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

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Authors:

Alexander de Tomás Pascual (UAB)

Miquel Sierra (UAB)

Rafael Nebot (ITC)

Ramin Soleymani-Fard (UAB)

Gara Villalba (UAB)

Cristina Madrid López (UAB)

Contact: cristina.madrid@uab.cat

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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 SEED 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.

Within the LIVEN group at ICTA-UAB, we are actively working on ENBIOS, a pythonbased 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 hyerarchical structure.

To further characterize the technologies compassed by the Calliope model, we conducted an analysis using ENBIOS 0.78 and data from ecoinvent 3.8. We analyzed the results for the following impact metrics: Global Warming Potential, Agricultural Land Use Occupation, Metal Depletion, Natural Land Occupation, and Water Depletion.

The first set of results shows a trend of lower impact in the categories of "agricultural land" (occupation and transformation) and water depletion. However, metal depletion shows a remarkable increase of 400-900% higher than the current situation.

The same results were normalized by TWh of electricity produced. Metal depletion is, on average, 125% times higher per TWh than the current situation. The other environmental indicators show a clear decrease tendence.

Finally, the best and worst spores were selected by adding the total difference of indicators compared with the current situation. The spore with the overall lower impact is predominantly composed of wind energy (wind onshore), whereas in the worst case, the use of solar energy was higher.

The findings presented in this report underscore the significance of incorporating multiple environmental indicators beyond the Global Warming Potential (GWP), when assessing energy transition pathways. These results reveal a substantial rise in metal depletion across all examined spores.

It is important to note that due to limitations in the available data, our comparison was solely based on electricity production and was compared with data from 2020. This assessment is a first insight into the environmental implications of different electricity configurations in Portugal.

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 model, participatory feedback from the local population, and an environmental analysis that seeks to go beyond carbon emissions.

In this report, we describe the methods and results of the environmental impact assessment energy scenarios for Portugal. The scenarios and indicators included in here take into account the participatory process carried out within the SEEDS project.

2 Methodology - ENBIOS setup

In the SEEDS project we further 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 MuSIASEM checker (D3.1).

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 is done with the energy system results of Calliope. With this information we create both the structure and quantitative relations of the MuSIASEM dendrogram within ENBIOS, as well as its grammar. 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 Deliverable 2.1.

The MuSIASEM perspective is then complemented with the perspective of the life cycle activities associated to each of the, from raw material extraction to manufacturing. For each energy technology, ENBIOS includes inventory data and calculate its associated impacts.



2.1 Scope and data

We used ENBIOS version 0.78 (*Enbios* \cdot *PyPI*) to conduct an analysis of the environmental impacts of over 260 scenarios of energy transition or *spores*. These spores are calculated with the Calliope energy model (Pfenninger, 2017) within the SEEDS project. We also used life cycle inventory data from Ecoinvent 3.8 (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, which haven't been yet included in our study. Therefore, this study has focused on examining the two general regions of Portugal as a first approach to solving the environmental model.

Regarding the energy system, we only consider energy extraction and transformation. We do not consider transmission and storage nor end use. Therefore, part of the impacts related to these categories are not covered in the assessment, being the emissions due to the burning of fossil fuels the most important emission that is left out.

The temporal line is year 2050, for which all the calliope SPORES are defined. Results of the environmental impact are related to a baseline for year 2020, in order to give an idea of the variation of impacts and trade-offs between them.

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*. For example, the impacts of the solar energy sector are calculated as the sum of the impacts of photovoltaic and thermal solar energy.

In ENBIOS impacts can be calculated by unit of generation (TWh) or capacity (TW). In SEEDS we calculate them normalizing by unit of generation (TWh) and upscaled according to the share of each technology in the upper level. The structure of the dendrogram is unique for the whole project, but the quantitative relations or shares between levels change with the SPORE. Consequently, we have one dendrogram for each of the SPORES analysed (260).

Figure 2 shows the dendrogram used in SEEDS where functional and structural processes are represented. The difference between functional and structural processes is explained in deliverable 2.1 (REF) and 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 an activity performed by the society to maintain itself (producing electricity). Levels n-3 are functional processes whereas level n-4 shows structural processes, which are indeed LCA-based activities, as explained below.

The MuSASIEM grammar is a mapping of the different semantic categories of energy flows included in an energy assessment. It covers the differences between energy flow types in order to guide the development of impact indicators. The SEEDS grammar is represented in Figure 3.

