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Holistic economic and environmental optimization of future energy systems

Master's thesis in Industrial Ecology
Supervisor: Edgar Hertwich
Co-supervisor: Schalk Cloete
June 2023

Master's thesis

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SINTEF

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Abstract

The energy transition requires secure, affordable, and sustainable solutions to mitigate climate change and other ecological damages. However, energy supply involves complex and diverse resource-intensive sectors in the value chains, requiring a holistic solution. An energy system model developed in GAMS, including a wide range of energy production, transmission, and storage technologies of electricity and fuels, is integrated with life cycle assessment (LCA) to meet the energy demand at minimal total economic-environmental cost of future energy systems with profiles of wind/solar resource in Germany. Twelve categories of monetized life cycle impact (LCI) assessed using Simapro with European Environmental Footprint (EF 3.0) methods, connected with LCI monetary valuation coefficients (MVCs). Results show that completing the full LCA instead of the conventional practice of only considering direct CO_2 emissions has a significant impact, increasing total system costs by around 50% and causing large changes to the optimal energy mix. Imposing the full LCA leads to nuclear power and natural gas (NGCC and decarbonized fuel production) increasing their shares while solid fuels (coal/biomass blend with CCS) and renewables (wind and solar) declining, where the inclusion of ecotoxicity and land-use impacts are the main drivers of these trends. Those results are generated under the assumptions of applying geometric mean of MVCs derived from literature data, which are subject to high uncertainty. An uncertainty quantification study reveals that, among the twelve impact categories considered, climate change, land use, ecotoxicity, and resource depletion MVCs dominate the outcome of the energy system optimization. The climate change MVC presents the largest effect on the optimal technology distribution but only a limited effect on the system cost. A higher CO_2 price strongly benefits nuclear and biomass with CCS at the expense of natural gas. The land use MVC has the highest effect on the system cost, reducing the shares of biomass and renewables while benefitting natural gas with higher values. Ecotoxicity has the second highest effect on the system cost as it is primarily related to mining/extraction processes that feature in the value chains of all technologies. Solid fuel is suppressed due to coal mining while natural gas gains from higher Ecotoxicity. A higher fossil resource depletion MVC reduces the share of natural gas while benefiting more abundant nuclear and solid fuels. Based on these results, consideration of full LCA is very important for energy system optimization. However, the optimal energy system changes greatly depending on the levels selected for the highly uncertain MVCs. Thus, there is a strong need for future research efforts to reduce the uncertainty bounds of these MVCs to facilitate effective energy system design. These efforts should focus on the most influential impact categories of land use, ecotoxicity and resource depletion.

Contents

Abbreviations

Abbreviation	Explanation
BOS	Balance of System
CC	Combined Cycle
CCS	Carbon Capture and Storage
CED	Cumulative Energy Demand
CSP	Concentrated Solar Power
EF	Environmental Footprint
EROI	Energy Return on Investment
ESP	Environmental Priority Strategies
GAMS	Generalized Algebraic Modelling System
GHG	Green House Gas
GSR	Gas Switching Reforming
LCA	Life Cycle Assessment
LCCA	Life-Cycle Cost Analysis
LCI	Life Cycle Impact
LCIA	Life Cycle Impact Assessment
LFP	Lithium Iron Phosphate
LiS	Lithium Sulfur Battery
LMO	Lithium ion Manganese Oxide
LTO	Lithium Titanium Oxide
MAWGS	Membrane-assisted Autothermal Reforming
NCA	Lithium Nickel Cobalt Aluminium Oxides
NEEDS	New Energy Externalities Developments for Sustainability
NG	Natural Gas
NGCC	Natural Gas Combined Cycle
NMC	Nickel Manganese Cobalt
O&M	Operating and Maintenance
PV	Photovoltaic
PEM	Polymer Electrolyte Membrane
PMG	Permanent Magnet Generator
RC	Recuperated Cycle
RES	Renewable Energy Source
SCPC	Supercritical Pulverized Coal
SMR	Steam Methane Reforming
TOC	Total Overnight Cost
VRE	Variable Renewable Energy
WTP	Willingness to Pay
ZEBRA	Sodium Nickel Chloride Battery

1 Introduction and background

1.1 Literature review

Sustainable and secure energy supply has gained great attentions due to the energy crisis, climate change and other environmental impacts. Meanwhile it requires continuing to uplift billions of impoverished world citizens. However, value chains involved in many resource-intensive sectors of the energy system are complex and diverse, requiring a holistic approach to provide meaningful strategy.

Energy system modelling offers such a comprehensive way to include a wide range of energy production, transmission, and storage technologies in the model, which then optimizes the construction and dispatch of each technology to meet energy demand at the lowest system cost [1]. While Life cycle assessment (LCA) is well acknowledged as an applicable method to evaluate process/product systems considering a wide range of environmental impacts [2]. Thus, integrating LCA into Energy system modelling is a promising route to obtain holistic solution.

There are massive studies on the life cycle impact of individual energy technologies. Electricity supply receives the most attentions. Turconi and colleagues compared life cycle assessment (LCA) of electricity generation technologies including coal, natural gas, oil, nuclear, hydropower, solar photovoltaic (PV), wind and biomass but they only evaluated GHG, NOx and SO_2 emissions [3]. Hertwich's group applied integrated life cycle assessment on the large-scale implementation of climate-mitigation technologies of electricity supply, covering twelve technologies and five impact categories [4]. Gibon and colleagues conducted life cycle assessment for environmental co-benefits and trade-offs of low-carbon electricity generation using a consistent set of methods for eleven technologies and addressing nine impact categories [2]. Besides electricity, fuel production such as hydrogen has obtained more and more investigations. Hermesmann and Müller applied life cycle assessment on different types of hydrogen production of green, turquoise, blue, and grey hydrogen with a wide range of impact categories [5]. Cetinkaya also analyzed five methods of hydrogen production within LCA, namely steam reforming of natural gas (SMR), coal gasification, water electrolysis via wind and solar electrolysis, and thermochemical water splitting with a Cu-Cl cycle but only focus on GHG emissions [6].

Energy storage and transmission also has gained increasingly notices. Hiremath performed a comparative life cycle assessment of battery storage systems for stationary applications in terms of cumulative energy demand (CED) and global warming potential (GWP) for four stationary battery technologies: lithium-ion, lead-acid, sodium-sulfur, and vanadium-redox flow [7]. Pellow and colleagues surveyed the existing studies in environmental life cycle assessments of lithium ion batteries for grid-scale stationary energy storage systems [8]. A life cycle assessment of three supply chain structures of hydrogen transport and distribution system is presented with fourteen impact categories by Wulf and colleagues:(a) Liquid Organic Hydrogen Carriers; (b) compressed hydrogen transported by pipelines and stored in salt caverns; and (c) pressurized gas truck transport, where the pipeline solution displays the least environmental impact [9]. Jorge and colleagues applied life cycle assessment of electricity transmission and distribution with twelve impact categories [10].

However, these studies of LCA on individual energy technologies are scattered, which need systemic integration to optimize economic-environmental energy system.

On the other side, there are numerous studies on energy system modelling optimization which mostly focus on decarbonization strategies with only considering the direct green house gas

(GHG) emissions [11][12][13][14]. Lopion and colleagues reviewed and investigated on the current challenges and trends in energy systems modelling [15] where most models are only aiming for cost-optimal low-carbon strategies without considering other environmental impacts [16][17]. There are very few studies are combining life cycle impact cost with the optimization of an energy system model.

While it has been claimed that employing low-carbon technologies may cause increasing other environmental impacts that does not benefit for sustainable energy system development [18][19]. In order to evaluate other environmental impacts, life-cycle assessment (LCA) has been recently integrated into the energy system modelling [20]. Electricity system was the first sector to be attempted. A multi-target model of electricity system was performed by Algunaibet and Guillén for quantification of the environmental load-shifting potentials from GHG emission reductions to other environmental impacts in the United States [19]. A case study of power generation in Norway is conducted by extending life-cycle indicators in energy optimisation models [21] Blanco and colleagues integrated LCA into the JRC-EU-TIMES energy system models for Power-to-Methane in the EU but the optimization is not including LCA[22]. Aiming for carbon neutrality in Switzerland in 2050, Li and colleagues established a new model to investigate the optimal carbon footprint of biomass and carbon capture and storage (CCS) [23]. But they only focus on impact of climate change without completing a full LCA [23]. Baumgärtner's group applies a holistic national energy model including LCA that assesses other environmental impacts as the consequence of meeting the climate mitigation goal towards 2050 in sectors of electricity, heat, and transport in Germany [24].

Although these energy system models have been integrated with LCA and present a comprehensive perspective on other environmental impacts, there are still two parts missing. Firstly LCA in most models does not participate in the optimization process, which only provide the burden-shifting potentials of other environmental impacts based on the low carbon scenarios. Or the model including LCA only optimizes climate change footprint in one technology. Secondly, these energy system models are not in a complete picture that do not cover production, storage and transmission of electricity and fuels considering the life cycle embodied energy of each technology supplied by the energy system itself with cross-sectoral interconnectivity. This study contributes to filling the gap.

1.2 Research questions and objectives

An energy model considering an integrated electricity-hydrogen system has been developed in SINTEF in Norway cooperating with Germany [1], which was upgraded to inclusion of steel production using clean electricity and hydrogen [25]. Recently, an optimized blue hydrogen production for future energy systems has been designed within the model [26].

In its existing status, the energy system model only accounts for the impact of direct CO_2 emissions in operation phase from all the technology options available for deployment. This cost is considered in the system cost minimization by putting a price on CO_2 emissions [26].

The objective of the study is to integrate life cycle environmental considerations into the existing model for optimizing the construction and dispatch of each technology at the lowest economic-environmental cost of future energy systems with the energy demand and profile of wind/solar resource in Germany towards the year of 2050, including generation, transmission, and storage of electricity, hydrogen, and other energy vectors.

Upgrades to the existing model are implemented in two steps: 1) Creation of a life cycle final energy demand inventory for each candidate technology to model the construction of new energy capacity using energy generated by the modelled energy system and 2) inclusion of the monetized life cycle environmental impacts in the optimization. These upgrades will provide answers to the following research questions:

1. How do life cycle assessment influence the optimal system cost and energy technologies deployment in the energy system, compared to only considering the direct GHG emissions?

2. How do different categories of life cycle impacts affect the energy system optimization?

1.3 Scope

1. Scope

The energy system in this study includes 35 candidate technologies of energy generation, transmission and storage described in detail in section 2.3.1. The flow chart of energy system integrating LCA including foreground and background system are displayed in Figure 1.

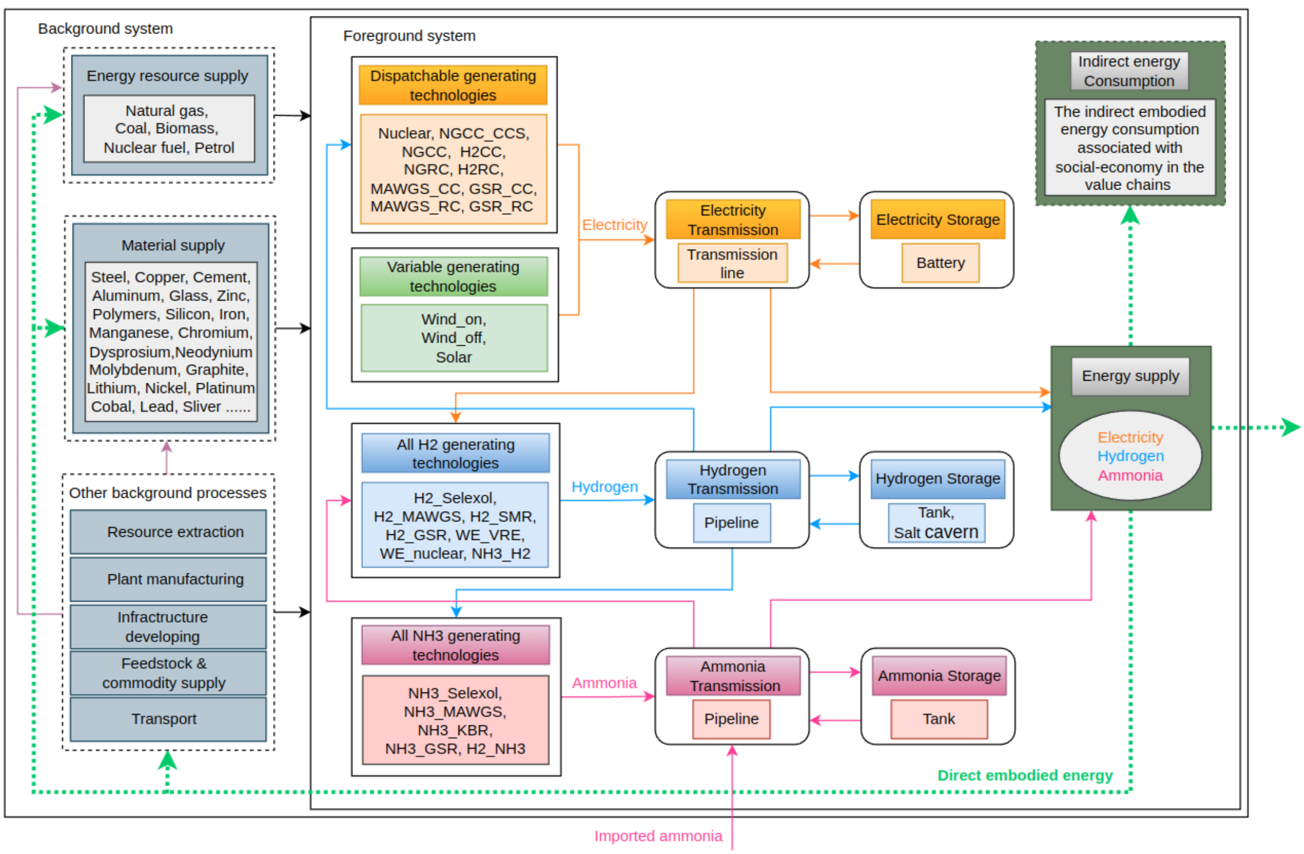

Figure 1: Energy system integrating life cycle assessment

There are 25 candidate technologies of electricity and fuel generation in four groups:

1) Dispatchable electricity generating technologies;

2) Variable electricity generating technologies;

3) Hydrogen generation technologies;

4) Ammonia generation technologies.

Nuclear, natural gas combined cycle (NGCC with/without CCS), hydrogen combined cycle (H2CC), wind and solar are the most important electricity generation technologies. Green hydrogen production (Electrolysis with renewables or nuclear power) and blue hydrogen (Steam Methane Reforming with CCS (SMR+CCS), Membrane-assisted Autothermal Reforming with CCS (MAWGS+CCS) fed by solid fuels (biomass/coal)) are the important fuel production technologies. Ammonia production has the similar technologies as hydrogen and they can convert to each other. Battery and transmission line are the typical electricity storage and transmission technologies, while hydrogen/ammonia tank and pipeline are the typical fuel storage and transmission technologies.

Twelve categories of life cycle impact are selected within LCA in this study due to their importance and availability in monetary valuation methods: climate change, ozone depletion, human toxicity cancer, human toxicity non cancer, particulate matter, ionizing radiation, photochemical, acidification, land use, ecotoxicity freshwater, fossils resource use and minerals resource use.

2. Methodology updated and loop process

The study on methodology was mainly conducted and documented in the master project report[27] last semester, including building a database of life cycle material and direct energy demands for constructing different energy technologies, using this database to derive the final energy demand and monetized life cycle impacts of each energy technology, as well as energy system scale model.

There are some updates of the methodology made in this thesis:

1) conducting the life cycle impact assessment of some more materials (Aluminium, Nickel, Epoxy and Concrete) and fuels (Petrol) in section 2.2.1;

2) exploring the foreground impacts of different candidate technology and distinguishing the important impacts in section 2.2.4;

3) further investigating on the monetary valuation coefficients (MVCs) of different impact categories, collecting more MVCs data from literature, identifying the different methods of MVCs and adjusting the methods of some important categories MVCs (land use, resource depletion) in section 2.2.2 and 2.2.5;

4) scenarios design is adjusted from 6 scenarios to 5 scenarios that no-coal scenario is removed from the energy system in section 2.3.1;

5) method of uncertainty quantification analysis is added in section 2.4.

A loop process developed in this study in order to catch the most important parameters of the energy system optimization. Firstly, modelling is conducted with the preliminary sets of database; Secondly, evaluation and identification are processed to discover the important parameters of the system optimization based on the preliminary results, and three impact categories MVCs of land use, ecotoxicity and resource depletion are found to have large effects on the energy mix; Then back to the methods, further investigation is carried on these three impact categories MVCs, where the methods and data are inspected, adjusted and estimated; Finally, modelling is conducted again with the updated methods and data.

2 Methodology

There are three stages in this section: life cycle final energy demand assessment, monetized life cycle impacts identifying and system scale modelling. Figure 2 presents the outline of the three sub-methods.

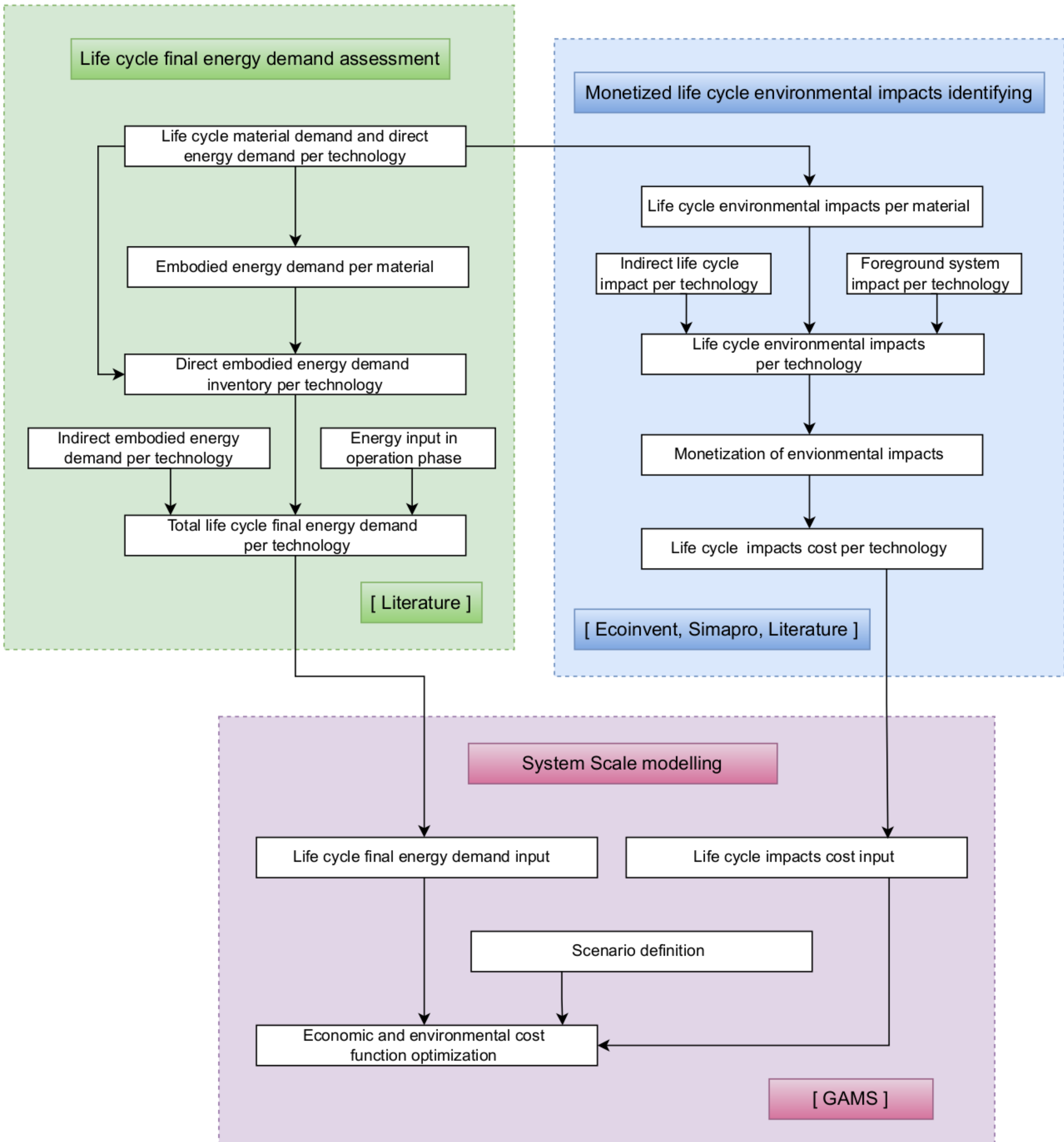

Figure 2: Schematic of the methodology and analysis tools applied in this study

In the first stage, a database of life cycle material and direct energy demands for constructing various energy technologies was collected based on literature data. Next, the embodied energy demand for each raw materials production was investigated in order to build a life cycle final energy demand inventory for each candidate technology to simulate the construction of new energy capacity using energy generated by the modelled energy system. This embodied energy is expressed in the final energy vectors of electricity, hydrogen (general fuel), and ammonia (transportation fuel). It consists of a direct component from energy and material consumption and an indirect component from general economic activity (e.g., energy required to sustain the lifestyles of all the people working along the value chain).

Secondly, a database of twelve life cycle environmental impacts of each important raw material production from Ecoinvent database 3.0 was explored by applying Simapro with LCA method of European Environmental Footprint (EF 3.0). Then a database of life cycle impacts of each technology was derived on the database of life cycle material demand of each technology in the first stage, with integrating the foreground system impacts. Indirect impacts from general economic activity associated with the energy system were also included. After identifying a reasonable monetary valuation for each impact category based on literature data, a database of life cycle impact cost of each technology was established for the system model.

Finally, these two set metrics of life cycle final energy demand and monetized environmental impacts database were transferred to the third stage where an energy system model developed in GAMS is used to optimize and seek a sustainable energy system economically and environmentally under different scenarios defined by technology availability. Environmental impact costs of each technology (externalized costs) are added to the standard (internalized) costs of each technology and fuel consumed, while the embodied energy involved in all parts of the energy system are supplied as electricity, hydrogen and ammonia within the model, increasing the overall energy demand.

2.1 Life cycle final energy demand assessment

Process-based life cycle assessment method is applied in this section based on literature data. The system scope contains the overall life cycles of energy generation, transmission or storage of each technology, including the phases of resource extraction, component manufacturing, construction, transportation, operation, maintenance, and disposal.

Functional unit:

1) For technologies of energy generation or transmission: 1 kW capacity of energy generation or transmission.

2) For technologies of energy storage: 1 kWh capacity of energy storage.

2.1.1 Life cycle material and direct energy demands of each technology

Renewable energy plays an essential role in the transition towards a sustainable energy system. However, significant raw material and energy demand of the renewable make crucial effects on investment feasibility, resource depletion and environmental impacts, which has been draw growing consideration in the study of energy economy and ecology.

1.Technologies of electricity generation

EU Science Hub recently reported that significant increase in raw material demand for wind and solar PV technologies are anticipated to achieve the goals of European Green Deal[28]. By 2050, within the deployment of wind turbines according to EU decarbonisation goals, the demand of both structural materials(concrete, steel, plastic, glass, aluminium, chromium, copper, iron, manganese, molybdenum, nickel and zinc) and technology-specific materials such as rare-earth elements (neodymium,praseodymium, dysprosium and terbium) and minor metals are expected to rise remarkably[28]. For solar PV technologies, the demand of silver, silicon, cadmium, gallium, indium, selenium and tellurium, germanium might increase up to 40-86 times in 2050. It reveals that EU's transition to green energy system could be endangered by deficiency of raw material supply in future[28].

Hertwich's group applied integrated life cycle assessment on different environmental impacts of low carbon technologies for electricity supply, in which life cycle material and direct energy demand of different technologies were investigated in the study period 2010-2050[4]. An elaborate life cycle inventory database of renewable (wind and solar) and conventional power (coal and natural gas with/without CCS) generation was created in their study, including foreground data and background data from ecoinvent 2.2 database[4]. Huang and colleagues conducted life cycle assessment and net energy analysis specifically on offshore wind power systems with a total power capacity of 104 MW offshore wind farms with 52 wind turbines[29]. Study from University of Oxford provided a global inventory of solar PV energy generating units installed in commercial-, industrial- and utility-scale with a nameplate capacity over 10 kilowatts by applying a longitudinal corpus of remote sensing imagery, machine learning and a large cloud computation infrastructure[30].

As most of functional unit of LCA system in literature is 1 kWh electricity produced from power station. The data of life cycle material and direct energy demand are further converted to demand per kW capacity based on the performance parameters such as life time and capacity factors. These are calculated by the equations:

$$M_{life,m} = \sum_{i,j} (M_{i,j,m} * C_f * T_{life} * 8760), \tag{1}$$

$$E_{life,direct,n} = \sum_{i,j} (E_{i,j,n} * C_f * T_{life} * 8760), \tag{2}$$

i: different processes in a phase of the life time cycle
j: different phases in a life time cycle (construction, operation, decommissioning etc)
m: different type of material (steel, copper, cement etc.)
n: different type of energy carries (electricity, natural gas, diesel etc.)
C_f: capacity factor (%)
T_{life}: lifetime (year)
8760: total hours per year (h/year)
$M_{i,j,m}$: material demand of type m in process i of phase j, per kWh energy generation
$M_{life,m}$: life cycle material demand of type m, per kW capacity of each technology
$E_{i,j,n}$ direct energy demand of type n in process i of phase j, per kWh energy generation
$E_{life,direct,n}$: life cycle direct energy demand of type n, per kW capacity of each technology

The key parameters of capacity factor and lifetime of each technology are listed in table 1 based on literature data.

Technology	Unit	Wind-onshore	Wind-offshore	Solar PV	Nuclear	NGCC	NGCC-CCS	SCPC	SCPC-CCS	Hydro
Lifetime Resource	year	20 [4]	25 [4][31]	25, 30(module) [4][31],[30]	up to 50 [32]	30 [4]	30 [4]	35 [33]	35 [33]	80 [4],[31]
Capacity factor Region Resource	%	30 Global average [34]	40 Global average IEA[35]	14 Global average IEA[35]	82.5 Global average [36]	55 US [37]	55 US [37]	50 US [37]	50 US [37]	50 Global average [38]

Table 1: The key parameters of various technologies

Deetman's group analysed the global trend of material stocks and flows in the electricity sector and projected material demand of the global electricity infrastructure including generation, transmission and storage towards 2050[39]. They applied dynamic stock modelling with a detailed review of material intensities of different technologies, including both bulk and critical materials such as steel, aluminium and neodymium. Their results display a significant growth with most materials in the electricity infrastructure due to the rising electricity demand and a shift from conventional electricity towards renewable technologies[39]. Furthermore, renewable technologies require higher material intensities than conventional infrastructures[39]. However, the material intensities value of wind and solar based on literature data in Deetman's study are mostly out of date, much higher than the data in Hertwich's study.

Considering the technologies of wind and solar develop rapidly over the time, while the conventional technologies such as coal, natural gas and nuclear are relatively mature, the material demand of conventional technologies are collected from Deetman's review.

For Wind onshore and offshore, the data of material and direct energy demand are collected based on Hertwich's study in NTNU[4], with the addition of the rare-earth elements of technology-specific materials such as neodymium, praseodymium, dysprosium and terbium from Carrara's study in EU Science Hub[28].

For solar PV, a combination of material and energy demand is made from three parts of data resource:

1) Energy consumption of the module in Kruitwagen's study in Oxford[30].

2) Energy consumption (exclude the module) from database of Hertwich's study in NTNU[4].

3) All the other materials from the MDS scenario in the year of 2050 in Carrara's study in EU Science Hub[28].

This combination considers the trend of technology development of solar PV module which leads the significant change on the material and energy demand of solar PV towards in the future, while the technology of the processes outside the module is relatively mature with little change in future. The combination of direct energy demand of solar PV can be expressed in the equation:

$$E_{life,direct,n} = \sum_{i,j}(E_{i,j,module,n} * C_f * T_{life,module} * 8760) + \sum_{i,j}(E_{i,j\_rest,n} * C_f * T_{life\_rest} * 8760), \quad (3)$$

The energy demand in transport of road, ship and airplane are calculated based on the data of transport type and energy consumption in the report of ecoinvent[40] and Treeze Ltd[41].

The life cycle material and direct energy demand of different energy technologies of electricity generation are calculated in table 1 in the Appendix based on literature data. In general, material demand of renewable are higher than that of conventional technologies, especially wind power has the additional demand for the rare-earth materials.

2. Technologies of electricity transmission and storage

The investigation of material requirements of electricity transmission and storage in Deetman's study was detailed reviewed including transmission line in three different voltage levels, the distribution of substations and transformers units and different types of battery[39].

The material demand of electricity transmission can be calculated by:

$$M_{total,m\_l} = (M_{line,m\_l} + M_{sub,m\_l} * N_{sub} + M_{trans,m\_l} * N_{trans}) / C_{line\_l} / 1000 * L_{line\_l} \quad (4)$$

m: different type of material (steel, copper, cement etc.)

l: different voltage level of transmission line (low, middle, high)

M_{total,m_l}: total material requirement of type m per kW capacity of level l electricity transmission, ton/kW

M_{line,m_l}: material requirement of type m per Km level l electricity transmission line, kg/Km

M_{sub,m_l}: material requirement of type m per unit of level l substation, kg/unit

N_{sub}: number of substation units per Km electricity transmission line, unit/Km

M_{trans,m_l}: material requirement of type m per unit of level l transformer, kg/unit

N_{trans}: number of transformer units per Km electricity transmission line, unit/Km

C_{line_l}: capacity of level l electricity transmission line, MW

L_{line_l}: length of level l electricity transmission line, Km

The lifetime of grid elements and the assumptions of electricity transmission parameter data in three voltage levels are listed in table 2 and 3 based on literature data.

Grid elements	**lines**	**transformers**	**substations**
Lifetime (year)	40	30	40
Resource	[42] ,[43]	[44],[10]	[42],[10]

Table 2: Lifetime of grid elements

Three level Voltage	**Unit**	**High voltage (HV)**	**Middle voltage (MV)**	**Low voltage (LV)**
Voltage	KV	200	50	0.5
Capacity	MW	3000	150	0.5
Length	Km	1000	250	2
Resource		[39], [42] ,[43]	[39],[44]	[39],[42]

Table 3: Assumptions of electricity transmission parameter data in three voltage levels

The material demand of VRE transmission is assumed applying middle voltage transmission, and the demand of general transmission is assumed the average of middle and high voltage transmission:

$$M_{total,m\_VRE} = (M_{line,m,mid} + M_{sub,m,mid} * N_{sub} + M_{trans,m,mid} * N_{trans})/C_{line,mid}/1000 * L_{line,mid} \tag{5}$$

$$M_{total,m\_General} = \frac{1}{2}\left(M_{total,m,mid} + M_{total,m\_high}\right) \tag{6}$$

The calculation results of material demand of VRE and General transmission are listed in table 2 in the Appendix.

In terms of electricity storage, different types of stationary battery are compared and those types with relatively low environmental impacts and high availability of the materials used are selected in this study. Li-ion battery - LFP (LiFePO4) and LTO (Li4Ti5O12), as well as advanced lithium-metal batteries - Lithium Sulphur (LiS) and Lithium air (LiO) are the main focus as those types of battery such as LMO, NMC, NCA, ZEBRA and Lithium Ceramic contain metals or rare elements of Co, Ni, Pb, Mn, Nd would be avoid to be used in our energy system.

Figure 3 shows the assumed development trend of market shares of grouped electricity storage technologies in year of 2018, 2030 and 2050, in which share of flywheels would decrease dramatically, flow batteries and Molten salt batteries would rise, advanced Li and hydrogen would start growing after 2030[39]. Besides the material demand, other performance indicators such as energy density, (dis)charge cycles, investment costs and round trip efficiency of different types of battery with technology in 2018 and towards 2030 were detailed reviewed in Deetman's study[39].

