Life cycle assessment integration into energy system models: An application for Power-to-Methane in the EU

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HIGHLIGHTS

- Study covers five energy sectors, 18 impact categories and 31 countries in Europe.
- Indirect CO_2 emissions can be one to three times higher than direct emissions.
- Electricity for PtM has to be below 123–181 gCO_{2eq}/kWh to achieve climate benefits.
- PtM has similar or lower impact than natural gas for 10 out of 18 categories.

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ABSTRACT

As the EU energy system transitions to low carbon, the technology choices should consider a broader set of criteria. The use of Life Cycle Assessment (LCA) prevents burden shift across life cycle stages or impact categories, while the use of Energy System Models (ESM) allows evaluating alternative policies, capacity evolution and covering all the sectors. This study does an ex-post LCA analysis of results from JRC-EU-TIMES and estimates the environmental impact indicators across 18 categories in scenarios that achieve 80–95% CO_2 emission reduction by 2050. Results indicate that indirect CO_2 emissions can be as large as direct ones for an 80% CO_2 reduction target and up to three times as large for 95% CO_2 reduction. Impact across most categories decreases by 20–40% as the CO_2 emission target becomes stricter. However, toxicity related impacts can become 35–100% higher. The integrated framework was also used to evaluate the Power-to-Methane (PtM) system to relate the electricity mix and various CO_2 sources to the PtM environmental impact. To be more attractive than natural gas, the climate change impact of the electricity used for PtM should be 123–181 gCO_{2eq}/kWh when the CO_2 comes from air or biogenic sources and 4–62 gCO_{2eq}/kWh if the CO_2 is from fossil fuels. PtM can have an impact up to 10 times larger for impact categories other than climate change. A system without PtM results in ~4% higher climate change impact and 9% higher fossil depletion, while having 5–15% lower impact for most of the other categories. This is based on a scenario where 9 parameters favor PtM deployment and establishes the upper bound of the environmental impact PtM can have. Further studies should work towards integrating LCA feedback into ESM and standardizing the methodology.

1. Introduction

The EU energy system has to change from fossil-based (71.5% in 2014 [1]) to renewable energy-based in order to decrease the environmental impact and contribute to limiting global temperature increase to less than 1.5 °C [2]. To achieve this, new technologies are needed across sectors to provide alternative ways to satisfy the energy demand. In these choices, it is important to consider a wide range of criteria that allow assessing the trade-offs of the consequences to weigh competing scenarios. These consequences are usually encompassed in

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economic, environmental and social aspects [3,4]. At the same time, due to the highly integrated nature of energy systems, changes will affect the entire system rather than a specific part, leading to a need to expand the boundaries of the evaluation. Ultimately, decisions in the energy system should target not only affordable, reliable and sustainable energy, but should also be put in the broader context of the Sustainable Development Goals and links with food, water, economic growth, employment, education and equality [5].

Life Cycle Assessment (LCA) has positioned itself as a widely used tool to assess environmental impact (damages to human health, ecosystem and resources) [6] throughout all the life cycle stages of a product or a process, from the extraction of the raw materials through production, operation, use and end-of-life [7,8]. It quantifies the energy and materials used, as well as the pollutants and wastes released [9]. The LCA methodology is recognized as a powerful sustainability assessment tool [10,11], mainly due to two advantages. First, it prevents shifting the burden from one life cycle stage to another (e.g. from operation of a power plant to the necessary infrastructure) aiding the impact allocation and establishing clear boundaries [12]. Second, by covering a wide range of impact categories (e.g. climate change, water use, land use, metal depletion, toxicity), it enables the identification of trade-offs across categories and ensures and reduces the risk of burden shifting from one category to another (e.g. improving climate change at the expense of a much higher water use). LCA has insofar mostly been applied to single technologies, with recent efforts targeted at enlarging the boundaries to cover sectors [13,14], national [15] and global systems [16], thus making an effort to have a broader scope and cover the entire energy system [17].

Energy system models (ESM) focus on cost-optimal pathways to achieve environmental and policy targets (introduced as user-defined constraints) [18,19]. Constraints can be added on emissions, energy consumption, efficiency targets, among others, which the final solution has to meet. They are technology-rich [20] and the main added value is the understanding of the possible evolution of the system over a long term horizon under various policies. The environmental aspect is covered by introducing constraints on energy use, CO_2 emissions or pollutants (NO_x, SO_2 and particulate matter) [21] or monetizing these emissions to take them into account as part of the cost optimization and make trade-offs with the investment and operational costs [22,23]. Similar to LCA, there is also a trend to expand the scope of ESM beyond pure economics. One of the most explored areas is the power sector, where the water implications for generation technologies have been assessed [24] and integrated in long term pathways [25]. ESM have also used life cycle emissions (rather than operational emissions only) [26–28], which is more relevant as renewable energy sources (RES) increase their share of electricity production. The specific ESM used in this study is JRC-EU-TIMES (The Integrated MARKAL-EFOM System) [29–32]. The reasons for this choice are: (1) the EU coverage; (2) it covers the entire energy system (residential, commercial, power, industry and transport) and (3) it has been used in the past to analyze the role of Power-to-Methane (PtM) [33]. The model covers CO_2 emissions from the energy system (i.e. excludes agriculture and land use) and it does not have other greenhouse gases (GHG) or pollutants. The energy use for all stages of the fuel cycle (upstream fuel production, conversion and end use) is covered and the corresponding emissions are accounted as CO_2 from fuel combustion. Emissions from plants construction and dismantling are not included. The boundaries of the system are the EU borders and CO_2 emissions from either imported fuels or manufactured assets are not included [29].