The grammar has two components: *Processes* and *Flows*. The first ones can be described as the activities or sources related to the energy system. The second ones are the energy flows considered from energy extraction from source to end use. Energy flow categories can be disaggregated according to their source or sink processes. The semantic categories of flows described in Figure 3 are:

Figure 2: MuSIASEM dendrogram used in SEEDS



- *Primary Energy Sources (PES).* They are the initial sources of energy that are extracted from natural resources (fossil) or natural gradients (typically renewable), and are expressed in physical units tones of wood, m³ of water, etc-. In a grammar is represented by the first part of the arrow between the natural gradients and the energy transformation processes. PES are only disaggregated by natural gradient (wind, solar, natural gas, etc)
- Gross Energy Requirements (GER). The total amount of energy contained in the primary energy sources that reaches the energy transformation processes. It is

expressed in units of energy (Joules, Watts-hour). GER are also only disaggregated by natural gradient (wind, solar, natural gas, etc)

- Net Energy Requirements (NER): This is the total energy provided by the energy transformation process, considering that from the total GER, some energy is lost due to transformation efficiency. Therefore, the NER discounts the inherent efficiency of the technology, as well as the required energy to operate and maintain the transformation. NER can be classified according to the natural gradient (eg.natural gas) entering the transformation process or the energy carrier produced (electricity).
- *End Use (EnU):* In SEEDS, we define the end use as the energy that reaches the final user after transmission losses have been discounted.

For example, take natural gas that is used in a power station to produce electricity which is later transmitted and reaches a household. The amount of natural gas in m³ is the PES that carries a fuel capacity in GER. After transformation, the electricity produced would be recorded in NER and the part of it that reaches the household would be the EnU.

Often, all energy flow categories are not known and a few of them must be calculated, using efficiency coefficients and losses. There are two approaches for this. The top-down approach departs from either PES or GER and calculates author NER or EnU. The bottom-up approach would start with data of EnU or NER and calculate wither GER or PES. This distribution allows us to, for example, identify the amount of natural gas that is needed for a certain electricity end use. For ENBIOS this is important as the energy flow that is actually impacting the environment la related to either the extraction of energy sources (PES) or emissions during transformation (GER to NER) or end use (in the case of fossil fuels or biomass).

In this work, we analyze the NER category, and we relate it to the PES to make the connection with the environment.

Figure 3: MuSIASEM grammar



Energy flows

2.3 Softlink with calliope

The data received from WP1 is divided into different files, containing information about the energy production mix, the storage capacity, the import dependency, among others. The data used in this study was sourced from one file, namely "*flow out sum*". The former file contained information on the energy mix of the system for each spore examined.

In SEEDS, we construct our dendrogram by considering the energy transformation technologies included in the Calliope output files. The "flow out sum" provides a portion of the required information, mainly in the form of NER, However, certain categories present in this file belong to the EnU category, and as a result, they have been excluded from our analysis.

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 included in the calliope scenarios and the inventory data it's presented in Annex 1. In SEEDS, inventory data is taken from ecoinvent 3.8 (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 the inventories are expressed in different ways.

Based on the grammar, the technologies falling into the *flow out sum* file are part of the energy system and are expressed in energy units, such as TWh or Joules. Since this data is given in "Net *energy requirements*", conversions between thermal and mechanical energy can be carried out with minimal conceptual errors, since the physical expression are equivalent, and no human valuations are involved. The annex provides a detailed explanation of these energy conversions.

As mentioned above, the technologies falling under the *Transmission* and *Demand* levels of the dendrogram have not been considered. While the transmission is occasionally included in LCI data, a thorough decomposition of each inventory is necessary to study it. As for the LCA of demand, assessing it requires linking to demand models, which ENBIOs does not currently have.

Finally, there are some technologies that have not been included yet due to the lack of life cycle inventories:

- Chp hydrogen
- Electrolysis
- H2 import/export
- Hydrogen to liquids
- Hydrogen to methane
- Hydrogen to methanol

2.4.1 Impact assessment methods

The impact assessment methods used in this study were sourced *from ReCiPe midpoint* H 3.7.1 (Huijbregts et al., 2017) focusing on the following impact categories: Global Warming Potential, Agricultural Land Use Occupation, Metal Depletion, Natural Land Transformation, and Water Depletion.

2.5 Scenario analysis

In order to have a reference for the change on the impacts, we completed a full assessment for year 2020. Data on electricity generation in Portugal (Peninsula) is used as proxy to the NER category and data from the Direção-Geral de Energia e Geologia (DGEG, 2022), and data extracted from Our World in Data (Ritchie et al., 2022), which is based on (BP Statistical Review of World Energy, Ember Yearly Electricity Data (2023) and (*Ember European Electricity Review*, 2022) were used to generate the energy mix.