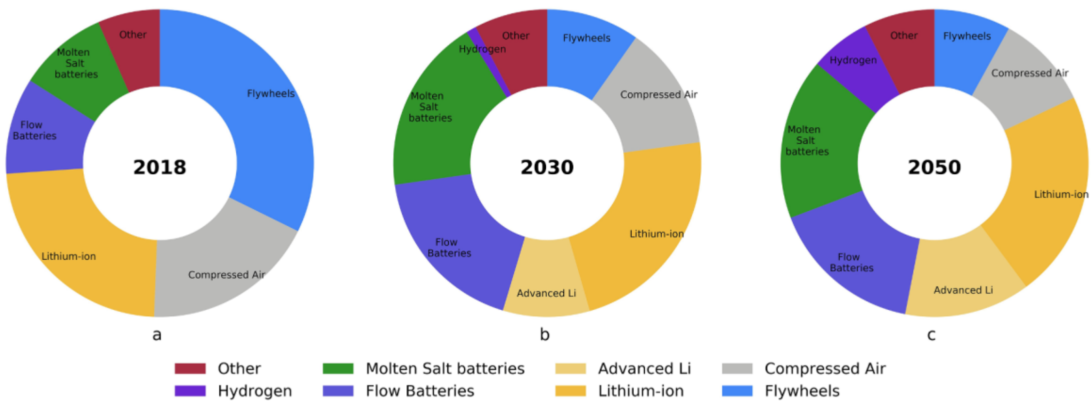

Figure 3: Assumed development of market shares for dedicated electricity storage technologies[39]

Bongartz and colleagues conducted criticality assessment of specific metal demand of LiB cell components for nine types of lithium-ion batteries including LFP, Lis and LiO in stationary storage applications in Germany by 2050 based on the mean value from data compiled from literature and their own assumptions[45]. Nelson's group applied battery performance and cost model (BatPaC) and built a material inventory per kWh for a module with a 10 kWh energy capacity in Argonne National Laboratory[46]. Carvalho presented the battery pack and battery cell mass composition by components, in which cells take the majority of the mass at 60% and followed by packaging at 32% [47]. They also defined and created an complete inventory of LFP pack and NMC pack in their life cycle assessment of stationary storage systems within the Italian electric network[47].

The cost and performance indicators for electricity storage technologies in 2030 are displayed in table 4. Both LiS and LiO have lower (dis)charge cycles around 1000 although LiS has higher energy density[39]. LTO has a outstanding performance of (dis)charge cycles at 20000 times but its investment cost is nearly double of LFP [48][49]. In addition, LTO contains 7.7% of manganese, which even higher than in NMC ans NCA battery[50]. Based on a trade-off between the environmental cost, investment cost and performance of these four types of batteries, LFP is selected as the represent of electricity storage in this study due to its relatively clean materials use, low investment and decent performance.

Technology	**Energy density**	**(dis)charge cycles**	**Investment costs**	**Round trip efficiency**
unit	Wh/kg	Nr. of cycles before end of life	USD/kWh (storage capacity)	%
LFP	212	5000	230	96
LTO	211	20000	400	99
LiS	750	1000	250	98
LiO	250	1080	275	85
Resource	[48],[49]	[48],[49]	[51],[52]	[53],[54]

Table 4: Cost and performance indicators for electricity storage technologies in 2030

A combined material and energy demand of LFP pack is built and listed in table 2 of the

Appendix:

1) The bulk material demand mainly are collected based on Deetman's review and converted from mass percentage (kg material /kg total battery) to mass per kWh (ton material/kWh capacity) by being divided by its energy density (Wh/kg)[39];

2) The values of Lithium and graphite are directly from Bongartz's[45] and Nelson's[46] study respectively;

3) The direct energy demand is calculated by using equation (2) based on the data of LFP pack inventory in Carvalho's study[47].

3.Technologies of hydrogen production, transmission and storage

Hydrogen has become an important role in the strategy of green energy transmission. Both green and blue hydrogen are considered as liquid fuel in our modelling. Electrolyzer and Steam methane reforming (SMR) are the typical technologies for green and blue hydrogen production, hydrogen pipeline is its energy transmission, hydrogen tank and salt cavern are the forms of energy storage.

Wulf and colleagues applied life cycle assessment on hydrogen transport and distribution system[9] based on published life cycle inventories of electrolysis[55] and pipeline[56]. Koj studied environmental impacts of industrial hydrogen production by alkaline water electrolysis with parameters in table 5[55].

Parameter	**Unit**	**Value**
AEL capacity	MW	6
System lifetime	year	20
Stack lifetime	year	10
Hydrogen production rate	kg H_2/h	118
Stacks per AEL system	pcs	4
Hydrogen energy carrier	MJ/kg	120
Electricity to hydrogen efficiency	%	65.7
Annual operation	h/a	8300

Table 5: Parameters data of alkaline water electrolysis[55]

The material and direct energy demand of AEL in construction phase are calculated by equations based on the LCI data in Koj's study:

$$M_{life,m} = \sum_{i,j}(M_{i,j,m}/(E_f * C_{AEL} * 1000)), \tag{7}$$

$$E_{life,direct,n} = \sum_{i,j}(E_{i,j,n}/(E_f * C_{AEL} * 1000)), \tag{8}$$

i, j, m, n are the same as in equations (1) and (2)
E_f: electricity to hydrogen efficiency, %
C_{AEL}: AEL capacity, MW
$M_{i,j,m}$: material demand of type m in process i of phase j, per AEL capacity MW
$M_{life,m}$: life cycle material demand of type m, per kW capacity of AEL
$E_{i,j,n}$: direct energy demand of type n in process i of phase j, per AEL capacity MW
$E_{life,direct,n}$: life cycle direct energy demand of type n, per kW capacity of AEL

j=construction phase

The material and direct energy demand of AEL in operation phase are calculated by equations based on the LCI data in Koj's study:

$$M_{life,m} = \sum_{i,j}(M_{i,j,m}/E_{H_2} * T_{life} * 8300), \tag{9}$$

$$E_{life,direct,n} = \sum_{i,j}(E_{i,j,n}/E_{H_2} * T_{life} * 8300), \tag{10}$$

i, j, m, n, T_{life} are the same as in equations (1) and (2)
E_{H_2}: hydrogen energy carrier, kWh/kg
8300: total operation hours per year, h/year
j=operation phase

Spath conducted a life cycle assessment on hydrogen production via natural gas steam reforming and created an inventory with parameter in table 6[57].

Parameter	Unit	Value
Plant size (hydrogen production capacity)	million Nm^3/day	1.5
lifetime	year	20
capacity factor	%	90
Hydrogen energy carrier	MJ/kg	120
Hydrogen density	Nm^3/kg	11.13

Table 6: Parameters data of Steam Methane Reforming (SMR) [57]

The material and direct energy demand of SMR in construction phase are calculated by equations based on the raw data of LCI in Spath's study:

$$M_{life,m} = \sum_{i,j}(M_{i,j,m} * d_{H_2} * 24/(E_{H_2} * C_{SMR} * C_f)), \tag{11}$$

$$E_{life,direct,n} = \sum_{i,j}(E_{i,j,n} * d_{H_2} * 24/(E_{H_2} * C_{SMR} * C_f)), \tag{12}$$

i, j, m, n, C_f are the same as in equations (1) and (2)
d_{H_2}: hydrogen density, Nm^3/kg
E_{H_2}: hydrogen energy density, kWh/kg
C_{SMR}: hydrogen production capacity, million Nm^3/day
24: 24h/day
j=construction phase

The direct energy demand of SMR in operation phase are calculated by equations based on the raw data of LCI in Spath's study:

$$E_{life,direct,n} = \sum_{i,j}(E_{i,j,n}/(E_{H_2} * T_{Life} * C_f * 8760)), \tag{13}$$

i, j, n, T_{life}, C_f are the same as in equations (1) and (2) j=operation phase

Wulf made LCI of 1km distribution and transmission of hydrogen pipeline with diameter of 100mm and 200mm respectively, adapted from Krieg's study on hydrogen pipeline system supply [56]and Faist's study on natural gas pipeline with long distance and high capacity[58]. Kuczyński specifically studied thermodynamic and technical issues of hydrogen pipeline such as flow rate of different pipeline diameters in table 7, pressure drop in pipeline length, energy carries and gas density [59].

Volume flow rate	**Pipeline diameter**
Nm^3/h	mm
12000	100-150
40000	150-250
80000	200-300
120000	250-400

Table 7: Recommended pipeline diameter for pure hydrogen transmission[59]

The energy carriers of hydrogen in distribution pipeline with diameter of 100mm and in transmission pipeline with diameter of 200mm are calculated by equations using thermodynamic data in kuczynski's study:

$$E_{c\_d} = Q_d * d * E_d, \tag{14}$$

E_{c_d}: energy carrier of hydrogen with diameter d, kWh/h
Q: volume flow rate of of hydrogen with diameter d, Nm^3/h
d: density of hydrogen, 0.08988 kg/Nm^3[60]
E_d: energy density of hydrogen, using lower heating value of hydrogen 33.33 kWh/kg

Then based on LCI data in the study of Wulf, Krieg and Faist, the material and direct energy demand of hydrogen pipeline are calculated by equations:

$$M_{life,m\_d} = \sum_{i,j} (M_{i,j,m\_d} / E_{c\_d} * L_{line\_d}), \tag{15}$$

$$E_{life,direct,n\_d} = \sum_{i,j} (E_{i,j,n\_d} / E_{c\_d} * L_{line}), \tag{16}$$

i, j, m, n are the same as in equations (1) and (2), E_{c_d} is the result from equation (14)
L_{line_d}: length of hydrogen transmission line with diameter d, Km, here the calculation of VRE H_2 pipeline is using distribution pipe line data with the length of middle voltage level of electricity transmission line in table 3, while general H_2 pipeline is using transmission pipeline data with average length of high and middle voltage level line.
M_{i,j,m_d}: material demand of type m in process i of phase j of the hydrogen pipeline with diameter d, per (kWh*Km) hydrogen transmission
M_{life,m_d}: life cycle material demand of type m of the hydrogen pipeline with diameter d, per kW capacity of a hydrogen transmission
E_{i,j,n_d}: direct energy demand of type n in process i of phase j of the hydrogen pipeline with diameter d, per (kWh*Km) hydrogen transmission

$E_{life,direct,n\_d}$: life cycle direct energy demand of type n of the hydrogen pipeline with diameter d, per kW capacity of hydrogen transmission

Wulf also collected a LCI of transport hydrogen tank with high pressure and small volume[9] based on literature data[61][62], while Moss studied the critical metals of hydrogen tank with 20000 kWh capacity and 10 hours of maximum operating time per cycle for evaluating the decarbonisation path of the EU energy sector[63]. Considering the capacity of hydrogen tank in the system-scale energy modelling should be higher than a transport tank, we collect the data of material and energy demand in Moss's study.

The calculation results of life cycle material and direct energy demand of different technologies of energy transmission, storage and hydrogen generation are summarized in table 2 in the Appendix.

2.1.2 Embodied energy demand of each material

The energy transition towards renewable energy is expected to boost demand of materials in construction of renewable infrastructure. On the other side, the embodied energy demand of material is contributing to the level of energy return on investment (EROI) of renewable energy in energy economy and ecology. Embodied energy is defined as the energy consumption of all the processes of the supply chain associated with the material production, including mining, extracting, refining, manufacturing and transport sector [64]. Embodied energy demand of different materials are various due to the different process route, technology choice and resource availability such as ore grade. The primary energy demand of various materials is readily available from LCA databases, but the system model demands final energy broken down into the three vectors of electricity, general fuel, and transportation fuel. Finding such detailed final energy demand data presents a considerable challenge, and the scope has therefore been limited to steel and copper, using a material cost scaling approach to extrapolate these results to other materials.

1. Steel

Steel is one of the most commonly used materials in the world, but steel is a material with high carbon intensity due to its high embodied energy consumption. Furthermore, steel production is a hard-to-abate sector for decarbonization [65]. Now days, steel is the largest industrial sector of CO_2 emission in Europe, contributing 22% of GHG emissions to European industry due to its high consumption of fossil energy such as coal and coke [66]. Wang analyzed the global steel production with different process paths from mining to casting to mill and their total GHG emission expressed in figure 4 [65]. A detailed life cycle inventory of output 1 kg steel including 7 stages and 19 processed was elaborately built to clarify its life cycle assessment in each path [65].

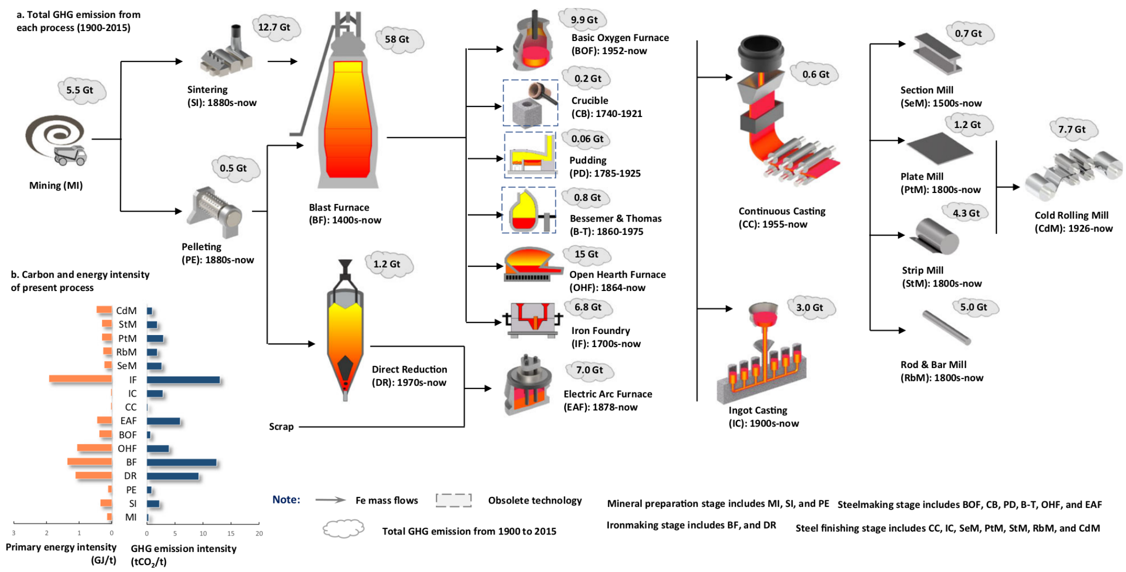

Figure 4: Steel production technologies and their total GHG emissions from 1900 to 2015, Abbreviations for steel production flows are: MI mining, SI sintering, PE pelleting, BF blast furnace, DR direct reduction, BOF basic oxygen furnace, CB crucible, PD puddling, B-T Bessemer & Thomas, OHF open-hearth furnace, IF iron foundry, EAF electric arc furnace, CC continuous casting, IC ingot casting, SeM section mill, PtM Plate Mill, StM strip mill, RbM rod bar mill, CdM Cold rolling mill. [65]

The calculation of embodied energy is the same as equation (2), but we conduct three different paths of steel production and gain three levels of embodied energy at 28.19 MJ/kg, 36.40 MJ/kg, 29.09 MJ/kg steel (7.83 MWh/kg, 10.11 MWh/kg, 8.1 MWh/kg) steel respectively :

Path NO	Path of Combination	Electricity	Diesel	natural gas	coal	Blast furnace gas	sum
1	MI+SI+BF+BOF+IC+PtM+CdM	2.04	2.91	5.66	17.56	-	28.19
2	MI+SI+BF+IF+IC+PtM+CdM	10.01	2.91	5.91	17.56	-	36.40
3	MI+PI+DR+EAF+CC+PtM+CdM	6.45	2.91	17.76	0.88	0.1	29.09

Table 8: Embodied energy (MJ/kg steel) of steel production in 3 different paths based on LCI data in Wang's study [65]

Steel production in path 3 has the lowest embodied energy consumption in coal, which is mostly contributed by the replacement of natural gas and electricity. Process of Direct Reduction (DR) with much lower mass of primary iron consumes much less energy than Blast Furnace (BF) and Electric Arc Furnace (EAF) uses electricity instead of coal/coke. Scrap is mixed with the primary iron after DR process then goes together to the next process of EAF. We assure that hydrogen and electricity are the main energy for steel production in year of 2050 in our energy system modelling. Thereby, the embodied energies of steel production in path 3 totally in 29.09 MJ/kg steel (8.1 MWh/kg) are applied in our modelling.

2. Copper

Copper is a vital metal to industrial application due to its excellent performance as a conductor of electricity with low corrodibility and high ductility [67]. Its continuously growing in global demand has been predicted to reach around 25 million tonnes of annual production by 2026 [68]. However, such a high demand of copper has been facing the resource depletion stress on the decline ore grades in recent decades, which lead to a supply constraint and the rise of its embodied energy consumption. It was reported that the global average copper ore grades are no higher than 0.53% in recently operational mines, while average grades are even no higher than 0.43% in new projects and in explored mines [69].

Koppelaar's group evaluated the relationship between the embodied energy demand of copper production and different ore grades and mine-depth [70].

Koppelaar made a historic analyses on copper energy input with different ore grade in two process routes based on literature [70]. The energy demands for a metric ton of copper product from mining to refining processes include constructing infrastructure, operational inputs, maintenance and transportation, while Koppelaar's study focus on operational inputs and transports [70].

Table 9 displays three process stages of copper production in two routes of hydrometallurgical and pyrometallurgical adapted from Koppelaar's study.

Process route	**Hydrometallurgical route**	**Pyrometallurgical route**
Phase 1	Mining, Crushing, Grinding	Mining, Crushing, Grinding
Phase 2	Heap leaching, Solvent extraction Electrowinning, Heap leaching SX–EW Heap leaching including embodied energy	Flotation, Smelting Electro-refining Beneficiation and smelting including embodied energy
Phase 3	Site transport, Product transport	Site transport, Product transport

Table 9: Phases of copper production in two different process routes adapted from Koppelaar's study [70]

Table 10 is the summary of the embodied energy demand of copper production with different ore grades in these two different routes based on Koppelaar's study. The energy demand of copper is dramatically rising when the ore grades drop to 0.25% [70]. Additional, the energy demand of copper in processing route pyrometallurgical has wide range due to its various smelting and Beneficiation process. Energy demands rise significantly when head grade is below 1%, while the influence of depth is much less. In surface mines, the energy demands of copper production in pyrometallurgy route appear higher than hydrometallurgy route [70].

Ore grade	**Energy demand in hydrometallurgical route**	**Energy demand in pyrometallurgical route**
1%	179.73	109.38-173.08
0.5%	267.28	187.88-316.28
0.25%	427.88	324.08-577.18

Table 10: The embodied energy demand (MJ/kg copper) of copper production with different ore grades in two different routes based on Koppelaar's study [70]

Rötzer and Schmidt evaluated the evolution of the cumulative energy demand (CED) of global copper production during the last eight decades and projected the future energy demand applying a holistic process-based modelling method [71]. They defined three main process steps including mining, processing and metallurgy with the two routes of pyometallurgical and hydrometallurgical, and then used foreground and background data to calculate the contribution of individual process to the average CED of global copper production in 1930, 1970 and 2010, where the contributions of mining and concentration were growing while the contributions of processes were decreasing[71]. Furthermore, their modelling result of the historic evolution of ore grade-CED and ore grade-GWP curves for the global copper production was presented in figure 5, in which the average CED are 70, 53, 69 GJ-eq/t Cu, and GWP are 5.7, 4.2, 4.5 CO_2-eq/t

Cu corresponding to ore grade in 1.7%, 1.3%,0.7% in the three time periods [71].

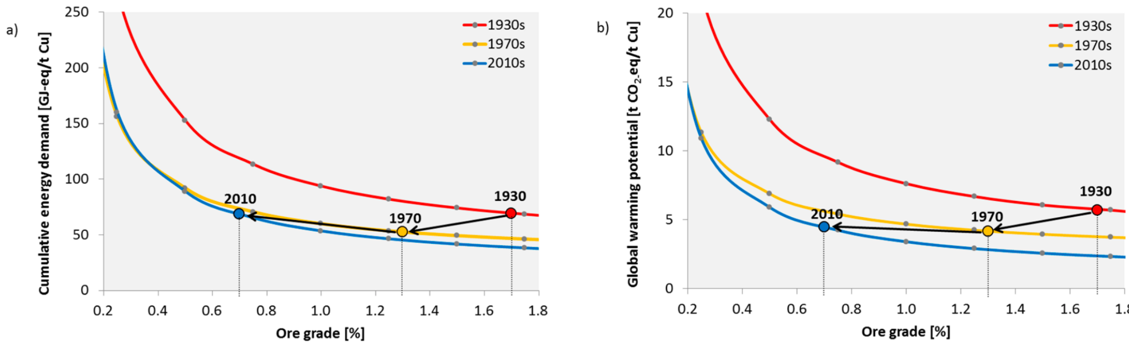

Figure 5: Evolution of relationship between cumulative energy demand (a), global warm potential (b) and ore grade for the global copper production [71]

Rötzer and colleague investigated how technological improvement had been able to counteract the declining ore grade and would compensate the increasing energy demand of copper production of the future scenarios, showing in figure 5 and 6 [71]. When geological factor of copper resource is keep going unfavorable, technology progress and renewable energy are crucial to reduce the increased CED due to the lower ore grade, which also influence the GWP in the similar trend. This explains that the CED in 2010 increased to 69 GJ-eq/t Cu from 53 GJ-eq/t Cu in 1970 but still slightly less than in 1930 although the ore grade kept dropping from 1.7% to 0.7% during the last eight decades as the energy demands associated with ore grade increased and energy demands associated with processes reduced [71]. Figure 7 outlined the relationship between ore grade and CED with different factors such as technology improvement and supply chain [71]. The world copper fact-book presented the evolution of the main smelting technologies of copper production between 1980 and 2010, where the numbers of flash continuous furnaces increase steadily while the reverberatory furnace declined due to the technology developing with higher efficiency and lower cost [72].

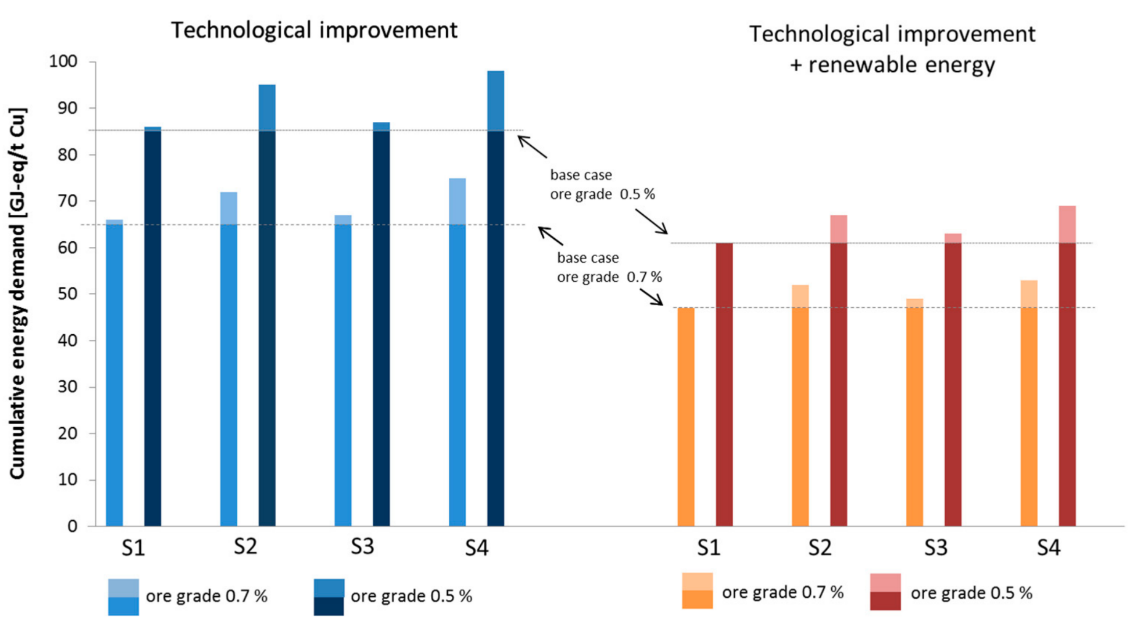

Figure 6: Cumulative energy demand of future scenarios[71]

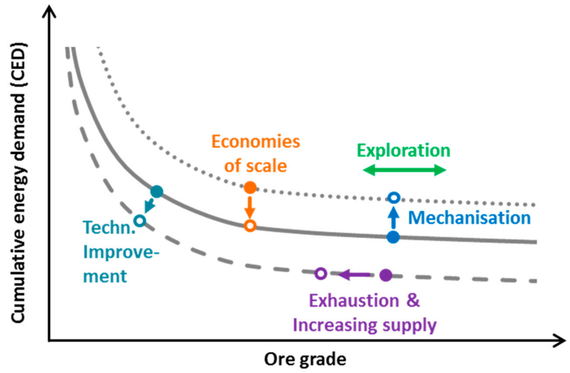

Figure 7: Schematic of the relationship between ore grade and cumulative energy with different factors [71]

In general, technology development of the copper production contributes the reduction of energy cost while the resource depletion with the declining ore grades makes it struggling to prevent the rising in energy costs.

There are large differences of the energy demand data of copper production in Koppelaar's study and Rötzer's study, where the system scopes of energy demand are different. The cumulative energy demand in Rötzer's study excludes transport sector and the embodied energy in the process which contributes 103 to 474 MJ/kg Cu to the total embodied energy demand [70]. While Rötzer's modelling results drew a picture of the possibility of technology improvement counteracting the resource depletion of copper. However resource depletion is irreversible. Recycle and secondary material is a real way out.

Considering the competition of the two opposite factors of ore grade drop and technology progress towards the year 2050, we apply the average value of the energy demand in two typical process paths at ore grade 0.5% Cu in year 2010 derived from the data of Rötzer's study, which is 46.4 MJ/kg displayed in table 3 of Appendix.

3. Other materials

Our strategy in this study is that the first step only model the important processes in detail, focusing on their full life cycle final energy demands. Steel, (aluminium), and copper are the most commonly used materials, then polymers, glass, carbon fiber, polysilicon are the possibly second set of materials applied in our energy system model. The trend of energy cost increases with ore grade declines of copper can be reasonable extended to other materials like nickel, chromium and rare earths. Our ultimate goal is to have a breakdown of embodied energy in electricity and fuels for each material. Doing this for each material will be impractical, but it could be reasonable to correlate energy demand with material prices. The energy cost rising with ore grade decline is particularly important because it will increase energy use over time. Processes like steel and aluminium that have essentially unlimited raw materials will not suffer from this effect.

Gibon and colleagues studied on a methodology of a hybrid life cycle assessment model integrating LCA databases with multi-regional input-output tables under large-scale technological change towards year 2050 in order to project the life cycle environmental impacts of products under a 2°C scenario [73]. They applied Ecoinvent key process inputs to calculate the energy demand of important materials of different technologies in 2010-2050 time frame based on LCA of background processes resource ESU, IFEU NEEDS [73].

Castro and Capellán-Pérez investigated the material requirements and their energy intensities for the five renewable energy source (RES) technologies including solar PV & CSP, wind onshore & offshore and large hydro power [74]. They estimated the present global average energy return on energy invested (EROI) for the five RES technologies at three defined energy system boundaries: standard (EROI-st), final consumption point (EROI-final), and extended to include indirect investments (EROI-ext) [74]. Their findings showed that only large hydro power would have a high EROI-ext around 6.5 at present, while all the rest of RES would be below 3, and CSP even below 1, which indicate the global average EROI-ext levels of variable RES are lower than those of fossil fuel combustion power [74]. The level of material requirements and their energy intensities influence the evolution of the energy system EROI, which is crucial to the viability of sustainable energy systems with the variable RES scale-up for the energy demand in modern societies chasing sustained economic growth [74].

However, literature data of energy demand of material in Castro's and Gibon's and other's study are far different and incomplete [73][74], which might due to the various scopes, resources and regions. The embodied energy demand and distribution for different materials are listed in table 4 of the Appendix based on literature data and assumptions. The assumptions mainly are according to the relationship between the embodied energy demand and its cost. Embodied energy of those materials with abundant resource is calculated based on data of steel, while material with limited declining resource is calculated based on data of copper. For instance, embodied energy demand of Zinc is calculated based on the embodied energy demand of copper and the ratio of material cost of copper and zinc. This intends to capture the trend of both supply chain and technology development of material which would have projection on embodied energy and cost of material in positive correlation.

Low ore grade materials of various technologies include Copper, Zinc, Lead, Cobalt, Nickel, Chromium, Manganese, Platinum, Sliver, Iridium, Lithium, Graphite, Dysprosium, Molybdenum, Neodynium, Praseodynium and Terbium.

2.1.3 Total fixed and variable embodied energy demand

Both fixed and variable embodied energy demand are comprised of direct and indirect embodied energy demand. The direct fixed embodied energy demand contains the part related to construction, fixed operation & maintenance, and decommissioning which include the life cycle direct energy input and the embodied energy in the life cycle materials input for investing each technology. The direct variable embodied energy demand includes the energy consumption during production and delivery of fuels (energy feedstock) for the power plant in operation phase. The indirect energy demand represents the part associated with general economic activity required to construct and maintain the energy system at an assumption of a general energy intensity of society (kWh/€).

1. Direct fixed embodied energy demand

Embodied life cycle final energy demand of technology, as called direct fixed embodied energy demand, includes the life cycle direct energy input and sum of all embodied energy demand of the life cycle materials input of various technologies, which is showed in equation (17).

$$E^{emb}_{life,final,n} = E_{life,direct,n} + \sum_{m} M_{life,m} * E^{emb}_{m,n} \quad (17)$$

m, n, $M_{life,m}$, $E_{life,direct,n}$ are the same as in equations (1) and (2)

$M_{life,m}$: life cycle material demand of type m per capacity of a technology, ton/kW

$E_{life,direct,n}$: life cycle direct energy demand of type n per capacity of a technology, MWh/kW
$E^{emb}_{m,n}$: embodied energy type n of material type m, MWh/ton
$E^{emb}_{life,final,n}$: total embodied life cycle final energy demand of type n per capacity of a technology, MWh/kW

In order to consider the factor of the low ore grade of material into the cost of each technology, the low ore grade materials cost share of each technology P_{lg} is calculated by equation (19). Then the updated price of each technology $P_{updated}$ is calculated by sum of the stated price P_{stated} and the increased price of the low ore grade materials using the factor of increased price due to declined ore grade F_{lg} in equation (20).

$$P_{stated} = P_{US}/C_{rate} \tag{18}$$

P_{stated}: stated price of each technology in Euro, €/kW, €2019
P_{US}: stated price of each technology in US dollar, USD/kW
C_{rate}: conversion rate 1.1 \$/€

$$P_{lg} = \sum_m M_{life,m,lg} * P_{M,m,lg} \tag{19}$$

P_{lg}: low ore grade materials cost share of each technology, €/kW
$M_{life,m,lg}$: life cycle demand of low ore grade material type m of each technology, ton/kW
$P_{M,m,lg}$: price of low ore grade material type m, €/ton

$$P_{updated} = P_{stated} + P_{lg} * (F_{lg} - 1) \tag{20}$$

$P_{updated}$: updated price of each technology in Euro, €/kW
F_{lg}: factor of increased price due to lower ore grades. Results presented in this report did not explore the effect of material depletion, i.e, F_{lg} was kept at 1 for all simulations. The updated price can be adjusted by adjusting this factor for potential study in future.

2. Total fixed embodied energy demand

Total fixed embodied energy demand of each technology not only includes the direct part, but also includes indirect energy demand. Aiming to quantify the indirect part of energy demand $E^{emb}_{indirect,n}$, the remaining cost of each technology $P_{remaining}$ associated general economic activity required to construct and maintain the energy system input is determined in equation (22) by using the updated price $P_{updated}$ deducting total price of life cycle final energy demand $P_{E,life,final}$, which is calculated by sum up of product of energy price and total final energy demand in equation (21). Then the indirect energy demand is assessed by multiplying the remaining cost of each technology $P_{remaining}$ with energy intensity of rest $E_{intensity}$ and energy ratio of type n R_n in equation (23). The total fixed embodied energy demand is estimated by adding up total embodied life cycle final energy demand with the indirect embodied energy demand in equation (24).

$$P_{E,life,final} = \sum_n E^{emb}_{life,final,n} * P_{E,n} \tag{21}$$

$P_{E,life,final}$: total price of life cycle final energy demand of each technology, €/kW
$P_{E,n}$: Price of energy type n, €/MWh

$$P_{remaining} = P_{updated} - P_{E,life,final} \quad (22)$$

$P_{remaining}$: remaining cost of each technology, representing the general economic activity other than direct energy supply needed to deploy a technology; €/kW

$$E^{emb}_{indirect,n} = P_{remaining} * E_{intensity} * R_n / 1000 \quad (23)$$

$E^{emb}_{indirect,n}$: indirect embodied energy demand of type n, MWh/kW
$E_{intensity}$: a general energy intensity of the society, currently with a assumption at 1 kWh/€, derived from global final energy demand and global GDP.
R_n: energy ratio of type n, %

$$E^{emb,fix}_{total,n} = E^{emb}_{life,final,n} + E^{emb}_{indirect,n} \quad (24)$$

$E^{emb,fix}_{total,n}$: total fixed embodied energy demand of type n, MWh/kW

Additionally, considering the change of energy price and energy type in future towards 2050, three current energy carriers of electricity, gas fuel and liquid fuel are transferring from electricity, natural gas and diesel to clean electricity, hydrogen and ammonia as the represented energy type in future. Future energy prices will be implicitly determined in the model, but some assumptions can be made here to illustrate the effects of this methodology on the total cost of various technologies. In equation (25) the residual price $P_{residual}$ independent of energy consumption is calculated the difference of updated price with the total current energy cost. Then the future updated price of each technology is estimated by adding the residual price with the total future energy cost in equation (26).

$$P_{residual} = P_{updated} - \sum_n E_{total,n} * P_{E,n} \quad (25)$$

$P_{residual}$: residual price, €/kW

$$P_{updated,future} = P_{Residual} + \sum_n E_{total,n} * P_{E,future,n} \quad (26)$$

n: different energy type n in future (electricity, hydrogen and ammonia)
$P_{updated,future}$: future updated price of each technology, €/kW
$P_{E,future,n}$: future price of different energy type n, €/MWh

Table 11 lists the assumptions of energy data including current and future energy price and energy demand ratio.

