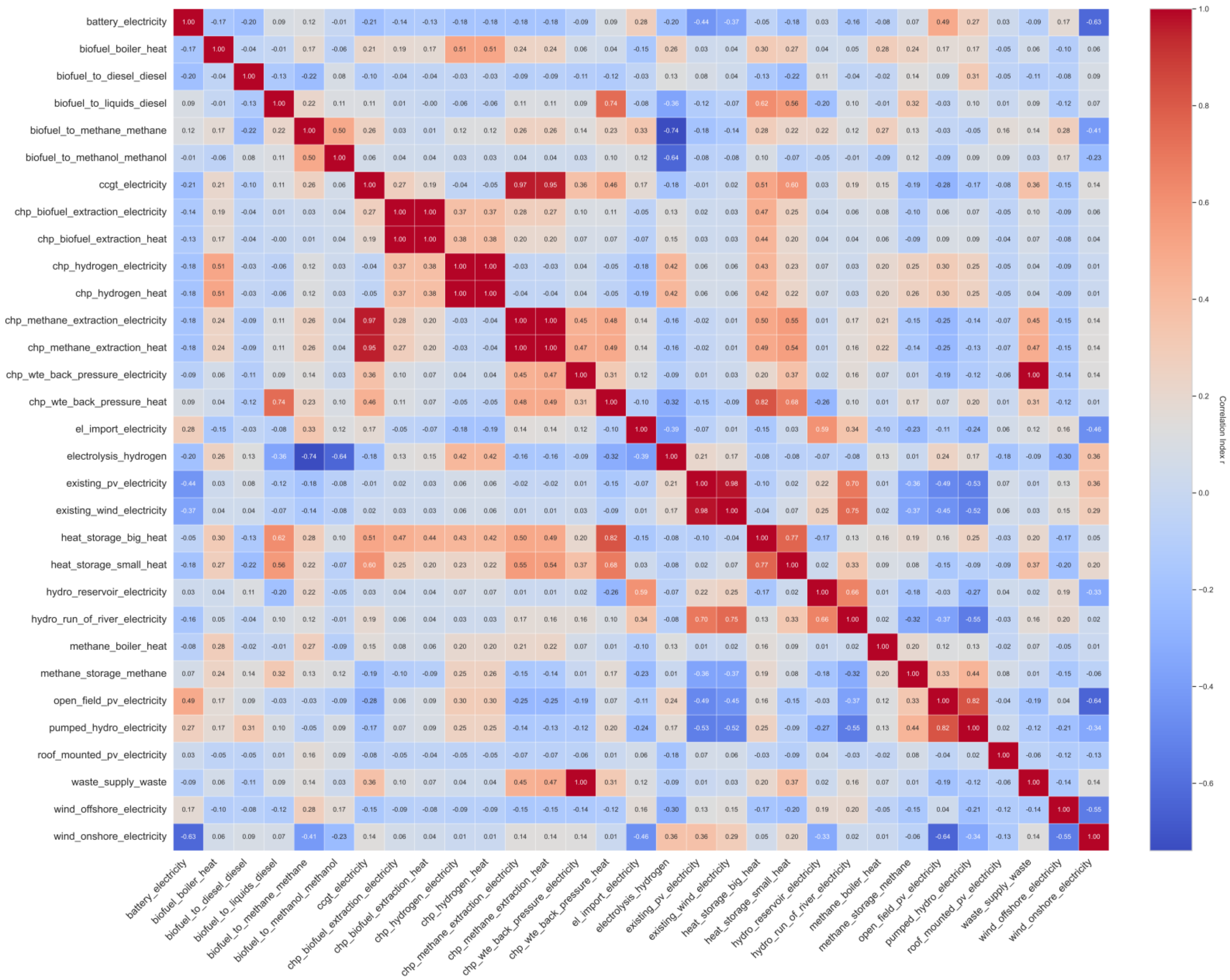

Figure 9: *Technological correlations at level n-3 in Spore definition for round 1*

3.2 Comparison between rounds 1 and 2

We compared the distributions of rounds 1 and 2 to look for differences and improvements after including the feedback of the participatory process (Figure 10). The first difference between rounds is the standard deviation: results from the second round tend to occupy a more restricted space. This might be due to the definition of the second round, which promoted and extended a specific group of alternatives based on participatory inputs.