The resulting impacts form the SPORE assessment were then compared with this baseline scenario. We calculated the difference between the value of the spore for an

impact category and the value of the spore. Total impacts as well as impacts by TWh produced were calculated to avoid the bias of differences in the energy production of the different spores.

2.6 Finding the best spore

To find the "*best spore*" or the "*n-best spores*" in terms of environmental impact, we searched for the scenario that maximizes the negative difference in the sum of the different outcomes. In other words, for each spore, the difference from the baseline for each scenario was added up, and the one with the lowest value was selected.

3 Results and discussion

We analyzed the environmental performance of over 260 energy transition scenarios in Portugal by the year 2050.

The first set of results aggregated the environmental impacts of electricity production of different spores across different regions (north and south) into a single region, Portugalcontinent. These results were compared with the energy mix results from 2020 and are shown in Figure 4. It can be observed that there is a trend of lower impact in the categories of "agricultural land" (both occupation and transformation), and water depletion. On the other hand, most scenarios have a lower global warming potential (GWP) compared to the 2020 result, but the distribution show cases where it can be doubled. The most striking fact is metal depletion, which is between 400-900% higher than the current situation.

The best spore (in electricity generation terms) is highlighted in red and corresponds to spore "89". By looking at the energy mix of the best spore (Figure 5 a), it's clear that the dominant technology of production is the wind onshore (84% of the total energy produced). The second biggest contributor is the import of electricity from Spain (8.8%), followed by the hydro-technologies.

The same study can be conducted by looking at the worst spore (Figure 5 b), which is "219". The first thing that stands out is the significant contribution of solar energy compared to the previous case, and it might be the reason for the higher metal depletion produced (this scenario is located between the 3rd quartile and the major value of the set).

Figure 4: Results of the different scenarios studied in Portugal. Comparison of percentage change with the 2020 energy mix. In red, the "best overall scenario"



The amount of energy produced can mislead the analysis of the environmental impacts. On average, the amount of energy produced by each spore is 3.15 times higher than the current situation. An option to study whether the energy mix performs better in environmental terms or not is to look at it by TWh produced.

As shown in figure 6, the distribution of results is similar, as expected. However, this figure indicates that the amount of metal depletion is on average 125% times higher than the current situation. The other impacts are generally lower compared to what is shown in figure 5.

The mix of the best and worst spores is marginally different from the overall case as the best and worst spores are not the same as the previous case, i.e., 81 and 171, respectively. Besides, the worst spore is driven by the maximum value from the set of

results in the metal depletion indicator. However, a clear trend can be observed from this comparison; the selection is mostly driven by the amount of electricity produced by wind or solar technologies, where the overall impact produced by wind is generally lower than solar, and they both significantly affect the amount of metal depletion produced.

The difference between the impact in the current situation and future scenarios may increase for positive differences (more impact produced) and decrease for negative ones. This is because we are accounting for different background processes in the 2020 results that need to be eliminated to achieve more precise results. Therefore, the manufacturing of various technologies used in the current scenario should be discounted as the impact was already generated in the past, and the horizontal bar referring to the current situation might become lower.

The results shown in this report highlight the relevance of considering multiple environmental indicators, not just the Global Warming Potential (GWP), when assessing energy transition scenarios. In a business as usual" case, scenario *191* may appear to be the best option due to its lowest GWP impact. However, this scenario has a high metal depletion (35th highest out of 260) and a high natural land transformation impact (49th out of 260).

Several steps are required in order to have a more in-depth comprehension of the results. First, the available data of the baseline is limiting the resolution of the study and only allows to analyse the production of electricity. More spatial resolution and data from the other levels of the system (n-1, Figure 3), would allow a better overall comparison of the spores produced by WP1.

On the other hand, it is relevant to notice that this set of results is lacking novel technologies, mainly hydrogen. The impact produced by these technologies could drive the results in a different direction.

Finally, to assess the causes of some phenomena and impacts, for instance, the apparently high contribution of solar to a higher overall impact, a more detailed study of the causes might be conducted using contribution assessment.







Figure 6: Environmental impacts of different spores in Portugal, normalized per TWh produced. In red, the best spore is highlighted.





Figure 7: Comparison between the best (*A*, spore 81) and worst (*B*, 171) energy mix based on the environmental impact produced per TWh.

4 Final remarks

Note that this method offers high flexibility in the study, as it can be studied at different levels of resolution. It also helps the user to understand the sources of the environmental impacts.