Energy type	**Unit**	**Electricity**	**Gas fuel**	**Liquid fuel**
Current energy price	€/MWh	60	30	60
Future energy price	€/MWh	100	100	150
Energy demand ratio	%	34	33	33

Table 11: Energy price and demand ratio

The calculation results of total fixed embodied energy demand and different prices of each technology are listed in table 5-7 of the Appendix. The observations show that renewable energy has significantly higher direct embodied energy demand than fossil technologies due to their high consumption of materials. Wind offshore has the highest direct embodied energy demand at 3.6 MWh/kW while natural gas power (NGCC) has only 0.3 MWh/kW. However nuclear has the highest indirect embodied energy demand at 4.1 MWh/kW which is nearly 9 times higher than its direct embodied energy demand. This is mainly because nuclear is a much more complicated technology involved with much more consumption of human activities behind the technology itself i.e., political decision, opinion poll and risk assessment. The indirect embodied energy demand of wind and solar are generally lower than fossil power. For the total fixed embodied energy demand, Wind offshore and nuclear take the first and second positions at 4.8 MWh/kW and 4.5 MWh/kW, whereas NGCC is with the lowest demand at 1.2 MWh/kW. Embodied energy demand is an fundamental factor affecting on energy system profile.

There are three factors considered in the energy system that affect the investing price of technology in future. One is the price increasing of Low ore grade materials due to the resource exhaustion. Low ore grade materials of these technologies include Copper, Zinc, Lead, Cobalt, Nickel, Chromium, Manganese, Platinum, Sliver, Iridium, Lithium, Graphite, Dysprosium, Molybdenum, Neodynium, Praseodynium and Terbium. The column with name "LG updated" in table 7 of the Appendix is the increased proportion of the updated price by double the price of Low ore grade materials (F_{lg} set 2). It shows that the updated prices of those technologies with heavy demand of Low ore grade materials rise notably. Electrolyzer, H_2 tank and battery rise nearly 20%; VRE transmission and solar grows 14% and 9% respectively. While nuclear, fossil, H_2 pipeline and SMR have little effect.

The second factor is energy price. The last column of table 7 of the Appendix is the increased proportion of the updated future price due to the energy price increasing from the current price to future price listed in table 11. It demonstrates that technologies with higher direct embodied energy demand such as wind and solar are very sensitive to the energy price. Hydrogen pipeline has highest increased proportion at 42%. This is a warning for those technologies with high intensive material consumption and high embodied energy may face the significant risk of soaring investment when the energy price increasing.

The third factor is the assumption of a general energy intensity of the society, currently assuming at a level of 1 kWh/€ based on global final energy demand and GDP data, but this is various in different regions. On the contrary, its reciprocal 1 €/kWh represents an economic efficiency of the society, which is applied for indirect environmental impact estimation in section 3. A higher economic efficiency of the society implies that the general economic activity other than direct energy demand for technology construction and material supply can be delivered consuming less energy.

3. Variable embodied energy demand of power plant in operation phase

Arvesen and colleagues studied global electricity supply of different technologies in different regions and scenarios towards 2050 and quantified energy requirements in a life cycle by deriving life cycle assessment coefficients for application in integrated assessment modelling [75]. Their results of energy input of electricity, gases, liquids and solids include freight transport, iron, cement and residual in construction, operation and end of life phases [75].

The calculation results of the energy input of different electricity supply technologies in life cycle and construction phase in China and Europe in 2050 derived from the data in Arvesen's study [75] are listed in table 8 of the Appendix. In a whole life cycle, the energy input of biomass with CCS is the highest at more than 20% energy consumption per electricity output, while biomass without CCS is close to 18%. Hydro and fossil fuel power are at level of 8-12%, followed by solar at 6-8%, nuclear at close to 5%. Wind power is at the lowest level around 3%. However in the construction phase, the energy input of fossil fuel and nuclear power are at the lowest level below 1%, biomass powers are at 2-3%. The energy input of renewable energy in construction phase take the majority part of the total energy input in a whole life cycle. It could be deduced that the energy consumption of fossil fuel power in operation phase takes the majority of the total energy input in a whole life cycle. This part of data are not directly applied into the energy system model but as a reference for better understanding the energy consumption and distribution in different phases of a life cycle for different generating technologies.

The principle of the energy consumption calculation in life cycle, in construction and operation phase are similar as equation (2).

$$E_{life,direct,n} = \sum_{i,j}(E_{i,j,n}) \tag{27}$$

i: different processes in a phase of the life time cycle (transport, iron, cement and residual)

j: different phases in a life time cycle (construction, operation, end of life)

n: different type of energy carries (electricity, natural gas, diesel and solid)

$E_{i,j,n}$: direct energy demand of type n in process i of phase j, GJ/MW

$E_{life,direct,n}$: life cycle direct energy demand of type n, GJ/MW

$$E_{life,direct,input,n} = \frac{E_{life,direct,n}}{C_f * T_{life} * 8760 * 3.6} \tag{28}$$

C_f: capacity factor (%)

T_{life}: lifetime (year)

8760: total hours per year (h/year)

$E_{life,direct,input,n}$: life cycle energy input of type n per electricity output, MWh/MWh

$$E_{con,direct,n} = \sum_{i}(E_{i,con,n}) \tag{29}$$

$E_{con,direct,n}$: direct energy demand of type n in construction phase, GJ/MW

$$E_{con,direct,input,n} = \frac{E_{con,direct,n}}{C_f * T_{life} * 8760 * 3.6} \tag{30}$$

$E_{con,direct,input,n}$: energy input of type n in construction phase per electricity output, MWh/MWh

The embodied energy demand of energy input of power plant in operation phase is calculated by equation (31) and (32):

$$E_{op,direct,n} = \sum_{i}(E_{i,op,n}) \tag{31}$$

i: different processes in operation phase

$E_{op,direct,n}$: direct energy consumption (GJ) of energy type n per coal/gas/biomass supply to power plant (kWh) in operation phase, GJ/kWh

$$E^{emb,var}_{direct,n} = E_{op,direct,n} * \eta_n / 0.0036 \tag{32}$$

$E^{emb,var}_{direct,n}$: embodied energy demand (MWh) of energy type n per coal/natural gas/nuclear fuel/biomass supply to power plant (MWh)in operation phase, MWh/MWh

η_n: energy efficiency of coal/gas/biomass power plant, %;

η_{coal}: 45%, η_{gas}: 60%, $\eta_{nuclear}$: 33%, $\eta_{biomass}$: 45% [76] [77]

The calculation results of variable embodied direct energy consumption (MWh) per coal/natural gas/biomass supply to power plant (MWh) in operation phase in China and Europe in year of 2050 derived from the data in Arvesen's study [75] are listed in table 9 of the Appendix. It shows biomass power has the highest embodied direct energy demand in the operation phase at 20% for crops and 14% for forest residue. Natural gas and coal power has much lower energy demand at 5.4% and less than 4% respectively. While nuclear has the lowest direct energy demand at less than 1.5%. In general, there is no big difference between these two regions but with slightly higher demand in electricity and slightly lower demand in liquid fuel for coal and natural gas power in Europe compared with in China due to their regional energy structure supply.

Same as the total fixed embodied energy, the total variable embodied energy demand includes direct and indirect two parts. The indirect part of embodied energy is scaled by the fuel cost, same method as fixed indirect embodied energy although the indirect part of variable embodied energy takes much lower ratio of direct energy demand.

2.2 Monetized life cycle environmental impacts identifying

In this section, life cycle impact of key materials and fuels from ecoinvent 3.0 database are investigated by applying Simapro with European Environmental Footprint (EF 3.0) method. Then the monetized impact cost are identified by using monetary valuation coefficients (MVCs) based on literature data. Finally, the monetized impact cost of each technology is obtained from the data set of impact cost of materials and fuels, as well as the data set of life cycle material and energy demand of each technology in section 2.1. Foreground impact and indirect impact are also considered.

2.2.1 Life cycle environmental impacts of typical materials and fuels

Some typical material production (steel, copper, Aluminium, Nickel, Epoxy and Concrete) and fuel market (coal, natural gas, nuclear fuel, biomass and petrol) in ecoinvent 3.0 database are chosen to assess their life cycle environmental impacts using Simapro. Those chosen processes are listed in table 12.

Material/Energy	Description
Steel	1 kg Steel, low-alloyed, hot rolled (RER)｜ production ｜ Cut-off, U [78]
Copper	1 kg Copper (GLO)｜ copper production, solvent-extraction electro-winning ｜ Cut-off, U [79]
Aluminium	1 kg Aluminium, primary, ingot IAI Area, Russia, RER w/o EU27 and EFTA｜ aluminium production ｜ Cut-off, U [80]
Epoxy	1 kg Epoxy resin, liquid RER｜ production ｜ Cut-off, U [81]
Nickel	1 kg Ferronickel, 25% Ni GLO｜ production ｜ Cut-off, U [82]
Concrete	1 m^3 Concrete, 40MPa RoW｜ concrete production 40MPa ｜ Cut-off, U [83]
Coal	1 kg Hard coal (Europe, without Russia and Turkey)｜ market for hard coal ｜ Cut-off, U [84]
Natural gas	1 m^3 Natural gas, high pressure (Europe without Switzerland)｜ market group for ｜ Cut-off, U [85]
Biomass	1 kg Wood chips, dry, measured as dry mass (RER)｜ market for ｜ Cut-off, U [86]
Nuclear fuel	1 kg Nuclear fuel element, for pressure water reactor, UO2 4.0% and MOX (GLO) market ｜ Cut-off, U [87]
Petrol	1 kg Petrol, unleaded RER｜ market for ｜ Cut-off, U [88]

Table 12: Process of material production and energy market in ecoinvent 3.0 database

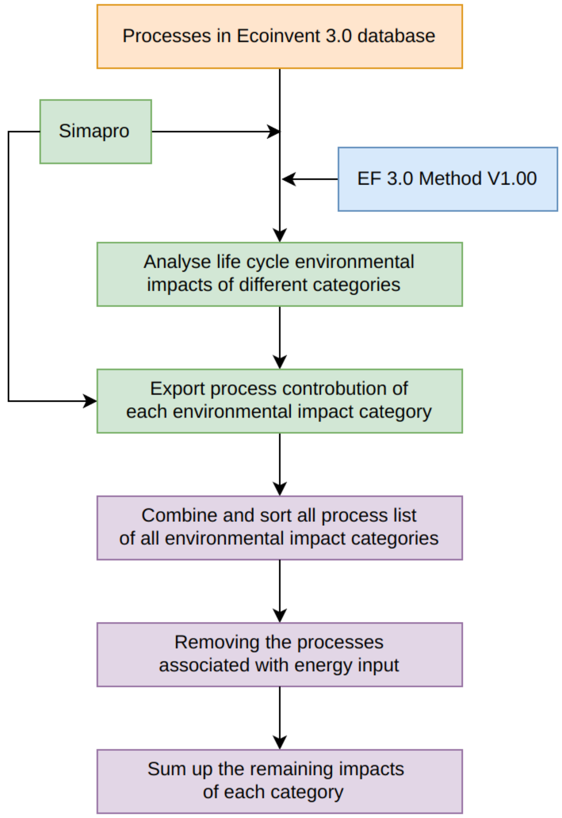

Figure 8: Process of life cycle environmental impacts of material, energy resource and technology

Figure 8 shows the process of analysing life cycle environmental impacts of material and energy resource. Firstly, calculate the life cycle environmental impacts of the chosen process of Ecoinvent 3.0 database and set the EF 3.0 method in Simapro. EF method is the impact assessment method of Environmental Footprint (EF), initiative introduced by the European Commission. The method included in the SimaPro Professional database includes a number of adaptations, which make it compatible with the data provided in SimaPro libraries. Secondly, export the list of process contribution of each category of environmental impact with setting characterisation as the indicator and a proper cut-off rate at 0.1%. Thirdly, combine and sort all the process lists of all environmental impact categories. Then removing those processes associated with the energy input including electricity, nuclear, natural gas, diesel, coal, coke, wood and renewable in the metal productions and energy resource market because the energy input are supplied by clean energy inside the energy system model. While for energy resource market, those processes associated with production of natural gas, coal and biomass are included. In terms of transport, the climate change impact is removed too but the other impacts are made assumptions at half of original value due to clean energy application in transport dose not eliminate other impacts. Finally, sum up the remaining of the impacts, ready for being monetized.

The remaining of the impacts of each category is calculated by equation as follow:

$$I_{i\_remain} = I_{i\_total} - I_{i\_energy} \tag{33}$$

i: impact category i

I_{i_remain}: the remaining impact of category i

I_{i_total}: the total impact of category i

I_{i_energy}: the impact from those processes involved in energy input (such as coal, natural gas, nuclear, biomass, heat etc which will supply from the energy system inside) in category i

The remaining impact of energy resource in each category is calculated with its energy intensity which is listed in table 13 of the Appendix:

$$I_{i\_e} = I_{i\_wv} / E_{int} \tag{34}$$

i: impact category i;
I_{i_e}: impact per GJ energy of category i;
I_{i_wv}: impact per kg or m$_3 energyofcategoryi$;
E_{int}: Energy intensity GJ/kg or GJ/m$_3$;

The remaining fractions and the remaining life cycle impacts of process of key materials and fuels are listed in table 10-12 and 14-16 in the Appendix. For the material production, it indicates that the remaining impact of fossils resource use of steel and copper production is very small fraction at 1-5% due to removing most processes of fossil fuel energy input, resulting in remaining impacts of climate change and ozone depletion also down to 9-21%. While impact of resource use of minerals is almost 100% remaining. When comparing the total life cycle impacts, almost all of impacts of copper production are larger than steel, especially impacts of Eco-toxicity freshwater and resource use of minerals being higher by 94 and 74 times. This is because that ore grade of copper is much lower than iron which leads to high impact of metal resource depletion. Also mining and extraction of copper with low ore grade needs higher embodied energy which cause higher impacts of climate change and other categories. Furthermore, the environmental standards of these two processes of metal production are different due to their difference regional reference of Europe and global.

However it is a different story for the processes of energy market. Impacts of resource use of fossils (MJ/per GJ energy) of natural gas, coal, nuclear fuel and petrol are mostly remaining while the impact of biomass only remain 10%. This shows that although the total impact of resource use fossils of biomass (wood chips) are lower than the other energy resources but it is involved with much larger fraction of energy input such as cutting and transport. It is noticeable that the impacts of land use of biomass are much higher than the other energy due to deforest for wood. Nuclear fuel has high impact of ionizing radiation.

The ecotoxicity of copper, nickel and coal is significant due to their mining/extraction process based on the contribution process list in Simapro.

2.2.2 Monetary valuation of life cycle environmental impacts

The monetary valuation of ecosystem services is obtaining attention in economy and policy bodies [89]. Monetary valuation applied in Life Cycle Assessment (LCA) enable to aggregate environmental impacts or cross-comparison between different categories with different units of measure, which facilitate the uniform standards in a comparable way with LCA results of different technologies in cost benefit analysis for policy-maker [90][91].

However, several challenges restrict its wide application in the field [90]. Pizzol's group performed a review of different monetary valuation methods in LCA with classification, definitions and evaluations of monetary valuation approaches and methods [90]. Cost perspective includes damage costs, market price, averting behaviour, travel cost, Hedonic pricing, contingent valuation, conjoint analysis with choice experiment, budget constraint, abatement cost, restoration cost and stated preference [90] [92]. Pizzol discovered that the methods of observed-preference, revealed-preference and the abatement cost have limitation to be applied in LCA, while the methods of conjoint analysis and budget constraint are the premier options for monetary valuation in LCA [90].

The classification of monetary valuation approaches and methods is provided by Pizzol [90] and Amadei [91] in Figure 9. Particularly, the approach of "damage cost" monetary valuation was contained, which estimated the damage to ecosystem and human caused by an emission or by other changes into ecology capital [91].

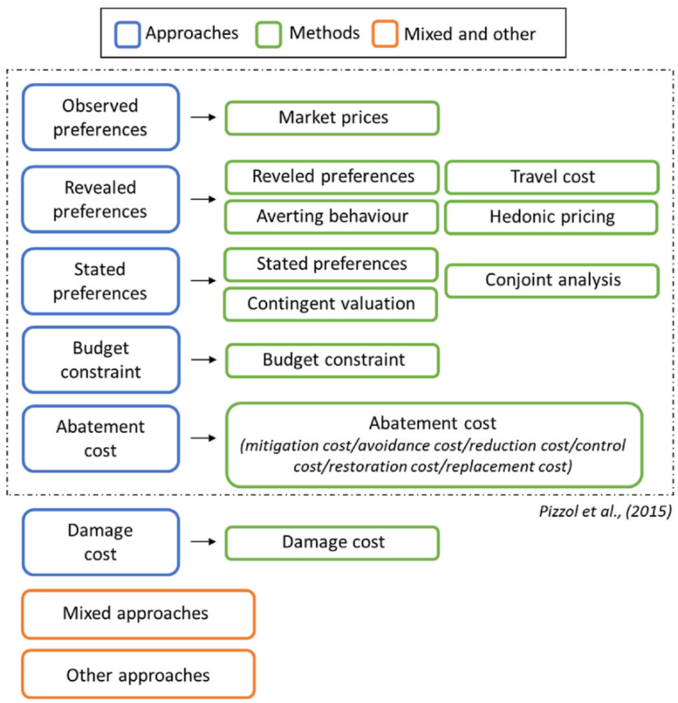

Figure 9: Outline of the classification of monetary valuation approaches and methods [90][91]

Amadei and colleagues systematically evaluated the available methods of monetary valuation and also investigated the future research demands of monetary valuation factors being applicable to life cycle impact assessment methods such as the European Environmental Footprint (EF) [91]. A wide range of monetary valuation coefficients (MVCs) was collected and compared with significant variability stemmed from the application of different approaches across impact categories including some frequently analyzed such as climate change and others with little information such as terrestrial euthrophication in their literature review [91].

Arendt's group also reviewed and quantitatively compared different monetization methods for LCA, namely Ecovalue12, Stepwise2006, LIME3, Ecotax, EVR, EPS, the Environmental Prices Handbook, Trucost and the MMG-Method [92]. Among these investigated methods, the ranges of monetary valuation factors of the same impact category are mostly within two orders of magnitude, while some have wider scope such as resources use mineral & metal within five orders of magnitude [92]. It is notable that the regional characteristics of per capita income has the largest affect on the monetary factors, which need cautiousness and range estimation of application various monetization methods [92]. In Arendt's study, unit conversion factors (UCFs) for converting all impact categories to the same units from different units based on different LCA methds are provided [92].

In this study, a range of monetary valuation coefficients of each impact category applicable to EF method is attempted to be established based on literature data. The challenge is to reconcile the unit-issues for MVCs related to different LCIA methods. Especially the MVCs of categories Particulate matter and Land use with units applicable to EF method are insufficient in literature and the unit conversion factors between EF and other LCIA methods are unavailable. A practical strategy is to assume that the environmental impact of a same process with the same functional unit in a same region should be the same in reality in the same category regardless of applying different LCIA methods, thus the unit conversion factors could be calculate by the impact value with different units based on different methods. The equations are as follows:

$$UCF_{i\_atb} = I_{i\_b} / I_{i\_a} \tag{35}$$

i: impact category i;
UCF_{i_atb}: unit conversion factor from unit a to unit b in impact category i;
I_{i_a}: impact of category i with unit a;
I_{i_b}: impact of category i with unit b;

$$MF_{i\_b} = MF_{i\_a} * UCF_{i\_atb} \tag{36}$$

MF_{i_a}: the monetary damage per unit of a in impact category i;
MF_{i_b}: the monetary damage per unit of b in impact category i;

However, there are limitations in this strategy of assumption. Different LCIA methods, even for the same impact category, possibly apply different rationales and assumptions. Thus, the coverage of modelled impact pathways and the associated parameters might differ. For instance impact category Particulate matter with unit of disease incidence in method EF is a regionally differentiated impact that depends on the population density around the release site. Moreover, factors like typical location or height of the chimney might influence the incidence. Such factors would not be considered in impact with the unit of PM2.5 eq in method ReCiPe.

Nevertheless, as we apply the same process in the same region for calculating UCFs between these two methods, the condition of the LCA target are exactly the same. Those different factors or different coverage between the different methods are reflected on the UCFs quantitatively.

Table 13 lists the range of collected monetary coefficient of different environmental impact category with min , max, average and mean values [91] [92].

Environmental impact category	Min	Max	Average	Arithmetic mean	Geometric mean	Median
Climate (kg CO_2 eq)	7.45E-03[93]	6.85E-01[94]	2.72E-01	1.26E-01	8.32E-02	9.47E-02
Ozone depletion (kg CFC11 eq)	3.20E+01[93]	7.56E+02[95]	5.55E+01	1.31E+02	7.06E+01	4.61E+01
Human toxicity, cancer (CTUh)	1.27E+05[93]	4.00E+06[96]	6.45E+05	1.16E+06	7.18E+05	8.12E+05
Human toxicity, non-cancer (CTUh)	2.53E+04[93]	7.95E+05[96]	1.28E+05	2.29E+05	1.43E+05	1.60E+05
Particulate matter (disease inc.)	1.71E+05[97]	4.82E+06[93]	2.96E+06	2.17E+06	1.62E+06	1.95E+06
Ionizing radiation (kBq U-235 eq)	5.87E-04[98]	4.86E-02[93]	2.13E-01	1.19E-02	2.86E-03	1.22E-03
Photochemical (kg NMVOC eq)	1.46E-01[93]	3.79E+01[93]	3.51E+00	6.70E+00	2.28E+00	1.53E+00
Acidification (mol H+ eq)	2.95E-03[95]	2.18E+01[94]	5.58E+00	4.33E+00	1.17E+00	2.44E+00
Land use (m²a)	1.78E-04[97][99]	2.80E-02[100]	1.88E-03	8.89E-03	2.83E-03	1.22E-03
Ecotoxicity, freshwater (CTUe)	4.09E-06[101]	5.80E-02[102]	6.41E-03	6.41E-03	1.76E-04	3.91E-05
Resource use, fossils (MJ)	1.1E-03[95]	1.79E-02[94]	1.10E-02	8.99E-03	7.03E-03	6.89E-03
Resource use, minerals (kg Sb eq)	1.65E+00[98]	8.21E+04[103]	4.39E+03	1.23E+02	8.75E+00	6.65E+00

Table 13: Monetary valuation coefficients of environmental impact categories, €2019/impact unit

It is found that the MVCs ranges of ionizing radiation, Ecotoxity freshwater, resource use minerals are bigger. According to mineral resources, only antimony was evaluated, because several methods just manage to monetized at inventory level rather than conducting to characterization [92]. The influence factors of the MVCs include the option in terms of cost perspectives methods, the regional characteristics such as geographical reference, the protection level of areas and resource scarcity, and the path to discounting, which heavily influence the magnitude of the monetary factors [92].

2.2.3 Life cycle monetized impacts of typical materials and fuels

In this study, the total monetized impacts of each technology not only contain the monetized life cycle impacts of direct material and energy input, but also include the indirect monetized impacts associate with social-economy consumption in the value chains of each technology, assumed at an economic efficiency of 1000 €/MWh.

In order to understand what monetized impacts are important and how is the total impact cost of the material and energy compared with their physical prices, the monetized impacts of each material or each energy resource are firstly calculated by their (remaining) impacts from section 2.2.1 and the MVCs from section 2.2.2 in the equations (37) and (38) as follows:

$$MI_{i,j} = I_{i,j} * MVC_i \tag{37}$$

i: impact category i;
j: type of material or energy resource j;
$MI_{i,j}$: the monetized impact of category i of material or energy carrier j;
$I_{i,j}$: the impact of category i of material or energy resource j;
MVC_i: the monetary valuation coefficient of impact category i;

$$MI_j = \sum_i MI_{i,j} \tag{38}$$

MI_j: total monetized impact of all categories of material or energy resource j;

The geometric mean of MVCs in table 13 is applied to calculate the monetized impact of materials and fuels, presented in table 21 of Appendix. In general, the total impact cost of copper is much higher than steel by more than 16 times, at 4.52€/kg copper to 0.276€/kg steel, due to the higher impact of copper production presented in table 10 of the Appendix. Among the energy resources, coal has the highest impact cost at 10.1 €/GJ coal, natural gas and nuclear fuel have the second high impact cost at 8.08 €/GJ natural gas and 7.9 €/GJ Uranium respectively, while biomass is lowest one at 3.06 €/GJ wood. This conforms the level of cleanliness and environmental friendliness of each energy resource that coal is the most polluting energy with higher emission during the process of mining, transport and combustion.

In terms of the proportion of each monetized impact category, Particulate matter is one of the monetized impacts with large proportion which takes 64%, 45% and 30% for steel, copper and biomass respectively mainly due to the refine processes for metal manufacture and urea production for wood, observed in the process contribution list from the LCA result in Simapro. Ecotoxicity is another import impact category especially in copper production which take 35% of the total impact cost due to the high impact in the blasting process of copper production in Europe and Rest of the world observed from process contribution of LCA result. Land use take 50% of total impact cost in biomass due to deforestation. After removing those processes associated with energy input, the monetized impacts of climate change are all no more than 10% of total impact cost for these 2 materials and 4 energy resources, among which nuclear fuel's monetized impacts of climate is close to 0%. Fossil resource use looks another important monetized impacts for energy resource which takes the majority proportion of natural gas, coal and nuclear fuel at 94%, 77% and 91% respectively. The monetary valuation method is market price for this impact category, however there is only about a century of oil & gas resources left but about a millennium of coal and nuclear left in the earth. Hence, coal & nuclear should technically have an order of magnitude lower fossil depletion impact than oil & gas because of their relative abundance (similar to 1 kg of steel having a much smaller metals depletion impact than 1 kg of copper).

2.2.4 Total monetized impacts of technologies and fuels

The total environmental impact cost includes direct and indirect parts. The direct impact cost is related to the direct impact which is the sum of the life cycle impact of different materials input of each technology. The indirect impact is related to the indirect impact which is associated general economic activity required to construct and maintain the energy system at an estimated general economy efficiency other than the material and energy demand of the technologies. For fuels, it is the similar concept as the direct, indirect and total impact cost of technology. The total impacts cost of technologies and each fuels are calculated by a few steps as follows:

1. The life cycle environmental impact of all other materials.

This is estimated on the assumption of the relationship between the impact of material and its cost being positive correlation. Impact of those materials with abundant resource is calculated based on impact of steel, while rare material with limited resource is calculated based on impact of copper.

$$I_{a,i} = I_{steel,i} \frac{C_a}{C_{steel}} \tag{39}$$

$$I_{r,i} = I_{copper,i} \frac{C_r}{C_{copper}} \tag{40}$$

i: impact category i;
a: material a with abundant resource;
r: rare material r with limited resource;
$I_{a,i}$: impact of material a in category i;

$I_{r,i}$: impact of material r in category i;
$I_{steel,i}$: impact of steel in category i;
$I_{copper,i}$: impact of copper in category i;
C_a: base cost of material a;
C_r: base cost of material r;
C_{steel}: base cost of steel;
C_{copper}: base cost of copper;

2. Life cycle impact of each category of each technology.

This is calculated by sum of products of each category of impact of each type material and the amount of the corresponding type of material input of each technology:

$$I_{life,direct,i} = \sum_{m}(I_{life,i,m} * M_{life,m}) \tag{41}$$

m: different type of material (steel, copper, cement etc);
$I_{life,i,m}$: the life cycle impact of category i of material m;
$M_{life,m}$: life cycle material demand of type m, per kW capacity of a technology;
$I_{life,direct,i}$: the life cycle impact of category i of each technology;

3. Indirect impact.

Indirect impact is the impact associated with general economic activities besides the direct material and energy resource input, per € of economic value added at an economic efficiency level (initially set to 1000 €/MWh). This is estimated based on the assumption of positive correlation relation between the indirect impact and indirect consumed energy associated general economic activity required to construct and maintain the energy system, which is further scaled by divided by its corresponding total overnight cost. This scaled indirect environmental impact was determined for each technology and averaged to get the general indirect environmental impact per € of general economic activity at an economic efficiency of 1000 €/MWh. The calculated values were reasonably consistent between different technologies, increasing confidence in this approach.

$$I_{indirect/cost,i} = \frac{I_{life,direct,i} * E_{indirect}/E_{total,direct}}{P_{TOC}} \tag{42}$$

$E_{total,direct}$: total direct energy demand including the life cycle direct energy demand and the embodied energy of the life cycle materials demand of each technology construction;

$E_{indirect}$: indirect energy demand associated general economic activity required to construct and maintain the energy system for each technology;

P_{TOC}: total overnight price of each technology in Euro, €/kW;

After the indirect environmental impact of each category of each technology is scaled with energy and its cost at an economic efficiency of 1000 €/MWh, its averaged value multiply back to its cost with this general economic efficiency.

$$I_{indirect,i} = \overline{I_{indirect/cost,i}} * P_{TOC} * 1000/E\eta \tag{43}$$

$E\eta$: a general economic efficiency based on GDP and energy consumption in an area. It is initially set to 1000 €/MWh and further conducted uncertainty study.

$\overline{I_{indirect/cost,i}}$: averaged indirect impact of different technologies in category i, per € of economic value added at a general economic efficiency $E\eta$;

4. Total impact of each technology including direct and indirect impact.

$$I_{total,tec,i} = I_{life,direct,tec,i} + I_{indirect,tec,i} \tag{44}$$

5. Monetized life cycle impact cost.

It is the sum of products of the total impact and the monetary valuation coefficient (MVC) of each category.

$$MI_{tec} = \sum_{i}(I_{total,tec,i} * MVC_i) \tag{45}$$

MVC_i is the same as in equation (37);

MI_{tec}: total monetized impact of all categories of each technology;

6. Monetized life cycle impact cost of fuel.

The life cycle impact costs of fuels (natural gas, coal, biomass and nuclear fuel) are calculated the same way as equation (43)-(45) as the sum of products of the life cycle impact of fuel and the monetary valuation coefficient of each category. The indirect impact of fuel is estimated based on the averaged indirect impact of different technologies and the market price of fuel at the general economic efficiency (initially set to 1000 €/MWh).

$$I_{indirect,i} = \overline{I_{indirect/cost,i}} * P_{fuel} * 1000/E\eta \tag{46}$$

$$I_{total\_fuel,i} = I_{life,direct\_fuel,i} + I_{indirect\_fuel,i} \tag{47}$$

$$MI_{fuel} = \sum_{i}(I_{total\_fuel,i} * MVC_i) \tag{48}$$

P_{fuel}: market price of fuel;

$I_{life\_fuel,i}$: the life cycle impact of category i of fuel;

MI_{fuel}: the monetized impact of all categories of each fuel;

The direct, indirect and total environmental impact of typical technologies and typical fuels in different categories are calculated and listed in the table 22-24 of the Appendix. In terms of direct impact, wind and solar generally have much higher direct environmental impacts than nuclear and natural gas power (NGCC) for all the categories, after removing the processes of energy input (which will be supplied by energy system inside) in all the material production applied in section 2.2.1. Especially wind offshore is the one with the highest impacts, by averagely 9 times of impacts compared with NGCC within all categories. This is for the fact that wind and solar are the technologies with much higher intensive material demand compared with nuclear and NGCC.

However, it is noticeable that the indirect environmental impact of nuclear power is much higher than its direct impact by averagely 17 times of all categories. NGCC is in the second position with larger difference between indirect and direct impact by averagely 3.3 times. Whereas the indirect impact of wind and solar are much lower with 30%-100% of their corresponding direct impacts. This matches the embodied indirect and direct energy demand profiles of different technologies. Fuels are in the similar situation that Uranium has much higher indirect impacts than coal and biomass.

Finally, the total impacts of nuclear power overtake those of wind offshore for all the categories. NGCC becomes the technology with lowest total impact among these 5 technologies. For fuels, coal still has the highest total impacts in categories of climate, human toxicity, photochemical ozone formation, acidification and ecotoxicity. Uranium has highest total ionizing radiation impact at 42.6 kBq U-235eq/GJ. Biomass has highest land use impact at 2570 Pt/GJ. The total fossil resource use impact of Uranium, natural gas and coal are all high at around 1000 MJ/GJ while biomass is at 17.3 MJ/GJ.