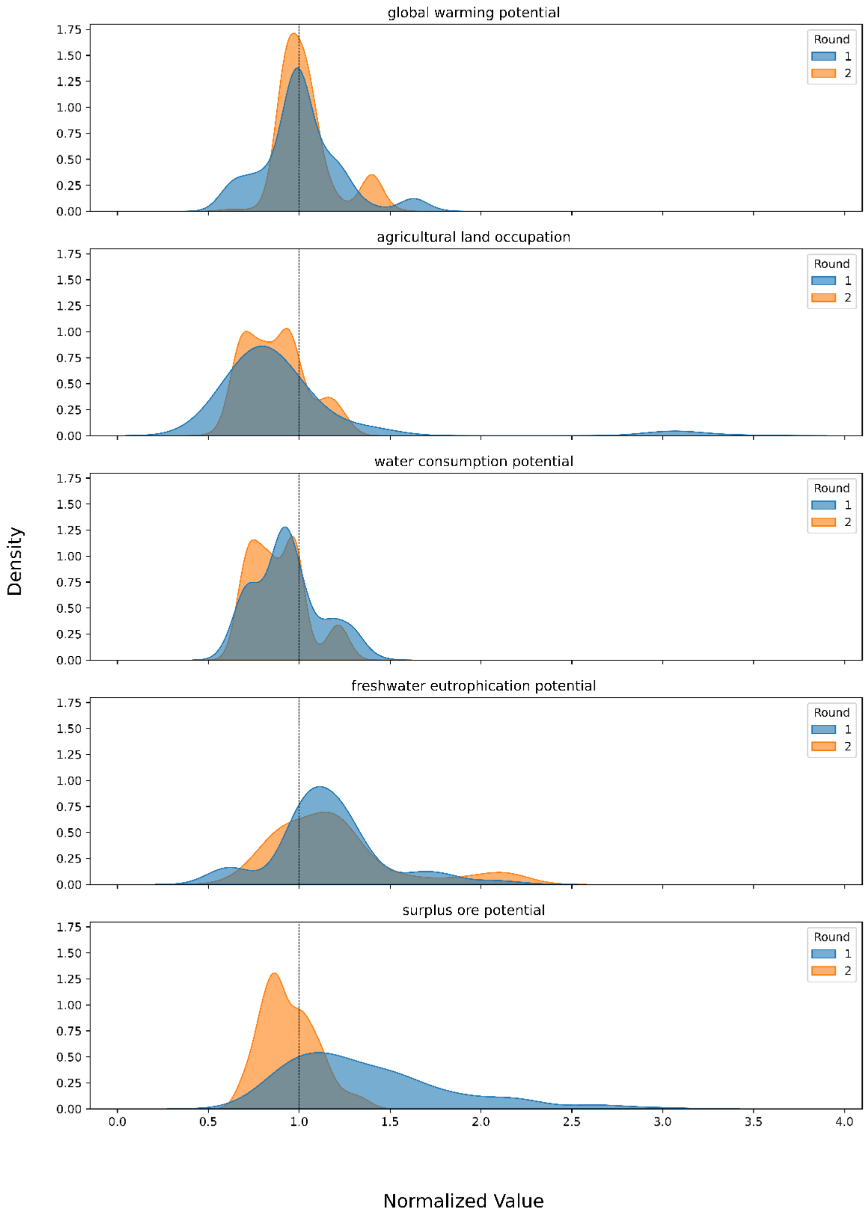

Figure 10: *Distribution of impacts normalized to spore 0 of the sets of energy system configurations in rounds 1 and 2.*

We performed a Wilcoxon singed-rank test to look for significant differences in the two sets of results. Only the surplus ore potential indicator presents significant p-values for the test (<0.01), indicating that the second round presents a significantly lower distribution.

Figure 11 presents a more detailed view of what is presented above. The second round tends to reduce the standard deviation (as mentioned above), avoiding extreme values in both directions. Nevertheless, the only indicator that presents better configurations is surplus ore potential.