However, this work presents some limitations. First, current data used as a baseline only permits assessing the electricity production, limiting the potential of Calliope and ENBIOS in assessing other categories like energy storage. On the other hand, the assessment of electricity production is incomplete, as it lacks hydrogen technologies included in Calliope. Additionally, this study is subjected to the inherence uncertainty of the different models and databases used, which has not been quantified yet.

To enhance these results, a thorough assessment of the underlying factors contributing to these results is necessary. That requires a contribution analysis to understand the sources of the impacts observed in some technologies. Furthermore, as mentioned above, the uncertainty needs to be computed to give more reliability to these results.

Finally, an improved version of these results will be implemented in the app that is being developed as part of this project.

5 Bibliography

BP Statistical Review of World Energy . (2023). Retrieved May 29, 2023, from https://www.bp.com/en/global/corporate/energy-economics/statistical-review-of-worldenergy.html

DGEG. (n.d.). Retrieved April 24, 2023, from https://www.dgeg.gov.pt/

- *Ember European Electricity Review*. (2022). https://emberclimate.org/insights/research/european-electricity-review-2022/
- Ember Yearly electricity data. (2023). https://ember-climate.org/data-catalogue/yearly-electricitydata/
- enbios · PyPI. (2023). Retrieved April 24, 2023, from https://pypi.org/project/enbios/0.78/
- *Energy data* 2020 edition Products Statistical Books Eurostat. (n.d.). Retrieved April 24, 2023, from https://ec.europa.eu/eurostat/web/products-statistical-books/-/KS-HB-20-001
- Heat values of various fuels World Nuclear Association. (2023). Retrieved April 24, 2023, from https://world-nuclear.org/information-library/facts-and-figures/heat-values-of-variousfuels.aspx
- Home Eurostat. (2023). Retrieved April 24, 2023, from https://ec.europa.eu/eurostat
- Huijbregts, M. A. J., Steinmann, Z. J. N., Elshout, P. M. F., Stam, G., Verones, F., Vieira, M., Zijp, M., Hollander, A., & van Zelm, R. (2017a). ReCiPe2016: a harmonised life cycle impact assessment method at midpoint and endpoint level. *The International Journal of Life Cycle Assessment*, 22(2), 138–147. https://doi.org/10.1007/s11367-016-1246-y
- Madrid-López, C., Nebot Medina, R., Martin, N., Talens Peiró, L., & Villalba-Méndez, G. (2022). ENBIOS. https://pypi.org/project/enbios/
- Martin, N., Talens-Peiró, L., Villalba-Méndez, G., Nebot-Medina, R., & Madrid-López, C. (2023). An energy future beyond climate neutrality: Comprehensive evaluations of transition pathways. *Applied Energy*, 331. https://doi.org/10.1016/j.apenergy.2022.120366
- Pfenninger, S. (2017). Dealing with multiple decades of hourly wind and PV time series in energy models: A comparison of methods to reduce time resolution and the planning implications of inter-annual variability. *Applied Energy*, 197, 1–13. https://doi.org/10.1016/J.APENERGY.2017.03.051
- Ritchie, H., Roser, M., & Rosado, P. (2022). Energy. Our World in Data.
- Statistical Review of World Energy | Energy economics | Home. (n.d.). Retrieved April 24, 2023, from https://www.bp.com/en/global/corporate/energy-economics/statistical-review-of-worldenergy.html
- Süsser, D., Martin, N., Stavrakas, V., Gaschnig, H., Talens-Peiró, L., Flamos, A., Madrid-López, C., & Lilliestam, J. (2022a). Why energy models should integrate social and environmental factors: Assessing user needs, omission impacts, and real-word accuracy in the European Union. *Energy Research & Social Science*, 92, 102775. https://doi.org/10.1016/J.ERSS.2022.102775
- *Technology Data | Energistyrelsen.* (2023). Retrieved April 24, 2023, from https://ens.dk/en/ourservices/projections-and-models/technology-data
- Wernet, G., Bauer, C., Steubing, B., Reinhard, J., Moreno-Ruiz, E., & Weidema, B. (2016a). The ecoinvent database version 3 (part I): overview and methodology. *The International Journal* of Life Cycle Assessment, 21(9), 1218–1230. https://doi.org/10.1007/s11367-016-1087-8