The environmental impact cost is called external cost relative to the investment of each technology and market price of fuels which called internal cost. These external costs are integrated into the total cost of each technology and fuel demand in energy system. Table 14 presents the internal cost (P_{stated}) and external cost (Monetized impact, MI) of these typical technologies and typical fuels are presented in the Appendix, in which the min, max, arithmetic mean, geometric mean and median of external cost, as well as the ratio of geometric mean external and internal cost are also detailed listed. The range of external cost is big due to the big range of MVCs, and the geometric mean values are close to the median values. The ratio of geometric mean external and internal cost shows that the renewable technologies has higher proportion of their external impact cost compared with their internal investment. Especially solar takes 30% external cost on its internal cost, wind onshore and offshore take 13% and 17%. While the external costs of nuclear and natural gas are only take 7% and 9% respectively. In terms of the energy resources, both Uranium and coal have much higher external cost at 10.8 and 5.34 times of their internal cost respectively; the second is natural gas at 1.4 times of its internal cost; biomass has the lowest ratio at 50%. The externalized cost of coal and (especially) nuclear is dominated by fossil resource depletion, which makes little sense due to the abundance of these resources. Hence, the fossil fuel depletion impact will be reduced in the default case presented later in the preliminary energy system model results.

Technology	Internal cost	External Min	External Max	Arithmetic mean	Geometric mean	Median	External/internal
Nuclear	4090.91	71.31	24999.05	3194.72	284.71	257.34	7%
NGCC	716.20	15.47	5133.58	658.63	60.95	55.58	9%
Onshore wind	1281.82	45.23	12817.57	1665.13	171.96	160.52	13%
Offshore wind	1200.00	54.95	14276.42	1868.97	205.25	193.88	17%
Solar	327.27	27.64	5964.68	795.50	99.79	96.44	30%
Uranium	1.00	3.63	466.94	36.72	10.79	10.17	1079%
Natural gas	6.03	1.62	60.87	15.68	8.47	8.14	141%
Coal	1.92	2.06	150.76	26.92	10.25	9.87	534%
Biomass	7.00	0.67	81.50	13.56	3.52	4.61	50%

Table 14: Internal cost and range, mean and median of external cost, €2019/kW, €2019/GJ

The foreground impacts are exploded using Simapro conducted LCA of some typical technologies in Ecoinvent database 3.0. The monetized impact cost distributions of seven typical technologies are displayed in Figure 10. However, there are some drawbacks of the impact and impact cost of these technologies that are not applicable for this study. Firstly, it is very difficult to separate the foreground impact from background. Secondly, the life cycle impacts of these technologies in Ecoinvent database are generally higher than expectation as they are existing old technologies that cannot present the technique level in future. In addition, some impact categories such as land use are far low for wind onshore and transmission as they are only considering the direct land use occupied by the infrastructure. After literature review and the preliminary modelling, land use is found as the most important foreground impact for wind, solar and transmission, which are further discussed in section 3.7.1.

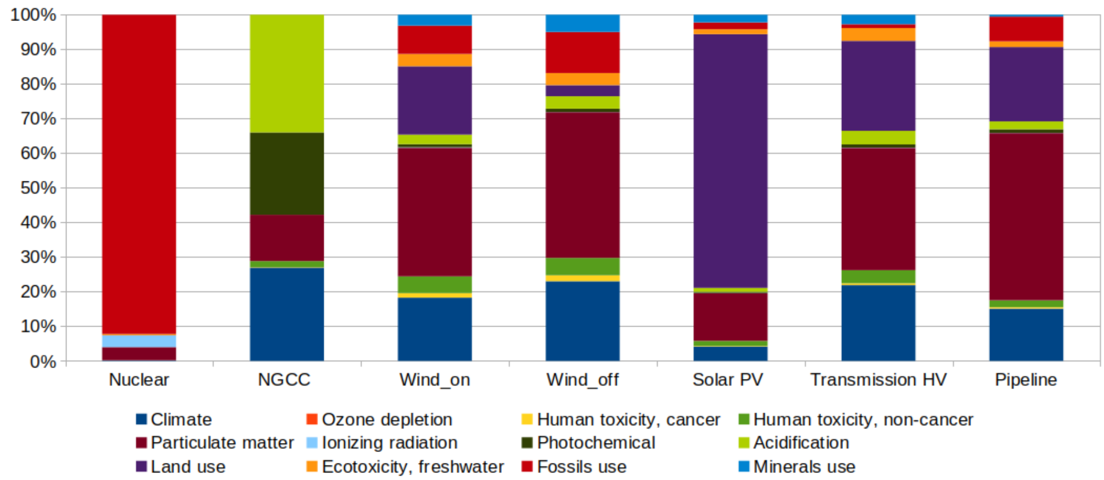

Figure 10: Life cycle impact cost contributions of technologies

2.2.5 Monetary valuation methods adjustment

After the first run of modelling, preliminary results reveal that besides climate change, MVCs of land use, ecotoxicity and resource depletion have large effects on the optimal energy mix. These three impact categories are discussed in detail both on the impact and impact cost in section 3.7.

Particularly, resource depletion impact and impact cost are re-evaluated with a complete new approach. The objective of a new approach of valuation of resource depletion is to derive a current value for future increases in costs and environmental damages to exploit finite resources. The damage to economy and environment is quantified by rising economic and resource depletion costs in future years as well as non-linear effects such as disruptive boom-bust cycles from over-exploitation of finite resources. The methodology is formulated to integrate the resource depletion cost from externality into internality as including the externality of depletion in the market price will moderate demand for finite resources, reducing the aforementioned damages. For some key materials, the rapidly expanding future demand strongly increases the externality. Thus, excessively rapid expansions in the exploitation of finite resources will be moderated more strongly by valuation of internalizing this externality to prevent potentially disruptive boom-bust cycles.

Figure 11 presents the resource depletion valuation modelling. Assumptions of base line are made to set the Original cost=1, Discount rate=5%, Increase (cost) per unit of use=0.02, Starting rate of use=0.5 and Increase in rate of use=0.02. The result of Weighted average price=2.5 and Discounted weighted average price=1.5.

The Top-left graph displays the trend of the cost of cumulative extraction which is assumed to increase with the cumulative amount of extracted material, under the assumption that the most accessible resources are exploited first. The Top-right graph shows the rate of use of the finite material can increase or decrease over time due to economic growth and changes in the technology or policy landscape. The Middle-left graph indicates the cumulative use over time which can be calculated based on the usage rate assumed in the top-right graph. The Middle-right graph exhibits that the assumed relationship between extraction cost and cumulative extraction (top-left graph) is now combined with the calculated cumulative use (middle-left graph) to calculate the increase in extraction cost over time. The Bottom-left graph shows the effect of discounting factor. A discount factor must be applied in this methodology for several reasons. Firstly, high extraction costs in the future are valued less than high extraction costs today because we can use resources extracted today to improve the economy, allowing us to economically exploit more expensive resources in the future. Secondly, if the current resource extraction is productively employed to make the economy more efficient (more value created from less resource consumption), higher extraction costs can be better absorbed in the future. Thirdly, some advances in extraction technology can also be expected to mitigate the increase in extraction costs in the future. The Bottom-right graph reveals that the rate of more expensive future extraction is discounted to account for the above-mentioned factors.

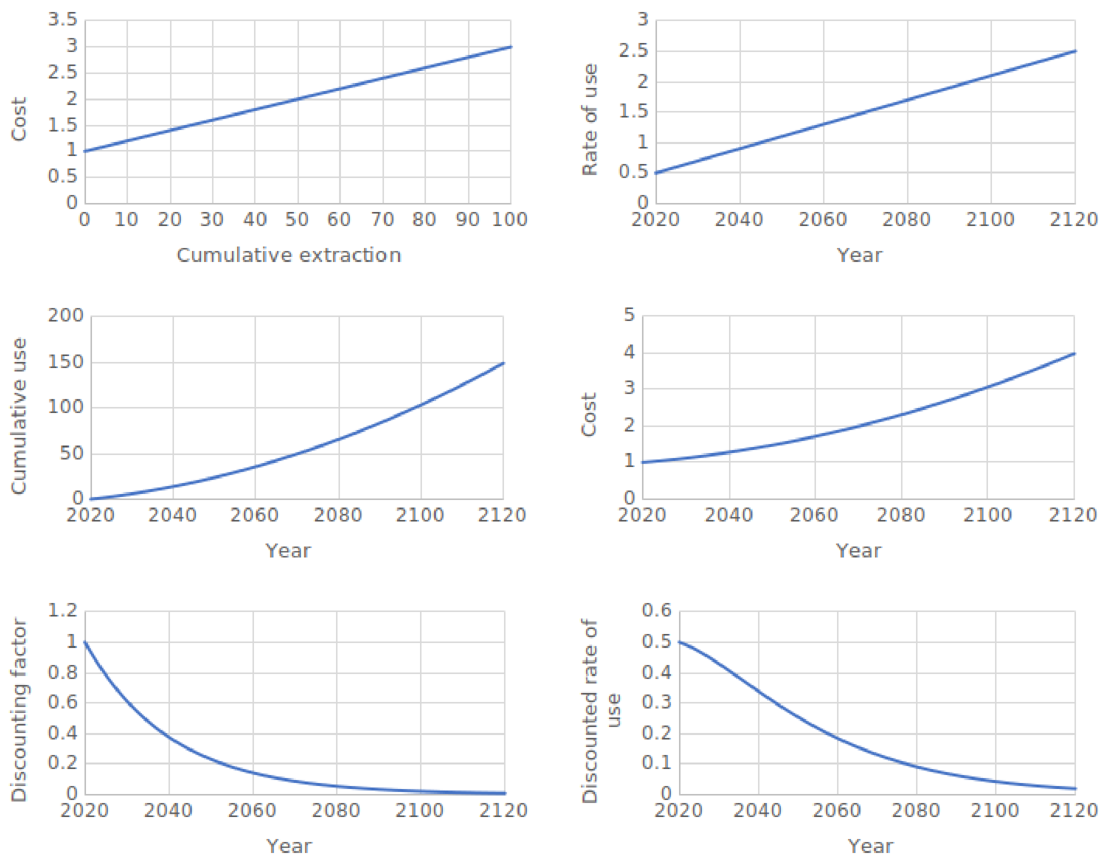

Figure 11: Resource depletion valuation modelling,baseline

Based on the graphs in the right-hand column, weighted averages can be calculated in two steps. Firstly, the simple weighted average cost $Cost_{wa}$ is calculated in Equation (49) from the top-right and middle-right graph in Figure 11. It represents the average cost of a unit of extracted material over the evaluated time period of one century without discounting future extraction.

$$Cost_{wa} = \frac{\sum_t Rate * Cost}{\sum_t Rate} \tag{49}$$

Secondly, the discounted weighted average cost $Cost_{diswa}$ is calculated in Equation (50) from the bottom-right and middle right graphs. It represents the average current value (by discounting future extraction) of a unit of extracted material over the evaluated time period.

$$Cost_{diswa} = \frac{\sum_t Rate_{dis} * Cost}{\sum_t Rate_{dis}} \tag{50}$$

Based on the discounted weighted average cost, the resource depletion externalized cost is calculated in Equation (51).

$$Cost_{ex} = Cost_{diswa} - Cost_{cur} \tag{51}$$

The discounted weighted average cost will always be higher than the current cost because future extraction is assumed to only become more expensive. Thus, the difference between the discounted weighted average cost and the current cost $Cost_{cur}$ is the externalized cost of resource depletion $Cost_{ex}$. In this baseline case, the discounted weighted average cost is 1.51, relative to the original current cost of 1. Thus the resource depletion externality cost is 51% of the internalized cost.

In this central case, historical extraction rates and inflation-adjusted market prices of oil and copper were used to estimate the two graphs in the top row Figure 11. The rate of extraction for both oil and copper increased by about a factor of five over the last 50-70 years. The inflation adjusted market price of oil and copper increased by roughly a factor of three over the same time period. Applying this central assumption to all fuels and minerals is obviously a very crude assumption, but it was not practical to estimate curves for each fuel and mineral in the assessment.

2.3 System scale model

In this section, the system scale model is depicted in respect of the equation system and the assumptions on technology cost and performance parameters. This is based on the exiting system-scale model of the optimizing blue hydrogen production for future energy systems in SINTEF [26], integrating with ammonia generation and storage, and energy transmissions, as well as the life cycle embodied energy demand and environmental impact cost of the technologies and fuels in the system. Hydrogen and ammonia represent the gaseous fuel and liquid fuel, together with electricity, for the energy supply towards the year 2050.

2.3.1 Energy system and scenarios

1. Energy system description

The energy system model applied in this study optimizes deployment and hourly dispatch of a range of electricity, hydrogen and ammonia production, transmission, and storage technologies, with energy supply to the embodied energy demand inside of the system, as outlined in Figure 12. Wind and solar conditions and electricity demand are extracted from German investigations, and performance of wind turbine, solar and battery and technology costs are adapted towards the year 2050[26]. The system model establishes a long-term perspective, with assumptions that all energy facilities in this system are invested in greenfield without restrictions from heritage infrastructure[26].

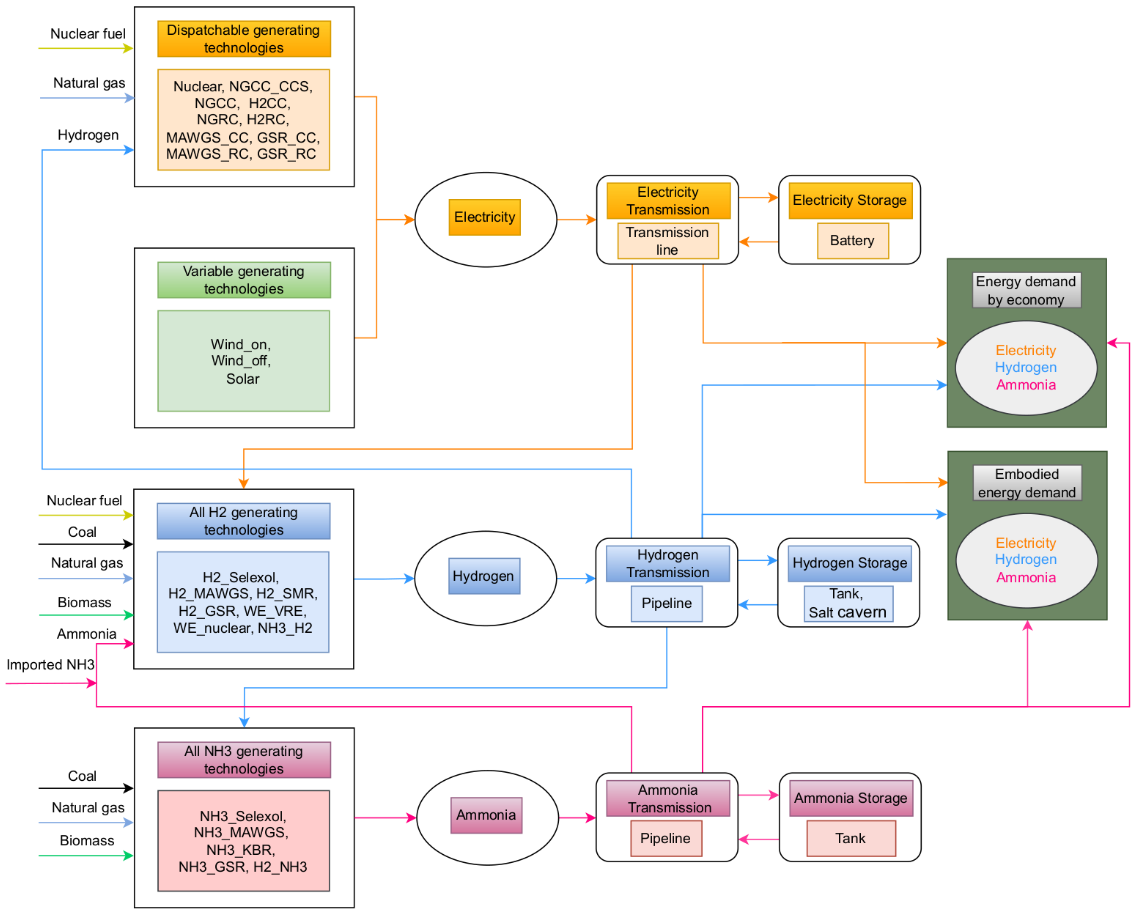

Figure 12: Flow chart of Energy system model towards the year 2050

The main technologies employed in the system is summarized as below:

•Electricity generation: 13 different power plants including dispatchable and variable generating technologies. The dispatchable group is comprised of nuclear, natural gas combined cycles (NGCC) with and without CCS, H_2-fired combined cycle (H2CC), natural gas and H_2 recuperated cycles (NGRC and H2RC), as well as combined and recuperated cycles specially customized for integrating into the GSR and MAWGS blue hydrogen technologies (GSR_CC, GSR_RC, MAWGS_CC, MAWGS_RC) [26]. The variable group includes onshore and offshore wind, and utility scale solar PV[26].

•Hydrogen production: 7 different hydrogen production technologies including blue, green and pink groups. Blue group is comprised of conventional blue hydrogen production from steam-methane reforming (H2_SMR) with MDEA CO_2 capture and coal/biomass co-gasification with Selexol CO_2 capture (H2_Selexol), advanced blue hydrogen production from natural gas applying gas switching reforming (H2_GSR), advanced gasification plants with membrane assisted water-gas shift technology fed by mixture of biomass/coal or pure coal (H2_MAWGS) [26]. Among these technologies, GSR plants are designed for electricity neutrality, and GSR plants have optional resistance heating for blue-green hydrogen production [26]. Both green and pink hydrogen are produced by electrolyzers but from renewable energy and nuclear respectively. The last technology is NH_3 cracking plant to produce hydrogen from ammonia (NH3_H2) [26].

•Ammonia production: 5 different ammonia production technologies including NH3_Selexol, NH3_MAWGS, NH3_GSR with same technical route as H2_Selexol, H2_MAWGS, H2_GSR that firstly produce H_2 then further synthesised with nitrogen, and directly using hydrogen to produce ammonia (H2_NH3), as well as NH3_KBR by KBR ammonia synthesis technology.

•Energy storage: Electricity storage in batteries, hydrogen storage in salt caverns or tanks and ammonia storage in tanks. Salt caverns are low cost but with restrictions of charge/discharge rate and location, requiring added H_2 pipelines to reach the cavern sites, while tanks are higher cost but with no requirements of extra transmission and limits of charge/discharge speed [26]. Ammonia storage is much cheaper due to its liquid phase containing much higher energy intensity.

•Energy transmission: Electricity transmission lines transporting wind and solar power through the spatial distance between good photovoltaic/wind resources and electricity demand, as well as pipelines for hydrogen, ammonia and natural gas supply to all generators and CO_2 pipelines for CCS facilities connecting the sites between carbon capture and storage [26].

2. Scenario definition

Five different scenarios are designed as below:

•S1-No CCS or nuclear: Neither CCS technologies nor nuclear are usable. Wind and solar are the only resource for electrolysis. The energy system is relying on wind, solar and imported ammonia, as well as the natural gas and standalone hydrogen power during periods of deficient wind and sun [26].

•S2-No nuclear: Nuclear is disabled for power generation.

•S3-No CCS: None of CCS technologies are available. Undiminished natural gas and selfstanding hydrogen power plants are able to generate electricity while wind and sun are insufficient. Electrolysis and imported ammonia are the only accessible resources for hydrogen generation [26].

•S4-No advanced CCS: The technology of NGCC-MEA as a conventional post-combustion CO_2 capture is available for power generation. In terms of hydrogen production, gasification with Selexol CO_2 capture from coal/biomass in form of Bio-Selexol and SMR-MDEA from natural gas are enabled [26].

•S5-All technologies: All technologies are available in the energy system. The main difference is the inclusion of advanced H_2 and NH_3 production technologies using gas switching reforming (GSR) and membrane-assisted water-gas shift (MAWGS). In addition, dedicated power cycles can be added to these plants to produce power from the low-carbon hydrogen whenever demand is high and/or wind/solar power output is low.

2.3.2 Equation system

The target of this study is to seek the minimum total costs integrated with embodied energy supply and environmental impact cost in the energy system model by optimizing deployment and dispatch as follows:

• Deployment of electricity, hydrogen and ammonia generators ($\hat{g}$) and storage volume ($\hat{v}$) [26] as well as transmission capacity ($\hat{fr}$)

• Hourly electricity, hydrogen and ammonia generating, consuming, charging, and discharging (g) from each energy production technology [26]

1. Total system costs

Total system costs are described in Equation (52), in which the right side is constituted by sum of annualized capital costs and fixed operating and maintenance (O&M) costs for energy generators (i), and transmission and storage technologies (j), variable costs of all related generating technologies and time-steps (t), costs regarding ramping dispatchable electricity, hydrogen and ammonia generators, displayed in Equation (77) [26], as well as the cost of imported ammonia.

$$C = \sum_i c_i^{fix} \hat{g}_i + \sum_j c_j^{fix} \hat{v}_j + \sum_{t,i} c_i^{var} g_{t,i} + \sum_{t,i} c_{t,i}^{ramp} + c_{imp}^{NH_3} \tag{52}$$

The life cycle environmental impact cost (c^{LCI}) is integrated into the capital costs (c^{cap}), together with the total overnight cost (c^{TOC}) in Equation (53).

In order to adjust the cost with time-value, capital costs (c^{cap}) are firstly adapted by using an assumed construction time (λ_{cons}) of each technology and a discount rate (d) in equation (53). Then it is further adjusted to an annualized cost by using the lifetime (λ_{life}) of each technology and the discount rate (d), expressed in Equation (54) [26].

Fixed costs are composed of annualized capital costs ($c^{fix,cap}$), fixed O&M costs ($c^{fix,O\&M}$), and fixed transmission and storage cost ($c^{fix,T\&S}$), but removing the cost of the embodied energy of each technology as it is supplied by the energy system itself, describe in Equation (55).

$$c^{cap} = \frac{(c^{TOC} + c^{LCI}) * ((1+d)^{\lambda_{cons}} - 1)}{\lambda_{cons} * lg(1+d)} \tag{53}$$

$$c^{fix,cap} = \frac{c^{cap} * d * (1+d)^{\lambda_{life}}}{(1+d)^{\lambda_{life}} - 1} \tag{54}$$

$$c^{fix,AFC} = c^{fix,cap} + C^{fix,O\&M} + C^{fix,T\&S} - \sum_n C_n^{en} * E_n^{material,emb} \tag{55}$$

Variable costs include variable O&M cost, variable fuel cost, CO_2 emission cost and CO_2 storage cost but removing the sum of cost of embodied energy demand in operation of the dispachable electricity, hydrogen and ammonia generating technologies in Equation (56). The variable fuel cost is consisted of its internal cost on market and external cost of monetized impact in Equation (57).

$$C^{var} = C^{var,O\&M} + C^{var,fuel} + C^{var,CO_2} + C^{var,CO_2 storage} - \sum_n (C_n^{en} * E_n^{fuel,emb}) \tag{56}$$

$$C^{var,fuel} = C^{var,fuel,market} + C^{var,fuel,LCI} \tag{57}$$

2. Energy balances

Energy balances of electricity (Equation 58), hydrogen (Equation 59) and ammonia (Equation 60) are defined for every hour of the year [26].

$$\delta_t^{el} = \sum_i g_{t,i}^{el} \qquad \forall\, t \tag{58}$$

$$\delta_t^{H_2} = \sum_i g_{t,i}^{H_2} \qquad \forall\, t \tag{59}$$

$$\delta_t^{NH_3} = \sum_i g_{t,i}^{NH_3} \qquad \forall\, t \tag{60}$$

In detail, energy production contains positive parts and negative parts that all generating technologies are positive production, storage charge is negative production and discharge is positive production, as well as consumption from electrolyzers is negative generation for electricity and H_2-fired power plants is negative generation for hydrogen. In terms of NH3_H2 plants (consume ammonia to produce hydrogen), it is negative generation for ammonia but positive production for hydrogen. For H2_NH3 plant, it is opposite to NH3_H2 plants. The embodied energy consumption of all the material input and energy input of all the technologies in the system and indirect embodied energy consumption associated general economic activity required to construct and maintain the energy system are negative generation. Imported ammonia is another form of positive production.

The energy load (δ) in each time-step must be equal to the sum of all these energy production of positive and negative parts[26]. The detailed energy balances including generation, feedstock consumption, energy stored, energy import and embodied energy supply of electricity, hydrogen and ammonia are expressed in Equations (61)-(63) respectively.

$$\delta_t^{el} = \sum_i g_{t,i}^{el} * Lo^{el} + \sum_i (g_{t,i}^{H_2} / \eta_{gnH_2}^{fuel} * \eta_{gnH_2}^{el}) + \sum_i (g_{t,i}^{NH_3} / \eta_{gnNH_3}^{fuel} * \eta_{gnNH_3}^{el}) + E_t^{el,store} - E_t^{el,emb} \qquad \forall\, t \tag{61}$$

$$\delta_t^{H_2} = \sum_i g_{t,i}^{H_2} * Lo^{H_2} + E_t^{H_2,store} - \sum_i (g_{t,i,H2gn}^{el} / \eta_{H2gn}^{el}) - g_{t,h2h3}^{NH_3} / \eta_{h2h3}^{fuel} - E_t^{H_2,emb} \qquad \forall\, t \tag{62}$$

$$\delta_t^{NH_3} = \sum_i g_{t,i}^{NH_3} * Lo^{NH_3} + E_t^{NH_3,store} + E_t^{NH_3,import} - g_{t,h3H2}^{H_2} / \eta_{h3H2}^{fuel} - E_t^{NH_3,emb} \qquad \forall\, t \tag{63}$$

3. Constrains on energy generation

In terms of all generators, hourly generation has to be restricted to the maximum availability (a) of capacity for every hour of the year [26]. For dispatchable generating technologies a is 1, shown that the available capacity of advanced natural gas plants reaches 100% [104]. Profiles of hourly available capacity for wind and solar is investigated in section 2.1.1 based on literature data.

$$g_{t,i} \leq a_{t,i} \hat{g}_i \qquad \forall\, t, i, n \tag{64}$$

The capacity factor of an entire year for any generating technology cannot be beyond 0.9 due to the requirement for plant shutdown for regular maintenance [26].

$$\sum_t g_{t,i} \leq 0.9 * 8760 * \hat{g}_i \qquad \forall\, i \tag{65}$$

Furthermore, the operation of the GSR and MAWGS plants has some extra restrictions [26]. There is limited amount of power that is able to be generated through dedicated power cycles integrated to GSR and MAWGS blue H_2 plants by the limited available amount of hydrogen produced from those plants, expressed in Equation (66) and Equation (67) [26]. The indices of GSPpower and MAWGSpower indicate the combined and recuperated cycles designed for their blue hydrogen plant respectively, while the index of MAWGS indicates either the pure coal or mixed biomass and coal co-gasification options of solid fuels for blue hydrogen generation [26].

$$\frac{g_{t,GSRpower,CC}}{\eta_{GSRpower,CC}} + \frac{g_{t,GSRpower,RC}}{\eta_{GSRpower,RC}} \leq g^{H_2}_{t,GSR} \qquad \forall\ t \tag{66}$$

$$\frac{g_{t,MAWGSpower,CC}}{\eta_{MAWGSpower,CC}} + \frac{g_{t,MAWGSpower,RC}}{\eta_{MAWGSpower,RC}} \leq g^{H_2}_{t,MAWGS} \qquad \forall\ t \tag{67}$$

For wind, there is a maximum allowable ratio (ε) between onshore and offshore wind capacity, stated that onshore wind is slightly higher economical but stands more public rejection [26].

$$\hat{g}_{wind,on} \leq \varepsilon * \hat{g}_{wind,off} \tag{68}$$

Also, there is an imposed force (f_{vre}) in the system to deploy at least a specified fraction of variable renewable energy (VRE, wind and solar) as % of total generation [26].

$$\sum_{t,i} g^{vre}_{t,i} \geq f_{vre} * \sum_{i} g^{gen}_{t,i} \qquad \forall\ t \tag{69}$$

Then, Equation (50) displays that the green hydrogen generation by electrolysis from VRE technologies should never exceed the total generation from VRE, where $g_{t,vre}$ is the negative generation by electrolyzers due to its consumption of electricity [26].

$$\frac{-\sum_i g^{H_2}_{t,i,vre}}{\eta^{H_2}_{vre}} \leq \sum_{i} g^{vre}_{t,i} \qquad \forall\ t \tag{70}$$

In these equations, the initial setting of these parameters are ε = 2, f_{vre} = 0.7.

4. Energy storage

In terms of energy storage, the total volume of stored energy (v) can never be beyond the installed capacity of energy storage ($\hat{v}$). Regarding salt caverns for hydrogen storage, there is a limit that the stored volume cannot be beyond half of the installed capacity due to the requirement of remaining storage volumes between 30 and 80% [105].

$$v_{t,j,n} \leq \hat{v}_{j,n} \qquad \forall\ t, i, n \tag{71}$$

The change of stored energy over time is displayed in equation (72)-(75) for batteries, hydrogen and ammonia respectively. Each equation is restricted in order that the stored energy must be matched in the first and last timesteps of the year [26]. Equation (73) and Equation (74) describe the hydrogen storage process, in which g^{H_2} is the storage charge (negative) or discharge (positive) rate regarded as a hydrogen generator in the hydrogen energy balance Equation (59) and (62) [26]. For ammonia storage expressed in Equation (72), g^{NH_3} is an ammonia generating technology in ammonia energy balance Equation (60) and (63).

$$v_{t,bat} = v_{t-1,bat} - (g^{in}_{t,bat} + \frac{g^{out}_{t,bat}}{\eta_{bat}}) \qquad \forall t \tag{72}$$

$$v^{H_2}_{t,cavern} = v^{H_2}_{t-1,cavern} - g^{H_2}_{t,cavern} \qquad \forall\ t \tag{73}$$

$$v_{t,tank}^{H_2} = v_{t-1,tank}^{H_2} - g_{t,tank}^{H_2} \qquad \forall\, t \tag{74}$$

$$v_{t,tank}^{NH_3} = v_{t-1,tank}^{NH_3} - g_{t,tank}^{NH_3} \qquad \forall\, t \tag{75}$$

Regrading salt caverns, the requirement for increased transmission capacity of hydrogen ($\hat{g}_{salt}$) in order to get these distant geographically restricted locations and the daily limit on charge/discharge rate at 10% of capacity are described in Equation (76) and (77)[26].

$$abs(v_{t,carven} - v_{t-1,carven}) \leq \hat{g}_{carven} \qquad \forall\, t \tag{76}$$

$$\hat{g}_{carven} = \frac{0.1 * \hat{v}_{carven}}{24} \qquad \forall\, t \tag{77}$$

The detailed energy storage of electricity, hydrogen and ammonia expressed in Equation (78)-(80). Electricity storage are composed of battery discharge and charge, as well as electricity consumption in H_2 salt cavern discharge and H_2 tank charge, in which the electricity efficiency of cavern transmission ($\eta_{cavern,trans}^{el}$) and tank compressor ($\eta_{tank,comp}^{el}$) are negative. For Hydrogen storage includes discharge and charge of salt cavern and tank. Ammonia storage only contains discharge and charge of tank.

$$E_t^{el,store} = g_{t,bat}^{out} * \eta_{bat}^{el} - g_{t,bat}^{in} + g_t^{H_2,out} * \eta_{cavern,trans}^{el} + g_t^{H_2,in} * \eta_{tank,comp}^{el} \qquad \forall\, t \tag{78}$$

$$E_t^{H_2,store} = g_{t,cavern}^{H_2,out} - g_{t,cavern}^{H_2,in} + g_{t,tank}^{H_2,out} - g_{t,tank}^{H_2,in} \qquad \forall\, t \tag{79}$$

$$E_t^{H_2,store} = g_{t,tank}^{NH_3,out} - g_{t,tank}^{NH_3,in} \qquad \forall\, t \tag{80}$$

5. Embodied energy

For the embodied energy demand for electricity, hydrogen and ammonia, each type of energy contains an annualized fixed part ($E_i^{el,fix}$, $E_i^{H_2,fix}$, $E_i^{NH_3,fix}$) and variable parts in Equation (81)-(83). The fixed part is estimated in table 5 and 6 of the Appendix. The variable parts are composed of the total embodied energy of the energy feedstock for all power, hydrogen and ammonia generation.

$$E_t^{el,emb} = \sum_i (E_i^{el,fix} * \hat{g}_i)/8760 + \sum_i (E_{gn,i}^{el,var} * g_{t,i}) + \sum_i (E_{gnH2,i}^{el,var} * g_{t,i}^{H_2}) + \sum_i (E_{gnNH3,i}^{el,var} * g_{t,i}^{NH_3}) \qquad \forall\, t \tag{81}$$

$$E_t^{H_2,emb} = \sum_i (E_i^{H_2,fix} * \hat{g}_i)/8760 + \sum_i (E_{gn,i}^{H_2,var} * g_{t,i}) + \sum_i (E_{gnH2,i}^{H_2,var} * g_{t,i}^{H_2}) + \sum_i (E_{gnNH3,i}^{H_2,var} * g_{t,i}^{NH_3}) \qquad \forall\, t \tag{82}$$

$$E_t^{NH_3,emb} = \sum_i (E_i^{NH_3,fix} * \hat{g}_i)/8760 + \sum_i (E_{gn,i}^{NH_3,var} * g_{t,i}) + \sum_i (E_{gnH2,i}^{NH_3,var} * g_{t,i}^{H_2}) + \sum_i (E_{gnNH3,i}^{NH_3,var} * g_{t,i}^{NH_3}) \qquad \forall t \tag{83}$$

6. Energy transmission

For energy transmission, all electricity, hydrogen and ammonia needed to be transmitted cannot exceed the capacity of transmission line, hydrogen pipeline and ammonia pipeline. The total energy transmission is calculated at the average of total energy supply and total energy demand, as described in Equation (84)-(86). Total energy supply includes energy generated, stored or imported. Total energy demand is composed of load, embodied energy demand as well as the energy consumption (negative) or generated (positive) within different technologies.

$$\begin{aligned} 0.5 * [\delta_t^{el} - E_t^{el,store} - \sum_i (g_{t,i}^{H_2}/\eta_{gnH_2}^{fuel} * \eta_{gnH_2}^{el}) - \sum_i (g_{t,i}^{NH_3}/\eta_{gnNH_3}^{fuel} * \eta_{gnNH_3}^{el}) + E_t^{el,emb}] \\ + 0.5 * (\sum_i g_{t,i}^{el} + E_t^{el,store}) \leq \hat{tr}^{el} \qquad \forall t \end{aligned} \tag{84}$$

$$\begin{aligned} 0.5 * [\delta_t^{H_2} - E_t^{H_2,store} + g_{t,H2CC}/\eta_{H2CC}^{el} + g_{t,H2RC}/\eta_{H2RC}^{el} + g_{t,h2h3}^{NH_3}/\eta_{h2h3}^{fuel} + E_t^{H_2,emb}] \\ + 0.5 * (\sum_i g_{t,i}^{H_2} + E_t^{H_2,store}) \leq \hat{tr}^{H_2} \qquad \forall t \end{aligned} \tag{85}$$

$$\begin{aligned} 0.5 * (\delta_t^{NH_3} - E_t^{NH_3,store} + g_{t,h3H2}^{H_2}/\eta_{h3H2}^{fuel} + E_t^{NH_3,emb}) \\ + 0.5 * (\sum_i g_{t,i}^{NH_3} + E_t^{NH_3,store} + E_t^{NH_3,import}) \leq \hat{tr}^{NH_3} \qquad \forall t \end{aligned} \tag{86}$$

7. CO_2 emissions

Equation (87) describes the CO_2 emission coming from three type of technologies: dispatchable power, hydrogen and ammonia generators. σ^{CO_2} is CO_2 intense (kg/MWh) of different technologies.

$$E = \sum_i g_{t,i,con}^{el} * \sigma_{con}^{CO_2} + \sum_i g_{t,i,gnH_2}^{H_2} * \sigma_{gnH_2}^{CO_2} + \sum_i g_{t,i,gnNH_3}^{NH_3} * \sigma_{gnNH_3}^{CO_2} \qquad \forall t \tag{87}$$

8. Other constraints

Finally, several additional constrains can be applied in the model. One extra restriction is applied due to the limits of the ramping abilities of thermal power cycles and blue hydrogen production facilities [26]. The definition of the ramp rate (MW/hour) is expressed in Equation (88), which cannot exceed the achievable ramp rate as described in Equation (89) [26]. Also the frequent ramping leads to added costs, expressed in Equation (90) [26]. The parameters r = 75000 €/MW/h and ρ= 5% are derived based on data in Kumar's study on different fossil-fueled generators [106].

$$r_{t,i} = abs(g_{t,i} - g_{t-1,i}) \qquad \forall\, t, i \tag{88}$$

$$r_{t,i} \leq \frac{r}{c_i^{cap}} * \hat{g}_{t,i} \qquad \forall\, t \tag{89}$$

$$c_{t,i}^{ramp} = \rho * c_i^{cap} * r_{t,i} \qquad \forall\, t, i \tag{90}$$

Equation (91) sets up the constraint of annual biomass amount at 150 TWh/year that can be consumed by the coal/biomass co-gasification technologies due to the limited availability of plants, wood or agriculture residues on earth [26]. λ = 0.22 is the proportion of the fuel heating value which comes from biogenic origin.

$$\sum_{t,i_{bio}} \frac{g_{t,i_{bio}}^{fuel}}{\eta_{i_{bio}}} \lambda \leq \mu \qquad \forall\, t, i \tag{91}$$

2.3.3 Technology cost and performance assumptions and identifications

The summary of assumptions of main technologies applied in this project are presented in this section. Table 15 lists the key data of cost and performance parameters of various technologies of energy generation, storage and transmission. Table 16 lists the transmission costs and embodied energy demand for extra VRE transmission and gases pipelines. All the numbers are chosen to be representative towards the year 2050.