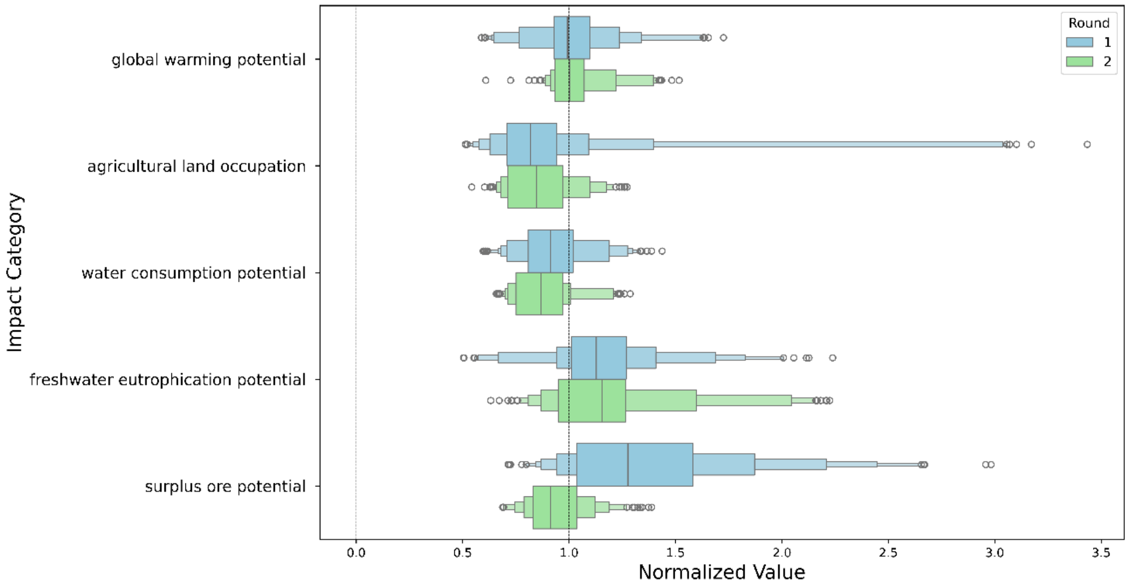

***Figure 11**: Boxen plot of impacts normalized to spore 0 in rounds 1 and 2. Vertical line at x=1*

3.3 Second round of spores

Regarding the analysis of the second round, there are signs of correlation between indicators; agricultural land occupation and global warming potential (r=0.8), agricultural land occupation and water consumption potential (r=0.79), global warming potential and freshwater eutrophication potential (r=0.79) (Figure 12).

The technologies driving the general impact present a different behaviour given the change of definition of the spores' search. We present in Figure 13 the Spearman rank correlations for the second round of spores. As mentioned above, these results depend on the established relations within the definition of the different energy configurations in Calliope.

In Figure 14, we find a higher number of technologies strongly correlated, which adds complexity to the analysis and interpretation of results. Nevertheless, batteries and solar PV technologies show the same patterns as in the first round. Additionally, we find new pairs such as electrolysis and biofuel to methane with the water consumption indicator. In this case, electrolysis has a higher impact on water consumption and its presence is negatively correlated with biofuel to methane. Pumped hydro, on the other hand, is strongly correlated with solar PV, and it also contributes to high impacts on water consumption.

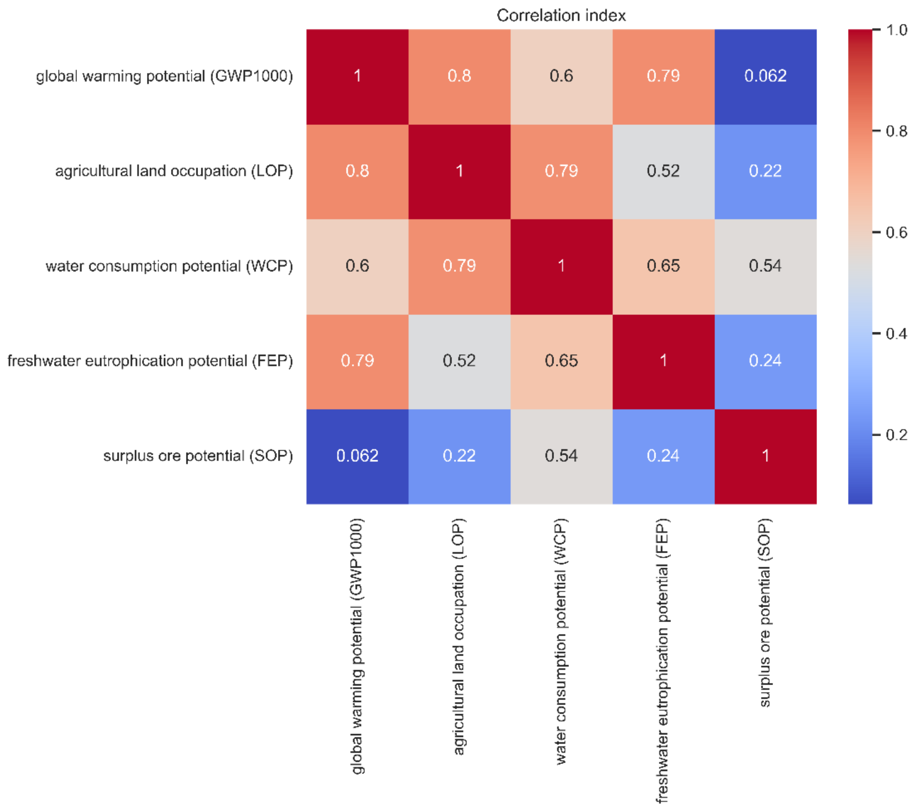

Figure 12: *Correlation index between impact indicators at level n. Second round of results*