6 Annexes

6.1 Summary of technologies and inventories used.

Technologies	Activity name	Location	Time- Period	Uni t	Calliope Unit	Conversio n
wind_onshore	electricity production, wind, 1-3MW turbine, onshore	РТ	2000-2021	kW h	TWh	1.00E+09
wind_offshore	electricity production, wind, 1-3MW turbine, offshore	РТ	2000-2021	kW h	TWh	1.00E+09
hydro_run_of_river	electricity production, hydro, run-of-river	РТ	1945 - 2021	kW h	TWh	1.00E+09
hydro_reservoir	electricity production, hydro, reservoir, non-alpine region	РТ	1945-2021	kW h	TWh	1.00E+09
ccgt	electricity production, natural gas, combined cycle power plant	РТ	2000 - 2021	kW h	TWh	1.00E+09
chp_biofuel_extractio n	heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014	РТ	2010-2021	kW h	TWh	1.00E+09
open_field_pv	electricity production, photovoltaic, 570kWp open ground installation, multi-Si	РТ	2008-2021	kW h	TWh	1.00E+09
existing_wind	electricity production, wind, 1-3MW turbine, onshore	РТ	2000-2021	kW h	TWh	1.00E+09

Technologies	Activity name	Location	Time- Period	Uni t	Calliope Unit	Conversio n
existing_pv	electricity production, photovoltaic, 570kWp open ground installation, multi-Si	РТ		kW h	TWh	1.00E+09
roof_mounted_pv	electricity production, photovoltaic, 3kWp slanted-roof installation, multi-Si, panel, mounted	РТ	2005-2021	kW h	TWh	1.00E+09
chp_wte_back_pressu re	electricity, from municipal waste incineration to generic market for electricity, medium voltage	РТ	2012-2021	kW h	TWh	1.00E+09
chp_methane_extracti on	heat and power co-generation, natural gas, combined cycle power plant, 400MW electrical	РТ	2000-2021	kW h	TWh	1.00E+09
waste_supply	electricity, from municipal waste incineration to generic market for electricity, medium voltage	РТ	2012-2021	kW h	TWh	1.00E+09
biofuel_supply	market for ethanol, without water, in 99.7% solution state, from fermentation, vehicle grade	СН	2000-2021	kW h	TWh	1.14E+08
chp_biofuel_extractio n	heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014	РТ	2010-2021	MJ	TWh	3.60E+09
chp_wte_back_pressu re	heat, from municipal waste incineration to generic market for heat district or industrial, other than natural gas	РТ	2008-2021	MJ	TWh	3.60E+09
chp_methane_extracti on	heat and power co-generation, natural gas, combined cycle power plant, 400MW electrical	РТ	2000-2021	MJ	TWh	3.60E+09
biofuel_boiler	heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014	РТ	2010-2021	MJ	TWh	3.60E+09
methane_boiler	heat and power co-generation, natural gas, combined cycle power plant, 400MW electrical	РТ	2000-2021	MJ	TWh	3.60E+09

Technologies	Activity name	Location	Time- Period	Uni t	Calliope Unit	Conversio n
battery	market for battery cell, Li-ion	GLO	2011-2021	kg	TWh	41600000 00
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	РТ	1945-2021	kW h	TWh	10000000 00
el_import	market for electricity, high voltage	ES	2014-2021	kW h	TWh	10000000 00
biofuel_to_diesel	market for fatty acid methyl ester	RoW	2011-2021	kg	TWh	13300000 0
biofuel_to_methane	market for biomethane, high pressure	СН	2000-2021	m3	TWh	23600000
biofuel_to_methanol	market for methanol, from biomass	СН	1995-2021	KG	TWh	15900000 0

6.2 Supplementary materials

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

6.2.1 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:

$1 TWh = 10^9 kWh$

The technologies that use this conversion are the following (based on Calliope's nomenclature):

- Wind onshore
- Wind offshore
- Existing wind
- Hydro run of river
- Ccgt
- Chp biofuel extraction

- Existing wind
- Existing pv
- Roof mounted pv
- Chp wte back pressure
- Chp methane extraction
- Waste supply

6.2.2 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

6.2.3 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.

6.2.3.1 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:

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

6.2.3.2 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 (*Technology Data* | *Energistyrelsen*, 2023).

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·°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. 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 amount of tanks needed to satisfy the requirements of a specific scenario.

6.2.3.3 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:

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

6.2.3.4 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 (*Technology Data | Energistyrelsen*, 2023), a plant of 200MW might be referred as a 2000 MWh plant capacity. Thus

$$1 TWh = 500 plants$$

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:

$$1 TWh = 10^9 kWh$$

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 Supply

The process chosen from ecoinvent is the production of biofuel by means of firstgeneration 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:

$$1TWh \frac{3.6 \cdot 10^9 MJ}{1TWh} \frac{1kg \ Bioethanol}{31.58 \ MJ} = 113.9 \cdot 10^6 kg$$

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

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

6.2.4.3 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:

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

6.2.4.4 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) (*Heat Values of Various Fuels - World Nuclear Association*, n.d.):

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