In table 15, capital cost, LC impact cost, operation & maintenance cost, construction/lifetime, energy efficiencies and CO_2 avoidance of various technologies are identified. Two efficiencies are specified for various technologies: an electric efficiency (η^{el}) that indicates the ratio of produced electricity to the fed fuel in low heat value (LHV) and a fuel production efficiency (η^{fuel}) that indicates the ratio of produced H_2 or NH_3 LHV to fed fuel LHV [26]. The former ratio is negative for some plants where electricity is consumed [26].

In terms of total overnight cost (TOC) of various generating technologies, nuclear is the most expensive one due to the high consumption of human activities involved behind; both NH3_Selexol and NH3_MAWGS are at the second high level with around half investment of nuclear; onshore and offshore wind power has the similar cost as NGCC_CCS. The integrated power cycles (MAWGS_CC, GSR_CC, MAWGS_RC, and GSR_RC) are cheaper and with higher efficiency than selfstanding power cycles due to the advantages of integration [26]. For energy storage and transmission technologies, specially the power-related cost of salt caverns and hydrogen increases from additional H_2 pipelines needed to connect geographically restricted cavern sites with the main transmission line and extra H_2 compressors [26]. Negative electric efficiencies are also employed to indicate the power consumption needed higher volume of storing hydrogen being over-pressurized in the storage facility than needed [26]. It is worth mentioning that practical utilization can only apply half of the storage capacity of salt cavern, which actually doubles the cost [105].

Regarding the LCI cost calculated based on the geometric mean of MVCs in table 13, the observation shows that the LCI costs of dispatchable technologies are lower than VRE technologies, at 6-8% of TOC. While on/off shore wind and solar take 13%/16% and 29% of ToC respectively. For the hydrogen and ammonia production technologies, LCI cost of electrolyzers with both VRE and nuclear take 22% of TOC, the other technologies take 8%. For hydrogen transmission and storage technologies, LCI cost of pipelines and tanks take 24-32% of TOC, batteries take 18% and electricity transmission lines take 8%. It is noticeable that the LCI cost is very sensitive with the monetary valuation coefficients. Also it has not completely covered the impact of foreground system such as emission from combustion in the operation of fossil power and it is estimated under the concept that all the embodied energy is supplied by electricity, hydrogen and ammonia produced in the energy system itself.

CO_2 intensity represents the CO_2 emission intensity of various technologies in operation phase, combined the CO_2 intensity of fuels (use phase in power plant) in table 17 and the CO_2eq intensity of fuel supply (life cycle of fuel market). CO_2 avoidance represents the percentage of CO_2 avoided in the operation phase due to CCS.

Technology	**TOC**	**Construction**	**Lifetime**	**LCI cost**	**El efficiency**	**Fuel efficiency**	**Fix O&M**	**Var O&M**	CO_2 **intensity**	CO_2 **avoid**	**Ref.**
unit	€/kW	years	years	€/kW	Wel/Win, %	Wfuel/Win,%	% TOC/yr	€/MWh	kg/MWh	%	
Nuclear	4,091	5	50	285	33.0	-	2.5	2.0	-	-	-
NGCC_CCS	1,234	3	40	105	54.5	-	2.6	1.9	33	91.2	[26]
NGCC	716	2	40	61	62.2	-	2.6	0.6	330	-	[26]
H2CC	716	2	40	61	63.3	-	2.6	0.6	-	-	[26]
NGRC	460	1	30	39	54.8	-	2.6	-	374	-	[26]
H2RC	460	1	30	39	55.8	-	2.6	-	-	-	[26]
MAWGS_CC	618	2	40	53	69.2	-	2.6	0.3	-	-	[26]
GSR_CC	677	2	40	58	65.2	-	2.5	0.6	-	-	[26]
MAWGS_RC	359	1	30	31	58.3	-	2.6	-	-	-	[26]
GSR_RC	412	1	30	35	56.5	-	2.5	-	-	-	[26]
Wind_on	1,282	2	25	172	100.0	-	2.0	-	-	-	[107]
Wind_off	1,200	3	25	205	100.0	-	2.0	-	-	-	[108]
Solar	327	2	25	100	100.0	-	1.5	-	-	-	[107]
H2_Selexol	1,392	4	40	118	-	59.4	3.1	1.8	-96	93.8	[26]
H2_MAWGS	1,078	4	40	92	-4.0	73.3	3.2	2.9	-107	100.0	[26]
H2_SMR	590	3	40	50	-1.0	74.8	3.9	1.6	34	87.6	[26]
H2_GSR	490	3	40	42	-6.9	92.5	3.8	1.0	9	95.9	[26]
NH3_Selexol	2,441	4	40	208	-0.3	50.9	3.2	1.9	-106	92.9	-
NH3,mAWGS	2,017	4	40	172	-2.5	62.3	3.2	2.9	-126	100.0	-
NH3_KBR	1,345	3	40	114	-0.1	65.5	3.8	0.5	54	82.8	-
NH3_GSR	1,011	3	40	86	-9.1	81.6	3.8	0.8	14	94.4	-
WE_VRE	344	1	25	86	-100.0	70.0	2.0	2.0	-	-	[109]
WE_nuclear	344	1	25	86	-100.0	70.0	2.0	2.0	-	-	[109]
H2_NH3	643	3	40	55	-2.6	87.3	2.0	-	-	-	[109]
NH3_H2	473	2	25	40	-4.5	99.0	4.0	-	-	-	[109]
Battery_vol	98	1	20	21	-	-	3.0	-	-	-	[109]
Battery_pow	98	1	20	21	90.0	-	10.0	-	-	-	[109]
H2_cavern	1	2	25	0	-	-	2.5	-	-	-	[105]
H2_tank	15	1	25	5	-	-	2.5	-	-	-	[105]
Cavern_trans	100	2	25	24	-1.5	-	5.0	-	-	-	[110]
Tank_comp	120	1	25	10	-2.0	-	2.5	-	-	-	[110]
Transmission	600	4	40	57	-	-	3.5	-	-	-	-
H2_pipeline	300	2	40	71	-	-	3.5	-	-	-	[109]
NH3_tank	1	2	25	0	-	-	2.5	-	-	-	-
NH3_pipeline	150	2	40	35	-	-	3.5	-	-	-	-

Table 15: Summary of technology assumptions for energy generation, transmission and storage, €2019

Table 16 shows the transmission costs including total overnight cost (TOC), LCI cost, total cost (CAPEX), operation (OPEX) and annualized fixed cost (AFC) for extra VRE transmission because of the branch transmission line needed to connect VRE sites to the main transmission centre, as well as natural gas, hydrogen, and CO_2 pipelines.

Natural gas transmission costs are identified with the assumption of a levelized natural gas cost at 2 €/GJ when the transmission facility is applied at a 40% capacity factor [26]. The price of large-scale hydrogen pipelines is around 1 €/kW/km [109], indicating that the assumption of TOC 150 €/kW in this study equivalents to around 150 km of pipeline [26]. The assumption of CO_2 transport and storage facilities is 150 €/tpa with an extra 5 €/ton of variable costs based on IEAGHG reports [111][112]. The cost of CO_2 emission from operation phase is set the same value as the monetized impact cost of climate change for the consistency. Imported ammonia price is selected at 500 €/GJ where the reason of setting so high price is to avoid its disturbance to energy system at this first stage of optimization. It is noted that Offshore wind transmission is set to higher cost due to its more highly restricted by geographical condition than onshore wind and solar PV [26]. Electrolysis is assigned negative cost because of the avoidance of this additional transmission by co-site with wind and solar infrastructures [26]. Although part of this avoided cost is balanced by the replacement of hydrogen pipeline, electrolyzers still provide a net benefit of energy transmission into the energy system [26].

In terms of LCI cost, offshore wind is the highest one by around 3 times of onshore wind and 5 times of solar. This also matches its highest embodied energy. The LCI costs of these VRE transmission and gases transmission take 15% and 14% of their TOC respectively.

VRE & Gases	**TOC**	**LCI cost**	**CAPEX**	**Lifetime**	**OPEX**	**AFC**	**Electricity**	**Gas**	**Liquids**
unit	€/kW	€/kW	€/kW	years	%CAPEX/yr	€/kWa	Mwh/kWa	Mwh/kWa	Mwh/kWa
Extra transmission									
Onshore wind	300 [113]	46.2	346.2	40	3.5	38.1	1.17E-02	1.04E-02	9.31E-03
Offshore wind	1000 [113]	154.2	1154.2	40	3.5	127.0	3.89E-02	3.47E-02	3.10E-02
Solar	200 [113]	30.8	230.8	40	3.5	25.4	7.78E-03	6.93E-03	6.21E-03
Electrolysis electricity	-300	-46.2	-346.2	40	3.5	-38.1	-1.17E-02	-1.04E-02	-9.31E-03
Gases transmission									
Natural gas	100	13.6	113.6	40	5	14.2	5.73E-03	1.25E-02	4.67E-03
Hydrogen	150 [109]	20.3	170.3	25	5	23.1	9.84E-03	2.15E-02	8.02E-03
CO_2 (€/(t/year))	150 [111] [112]	20.3	170.3	40	3	17.9	8.60E-03	1.88E-02	7.01E-03

Table 16: Cost and embodied energy of extra VRE transmission and gases transmission, €2019

Table 17 displays the price and CO_2 intensity assumptions of natural gas, coal, Uranium and biomass. The internalized price represents the physical price of fuel, while the externalized price represents its life cycle impact cost. The reduced externalized price is adjusted by reducing the fossil resource depletion of natural gas to 50% of mean value, Coals & Uranium depletion to 20% of natural gas depletion. Such assumptions are based on the facts of their different relative abundance that the remaining natural gas resource is only left for about a century while coal and Uranium are left for about a millennium, as listed in Table 18. Furthermore, the monetary valuation method of fossil resource depletion applied is market price, which is far higher and covering other categories of monetized impact. It is notable that even the fossil depletion impact reduced for natural gas, coal and Uranium, their externalized prices are still significantly high at 70%, 170% and 180% of their internalized price respectively. CO_2 intensity represents the CO_2 emission intensity of various fuels in process of power generation.

Fuel	**Internalized price**	**Externalized price**	**Reduced externalized price**	**Total price**	**CO_2 intensity**
unit	€/GJ	€/GJ	€/GJ	€/GJ	kg/GJ
Natural gas	6.0	8.08	4.5	10.5	57
Coal	1.9	10.1	3.2	5.2	96.4
nuclear	1.0	7.9	1.8	2.8	-
biomass	7.0	3.1	3.1	11.6	100

Table 17: Cost and CO_2 intensity assumptions of fuels, €2019

Fuel	Oil	Gas	Coal	Uranium
Unit	billion barrels	trillion m3	billion tons	thousand tons
Resources	6192	806	20803	13684
Consumption	33.9	4.1	5.8	54.0
R/C ratio	183	194	3571	253

Table 18: The resources and consumption of fuels

2.4 Uncertainty quantification analysis

The uncertainty quantification analysis is based on Monte Carlo simulation with Latin Hypercube sampling for 1000 trials. Variation of the 12 life cycle impact (LCI) categories between their minimum and maximum values (five outliers are removed from the data that were more than an order of magnitude from any other point). The trials are arranged according to a skewed log-normal distribution with 99% of cases between the minimum and maximum value of the MCV and the median at the geometric mean of all the cases. Figure 13 is an example of a histogram of the distribution of climate change MVCs, where the geometric mean was 83.2 €/ton, the minimum value was 7.5 €/ton, and the maximum value was 685.0 €/ton.

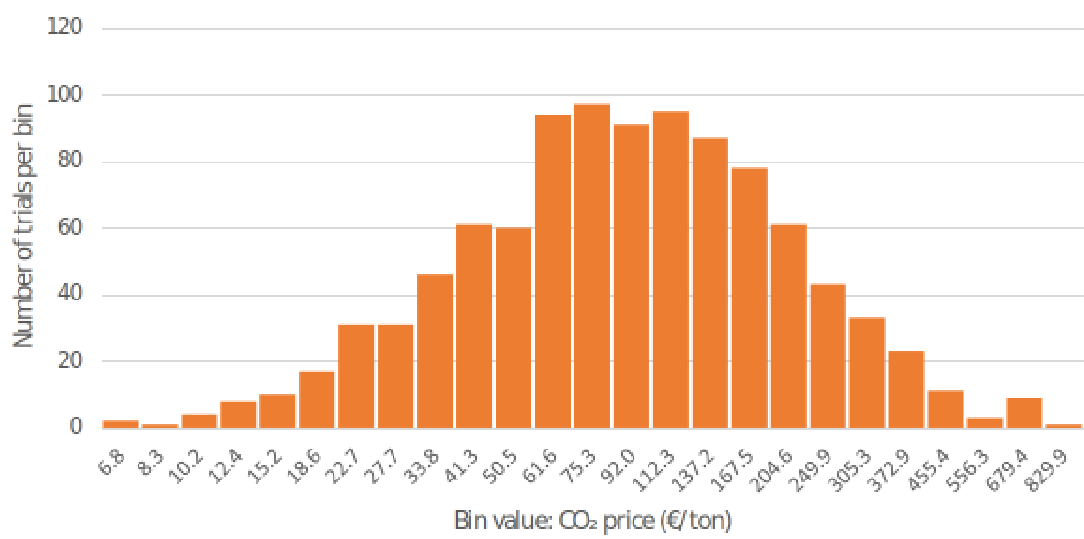

Figure 13: Histogram showing the distribution of the 1000 Monte Carlo trials for the climate change MVC

The data is processed in three ways:

1) Histograms of the market shares of different technology groups;

2) Linear regression to isolate effects of varying individual MVCs on the total system cost and technology distribution;

3) A simple correlation matrix identifying the strength and direction of correlations between all the parameters in the analysis.

3 Results and Discussion

3.1 Total cost of fuels and technologies

These results are compiled using the geometric mean of all MVCs. Different assumptions for the MVCs can cause large changes to all the figures in this subsection.

The total cost of primary fuels including natural gas, petrol, coal, uranium and biomass consists of internalized, externalized and extra penalty cost towards 2050, presented in Figure 14. Petrol has the highest total cost at 37.6 €/GJ, Uranium has the lowest cost at 2.1 €/GJ. The internalized cost is the assumed future economic price based on the law of historical development applying fossil fuel as the embodied energy input without considering environmental impact cost. Petrol, biomass and natural gas have relatively higher internalized price compared with coal and uranium. The extra penalty is considered the energy security factor due to the dependence on imports of fossil fuels. The life cycle impact (LCI) cost includes direct and indirect impact cost. The direct climate impact cost (CO_2 emissions from fuel combustion) is significant in coal, petrol and natural gas, taking 50%, 16.6%, 22.2% of their total cost respectively. While biomass has notable Land Use cost, contributing 36.7%. Fossil depletion cost is considered a few factors including discount rate and increase in the rate of use. Both direct and indirect energy cost refer to the difference between the future clean energy input cost calculated by the energy system modelling including LCI cost and the base line of the fossil fuel cost included in the internalized price.

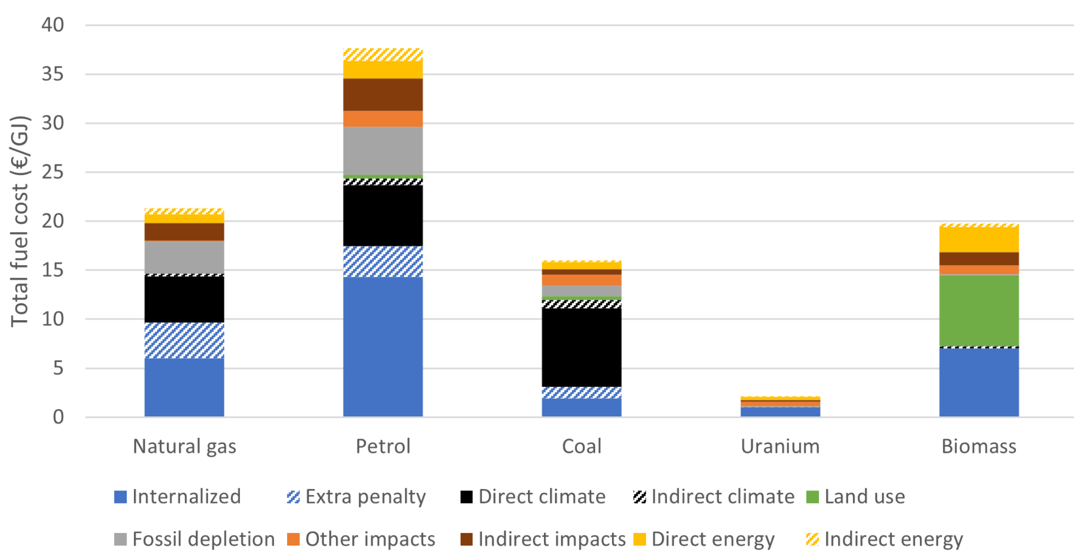

Figure 14: Total cost of Primary fuels

Figure 15 displays that the total cost of final fuels including conventional fossil fuels (natural gas and petrol) and clean fuels (blue hydrogen and blue ammonia made from natural gas or solid fuels) is comprised of internalized, LCI and energy cost in different phases of capital, connection and operation towards 2050. Overall, natural gas has lower total cost than blue hydrogen by 23-27%, while petrol has higher total cost than ammonia by 8-11%. Both blue hydrogen and ammonia made from natural gas is 3% more expensive than those made from solid fuels (70% coal and 30% biomass) respectively. Among different categories of LCI, direct CO_2 emissions is presented separately due to its strong traits in the production of fossil fuels and clean fuels. Natural gas and petrol have remarkable direct CO_2 emissions at 4.7 €/GJ and 6.2 €/GJ respectively. While blue hydrogen and ammonia from solid fuels have negative CO_2 emission cost at -2.5 €/GJ and -2.9 €/GJ respectively due to biomass CCS, which contributes a lower total cost than gas-made hydrogen and ammonia. Among the energy input, electricity is also displayed alone due to its significance in the production of hydrogen and ammonia. Blue hydrogen and ammonia made from solid fuels have lower primary fuels and electricity cost but higher internalized cost than blue hydrogen and ammonia made from natural gas respectively. Plants processing solid fuels are generally more capital and maintenance intensive than plants processing natural gas. In addition, they produce large quantities of captured CO_2, leading to significant connection costs for CO_2 transport and storage.

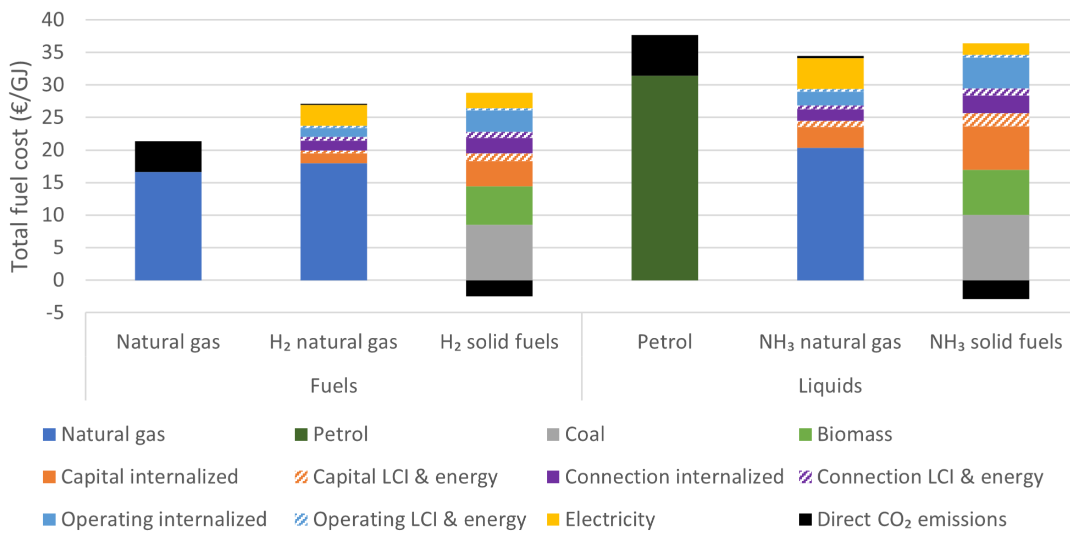

Figure 15: Total cost of final fuels

Figure 16 exhibits that the total cost of power generation technologies consists of primary fuel, internalized, LCI and energy in different phases of capital, connection and operation. In general, among the typical four technologies of onshore wind, solar PV, nuclear and NGCC with the renewable resource profile in Germany, solar has the lowest total cost at 87.5 €/MWh and NGCC has the highest total cost at 165.2 €/MWh. In order to consider the energy security factor, penalty cost is added on nuclear power due to the local people's opposition. The total original cost of nuclear (93.9 €/MWh) is lower than onshore wind (124.1 €/MWh), but it exceeds wind after considering penalty. Capital internalized cost is significant for wind, solar and nuclear, accounting for 35.4%, 27.7% and 34% respectively. Considering the resource of wind and solar is mostly located in the northern part while the industries located in the south of Germany, connection internalized cost of wind and solar is relatively high. While fuel is the largest share for NGCC total cost at 58%. In terms of LCI cost, Land Use cost is notable for wind and solar at 28% and 7.5%, while direct CO_2 emissions is significant for NGCC at 16.6%.

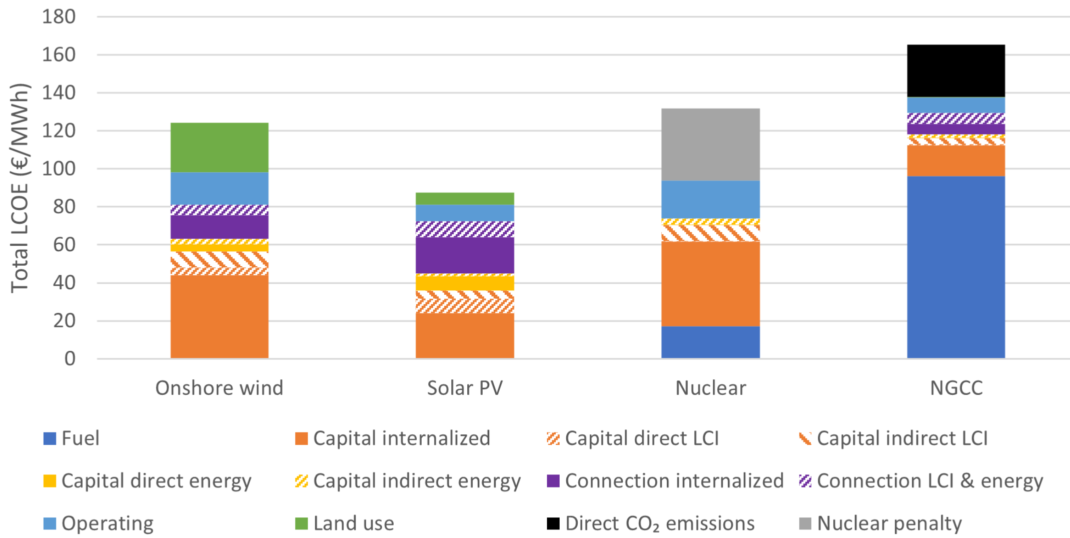

Figure 16: Total cost of power generation technologies

3.2 Total system cost within five scenarios

This section presents the general comparisons of electricity generation, fuel production and total system cost under two conditions of considering between only direct CO_2 emissions and full life cycle impacts assessment within five scenarios which is listed in table 19 and described in detail in section 2.3.1. Several parameters are specified as the base settings in the model that the energy economic efficiency is assigned at 1000 €/MWh, and the monetized environmental impact averaging values of various technologies and fuels are applied the geometric mean.

S1	S2	S3	S4	S5
No CCS or nuclear	No nuclear	No CCS	No advanced CCS	All technologies

Table 19: Five scenarios designed for the energy system model

3.2.1 Conventional fossil fuels permitted in the system

Figure 17-19 displays the electricity mix generation, fuels production and the total system cost when both conventional fuels (natural gas and petrol) and clean fuels (hydrogen and ammonia) are available in the energy system.

Firstly, in the electricity mix shown in Figure 17, when only direct CO_2 is considered, renewables combining with unabated (CCS) thermal power for balancing take the dominant position. While with full LCA, the optimal solution is to displace natural gas, coal-derived H_2, and renewables with nuclear in S3-S5, which has a low total environmental footprint. This result partly agrees with the findings from a study of LCA on environmental trade-offs of low-carbon electricity mix by Gibon and colleagues that both renewable and nuclear power cause a decrease of a wide range of environmental impacts [2]. But the result of electricity generation with CCS is driven out of the energy system under full LCA, which matches Gibon's conclusion that CCS causes increased non-GHG impacts [2]. Under only direct CO_2 considered, there are some notable amounts of negative electricity generation consumed by fuel production in S2 and S5 due to a large amount of blue fuels production when advanced CCS available.

Secondly, the level of CO_2 emission in the operation phase related with fossil fuel utilization is directly connected with the power generation from unabated (without CCS) thermal power plants (NGCC). S1 relies more on wind and solar backed up by natural gas power, which involves considerable CO_2 emissions. It is notable that the CO_2 emission is significant at around 400 Mton/year in S1, then gradually drops to 67 Mton/year in S5 under full LCA. While in S2 and S5 when only direct CO_2 considered, the CO_2 emission gains avoidance at -125 Mton/year due to the biomass with CCS. This is because cases allowing advanced CCS displace NGCC with coal/biomass-derived H_2, but the environmental footprint of coal and biomass drives this option out in the full LCA.

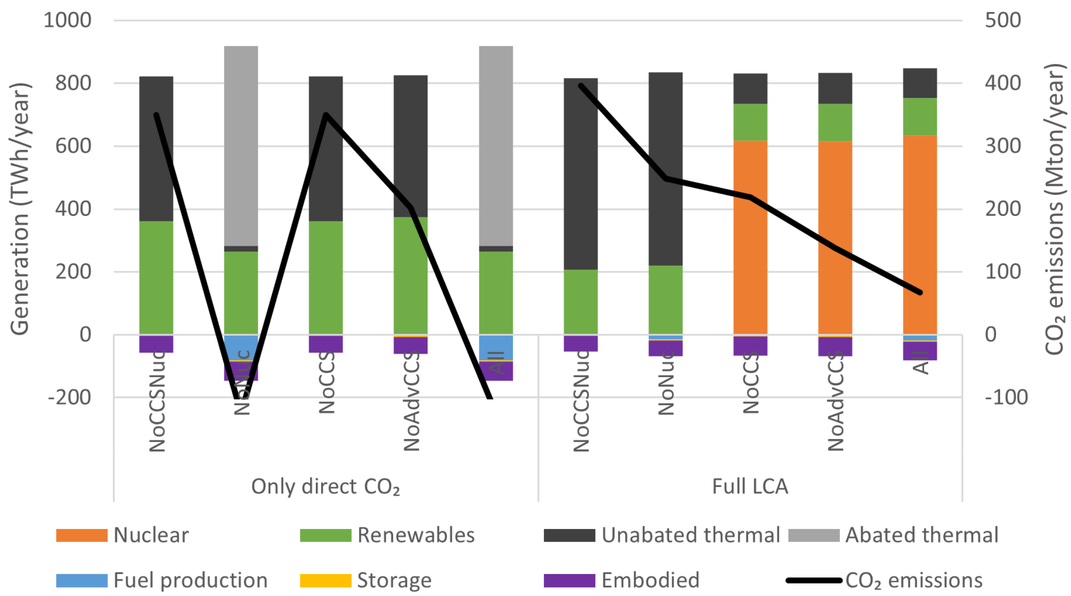

Figure 17: Electricity generation of energy system applying renewable resource in Germany with conventional fuels permitted

In the fuel production displayed in Figure 18, when only direct CO_2 emission is considered, blue fuels made from coal/biomass takes a large share in S2 and S5 with advanced CCS available. While around 80% of the blue H_2 are consumed to generate power (negative) with the advantage of negative CO_2 emission. When completing full LCA, blue H_2 is displaced by natural gas which has a lower environmental footprint than solid fuels in full LCA. Blue NH_3 displaces petrol when CCS technologies are available, otherwise only direct natural gas and petrol are used. This is because the total cost of blue NH_3 is lower than petrol but blue H_2 is more expensive than natural gas shown in Figure 18.