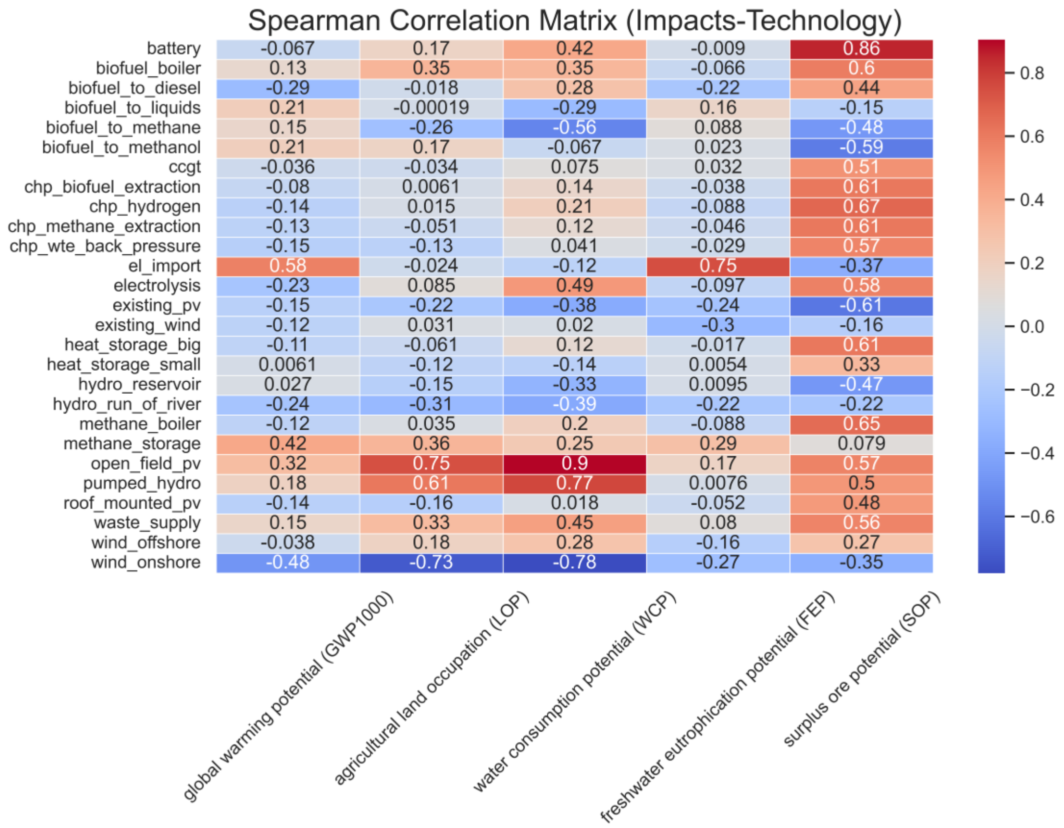

Figure 13: *Spearman rank correlation index between impacts at level n and technologies at level n-3. Second round of results*