In the energy system, imported fuels including natural gas, petrol and ammonia is considered due to the large difference of the availability and production cost between the local and the rich-resourced location such as Saudi Arabia. When only CO_2 emission considered, in S1 and S3 without CCS technologies, the import share is reaching 100%, otherwise the import share decreases to 13% and 54% in the scenarios with advanced CCS available (S2 and S5) and without advanced CCS (S4). With full LCA, the import share decreases to 52% and 54% in the scenarios with advanced CCS available (S2 and S5), while it keeps at 100% in S4.

The level of import fuel share depends the combinations of different types of technologies and the type of fuel production in each scenario. If the technologies using coal/biomass as primary energy input to generate electricity or produce fuels, the import fuel is low as coal/biomass are assumed to be produced locally. While natural gas is imported to generate electricity or produce blue hydrogen/ammonia, or natural gas/petrol/ammonia is directly imported as final fuels, the level of import fuel share will be increased.

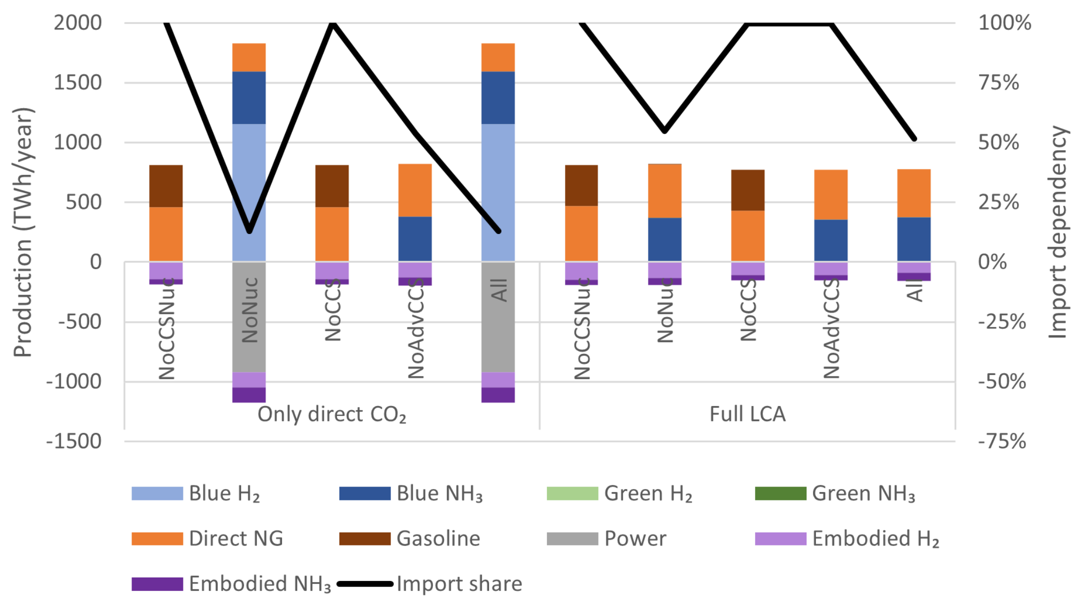

Figure 18: Fuel production of energy system applying renewable resource in Germany with conventional fuels permitted

In terms of the total system cost indicated in Figure 19, completing the full LCA rather than just direct CO_2 emissions increases system costs by about 50%. Total system costs in the different scenarios are similar because the trade-offs between the different technologies are quite close, with slight difference between the lowest total system cost at 178 G€/year in S5 and the highest one at 190 G€/year in S1. In scenario 2 and 5 with advanced CCS technologies available when only direct CO_2 considered, there are 65 G€/year internal cost (negative) due to the blue fuels consumption to generate electricity.

For the energy price in the system, electricity is the most expensive but gas fuel (natural gas or hydrogen) is the lowest, liquid fuel (gasoline or ammonia) is in the middle. The energy price with full LCA is higher compared with the price with only direct CO_2 emission considered. While there is no significant difference in electricity and gas fuel price in S1-S5 respectively. In S5 with full LCA, the price of electricity, gas fuel and liquid fuel is 155 €/MWh, 85 €/MWh and 123 €/MWh respectively. These costs are considerably higher than historical values because of all the externalities that are monetized in the model.

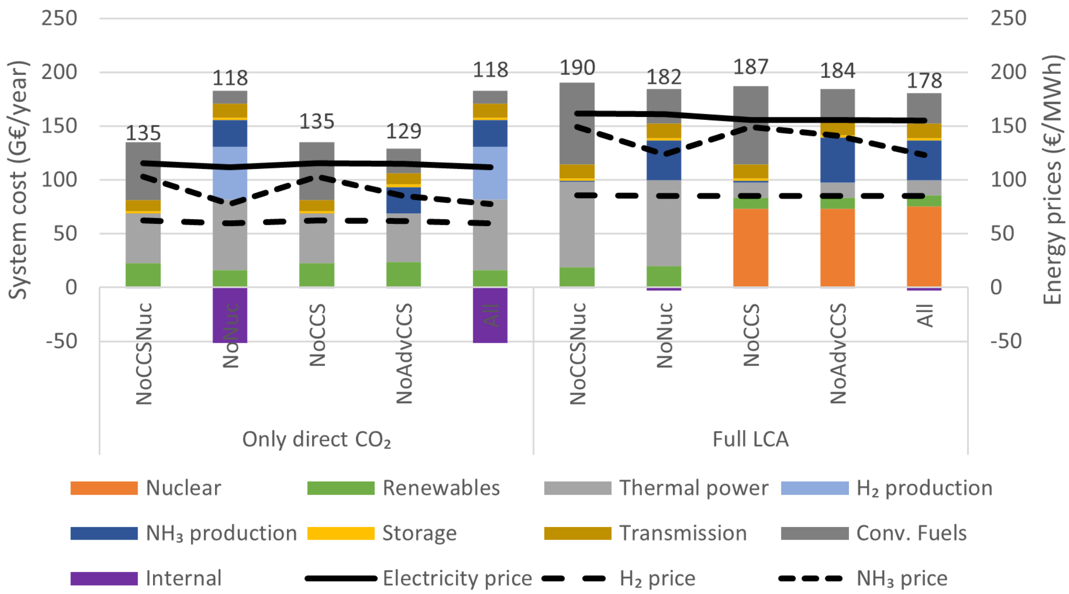

Figure 19: Total system cost of energy system applying renewable resource in Germany with conventional fuels permitted

3.2.2 Only clean fuels permitted in the system

Figure 20-22 presents the electricity generation, fuels production and the total system cost when only clean fuels are permitted as the final fuels in the energy system.

In the electricity generation shown in Figure 20, there are no large differences of the electricity mix profiles between under the conditions of conventional fuels permitted in Figure 20 in section 3.2.1 and only clean fuels permitted here. But when no direct use of natural gas and petrol is permitted, there are some more electricity generation (negative) consumed by blue fuel production.

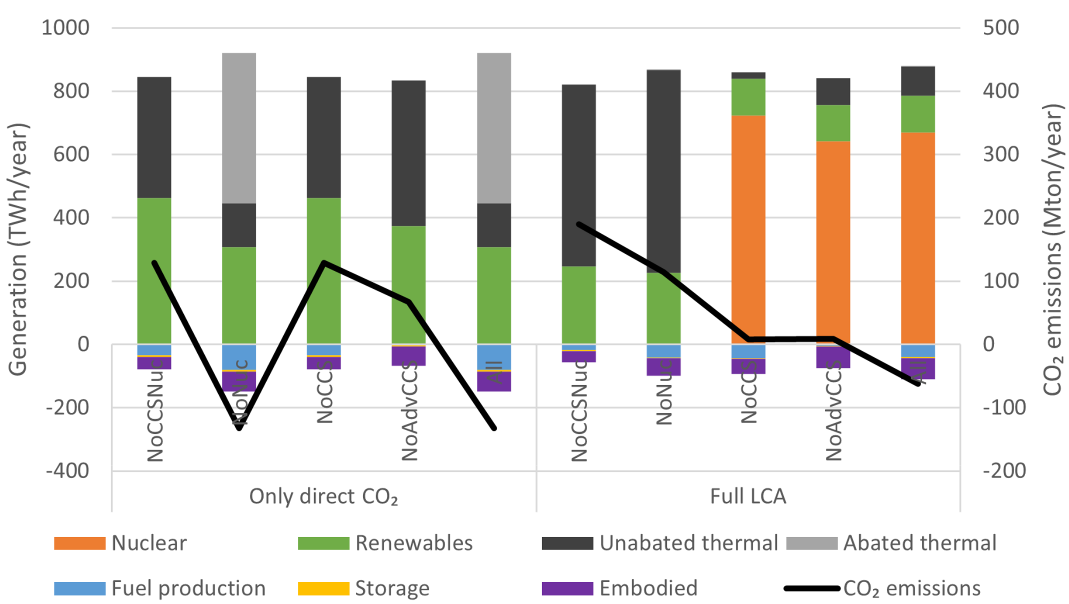

Figure 20: Electricity generation of energy system applying renewable resource in Germany with only clean fuels permitted

Since direct use of natural gas and petrol are disabled, CO_2 emission decreases significantly in all scenarios compared with conventional fuels permitted in the system in Figure 20. For instance, with full LCA, the CO_2 emissions drop 52% in S1 and even drop to -63 Mton/year in S5 due to lower or negative CO_2 emissions in clean fuel production compared to direct use of fossil fuels.

In fuel production displaced in Figure 21, only hydrogen and ammonia are allowed to be directly used as final fuels while natural gas and petrol are excluded in the system.

Green hydrogen and ammonia are produced by electricity from renewables or nuclear power in scenarios without CCS technologies available. While blue fuels displace green fuels in the scenarios with CCS due to the lower cost. There might be two main reasons: Firstly, blue hydrogen is produced directly from fossil fuels by chemical reaction with higher energy efficiency, while green hydrogen is produced through two processes of energy conversion from renewable/nuclear to electricity then from electricity to hydrogen by electrolysis. Secondly, green hydrogen production requires a large scale of additional capacity of renewable/nuclear[17], which is very expensive due to their increased investment, embodied energy consumption and impact cost. As a result, green hydrogen with resource in Germany is much costly then blue fuels from fossil fuels. This effect is intensified because a most of the embodied energy in new energy is required in the form of fuels. Hermesmann and Müller conducted a comprehensive comparison within LCA on green (from wind power in Germany) and blue hydrogen (from natural gas steam reforming, SMR+CCS) production, where green hydrogen has much low climate impact and fosil depletion but higher ecotoxicity, human toxicity, land use and water use compared with blue hydrogen [5]. However, without aggregating different categories of impact of these two technologies, it is difficult to achieve quantitative comparison.

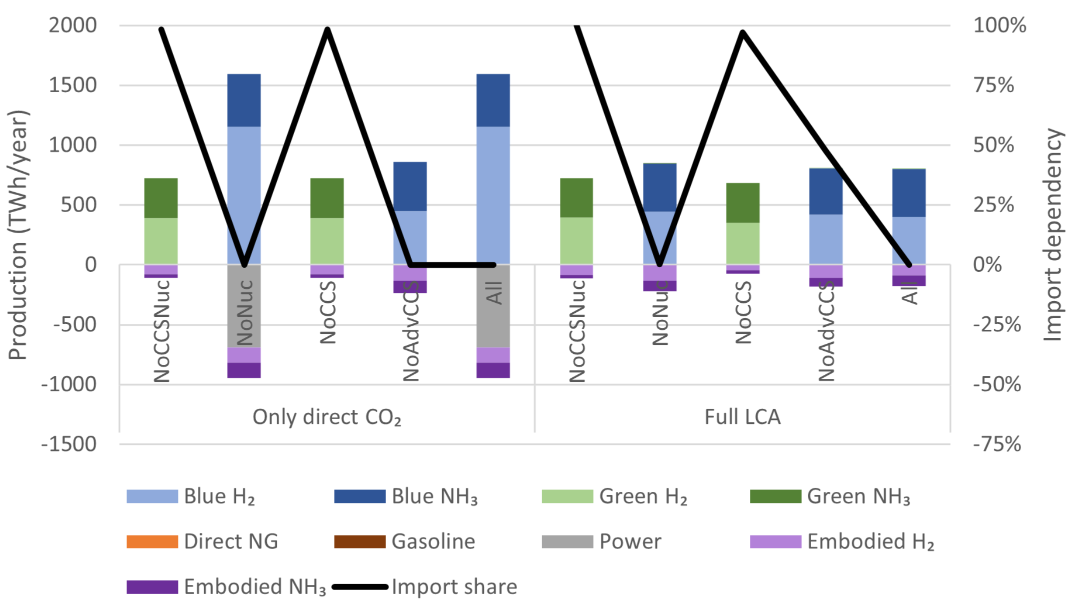

Figure 21: Fuel production of energy system applying renewable resource in Germany with only clean fuels available

In scenarios without CCS, the expensive green fuel production is the only option. The import fuel share nearly reaches 100% because the local green fuel production in Germany is much higher cost than the production in resource-rich location. The price of imported green ammonia from Saudi Arabia is set at 42.6 €/GJ derived from the techno-economic assessment of green ammonia as energy carriers in a low-carbon future and augmented with the LCI costs assessed in the present work [114]. In scenarios with advanced CCS, the import fuel share is 0% due to the blue hydrogen production from coal/biomass locally. Scenario without advanced CCS has a middle level of import share around 48% because of partly natural gas imported for blue hydrogen production.

Figure 22 exhibits the total system costs with only clean fuels permitted. The scenarios with CCS are similar to those with conventional fuels permitted in section 3.2.1, indicating that blue ammonia and hydrogen from fossil fuels is almost competitive with natural gas and petrol when all externalities are accounted for in full LCA. However, the total cost of scenarios without CCS doubles due to the high cost of producing large quantities of green fuels even imported from resource-rich location. With full LCA cost, the lowest total system cost is 184 G€/year in S5 and the highest one is 230 G€/year in S1. It is notable that there are significant internal cost in the scenarios without CCS due to the electricity consumed in the green fuels production.

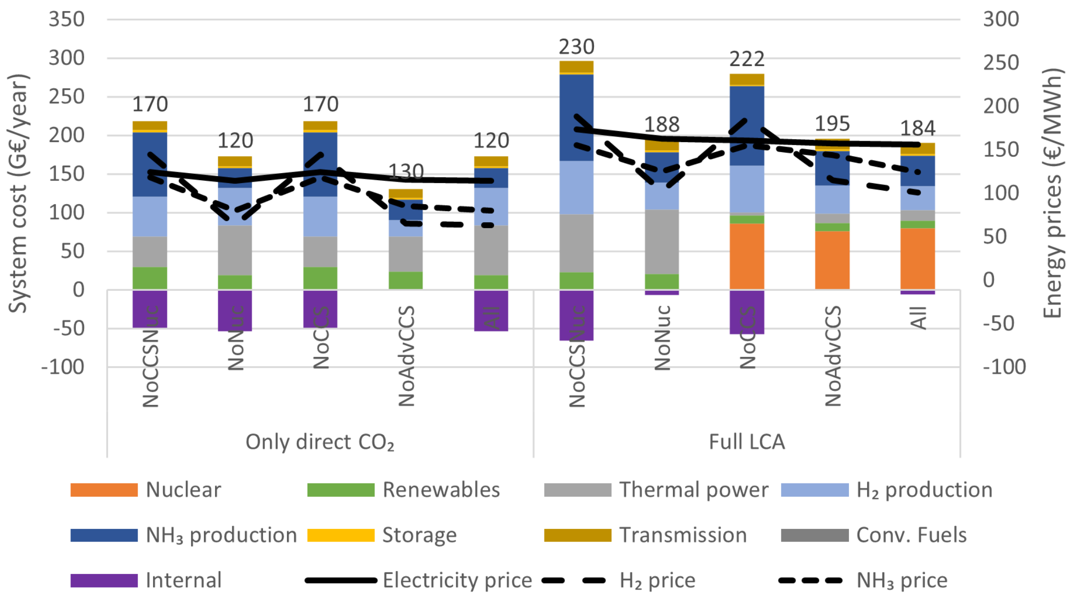

Figure 22: Total system cost of energy system applying renewable resource in Germany only with clean fuels available

In terms of the price of electricity and fuels, the hydrogen's price exceeds the ammonia's and the electricity's price in the scenarios without CCS because green hydrogen is produced from imported ammonia by adding one more process and extra cost. Otherwise, blue hydrogen is the cheapest compared with blue ammonia and electricity. In S5 with full LCA, the price of electricity, gas fuel and liquid fuel is 156 €/MWh, 100 €/MWh and 124 €/MWh respectively, with no big difference from the price of conventional fuels shown in Figure 22.

3.3 Comparison within nuclear penalty scenarios

Five scenarios are designed for the different levels of nuclear penalty from 0% to 80% in table 20 in order to investigate how much penalty added on the nuclear power (representative of the socio-political challenges facing nuclear deployment) will drive it out of the system. This comparison is conducted under the condition of S5 all technologies available with full LCA and the same parameters setting of LCI cost averaging method, economic efficiency and fossil depletion adjustment as in section 3.2.1.

SN1	SN2	SN3	SN4	SN5
0%	20%	40%	60%	80%

Table 20: Five scenarios designed for the different levels of nuclear penalty

Figure 23 shows the electricity generation in scenarios of nuclear penalty. In S1 without the nuclear penalty, it is optimal to generate essentially all power with nuclear due to its low cost of full life cycle environmental footprint. As nuclear gets more expensive, it gradually loses market share. Then there is a sudden drop from 60% to 80% penalty as the combination of renewables and natural gas (VRE+NGCC) becomes more economical. It is notable that with the growing share of VRE+NGCC, the share of NGCC rises faster than renewables because it replaces nuclear for balancing the renewables.

The amount of negative electricity consumed by fuel production gradually decreases due to the green hydrogen production. When NGCC is very limited in the electricity system, electrolysis is used to assist in power system balancing by consuming electricity when it is available in excess.

For the direct CO_2 emission, it gradually increases from 0% to 60% then soars from 60% to 80%, which directly connected with the share of unabated thermal (without CCS).

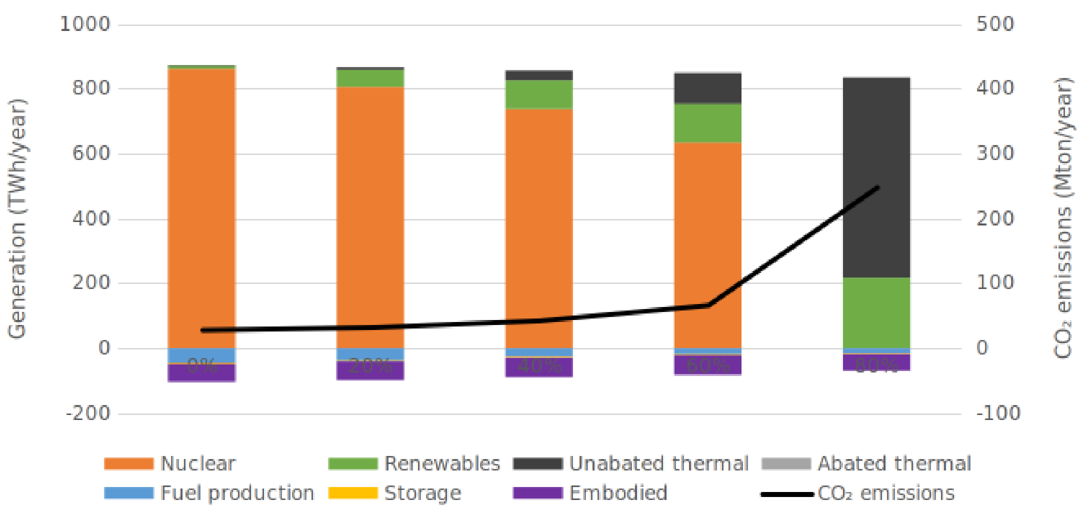

Figure 23: Electricity generation of energy system within nuclear penalty

In terms of fuel production shown in Figure 24, natural gas and blue ammonia take the dominant position with small share of green hydrogen in SN1-SN3 due to the surplus high capacity of nuclear power. The embodied gas fuel in SN5 with 80% nuclear penalty is almost doubles of that in SN1 with 0%. This is because the renewables require much high materials demand than nuclear, which causes higher embodied energy demand.

The import share is slightly climbing from 48%-54% due to the growing embodied fuel demand in the system.

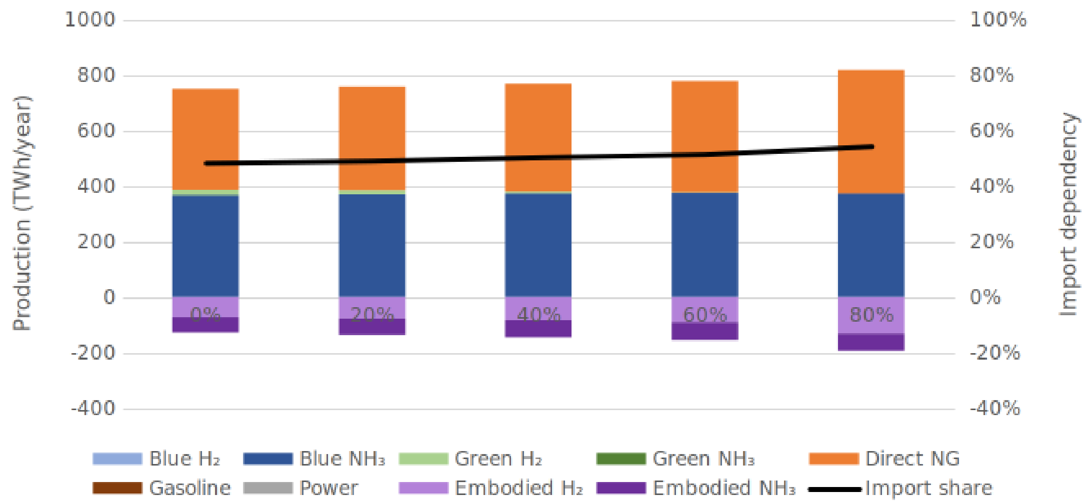

Figure 24: Fuel production of energy system within nuclear penalty

The total system cost displayed in Figure 25 gradually rises from 146 G€/year in SN1 to 182 G€/year in SN5 due to the growing share of the combination VRE and NGCC which has more expensive cost than nuclear with full LCA.

The price of gas and liquid fuels are almost stable at around 85 €/MWh and 122 €/MWh respectively in the five scenarios because these fuels are produced independently from the changes in the electricity mix caused by the changing nuclear penalty. However, the price of electricity rises from 109 €/MWh to 161 €/MWh due to the rising cost of the technologies moving from nuclear (with no penalty) to the combination of renewables and NGCC.

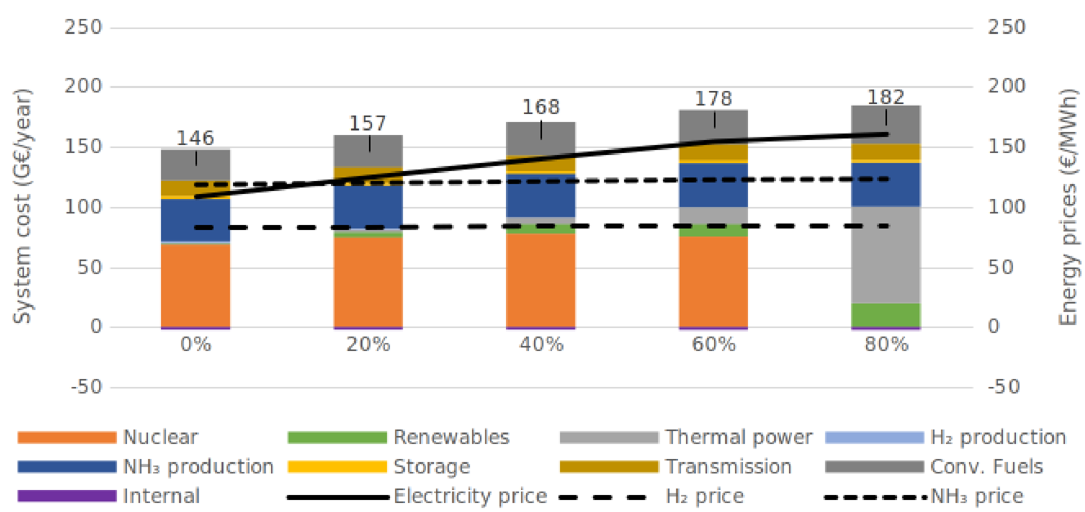

Figure 25: Total system cost of energy system within nuclear penalty

3.4 Comparison within renewable mandate

Five scenarios are designed for the different levels of renewable mandate from 1% to 90% in table 21 in order to investigate how the growing share of renewable effects the whole system. This comparison is conducted under the condition of S5 with full LCA and the same parameters setting in section 3.2.1.

SR1	SR2	SR3	SR4	SR5
1%	30%	50%	70%	90%

Table 21: Five scenarios designed for the different levels of renewable mandate

Figure 26 indicates the comparison of electricity generation within five assumptions of renewable mandate at 1%, 30%, 50%, 70% and 90% respectively. Mandating higher shares of wind and solar has a moderate effect up to 70% from SR1 to SR4 and a larger effect up to 90% in SR5. More renewables also bring more NGCC for balancing. That is why Nuclear is gradually displaced with the combination of renewables and NGCC as NGCC has more superior ramping capability to adapt the fluctuation of electricity generation of wind and sola than nuclear. When renewable mandate researches 70%, nuclear is completely out of the system. At 90% of VRE mandate, wind and solar are backed by a broader mix of natural gas, storage, and electrolysis.

Direct CO_2 emissions slowly increase from 67 Mton/year at 1% VRE to 130 Mton/year at 70% VRE as unabated natural gas (NGCC without CCS) backup replaces nuclear backup. There are very small amount of the negative electricity generation for fuel production up to 70% VRE until setting renewable mandate at 90%. Low CO_2 emissions at 1% and 90% of VRE mandate are caused by the lower share of NGCC.

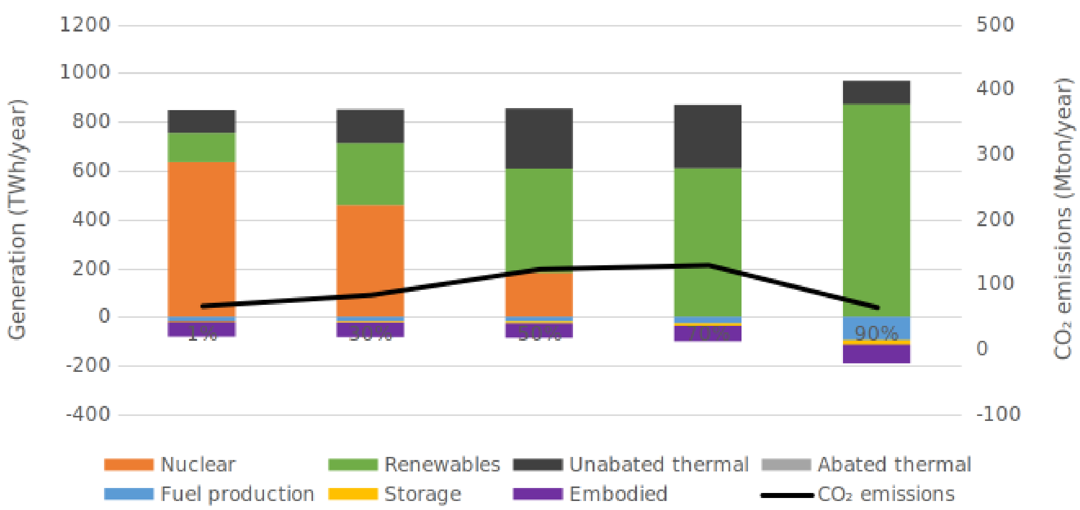

Figure 26: Electricity generation of energy system within renewable mandate

Figure 27 indicates that the fuel production mainly consists of direct natural gas and blue ammonia. At 90% VRE some green hydrogen production is used for balancing because only 10% of power output is left for NGCC, as the green H_2 production can use the surplus electricity generation from the renewables in large-scale capacity. Increasing VRE mandates lead to gradually increasing embodied energy demand because wind and solar requires higher material intensity with more embodied energy to be constructed.

The import share is stable at 52% from 1% to 70% VRE until 90% VRE where it drops to 46% due to the green hydrogen production.

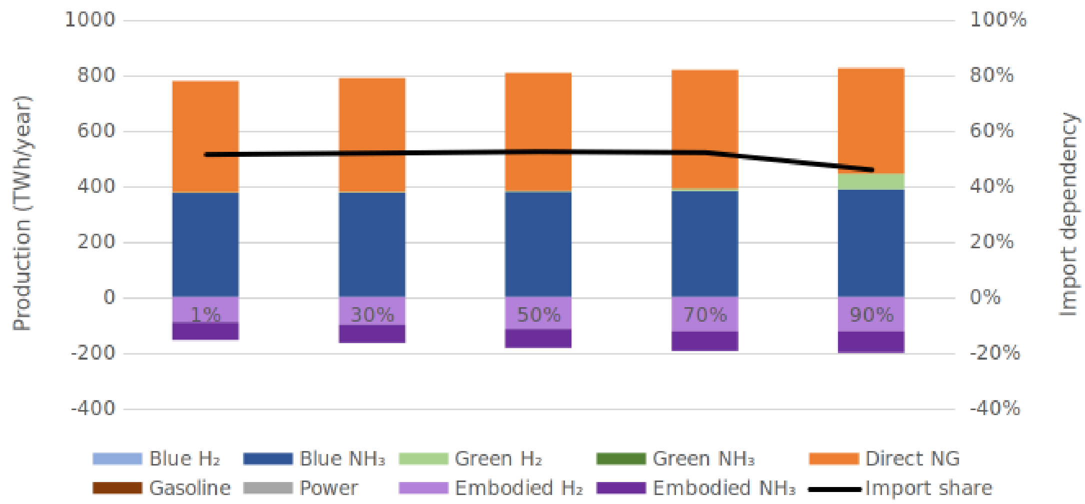

Figure 27: Fuel production of energy system within renewable mandate force

In terms of total system cost shown in Figure 28, increasing the renewable share to 70% is not very expensive in the range of 178 G€/year and 186 G€/year. While climbing from 70% to 90% begins to be a little costly from 186 G€/year to 199 G€/year. It is notable that the storage cost significantly increases at 90% of VRE mandate, which has a large contribution to the rise of total cost.

The price of gas fuel (natural gas and hydrogen) and the liquid fuel (ammonia) are 85 €/MWh and 125 €/MWh with no big difference in section 3.2.1. However, the price of electricity rises by 22% from 155 €/MWh to 189 €/MWh due to the higher cost of 90% renewables system including storage and electrolysis with full LCA.

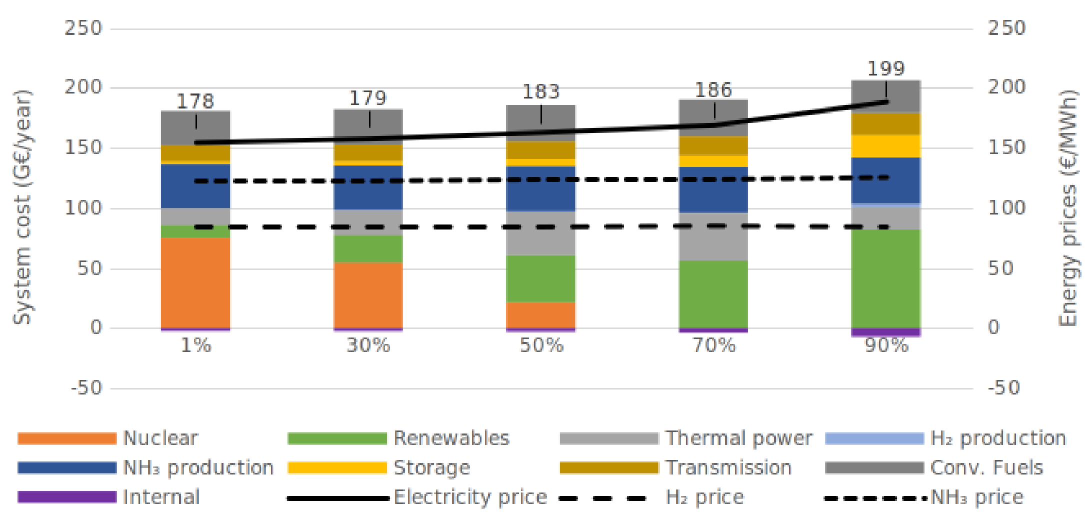

Figure 28: Total system cost of energy system within renewable mandate force

3.5 Comparison with applying resources in Spain

In order to investigate how wind and solar profile effects the energy system, resource in Spain is applied in the energy system modelling. It is noted that this is an artificial scenario because Spanish wind/solar resources are combined with German energy demand profiles. The purpose is only to quantify the increase in wind/solar deployment when excellent resources are.

Figure 29 displays the total cost of four typical power generation technologies with applying resources in Spain. The costs of onshore wind and solar PV are lower than the cost with resources in Germany by 16% and 25% respectively. This is mainly because the capacity factors of wind and solar power are higher with better resource, which lead to the lower requirements of capacity for the same amount of electricity generation supply. The costs of internalized, LCI and energy in capital, connection and operation all decrease in different levels with better renewable resource.

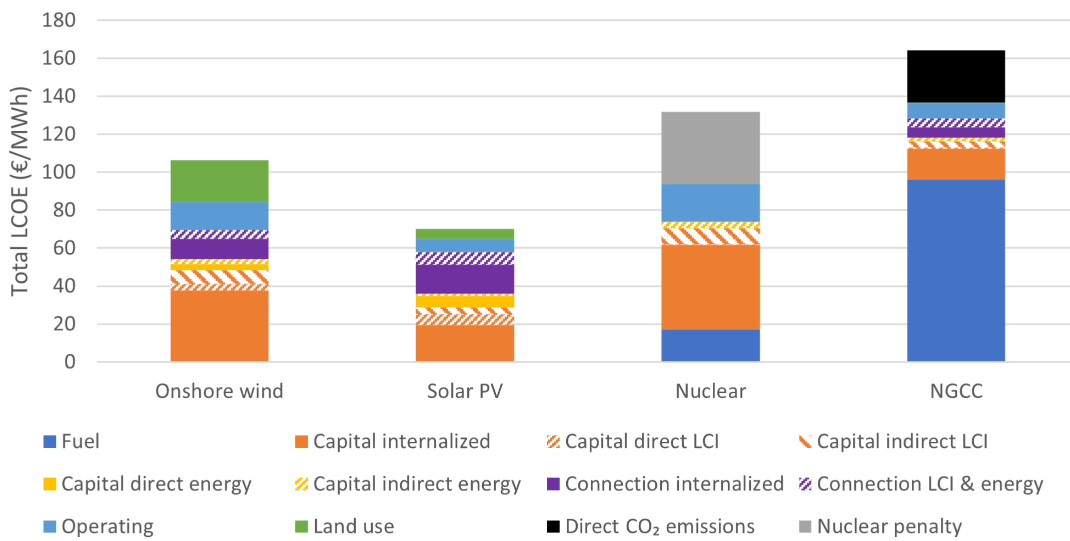

Figure 29: Total cost of technologies with applying resource in Spain

Figure 30-32 reveal the different characteristics of electricity generation, fuel production and total system cost after applying the resources in Spain under the same assumptions of renewable mandate at 1%, 30%, 50%, 70% and 90% VRE.

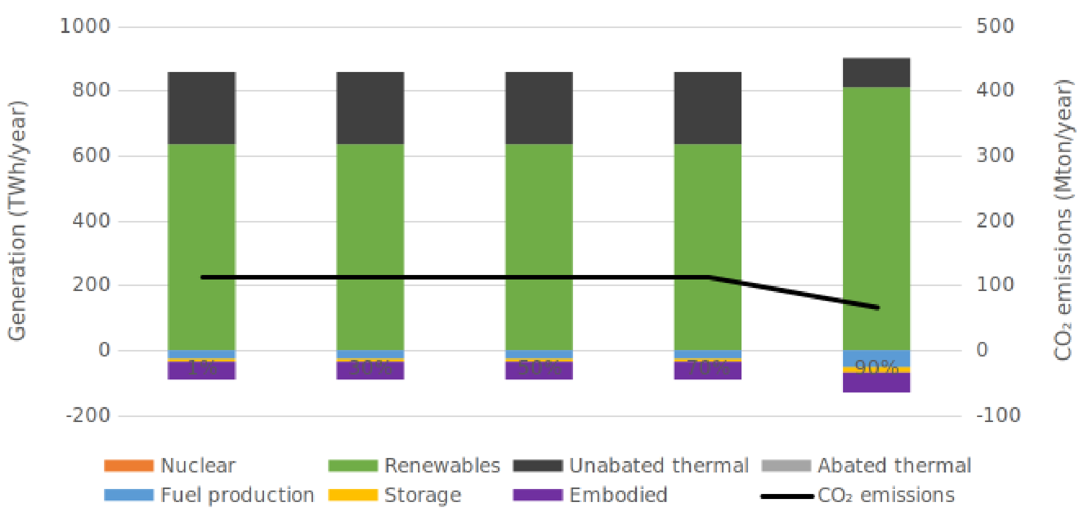

Figure 30: Electricity generation of energy system applying Spain resources within renewable mandate

With Spanish wind/solar resources, for the electricity mix shown in Figure 30, nuclear is automatically driven out of the system and displaced with the combination of renewable and NGCC due to the cheaper cost even at 1% mandate VRE. The optimal wind/solar share is 74%.

Direct CO_2 emission is stable at 114 Mton/year up to 70% VRE and drop at 67 Mton/year at 90% VRE due to the share of unabated thermal (NGCC).

For the fuel production exhibited in Figure 31, there are generally no differences on the productions of natural gas and blue ammonia among 1%-90% VRE except some green hydrogen produced from the surplus renewables power at 90% VRE. The amount of green hydrogen is 55% lower than that with German resources due to the lower requirement of the renewables capacity with Spain resources for the same demand as Germany. The import share is slightly drop at 90% VRE because of this small amount of green hydrogen production.

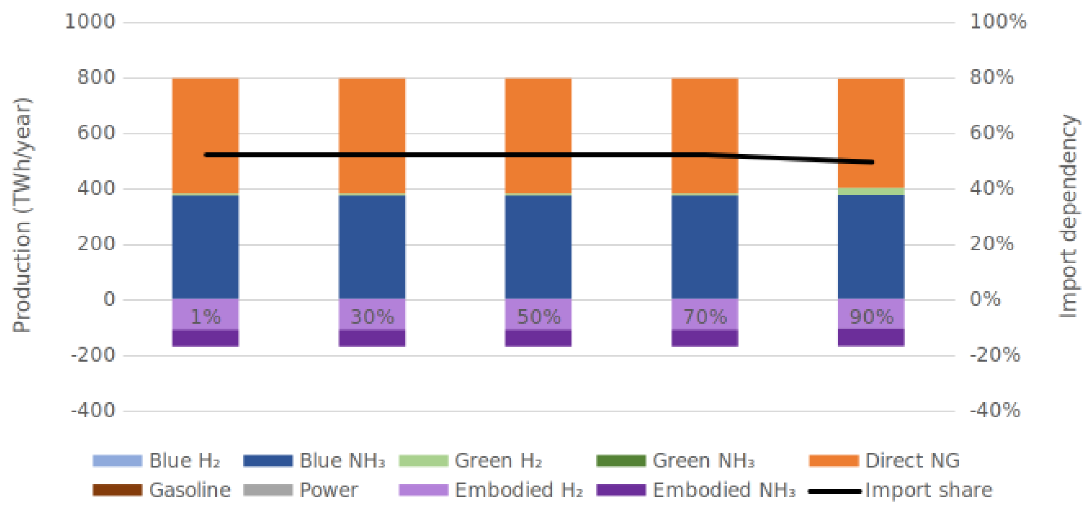

Figure 31: Fuel production of energy system applying Spain resources within renewable mandate

Regarding the total system cost shown in Figure 32, 90% VRE can be achieved at 173 G€/year with a very small added cost by 1 G€/year from 70% VRE. 90% VRE with Spanish resources reduces system costs by 13% relative to 90% VRE with German resources.

The prices of gas fuel (natural gas and hydrogen) and liquid fuel (ammonia) are almost keeping at 85 €/MWh and 123 €/MWh in the five different levels of VRE mandate without big difference from German resources. The electricity price of 90% VRE drops by 20% compared to 90% VRE with German resources.

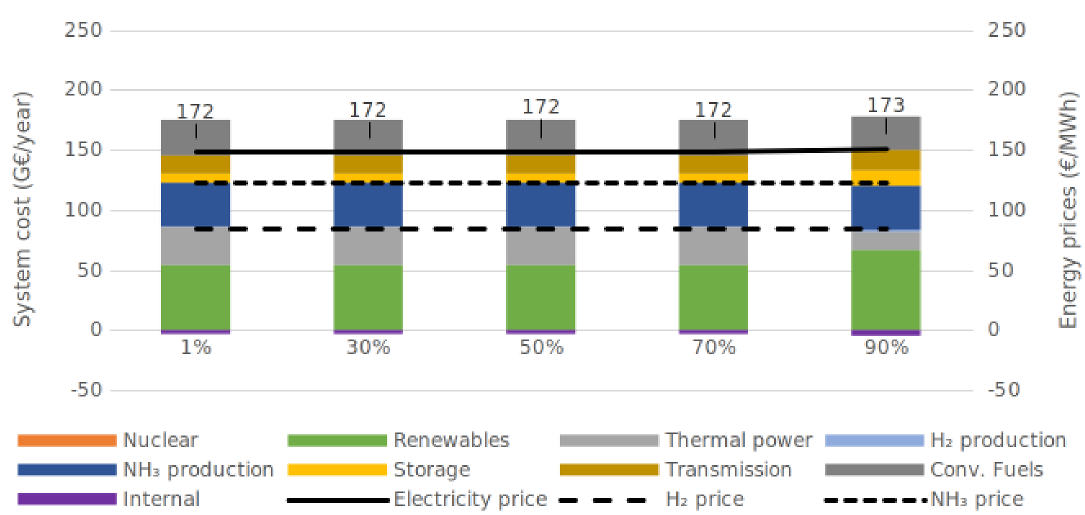

Figure 32: Total system cost of energy system applying Spain resources within renewable mandate

Figure 33 shows the electricity generation profile for nuclear penalty with Spanish resources that nuclear still displaces renewables when the penalty is low. However, when the penalty is growing to 60%, renewables combined with NGCC replace nuclear completely. This reveals that renewables with Spanish resources is already more economical than nuclear with penalty 60% which is still economical when with German resources in figure 28. It is also notable that the share of NGCC combined to renewables with Spanish resources is much lower than with German resources. Because Spanish resources is not only in higher intensity but also distribute more evenly which need less NGCC for balance and lead to less CO_2 emission.

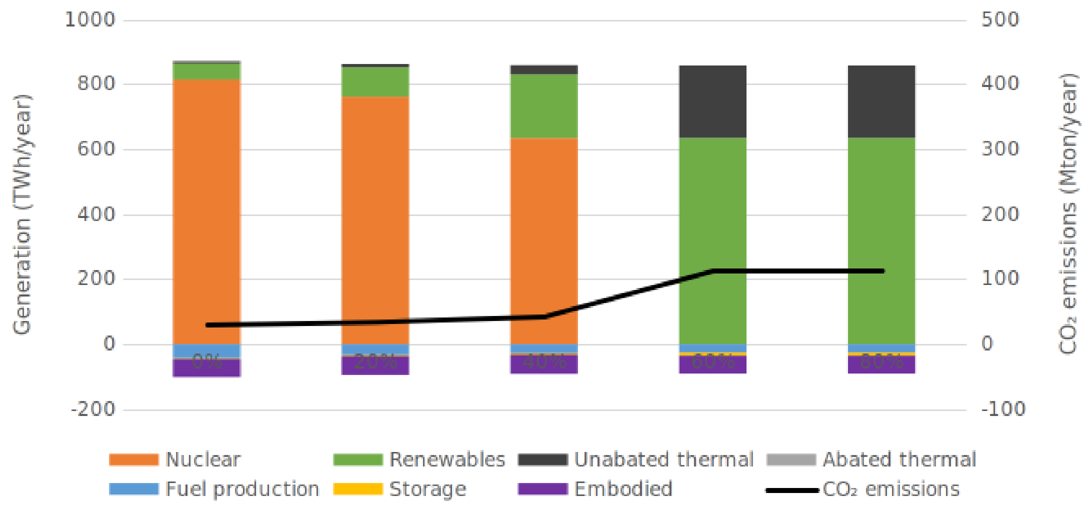

Figure 33: Total system cost of energy system applying Spain resources within nuclear penalty

3.6 Uncertainty quantification analysis

3.6.1 Life cycle impact MVC

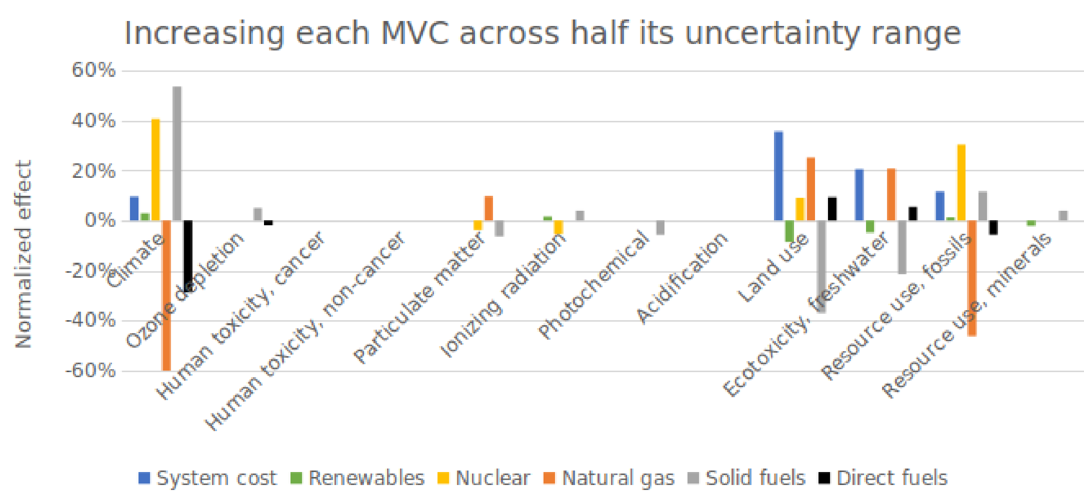

Figure 34: Linear regression results of effect to technologies when increasing each category of MVC across half its uncertainty range (For the system cost, the y-axis displays the change relative to the average system cost across all cases. The change in technology contribution is expressed as a percentage of the total final energy demand of the system.)

Although the geometric mean of monetary valuation coefficient (MVC) is applied for life cycle impact (LCI) cost in section 2.2 in order to obtain the most representative value, there are still large uncertainty of MVCs collected from literature data. It is important to analyze quantitatively on the uncertainty of MVC which is sensitive to the total system cost.

Figure 34 exhibits how different LCI categories of MVCs affect the system cost and different technologies in the energy system.

1. Climate change

The climate MVC has a relatively small effect on the system cost at +10%, but a large effect on the technology distribution. Thus, avoiding emissions from NGCC power plants and direct use of natural gas and petrol is not so expensive. This is partly because extremely high CO_2 prices actually start reducing system costs due to the CO_2 credit earned by the biomass in the solid fuel plants.

Nuclear acquires big gains at +41% from higher CO_2 prices since it outcompetes NGCC with CCS. Natural gas falls significantly at -76% as it can be displaced by nuclear cheaply in electricity generation, also displaced by solid fuels in fuel production sector. Because solid fuels are used for fuel production with CCS, leading to negative emissions due to a 30% biomass fraction, which makes it benefit at +54% from higher CO_2 prices. Renewables only gain a small improvement at +3% with higher CO_2 taxes due to their dependence on NGCC for balancing. Direct fuels which consists of majority of natural gas and smaller amounts of petrol and imported ammonia decline at -29% with higher climate MVC as they are replaced by blue hydrogen and ammonia with lower CO_2 emissions.

2. Particulate matter and ionizing radiation

Particulate matter makes anything with mining more expensive, impacting on coal , uranium and material mining. This leads to the increasing cost of the technologies such as solid fuels (70% coal), nuclear and renewables due to their value chain involved with mining. While natural gas has relatively low particulate emissions, which is why it gains at +10% from a higher particulate MVC. Therefore, the combination of different technologies such as renewables and NGCC with different direction of the influences comprehensively counteracts the effect on the system cost.

Radiation affects nuclear power negatively at -5%, although the effect is quite small.

3. Land Use

Higher Land Use MVCs hit renewables and solid fuels at -9% and -37% respectively, as both have higher Land Use impact, especially the biomass fraction in the solid fuels. While nuclear, natural gas, and direct fuels benefit at +9%, +25%, +9% respectively from the decline in renewables and solid fuels due to their relatively lower Land Use impact.

The high rise in system cost at +36% is partly related to the large indirect Land Use impact associated with each € of GDP added at a general economic efficiency in equation (43).

4. Ecotoxicity Freshwater

A higher Ecotoxicity MVC has double the uncertainty effect of a higher climate MVC, on system cost at +21%. However, the effects on the optimal technology distribution is smaller because every option has significant Ecotoxicity impacts mainly due to material mining process.

While natural gas has the lowest Ecotoxicity problems, thus it gains at +21% from a higher

Ecotoxicity MVC. Direct fuels have the similar characteristic with lower Ecotoxicity impact and earn +5%. Whereas, coal mining and minerals drag down solid fuels and renewables at -21% and -5% respectively. Coal mining has more than four times impact on solid fuels than minerals on renewables.

5. Resource use

A higher MVC of fossil resource use strongly affects natural gas and nuclear in opposite direction at -46% and +30% respectively as natural gas has high impact of fossil resource. Nuclear gains from the drop of natural gas. Since it is expressed as a percentage of the internalized cost, natural gas is observed a significant rise in price while uranium is relatively unaffected. Solid fuels receive both positive and negative effects from a higher MVC of fossil resource. The coal fraction causes a fall somewhere in the middle while solid fuels obtain modest rises by displacing natural gas for fuel production, which lead to a comprehensive gain at +12%. Direct fuels fall at -6% due to its similar feature as natural gas. Mineral resource use has a small negative effect on renewables at -2%. Because renewables have relatively higher demand of some materials facing ore grade declining such as copper.

The system cost rises at +12% from increasing the MVC of fossil resource use due to higher cost of electricity and fuel production. While mineral resource has negligible effect on the system cost.

6. Other categories of MVCs

The rest categories of MVCs including ozone depletion, human toxicity, photochemical, acidification have slight effect on system cost and technologies.

7. summary

Besides climate change, Land Use, Ecotoxicity and Resource Use are the other three most important categories of MVCs for the energy system modelling considering life cycle environmental impact. Particulate matter and ionizing radiation have modest effects. These six categories of MVCs are worthy to be investigated deeply in order to obtain more accurate monetary valuation of LCI cost for sustainable energy system modelling.

3.6.2 Feature of technologies distribution

Figure 35 indicates the histograms of technologies distribution. Most technology classes follow multi-peak distributions, especially solid fuels and direct fuels. These two classes have relatively sharp transitions in competitiveness when producing gas fuels and liquid fuels. For example, as the CO_2 price crosses over a relatively narrow range, 400 TWh of petrol will be displaced by 400 TWh of ammonia. Ammonia displaces petrol before hydrogen displaces natural gas as total cost of blue ammonia is lower than petrol while the total cost of blue hydrogen is higher than natural gas in section 3.1. Also solid fuels is used to produce hydrogen for use in the power sector. Hence there three peaks for solid fuels around 400, 800 and 1400 TWh/year.

Natural gas is very versatile and competes in electricity, hydrogen, and ammonia production, giving a more complicated distribution.

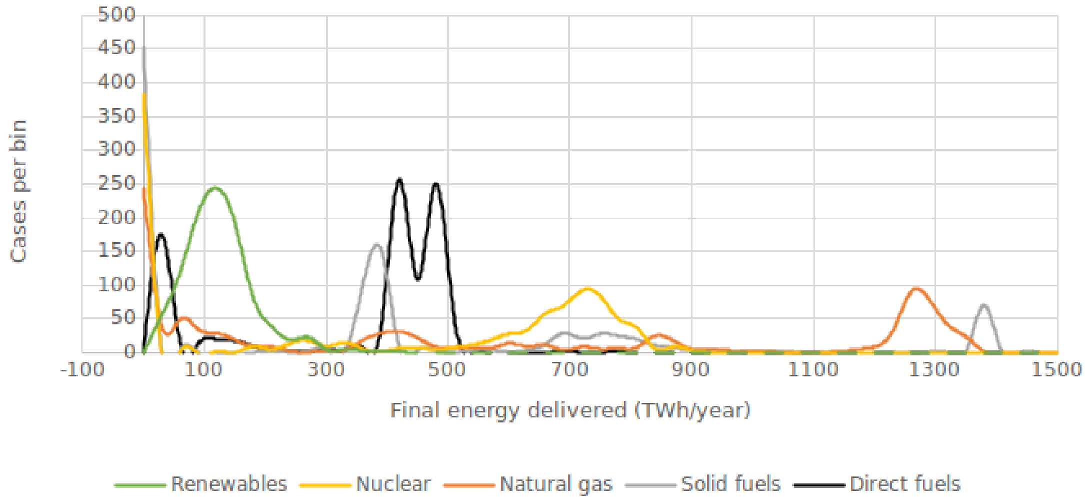

Figure 35: Histograms of technologies distribution across the 1000 simulated cases. The bin size is 30 TWh/year.

On average, nuclear is observed more deployment than renewables, although about a third of cases does not deploy nuclear while some renewables is always deployed. As illustrated earlier in Figure 26, there is a relatively sharp threshold over which the system flips from a high nuclear share to no nuclear because nuclear does not perform well with renewables in a balancing role. Renewables and nuclear compete mainly in the electricity sector as green hydrogen from electricity is considerably more expensive than blue hydrogen from fuels.

3.6.3 Correlations between different energy technologies

Figure 36 shows the correlations among different technologies.

	objective	Renewables	Nuclear	Natural gas	Solid fuels	Direct fuels
objective		-0.469			-0.298	
Renewables				-0.466		-0.355
Nuclear	0.276			-0.825		-0.455
Natural gas					-0.709	
Solid fuels		0.582	0.248			-0.864
Direct fuels	0.105			0.698		

Figure 36: Correlations between different energy technologies

Solid fuels correlate well with renewables because they both exhibit similar responses to Land Use (due to the biomass fraction), Ecotoxicity (due to coal and copper mining) and fossil resource depletion. Similarly, solid fuels positively correlate with nuclear because of similar responses to climate and fossil depletion MVCs.

There is a strong negative correlation between solid fuels and direct fuels because blue H_2 and NH_3 from solid fuels compete directly with direct use of natural gas and petrol. Solid fuels and natural gas also have a negative correlation because they are in competition for producing blue H_2 and NH_3.

Natural gas and renewables are negatively correlated mainly due to their opposite responses to Land Use and fossil depletion MVCs. Natural gas and nuclear have a large negative correlation as they compete directly in the electricity sector with large and opposite responses to climate and fossil resource MVCs. Natural gas (which only represents fuel use in power, H_2, and NH_3

production plants) and direct fuels are positively correlated because half of the direct fuels is directly used natural gas (the other half is petrol).

Although they are not in direct competition, a large negative correlation between nuclear and direct fuels exists mainly due to the very large opposite response to the climate MVC.

3.7 Three important categories of life cycle impacts besides climate

Climate change impact has received great attention in the energy sector. Numerous studies focus on how to reduce the climate change impact by energy system modelling. However, it is discovered in this study that Land Use, Ecotoxicity and resource depletion are three other important categories of life cycle impacts which have effect on sustainable energy system design on a magnitude similar to climate change. Since these categories enjoy much less attention than climate change in the open literature, they will be investigated in more detail in this section.

There are two dimensions of effects on the energy system from the life cycle environmental impacts, which is worthy to be further investigated. One is refer to the value of the life cycle environmental impact itself: how it presents the practical impact according to different levels of impact with different LCIA methods? The other side is refer to MVCs: how the monetary valuation of LCI presents the practical LCI cost in different levels and in different MVC methods?

3.7.1 Land Use

Land Use impact has the most sensitive effect on the total system cost as every technology is involved with direct and indirect Land Use, especially renewables and solid fuels.

Land Use of typical wind, solar, transmission line, and pipelines are firstly conducted by Simapro using Ecoinvent database.

However the land use impact of solar PV is higher than the expectation possibly because it was using older, much less efficient solar technology that occupies more land to generate a certain amount of electricity. Also land use of modern solar PV could combine livestock (such as sheep) farming between the solar PV facilities, which decrease the land use impact of solar.

While land use impact of wind power and transmission of Ecoinvent database are much smaller than the expectation. Because there only the direct occupied land of the infrastructure is considered in some technologies in Ecoinvent. For instance, Land Use of wind power in Ecoinvent only presents the Land Use area of a wind turbine rather than a wind farm. Similarly, the Land Use of the electricity HV transmission line is in the order of 1000 m^2 a/km of HV transmission in Ecoinvent, which is much smaller than the impact when considering a typical 50m wide corridor of the line. Furthermore, the corridor of impact for transmission lines and pipelines depends greatly on the type of land. In sensitive areas like the Amazon, this can be very large. Hyde and colleagues found that 39625 km of transmission lines in the Amazon directly impact 23467 km2 of land that amounting to an average corridor of about 600m [115].

Taking wind as an example, its Land Use is relatively complicated and involved with different levels. Recording the suggestions from researchers, a 150 meters of distance between wind turbines and the adjacent obstructions is sufficient[116]. In terms of wind farm spacing, there is a need of at least 7 times of rotor diameters of turbines away from each other[116]. The National Renewable Energy Laboratory (NREL) in the US investigated the direct Land Use of wind turbines including the concrete tower foundation, the power substations and new access roads, and found that 1.5 acres of land would be required for a 2-megawatt wind turbine[116]. For total wind farm area, The space between the wind turbines is not directly occupied by wind turbine, but some of its function is to minimize turbulence, or to follow ridge lines, or to avoid other obstacles, or to be used for agricultural farms[116]. Hence, there would be Land Use impact on some of those indirect Land Use due to the losing function of the natural land. NREL also did survey on the total wind farm area and roughly estimated an average of 4 megawatts per square kilometer[116]. Further more, there are noises and dynamic shadows from the rotation of the blades, as well as some potential disadvantages or dangers of siting turbines close by other structures, which has the impact on a wider Land Use and lead to the regulatory requirements of a minimum distance for wind turbines located from property lines, setting a uniform 304.8 meters in the US[116].

Hence, four levels of Land Use of wind can be distinguished:

1) a small footprint of complete direct Land Occupation by the turbines and their service roads;

2) a 10-100x larger area between the turbines that could still be productively used for purposes like agricultural farming;

3) a radius of about 1 km around the wind farm where effects like noise and shadows degrade the value of the land;

4) a radius of 10 or more km around the wind farm where the natural beauty of the land can be spoilt and bird species can be driven out by the wind farm.

Clearly, the monetary valuation per m² of land influenced should drastically reduce from level 1 to level 4. However, it is difficult to find existing methods of monetary valuation to convert between these different types of Land Occupation.

Eleven Land Use MVCs were collected from literature data in a range from 8.91E-02 €/m²a[99]to 3.70 €/m²a[100]. Nine numbers are applied methods of damage cost; the remaining two are applied methods of abatement cost and societies' WTP respectively which are covered in the range of those damage cost MVCs. The lowest MVC derived from "Environmental Prices Handbook EU28" integrates characterization models, impact route evaluation and monetized methods to achieve at a consistent estimation of the well-being costs associated with harmonized characterization from midpoint to endpoint[99]. The largest MVC applies the method of Environmental Priority Strategies (EPS), which assesses the impact on biodiversity and agricultural damage for industrial use[100]. All of the eleven MVCs only cover the concept of impact level 1 and level 2 in terms of Land Use of wind.

So far, the aggregated damage level of impact categories in LCIA has only included human health, ecosystem quality and natural resources and has not operationalized with ecosystem services, socio-economic assets, cultural heritage and natural heritage.

Some studies exploded the socio-economic valuation of the Land Occupation by the wind farm applied the method of willingness to pay (WTP). One case was the Environmental Impact Assessment conducted on proposals of a wind farm with capacity of 200 MW siting at Búrfellslundur on the verge of the Icelandic highlands considered about the visual impacts on the nearby landscape[117]. They applied the method of interval regression using log-transformation to evaluate mean willingness to-pay at around US $128 and the total economic value of reserving Búrfellslundur at around $32.3 million when expending to the all Icelandic tax-payers[117].

The other case was the study on the willingness to pay for diminished visual unpleasantness from offshore wind farms in Denmark[118]. Ladeenburg and Dubgaard estimated the willingness to pay for moving turbines from an 8 km baseline further to 12, 18 or 50 km away from shore reaching at 46, 96 and 122 Euros per year per household respectively based on the survey[118]. A similar study conducted on offshore wind and the Cape Cod economy suggest by the survey data that generally the public considers offshore wind farms as unfavourable visual circumstance and the average net willingness to pay for windmills to not be built was$75 per person at a onetime cost[119].

Westlund and Wilhelmsson inspected the socio-economic cost of wind turbines in Sweden[120]. Their conclusions clearly revealed a significant negative capitalization of wind turbines imposed a socio-economic cost on lower values properties within 8 km of the wind power plant[120].

Besides the different levels of impacts of wind turbines that devalue the land in different levels, the impact cost of Land Occupation of wind/solar has a rising trend as the land depletion increase with the growing capacity of renewables in future. More and more land will be used for wind/solar in order to meet the requirement of green energy transition by renewable policy, the possibility of use higher value land rises. There is similar tendency on the land use of biomass. Initially, there is no land use impact (or it could even be negative) from using waste biomass stream that would need to be sent to landfill or burned otherwise. But the land use impact starts to increase rapidly if land needs to be dedicated to energy crops. Therefore, the impact cost of Land Use should be dynamically adjusted over the time rather than a constant value (a topic for future work). Additionally, different location of Land Use, different types of the original land (agriculture, forest or wetland etc.) and different level of the biodiversity and precious species all lead to different monetary valuation of Land Use.

In this study, adjustment for the Land Use of wind power is made by considering the whole area of wind farm instead of a single wind turbine. The basic assumption is that the positive effect of being able to utilize land between the turbines for selected purposes is canceled out by the negative effects of wind turbines on the land surrounding the wind farm. Also the Land Use of transmission is expanded by considering the corridor width of the line. But the Land Use MVCs are still simplified to use a constant value of the geometric mean of the eleven MVCs. Land Use impact and impact cost need to be investigated further in future work.

Table 22 presents the key data related to the land use of wind, solar and transmission using factors using multiplier and corridor width, where the extra transmission externality of wind and solar is not the same as the general transmission and pipeline land use externality in the two bottom rows. Instead it represents the additional transmission required by wind and solar because they are often located relatively far from demand centers in regions with good resources and low public resistance.

The adjusted land use impact of wind, solar, transmission line and pipeline are 166.7 m^2/kW, 10 m^2/kW, 30 m^2/kW and 10 m^2/kW respectively. The range of Wind's land use impact could be large, so its multiplier is set from 10% to 5 times of the baseline. Solar's multiplier is smaller and assumed from 50% to 2 times of the baseline due to the uncertainty is much lower for solar than for wind. Because the layout of solar PV is relatively intensive with no need space between each other. While the range of transmission line's corridor could be wide from 5m to 600m depending on the type of the land passing through and the way of installation. It could be only a few miters of the width of the transmission line itself when passing through in an empty remote badlands or up to 600m when passing through an original ecology region such as Amazon[115].

Figure 37 reveals the sensitivity of those factors to total price of wind and solar. The Wind's land use impact has strong effect on the wind's total price from negative 20% to positive 85%, while solar's land use has much lower effect from -2% to 4%. Transmission line has large positive effects on the cost of wind and solar at 21% and 34% respectively as the corridor factor of transmission line could be very wide in some special region.

	Energy density	Multiplier	Land use	Externality	Extra transmission externality
Unit	W/m2		m2/kW	€/kWa	€/kWa
Wind on	6	1	166.7	62.3	5.6
Solar	100	1	10.0	3.7	3.7
	Length	Wattage	Corridor	Land use	Externality
Unit	km	MW	m	m2/kW	€/kWa
Transmission	600	1000	50	30.0	11.2
Pipeline	600	3000	50	10.0	3.7

Table 22: Adjusted Land Use impact of wind, solar and transmission technologies

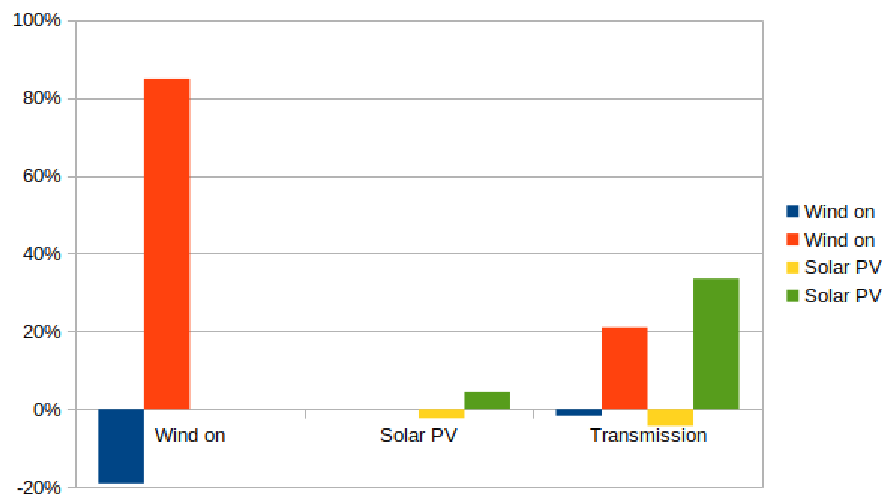

Figure 37: Sensitivity analysis of Land Use impact of wind, solar and transmission technologies (wind's multiplier set from 0.1 to 5, solar's multiplier set from 0.5 to 2, transmission's corridor set from 5m to 600m)

3.7.2 Ecotoxicity

The results show that Ecotoxicity is an important contributor to the life cycle impact costs, for instance the monetized Ecotoxicity Freshwater impact of Copper takes 41% of its total LCI cost of 12 categories when applying LCIA methods of Environmental Footprint (EF 3.0) and geometric mean of MVCs in table 13. Uncertainty analysis also reveals Ecotoxicity Freshwater is the second most sensitive impact category to the energy system. It is consistent with the result of a sector-coupled energy system modelling integrating LCA that full LCA increases freshwater ecotoxicity and minerals depletion impact as the environment impacts shift from operation to infrastructure of the energy system [24].