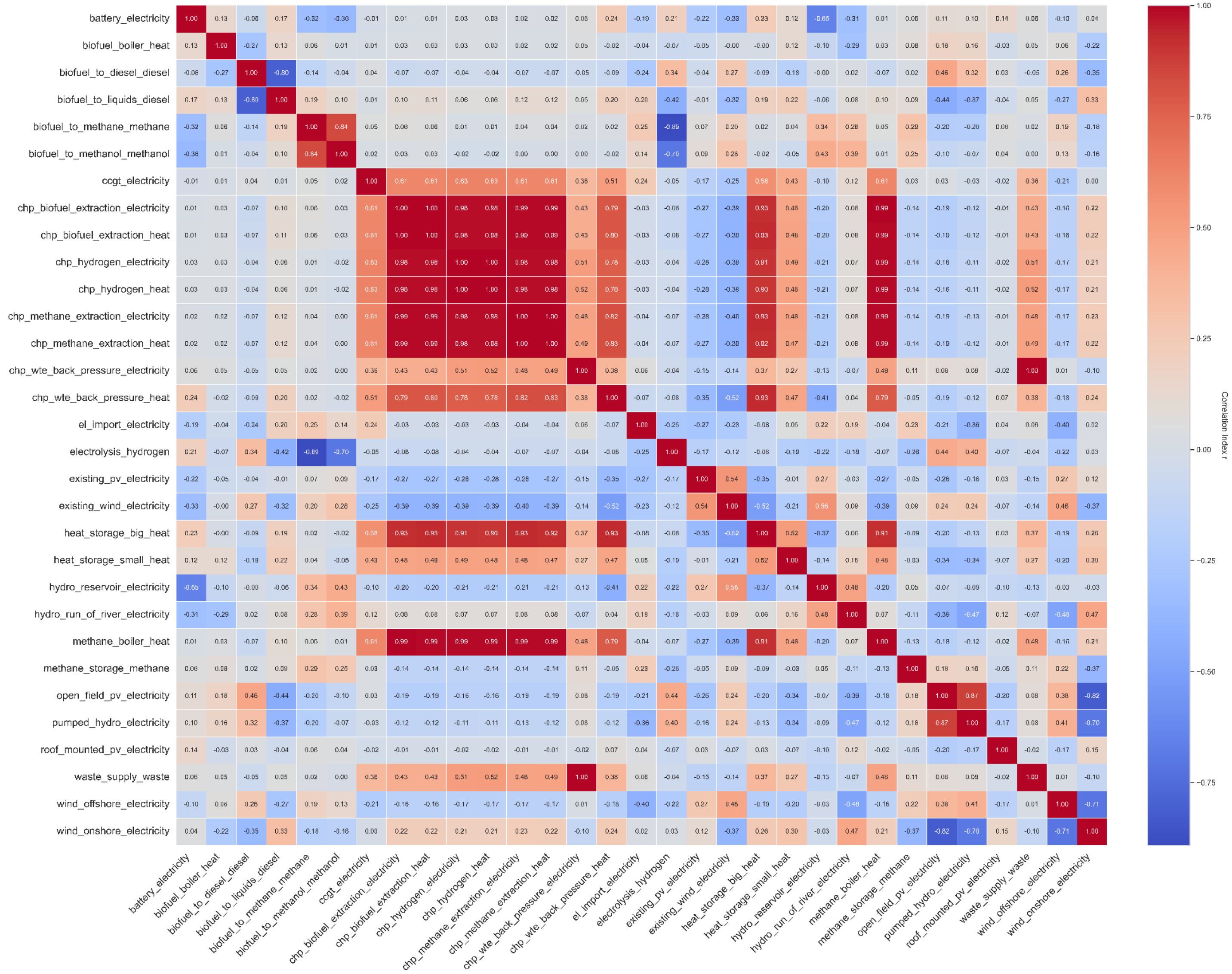

Figure 14: *Technological correlations at level n-3 in Spore definition for round 2*

4 Final remarks

This study is subjected to the inherence uncertainty of the different models and databases. For the uncertainty and sensitivity analysis of the whole human-computer loop, see (de Tomás-Pascual et al., 2024)

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6 Annexes

6.1 Summary of technologies and life cycle inventories

PROCESSOR	PARENT PROCESSOR	FACTOR	UNITS	ACTIVITY NAME	LOCATION
WIND_ONSHORE	Electricity_generation	1000000000	kWh	electricity production, wind, 1-3MW turbine, onshore	PT
WIND_OFFSHORE	Electricity_generation	1000000000	kWh	electricity production, wind, 1-3MW turbine, offshore	PT
HYDRO_RUN_OF_RIVER	Electricity_generation	1000000000	kWh	electricity production, hydro, run-of-river	PT
HYDRO_RESERVOIR	Electricity_generation	1000000000	kWh	electricity production, hydro, reservoir, non-alpine region	PT
CCGT	Electricity_generation	1000000000	kWh	electricity production, natural gas, combined cycle power plant	PT
CHP_BIOFUEL_EXTRACTION	Electricity_generation	1000000000	kWh	heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014	PT
OPEN_FIELD_PV	Electricity_generation	1000000000	kWh	electricity production, photovoltaic, 570kWp open ground installation, multi-Si	PT
CHP_HYDROGEN	Electricity_generation	1000000000	kWh	heat and power co-generation, hydrogen, combined cycle power plant, 400MW electrical	RoW
EXISTING_WIND	Electricity_generation	1000000000	kWh	electricity production, wind, 1-3MW turbine, onshore	PT
EXISTING_PV	Electricity_generation	1000000000	kWh	electricity production, photovoltaic, 570kWp open ground installation, multi-Si	PT
ROOF_MOUNTED_PV	Electricity_generation	1000000000	kWh	electricity production, photovoltaic, 3kWp slanted-roof installation, multi-Si, panel, mounted	PT
CHP_WTE_BACK_PRESSURE	Electricity_generation	1000000000	kWh	electricity, from municipal waste incineration to generic market for electricity, medium voltage	CH
CHP_METHANE_EXTRACTION	Electricity_generation	1000000000	kWh	heat and power co-generation, natural gas, combined cycle power plant, 400MW electrical	PT
WASTE_SUPPLY	Electricity_generation	1000000000	kWh	electricity, from municipal waste incineration to generic market for electricity, medium voltage	CH
CHP_BIOFUEL_EXTRACTION	Thermal_generation	3600000000	MJ	heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014	PT
CHP_HYDROGEN	Thermal_generation	3600000000	MJ	heat and power co-generation, hydrogen, combined cycle power plant, 400MW electrical	RoW
CHP_WTE_BACK_PRESSURE	Thermal_generation	3600000000	MJ	heat, from municipal waste incineration to generic market for heat district or industrial, other than natural gas	CH
CHP_METHANE_EXTRACTION	Thermal_generation	3600000000	MJ	heat and power co-generation, natural gas, combined cycle power plant, 400MW electrical	PT
BIOFUEL_BOILER	Thermal_generation	3600000000	MJ	heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014	PT
METHANE_BOILER	Thermal_generation	3600000000	MJ	heat and power co-generation, natural gas, combined cycle power plant, 400MW electrical	PT
BATTERY	Electricity_storage	60490000	kg	market for battery, Li-ion, NCA, rechargeable, prismatic	GLO
HEAT_STORAGE_BIG	Thermal_storage	2630	unit	market for heat storage, 2000l	GLO
HEAT_STORAGE_SMALL	Thermal_storage	5230	unit	market for hot water tank, 600l	GLO
METHANE_STORAGE	Thermal_storage	1.88	unit	compressed air energy storage plant construction, 200 MW electrical	RER
PUMPED_HYDRO	Electricity_storage	1000000000	kWh	electricity production, hydro, pumped storage	PT
EL_IMPORT	Imports	1000000000	kWh	market for electricity, high voltage	ES

BIOFUEL_TO_DIESEL	Conversions	133000000	kg	market for fatty acid methyl ester	RoW
BIOFUEL_TO_LIQUIDS	Conversions	133000000	kg	market for fatty acid methyl ester	RoW
BIOFUEL_TO_METHANE	Conversions	23600000	m^3	market for biomethane, high pressure	CH
BIOFUEL_TO_METHANOL	Conversions	159000000	kg	market for methanol, from biomass	CH
ELECTROLYSIS	Conversions	30084235	kg	Group_market_for_hydrogen	GLO

6.2 Unit conversions

This file presents the unit conversions to link inventory data with Calliope outputs (WP1).

6.2.1 Electricity generation

To connect the various technologies and inventories of the dendrogram's "*electricity generation*" level, we made a conversion between Calliope outputs, in TWh*,* and the reference flow of the inventories, in kWh.

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

6.2.2 Thermal generation

Thermal generation technologies in Calliope also use TWh. To match ecoinvent inventories, we converted them into MJ:

$$1\ \mathrm{TWh} = 3.6 \cdot 10^{9}\ \mathrm{MJ}$$

6.2.3 Storage

Calliope outputs for storage are given in TWh. These do not match reference flows in ecoinvent, which are related to the structural elements in terms of either size or unit. Then, we need to generate connections between those sizes and the TWh of stored and delivered energy determined by the Calliope scenarios. Then, we need to know:

a) Energy stored per year per item (assumption of stored and delivered energy per day/week and multiplication by 365 days or 52 weeks)
b) Number of items needed (total energy stored/energy stored per year per item)
c) Impacts per one year (divided by lifetime)

6.2.3.1 Batteries

a) Energy stored per year per item:

Assumption: batteries are discharged and charged 2 times per week. The diversity of uses for batteries means that the "full equivalent cycles" are diverse.