Based on the structure analysis of LCA on various materials, it is observed that mining/extraction processes are the main contributors to Ecotoxicity. Technologies such as renewables and solid fuels involved with mining process (such as Copper and Coal mining) has high Ecotoxicity impact and impact cost. As mining processes are necessary process for most material production, it is universal in the value chain of various technologies. Thus, Ecotoxicity impact is significant in many materials and technologies. Especially, low-carbon technologies have higher demands of metals than conventional fossil power [2]. Minerals extraction leads to both impacts of ecotoxicity and minerals depletion.

However, there is only Ecotoxicity Freshwater in EF LCIA methods. EF service replied our inquiry that Terrestrial Ecotoxicity and Marine Ecotoxicity have not been included in the current set of EF LCIA Methods, as there was no sufficiently robust method identified so far when compiling the methods. Then, further investigation is conducted on the assessment using ReCiPe, with which the three categories of Freshwater, Terrestrial and Marine Ecotoxicity are completed.

The Ecotoxicity impact comparison of some typical materials and primary fuels using ReCipe 2016 V1.03 Midpoint (H) and EF3.0 methods from Ecoinvent database are listed in table 23, applying the unit conversion coefficient 983 CTUe/kg 1,4 DCB eq[92] to convert CTUe to kg 1,4 DCB eq. In terms of ReCipe method, the Ecotoxicity Terrestrial is several orders of magnitude larger than the Ecotoxicity Freshwater for the same process except Copper, while Ecotoxicity Marine are slightly higher than Ecotoxicity Freshwater with the same order of magnitude. Comparing Ecotoxicity Freshwater with these two methods, most process has the same order of magnitude value except Copper. Copper has the same order of magnitude of the three Ecotoxicity categories in ReCipe, while it has 10 times lower of Ecotoxicity Freshwater of EF than of ReCipe. These seven processes are mostly located in Europe except Copper located globally considering the distribution of copper mine and mining process in the world.

Methods	ReCiPe 2016 v1.03 Midpoint (H)			EF 3.0	
Environmental impact categories	Ecotoxicity Freshwater	Ecotoxicity Terrestrial	Ecotoxicity Marine	Ecotoxicity Freshwater	
Process/Unit	kg 1,4-DCB-Eq	kg 1,4-DCB-Eq	kg 1,4-DCB-Eq	CTUe	kg 1,4-DCB-Eq
1 kg steel production	0.189	13.3	0.265	86.4	0.0879
1 kg aluminium production	0.328	11.1	0.45	146	0.148
1 kg copper production	102	151	127	10700	10.9
1 m3 Natural gas	0.00518	0.404	0.00745	10.1	0.0103
1 kg Coal market	0.042	0.455	0.0581	47	0.0478
1 kg Biomass market	0.00227	0.543	0.00325	2.06	0.0021
1 kg market for nuclear fuel element	272	99200	405	732000	745

Table 23: Ecotoxicity impacts comparison of ReCipe 2016 V1.03 Midpoint (H) and EF3.0 methods from ecoinvent database 3.0

The impacts pathway and region scope are different between ReCipe and EF methods. ReCipe methods are in a global context while EF is for Europe. The different effect factors and impact route in these two LCIA methods model might be the main reasons for the difference in Ecotoxicity Freshwater.

ReCipe applies a linear function of concentration–response in aquatic environment which is determined by EC50 data as the first step of the average toxicity[121]. For the terrestrial Ecotoxicity, its effect factor was deduced from data of aquatic toxicity integrating the method of equilibrium partitioning[122]. While EF methods made some adaptations on Ecotoxicity effect modelling which is based on HC20 (instead of EC50) derived from EC10-equivalents[123].

There are two questions raised: 1) How large would be the deviations when using aquatic toxicity data to extrapolate the terrestrial environmental effect factor for Terrestrial Ecotoxicity in ReCipe methods? 2) How big difference would be caused in the applications between the two Ecotoxicity effect modelling based on EC50 and HC20 respectively for ReCipe and EF methods?

However there are few studies inspected deeply on the Ecotoxicity between different methods. Pizzol and colleagues investigated the Ecotoxicity impact of “metals” on the aquatic and terrestrial environment by conducting evaluations among eight different LCIA methods but excluding EF methods[124]. Their results reveal that there is a low consistency between methods for identifying the total ecotoxicity impact from metals, which is critically determined by the characterization phase between methods[124].

Regarding the monetary valuation of Ecotoxicity, the concept of Ecotoxicity is a midpoint impact category which leads to the damage to ecosystems at the endpoint through the damage pathways of the damage to freshwater/terrestrial/marine species. The cost of the damage to ecosystems is general concept of the monetized Ecotoxicity impact.

Further investigation is conducted on the monetized Ecotoxicity applying ReCipe methods. Whereas, the monetized Terrestrial Ecotoxicity impact becomes dominant of all other life cycle impacts after integrating Terrestrial and Marine Ecotoxicity. For instance, the monetized Terrestrial Ecotoxicity impacts of Copper, Steel and Nickel account for 91%, 99% and 100% of their total LCI cost respectively. This massive Recipe Terrestrial Ecotoxicity effect lead to obviously unreasonable results. For instance, the externalized cost of copper rises to 500 €/kgCu from 9.4 €/kgCu using EF methods; that of Nickel soars to 1652 €/kgNi from 1 €/kgNi using EF methods.

The largest factor influencing the huge Terrestrial Ecotoxicity impact cost is due to both of its much higher impact value and its much higher geometric mean of MVC than freshwater and marine by 10 times and nearly three orders of magnitude respectively.

But MVCs of Terrestrial Ecotoxicity are very limited in literature compared with MVCs of Freshwater Ecotoxicity. It is surprising that this apparently important impact has been investigated so much less. There are only three typical methods for the MVCs of Terrestrial Ecotoxicity in literature: Ecotax 2006[125], Environmental Prices[99] and Stepwise 2006[126][127]. Ecotax is the highest one at 17 €/kg 1,4-DCB-Eq which is derive from the method of Societies' willingness to pay based on the ecotax in Sweden on exceeding amount of cadmium in fertilizer[125]. Environmental Price has the medium value at 9.11 €/kg 1,4-DCB-Eq, which is monetized on the damage cost estimated through ReCiPe 2016[99]. Stepwise has a much lower value at 0.46 €/kg 1,4-DCB-Eq also assessed on damage cost but through Impact 2002+[126][127]. Different impact assessment methods lead to different monetized values as the different impact pathway, characteristic factor and scope have effects on the monetized modelling. The geometric mean MVC of Terrestrial Ecotoxicity is 1.58 €/kg 1,4-DCB-Eq.

MVCs data of Ecotoxicity Marine are also limited in the literature with a much lower geometric mean of 5.89E-03 €/kg 1,4-DCB-Eq, which evaluated with three typical methods: Ecotax 2006[125], Ecovalue [128]and Environmental Prices[99]. Ecovalue method is assessed on tributyline pollution in Sweden but with no information of transferring from tributyline to 1,4-DCB equivalents[128].

Ecotoxicity Freshwater has attracted more research attention but in a wider range of four orders of magnitude from 1.34E-03 €/kg 1,4-DCB-Eq (1.36E-06 €/CTUe) [101] to 5.7E+01 €/kg 1,4-DCB-Eq (5.8E-02 €/CTUe)[102]. The minimal MVC of Ecotoxicity Freshwater is assessed with the method of Societies' WTP using budget constraint and the valuation of environmental impacts with indicators of quality-adjusted life year (QALY) and biodiversity-adjusted hectare year (BAHY) in Thailand[101]. Considering they use Thai GDP per capita for calculating the valuation of QALY and BAHY, it is adjusted to 4.02E-03 €/kg 1,4-DCB-Eq (4.09E-06 €/CTUe) by tripling as European GDP per capita is roughly 3 times of Thai's[129]. The largest one of Ecotoxicity Freshwater is estimated with method of abatement cost which is the price to reduce the environmental pollution or materials depletion using Life-Cycle Cost Analysis (LCCA) in sector of construction and buildings[102]. There are totally 14 MVCs of Ecotoxicity Freshwater collected in literature with geometric mean 1.73E-01 €/kg 1,4-DCB-Eq, seven are evaluated with methods of damage cost, five are with the method of Societies' WTP, the rest three are with abatement cost. Generally, MVCs assessed with methods of damage cost are three orders of magnitude lower[130][99][131][126][127]. While MVCs estimated with methods of Societies' WTP or abatement cost swing from the similar value as the MVCs applying the damage cost methods [131]to the highest one[102]. Two of Societies' WTP are the second highest ones over 12 €/kg 1,4-DCB-Eq, which are provided by Ecotax method based on pollutants discharge to fresh water[125].

Figure 38 displays the collected MVCs of Ecotoxicity, in which there are three typical technical routes of methods: Damage cost, Societies' WTP and Abatement cost. The damage cost MVCs generally has lower value while the other two methods have large swinging ranges.

The possible reasons could be:

1) The knowledge of understanding the biodiversity and species are limited, especially in marine ecosystems, which leads to the damage cost methods missing some unknown damage effects on the ecosystem.

2) Damage cost methods might not include all effects of damage due to some unavailable quantitative data.

3) MVCs with Societies' WTP and Abatement cost methods can be effected by many factors: type of pollutants, standard of emissions in environmental policy, technology level of reducing pollutants, regional characteristics etc, which lead to their value fluctuating greatly.

In this study, three strategies are taken:

1). Collect MVCs data as many as possible and apply the geometric mean values of MVCs with all mixed methods for LCI cost integrating into the energy system modelling, as damage cost methods likely incompletely cover all the damage to the ecosystem due to the knowledge missing and data availability. Other methods provide complementary, because damage cost methods mostly only consider the damage to species/biodiversity. While there are some other costly damages such as agricultural/fishery yield declines, ecosystem services degradation and natural heritage destruction, which could be compensate by other methods at some levels.

2). Some adjustments have made on MVCs in order to adapt the monetized methods to European context such as applying European GDP per capita instead of Thai's.

3). Terrestrial and Marine Ecotoxicity from ReCipe have been abandoned and only Ecotoxicity Freshwater from EF is applied in this study. Because the monetized impact cost of Terrestrial Ecotoxicity makes the externalized cost of materials and technologies unreasonably expensive. Also the energy system optimization may get benefit from the consistency of LCIA methods with different impact categories. The attempt to account for the missing Terrestrial and Marine Ecotoxicity impacts in the EF method was considered through multiplying the Ecotoxicity Freshwater impact by some factor to scale up. However, EF service denied this approach as they explained there are completely different impact pathways and likely different emissions between Terrestrial and Freshwater Ecotoxicity. Hence this will not improve the result from energy system. All considered, however, it is likely that ecotoxicity impacts are underestimated in the present study.

Finally, there is an important issue related Ecotoxicity emerged on social justice involved in the energy transition: To which degree are these Ecotoxicity effects confined to the country where the mining and mineral processing is being done? As many materials or technologies imported to Europe from developing countries where most mining processes located there. Will the green energy transition in Europe is established on the expensive cost of damage to ecosystems, human health and resource availability on the other corner of the world? There is little studies on this issue which needs to be deeply investigated and inform commenting.

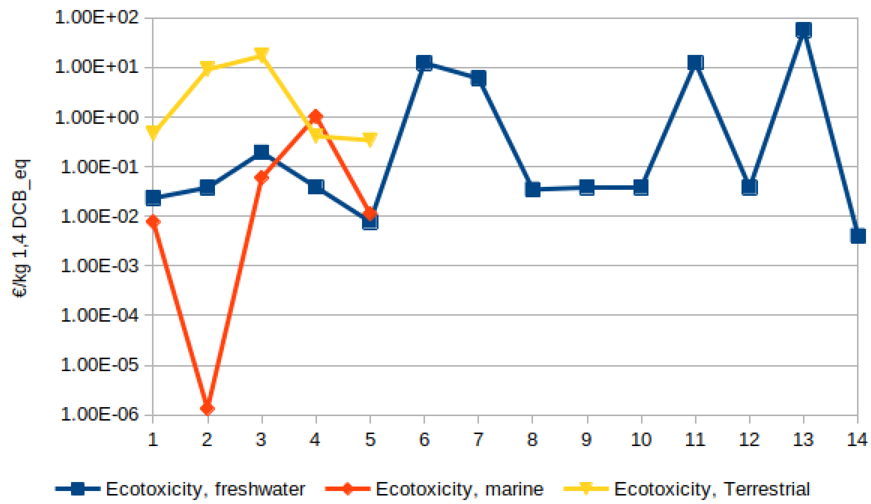

Figure 38: Monetary valuation coefficients of Ecotoxicity[125][99][126][127][101][102][128][131][130]

3.7.3 Resource depletion

Resource depletion impact represents the level of scarcity of that type of resource, which causes the tendency to exploit easily accessible resources first. Hence, current exploitation of a finite resource will increase the cost and environmental impact of exploiting that resource in the future.

In the EF method connected with the geometric mean of MVCs, the fossil fuel depletion impact cost is assessed at reasonable values which is similar to the internalized cost of natural gas. However, there is a drawback in the method that this constant value is applied to all fossil fuels and uranium. Clearly, depletion is a much bigger concern for oil and gas than it is for coal and uranium, which are about an order of magnitude more abundant and therefore much cheaper (per unit exploitable energy) to extract. The fossil resource depletion impact should reflect this large difference in resource availability. Furthermore, the mineral depletion impact with EF method from the ecoinvent database is unreasonably low. For example, the depletion impact of 1 kg of primary copper is only about 0.002 kgSb, which is surprising because the production cost of Copper is similar to that of Antimony. These values in the EF methodology are derived from 1999 values of ultimately recoverable resources and exploitation rates, and need to be revised. In addition, the EF methodology presents no clear path to impact monetization.

For these reasons, a simpler approach is created to monetize the resource depletion impacts in the present study in sector 2.2.5, which considers the factors of the trend related to the discount rate, use rate of resource and the acceleration of use rate over the time to predict the discounted weighted average price in future. Table 24 displays the resource depletion impacts under different assumptions of the key parameters in the resource depletion valuation modelling with the situations of baseline, rapid mineral expansion and fossil phase-down in this approach. The factors of Discount rate, Increase per unit of use and Starting rate of use are still are set the same values as the baseline. While the factor of the Increase in rate of use are largely different for different resources. One example of rapid mineral expansion is assumed its increase in rate of use at 20% per year based on the information of IEA's prediction on the soaring demand of some key materials such as Lithium, Nickel and copper in the future[132]. Considering the increasing recycle rate of the mineral in the future, Decline in rate of use after recycle is added to this resource depletion valuation modelling. The assumption of decline rate is set to the same rate of increase for the example of mineral. Whereas fossil resource use has different trend that it's rate of use declines first due to the replacement from other energy. After those easy substitutions of fossil sectors displaced, the decline rate of use of fossil becomes slower. That is why the factors of increase and decline in rate of use of fossil resource use are set to -0.5% and -0.2%. Based on equation (50), the discounted weighted average prices of baseline, mineral and fossil are 1.5, 3.51 and 1.15 respectively which means the future price presented at current price after considering the discount rate, start point of use, increase/decline rate of use and cost increase. Thus, the resource depletion costs of baseline, mineral and fossil is 0.5, 2.51 and 0.15 as the original current price is set to 1, according to equation (51).

Factors	Baseline	Rapid mineral expansion	Fossil phase-down
Discount rate	5%	5%	5%
Increase cost per unit of use	0.02	0.02	0.02
Starting rate of use	0.5	0.5	0.5
Increase in rate of use	0.02	0.2	-0.005
Decline in rate of use after recycle	0	-0.2	-0.002
Results			
Weighted average price	2.50	6.23	1.29
Discounted weighted average price	1.50	3.51	1.13

Table 24: Key factor assumptions and results of the resource depletion valuation modelling, baseline, mineral and fossil

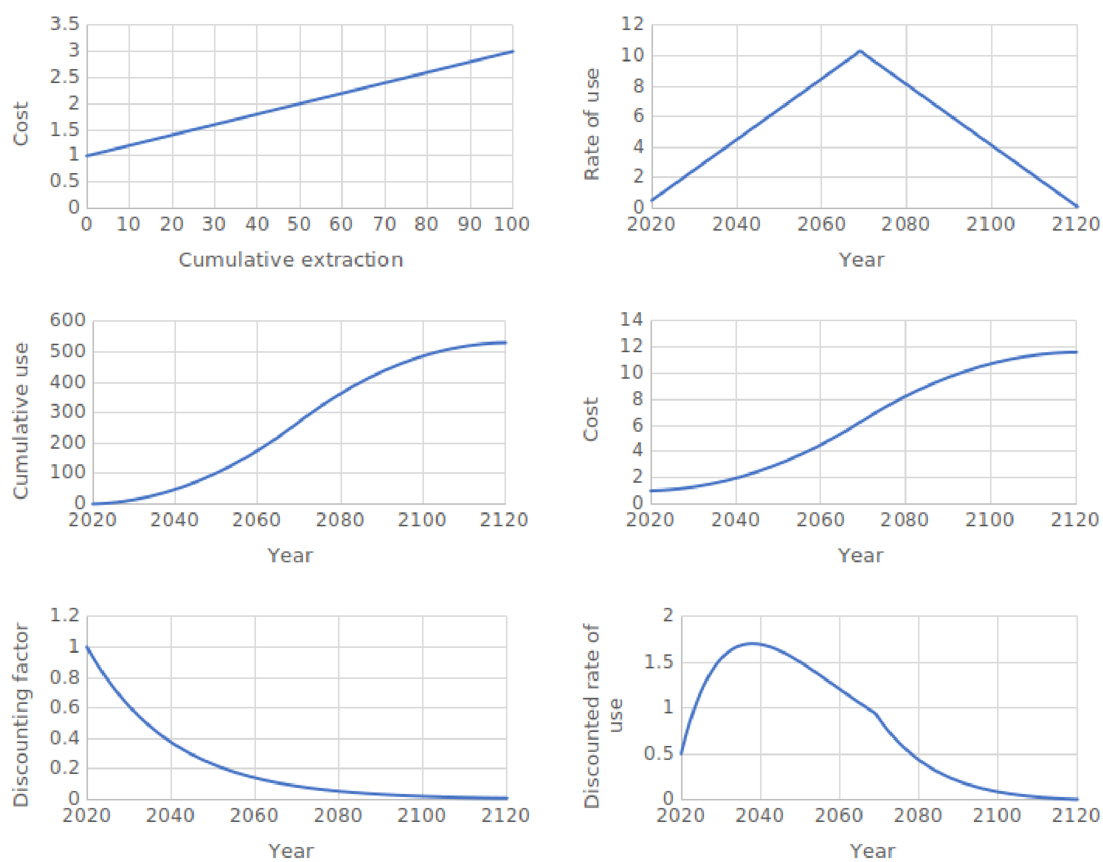

Figure 39: Resource depletion valuation modelling of rapid mineral expansion

Figure 39 illustrates the resource depletion valuation modelling of rapid mineral expansion under the various tunable parameters in the next century. There may be a large neglected externalized cost of resource depletion impact involved in such a rapid green transition scenario as key minerals become much more expensive and environmentally destructive in the future. This rapid rate of change in complex value chains cause costly and economically disruptive boom-bust cycles. Thus, internalizing this externalized cost would moderate the rate of expansion to more manageable levels to mitigate these potentially very large future costs.

Technologies with high consumption of low ore grade materials such as electrolyzer, battery, hydrogen tank, VRE transmission and solar PV are facing the risk of rapidly increased mineral resource depletion impact cost due to the growing cost of material and environmental impact in future.

Figure 40 presents the resource depletion valuation modelling of fossil. Such a declining rate in the use of fossil fuels means that they will be phased out long before they are depleted. Thus, the externality of resource depletion cost is low and would not make much difference if it is internalized in the market price. Unless suitable alternatives are found that are genuinely cheaper and more practical than fossil fuels in all sectors of the economy, such a phase-out well before the fossil resource is depleted may not be advisable, especially since about half of the global population still lives on less than 200 \$/month[133]. The results presented earlier show that renewables and nuclear cannot compete with fossil fuels + CCS outside the electricity sector, such as fuel production, casting doubt on calls to rapidly phase out fossil fuels.

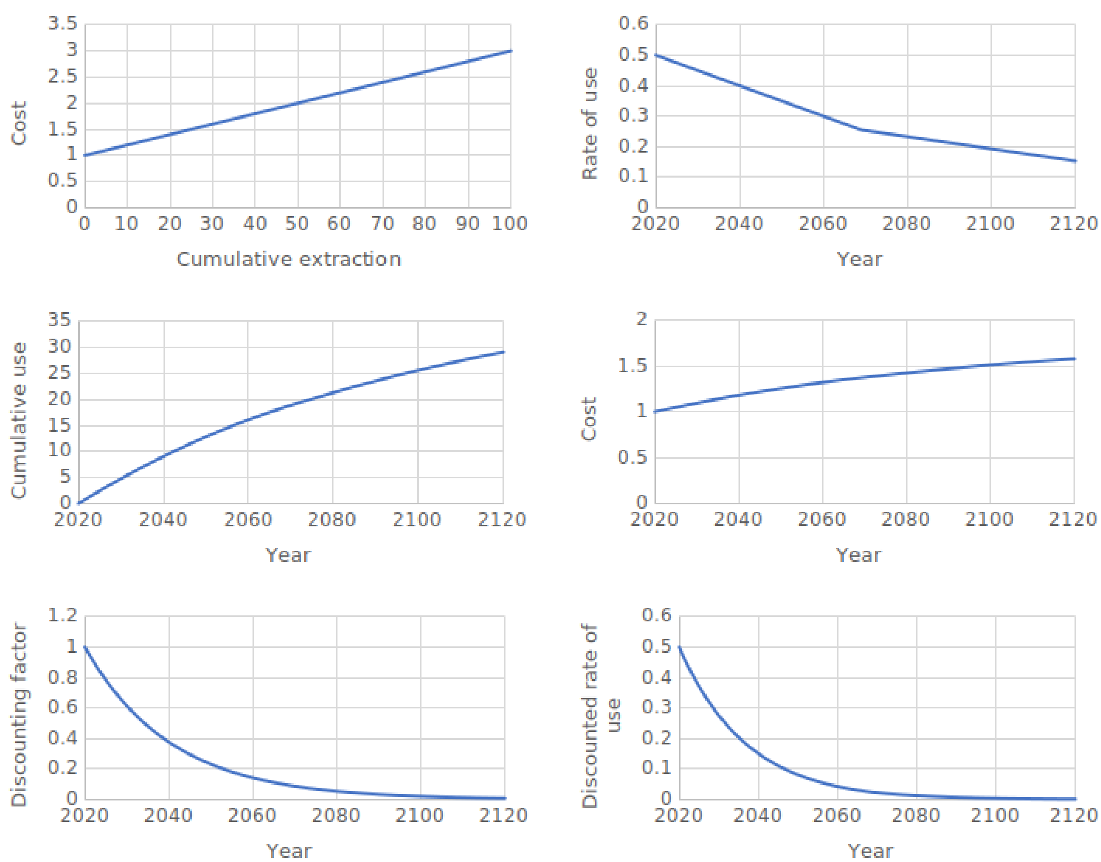

Figure 40: Resource depletion valuation modelling of fossil

4 Conclusions

1. Total system cost and optimal energy mix

An energy system model is integrated with life cycle assessment (LCA) using European Environmental Footprint (EF 3.0) methods with twelve impact categories, showing comprehensive pictures of optimization with different scenarios and parameter assumptions with the energy demand and the profile of wind/solar resource in Germany.

The optimization of total system cost are effected by several factors of the availability of technologies, life cycle impact monetization, social economic efficiency, energy penalty, renewable mandates under the assumptions of using geometric mean of monetary valuation coefficients (MVCs), which are subject to high uncertainty. Considering the full LCA rather than the conventional practice of only covering the direct CO_2 emissions is very important in energy system modelling, which increases the total system cost by around 50%. In addition, including the full LCA causes large changes to the optimal energy mix that nuclear power and natural gas (NGCC and decarbonized fuel production) gain their shares while solid fuels (coal/biomass blend with CCS) and renewables lose their shares, where the inclusion of ecotoxicity and land-use impacts are the main drivers of these trends. Because 70% coal in solid fuels lead to high ecotoxicity mainly from the coal mining process and 30% biomass causes high land-use impact. Renewables also have high ecotoxicity due to their high material consumption related to the minerals extraction processes and large land occupation. While nuclear and natural gas has a relatively lower full environmental footprints.

As there are large uncertainties of the twelve categories of LCI MVCs, it leads to different levels of the sensitivity to the system cost. Based on the uncertainty quantification analysis, land use has the highest effect on the system cost by +36% (measured on a logarithmic scale) when increasing the MVC across half of its uncertainty range. Ecotoxicity, fossil resource use and climate change have the second and the third effects on the system cost by +21%, +12% and +10% respectively. Other categories of MVCs have little effect on the system cost.

The absence of CCS technologies has a large impact on the system cost due to the unavailability of blue hydrogen production. Because green hydrogen and ammonia is much more expensive than blue fuels produced locally under all the assumptions and conditions, which leads to the imports of green ammonia from resource-rich area optimized by the energy system. This import green fuel limits the high cost of green hydrogen and ammonia in noCCS scenarios at the expense of near-complete import dependence. The effect of the scenarios also reveals that CCS technologies for fuel production is more superior than CCS for electricity generation.

2. Important life cycle impact categories

The optimal energy system changes greatly depending on the levels selected for the twelve categories MVCs. The total system cost and energy technologies deployment receive the effects with different directions and degrees.

Four impact categories of climate change, land use, ecotoxicity, and resource use dominate the picture. Climate change MVC presents a relatively low effect on the system cost, mainly because very high CO_2 prices start reducing the system cost due to negative emissions form biomass with CCS, but it has a strong effect on the technology distribution. Nuclear power and Solid fuel (coal/biomass blend with CCS) production gain large benefits from higher CO_2 price. Natural gas (NGCC and decarbonized fuel production) and Direct fuels (mainly direct use of natural gas in the economy) fall significantly from higher CO_2 taxes. Renewables obtains only a small improvement with higher CO_2 taxes as they are dependent on NGCC for reliable electricity supply. Land Use is the most sensitive impact category to the energy system as it is widespread in every technology. Higher Land Use MVC negatively impacts renewables and biomass due to their higher Land Use impact. Nuclear, natural gas, and direct fuels gain because of their relatively lower Land Use impact. Ecotoxicity Freshwater MVC has double the effect on total system cost than climate MVC. While it displays smaller effects on the optimal technology distribution as every option has significant Ecotoxicity impact, which mostly come from the mining/extraction process. Coal mining and minerals drag down solid fuels and renewables from higher Ecotoxicity MVC, while natural gas and direct fuels gain due to their low Ecotoxicity. In terms of resource use, technologies consuming scarcer fossil fuels such as natural gas and oil lose ground from a higher fossil resource MVC. More abundant nuclear gains from the drop of natural gas. Solid fuels receive a small negative effect from its coal fraction and a large positive effect for compensating the decline of oil and gas. Mineral resource use has a small negative effect on renewables due to its higher material intensity.

A key finding from this study is that besides climate impact, land use, ecotoxicity, and resource depletion are crucial to the energy optimization but do not obtain enough attentions. There are substantial uncertainties in each of these three categories. They need further detailed investigation to ensure that energy systems are designed optimally.

Land use impact of some technologies, such as wind and transmission line, involves several different levels of degrading land value that can extend far beyond the borders of the infrastructure, which lead to the complexity of different levels of land use impact and impact cost. The uncertainty of land use impact of wind, solar and transmission has been estimated with different degrees of range respectively based on literature. Ecotoxicity impacts vary widely in different LCA methods for the same process in Ecoinvent database. There are few studies to investigate and compare Ecotoxicity in different LCA methods. The MVCs of terrestrial and marine ecotoxicity are also less widely studied, and those studies focusing on terrestrial ecotoxicity show surprisingly large values. The attempt to integrate the three categories of monetized ecotoxicity from Recipe methods into the energy system results in unreasonably expensive materials and technologies by the dominant cost from terrestrial ecotoxicity. Thus, the EF method that neglects all terrestrial and marine ecotoxicity impacts had to be adopted. Fossil resource depletion has some drawbacks that a constant value applied to all fossil fuels and uranium without reflecting the large difference in resource availability and without considering discount rate and trend of use rate. The mineral depletion impact with EF methods from the ecoinvent database is unreasonably low. A new approach of resource depletion is created to predict the discounted weighted average price considering the factors of discount rate, increase cost per unit of use, and changes in rate of use over the time.

5 Limitations and Future work

There are some limitations and recommendations for future work based on the finds in this study. Although the uncertainty analysis provides us a much clearer picture on how different categories of life cycle impact MVCs affect the energy system, further deep investigations need in several sectors.

1. Three important impact categories need more attentions.

1) Land use

There are few studies on different levels of land use impact and impact cost (MVCs) according to different types of land occupation/transformation and land devaluation such as noise, shadows and nature view destruction from energy facilities. The subdivided MVCs of different profiles of land use including its function, location and surrounding need deep investigations. Wind, solar and transmission expand rapidly all over the world during the energy transition, which are frequently encountering public resistance challenges. Thus, Willingness-to-pay should be the most appropriate MVCs method to obtain clarity on the monetized land use impact. Also many opportunities for such studies are now emerging. A standardized methodology is required to quantify the amount that wind/solar/transmission investors need to pay local stakeholders based on the installed capacity and land use to compensate the impacts from building the infrastructure nearby, where the classification of land use needs to be considered according to land function/type/location.

2) Ecotoxicity

Monetary valuation methods of Terrestrial and Marine Ecotoxicity requires more investigations. The unreasonably high cost of Terrestrial Ecotoxicity in the Recipe methods need to be further inspected. There are large differences of Ecotoxicity impacts in different LCIA methods for the same process, eg. Ecotoxicity freshwater of copper is 10 times higher in Recipe methods than in EF methods. Thus, systematic evaluations of different LCIA methods need to be conducted in order to understand their commonalities and differences, advantages and disadvantages, as well as their applicability.

3) Resource depletion

The relationship between resource depletion impact, impact cost, resource abundance, rate of use and discount rate need to be further studied. Moderating effect of resource depletion impact monetization should be included in models. In rapid decarbonization scenarios, the potential rapid expansions in several critical minerals extraction requires 10-50 times increase on their extraction rates. Such extensive expansions will rapidly deplete the most easily accessible stocks, increasing the cost and environmental impact of future resource extraction. As a result, a high mineral depletion MVC should be applied to moderate the expansion rate and prevent economically destructive boom-bust cycles. Historical market data of resources could be studied to better quantify important parameters such as the cost evolution with rising cumulative extraction and the discount rate applied to future cost increases.

2. Dynamic modelling of land use

Assumptions of constant valuations of land use, fossil resource depletion and mineral resource depletion are made to simplify their impact cost to integrate into the energy system modelling. However, land and resource depletion impact and impact cost will rise over the time that need to be further investigated.

Spatial resolution could be included in the energy system model with land valuation coefficients for various locations according to ecological sensitivity and population density. The model will then automatically choose the locations with the lowest land use impacts and MVCs first to build infrastructure before moving to more sensitive locations when the low-cost locations are depleted. More detailed spatial modelling of transmission could also be included to conduct the trade-off between building wind/solar infrastructures at distant locations with low land use costs but high cost for transmitting the power in a long distance, or building wind/solar capacity closer to demand in more sensitive areas to reduce transmission cost.

However, such a more resolved modelling effort would require much more data, making it a challenging task.

3. Social justice issue related to Ecotoxicity and Climate

Ecotoxicity impacts mainly come from the mining processes which are mostly located in developing countries. Thus, there is an social justice issue emerged during the evolution of the energy transition: to which degree are these Ecotoxicity impacts limited to the mining countries? Is the clean energy expansion in Europe at the serious Ecotoxicity cost in some developing countries? There are carbon leakages between the international trade; there are also Ecotoxicity leakages between the international trade especially in green energy transition. This needs further study.

Climate change has the parallels, where the rich world enjoys most of the benefits of a long history of fossil fuel consumption, while the developing world is much more vulnerable to a more volatile climate caused by all those historical emissions.

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