The mean energy density of the battery according to ecoinvent is 240 Wh/kg.

$$\text{year of functioning of 1kg of battery} \cdot \frac{52\ \text{weeks}}{1\ \text{year}} \cdot \frac{2\ \text{cycles}}{1\ \text{week}} \cdot \frac{0.159\text{kWh}}{1\ \text{cycle}} = 16.53\,\frac{\text{kWh}}{\text{year} \cdot \text{kg}}$$

b) Number of items needed per TWh:

$$\frac{10^{9}\ \text{kWh (1 TWh) of energy stored in a year}}{16.53\ \text{kWh per year and kg of battery}} = 6.05 \cdot 10^{7}\ \text{kg of battery for providing 1 TWh in a year (fund of batteries)}$$

c) Divide by lifetime and get the conversion factor:

$$\text{Impacts of 1 TWh of stored energy} = \frac{\text{impact of } 6.05 \cdot 10^{7}\ \text{kg of battery}}{10\ \text{years of lifetime}}$$
$$= \mathbf{impact\ of\ 6.05 \cdot 10^{6}\ kg\ of\ battery}$$

6.2.3.2 Heat storage big

a) Energy stored per year per item:

In Calliope, this technology is described as a "hot water tank 3000 l". In the selected inventory from Ecoinvent, the reference unit is a 2 m^3 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 (Technology Data | Energistyrelsen, 2023). The energy or capacity of a system can be described as:

$$\mathrm{E\ (kJ)} = \mathrm{c_p} \cdot \mathrm{m} \cdot \Delta\mathrm{T}$$

Where C_p corresponds to the calorific capacity of water at constant pressure (4.2 kJ/kg·°C), m is the mass of water and ΔT is the difference of temperature between the water and the surroundings, where 90°C of water and 20°C of the surroundings have been assumed for the calculations. Then, the capacity of the system is 163.33 kWh per tank.

Assumption: heat storage is discharged and charged 2 times per week.

$$\text{1 year of functioning of 1 tank} \cdot \frac{\text{52 weeks}}{\text{1 year}} \cdot \frac{\text{2 cycles}}{\text{1 week}} \cdot \frac{\text{163.33 kWh}}{\text{1 cycle}} = 16983.2 \frac{\text{kWh}}{\text{year} \cdot \text{tank}}$$

b) Number of items needed per TWh:

$$\frac{10^9 \text{ kWh (1 TWh) of energy stored in a year}}{\text{16983.2 kWh per year and tank}} = 5.89 \cdot 10^4 \text{ tanks for providing 1 TWh in a year (fund of large tanks)}$$

d) Divide by lifetime and get the conversion factor:

Lifetime provided by Ecoinvent metadata (25 years).

$$\text{Impacts of 1 TWh of stored energy} = \frac{\text{impact of } 5.89 \cdot 10^4 \text{ tanks}}{\text{25 years of lifetime}} = \mathbf{impact\ of\ 2.36 \cdot 10^3\ tanks}$$

6.2.3.3 Heat storage small

a) Energy stored per year per item:

In the selected inventory from Ecoinvent, the reference unit is a 600 l 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 (Technology Data | Energistyrelsen, 2023). The energy or capacity of a system can be described as:

$$\mathrm{E\ (kJ)} = \mathrm{c_p} \cdot \mathrm{m} \cdot \Delta\mathrm{T}$$

Where C_p corresponds to the calorific capacity of water at constant pressure (4.2 kJ/kg·°C), m is the mass of water and $\Delta\mathrm{T}$ is the difference of temperature between the water (90°C) and the surroundings (20°C). Then, the capacity of the system is 49 kWh per tank.

$$\mathrm{E\ (kJ)} = 4.2 \frac{\mathrm{kJ}}{\mathrm{kg \cdot {}^\circ C}} \cdot 600\ \mathrm{kg} \cdot (90 - 20) = 49\ \mathrm{kWh/tank}$$

Assumption: heat storage is discharged and charged 3 times per week.

$$\text{year of functioning of 1 tank} \cdot \frac{\text{52 weeks}}{\text{1 year}} \cdot \frac{\text{3 cycles}}{\text{1 week}} \cdot \frac{\text{49 kWh}}{\text{1 cycle}} = 7644 \frac{\text{kWh}}{\text{year} \cdot \text{tank}}$$

b) Number of items needed per TWh:

$$\frac{10^9 \text{ kWh (1 TWh) of energy stored in a year}}{7644 \text{ kWh per year and tank}}$$
$$= 1.31 \cdot 10^5 \text{ tanks for providing 1 TWh in a year (fund of small tanks)}$$

a) Divide by lifetime and get the conversion factor:

We assume the same lifetime as the large hot storage (25 years)

$$\text{Impacts of 1 TWh of stored energy} = \frac{\text{impact of } 1.31 \cdot 10^6 \text{ tanks}}{25 \text{ years of lifetime}} = \mathbf{impact\ of\ 5.23 \cdot 10^3\ tanks}$$

6.2.3.4 Methane storage

a) Energy stored per year per item:

We use the inventory "compressed air energy storage plant construction, 200MW, electrical", which comes from Bouman et al. (2016). This refers to a reservoir that stores compressed air and has a power plant that provides electricity. For us, the important thing is the storage in this kind of facilities, since it is the most similar to the typical underground storage for natural gas, and we expect the same type for methane.

First, we calculate the pressure in the reservoir. Assuming 0.01 MPa/m (Université Grenoble Alpes) and a well length of 680m:

$$\text{p} = 0.01 \frac{\text{MPa}}{\text{m}} \cdot 680\text{m} = 6.8 \text{ MPa} = 68 \text{ bar}$$

Then, we calculate the number of moles, assuming an ideal gas and the volume of the reservoir in the inventory ($7.97 \cdot 10^6$ m^3):

$$\text{n} = \frac{\text{V} \cdot \text{p}}{\text{R} \cdot \text{T}} = \frac{7.97 \cdot 10^6 \text{ m}^3 \cdot 68 \text{ bar}}{0.083 \frac{\text{bar}}{\text{mol} \cdot \text{K}} \cdot 273 \text{ K}} = 23918090 \text{ mol}$$

Through the number of moles, we can calculate the stored mass and therefore, the energy stored:

$$\text{E} = 23918090 \ \frac{\text{mol}}{\text{reservoir}} \cdot 0.016 \frac{\text{kg}}{\text{mol}} \cdot 50 \frac{\text{MJ}}{\text{kg}} = 19.18 \text{ TJ/reservoir} = 5.33 \cdot 10^6 \text{ GWh/reservoir}$$

We assume that each year we fill it and empty it only once like it happens nowadays with natural gas storage.

b) Number of items needed per TWh:

$$\frac{10^9 \text{ kWh (1 TWh) of energy stored in a year}}{5.33 \cdot 10^6 \text{ kWh per year and reservoir}}$$
$$= 188 \text{ reservoirs for providing 1 TWh in a year (fund of reservoirs)}$$

We must consider that current natural gas reservoirs are way larger than the ones in the inventory and that this inventory does not match the technology at hand.

a) Divide by lifetime and get the conversion factor:

The air storage is modelled with a lifetime of 100 years by Bouman et al. (2016).

$$\text{Impacts of 1 TWh of stored energy} = \frac{\text{impact of 188 reservoirs}}{100 \text{ years of lifetime}} = \mathbf{impact\ of\ 1.88\ reservoirs}$$

6.2.3.5 *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:

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

6.2.4 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.

6.2.4.1 *Biofuel to diesel and liquids*

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 (Energy Data — 2020 Edition - Products Statistical Books - Eurostat.) , the conversion can be expressed as follows:

$$1\ \text{TWh} \cdot \frac{3.6 \cdot 10^9 \text{MJ}}{1\text{TWh}} \cdot \frac{1\text{kg bioethanol}}{27\text{MJ}} = 113.3 \cdot 10^6 \text{kg}$$

6.2.4.2 *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:

$$1\ \text{TWh} \cdot \frac{3.6 \cdot 10^9\ \text{MJ}}{1\ \text{TWh}} \cdot \frac{1\ \text{kg}\ \text{CH}_4}{46\ \text{MJ}} \frac{1\ \text{m}^3}{3.31\ \text{kg}} = 2.64 \cdot 10^6\ \text{m}^3$$

6.2.4.3 *Biofuel to methanol*

Methanol is produced through the gasification of biomass, and the inventory “market for methanol, from biomass” is reported as 1 kg of pure methanol. Considering the calorific power of methanol (22.7MJ/kg) (Heat Values of Various Fuels - World Nuclear Association, n.d.)(Heat Values of Various Fuels - World Nuclear Association, n.d.):

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

6.2.4.4 *Market for hydrogen production*

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

6.3 Additional inventories

6.3.1 Market for hydrogen production

The hydrogen production inventories were extracted from (Gerloff, 2021; Sacchi et al., 2023). We combined the three main technologies (AWE, SOEC and PEM) into one single activity with 1 kg of hydrogen as a functional unit. It receives 0.33 kg of each of the three hydrogen production activities.

6.3.2 CHP hydrogen

The inventory for *CHP hydrogen* plant was adapted from a conventional CHP plant in Portugal. We removed the natural gas input and removed all the biosphere flows except NOx emissions, and water vapour, which was adapted according to stoichiometry relations. Given that the impacts of the production of hydrogen are already deleted as an input for other activities, there is no need to use the market for hydrogen as an input.