In this study, the environmental performance of PtM is explored. PtM refers specifically to the pathway from electricity to hydrogen and subsequent methane production [34]. PtM is seen as an option to satisfy gas demand while decreasing the emissions of the gas system. At the same time, it provides a source of flexibility to the power system and makes possible the integration of a larger fraction of variable renewable energy (VRE) [35]. Its environmental impact is largely defined by the

sources of electricity and CO_2 [36], hence the need for a life cycle approach in its assessment. The electricity mix depends on the constraints chosen for the system (e.g. no nuclear) and has a temporal variation (e.g. nights when there is no solar contribution). JRC-EU-TIMES is suitable to capture both of these components. Furthermore, JRC-EU-TIMES allows looking beyond the process itself and considering the changes in the rest of the system in alternative future scenarios [37]. Research on the technology has greatly increased in the last decade [38] with a continuous growth in demonstration plants [39,40].

There are multiple benefits of combining LCA into ESM and there is an increasing need to use methods that are overarching and considering trans-disciplinary issues [41]. LCA can benefit from ESM since the latter includes the learning curve and technology developments over time (i.e. efficiency), but also the evolution of electricity mix and material demand over time. It also allows making the bridge with the economic dimension by considering the relation with different supply and demand curves that will lead to different technology mixes with varying environmental impact. Lastly, ESM provide the means to relate the effects of policies in various sectors, assessing the consequences of changes across the energy system and the evolution in time on the environmental impact for alternative energy pathways [37]. On the other hand, the added value LCA gives to ESM includes the consideration of the other life cycle stages of the assets (construction and dismantling), other impact indicators besides climate change and the impact associated to imported commodities beyond the ESM boundaries [42]. As the CO_2 emissions decrease, the indirect emissions from these background processes will become more relevant [43].

LCA has already been used before in combination with ESM. Hitherto, most of the studies have focused on the power sector [44–46], which has the advantage of fewer technologies to match between the model and the life cycle data, but it limits the feedback from other sectors (e.g. industry for supply of materials). Most of the studies have conducted ex-post analyses [14,16,46–48], either as stand-alone analyses, where results from the ESM are used to estimate the life cycle impact or as part of a wider methodology like Multi-Criteria Decision Analysis (MCDA) [49]. Studies that have made the LCA endogenous have either been limited to CO_2 emissions [50] or to the power system [51]. The two approaches for endogenization have been multi-objective optimization [50] and monetization of externalities [51]. A third approach where reduction targets are set in the ESM for impact categories has not been found in literature.

The novelty of this study is the combination of both tools with an EU-scope (rather than a single country), covering the entire system (residential, commercial, power, industry and transport rather than a single sector), 18 impact categories (beyond climate change) and exploring deep decarbonization scenarios (80–95% CO_2 reduction by 2050 vs. 1990 [52]). Previous studies have made a compromise in at least one of these areas (sectoral coverage, geographical scope, impact categories covered or CO_2 emission target ambition). Thus, this study contributes to a more holistic approach used to evaluate alternative pathways towards a sustainable, affordable and secure low-carbon society. The focus is on the EU, given the ambitious climate targets, but the same methodology can be applied to other regions, where many of the technologies (and corresponding data) are similar, being differentiated by the specific technology mixes and policy frameworks. Therefore, the contribution of this study lies in both the methodological developments and the specific results that will benefit future research on overarching evaluations and provide insights to inform policy-making. The focus on 2050 is considered owing to the larger changes in the system and higher PtM capacities envisioned due to more ambitious CO_2 reductions [33], establishing an upper bound for the changes in environmental impact across categories.

The key questions to be answered in this study are divided in two major aspects, the LCA integration into ESM and the PtM evaluation with focus on 2050. Research questions in the LCA-ESM integration are: (1) what is the ratio between direct and indirect emissions for an energy

system with low CO_2 emissions; (2) what is the scenario with the lowest impact across categories; (3) are there specific technologies that drive the environmental impact for some impact categories or is the environmental burden evenly spread across a multitude of technologies? The research questions related to the PtM evaluation are: (1) what is the environmental impact of PtM considering the spatial and temporal differentiation of the electricity mix in future low carbon scenarios; (2) how does PtM environmental impact compare with natural gas; (3) what is the environmental impact of not having the technology available.

The rest of the publication is organized in the following manner: Section 2 goes through the literature to identify the main studies done in this area, scope of the work to establish a basis for benchmarking the current study; Section 3 addresses the methodology, this includes sources used, ESM background, description, issues found, changes made and solutions adopted; Section 4 goes through the scenarios analyzed that have been selected based on PtM characteristics and previous assessment [33]; Section 5 goes through the analysis of results and Section 6 summarizes the conclusions, remaining gaps and subjects for further study.

2. Literature review

The objectives of this section are to discuss the alternative approaches to integrate the environmental aspect in energy models and understand how LCA integration to comparable models can shed light into the LCA-ESM combination. Since this study analyzes PtM, previous studies on LCA for PtM are summarized. For both areas, the gaps in literature are identified. The separate reviews of policy with LCA [6,53,54] or policy with ESM [55–57] are not included since that is the more conventional approach (stand-alone), while the novelty of this study lies in their combination.

2.1. Approaches to assess the environmental impact from ESM

There are trade-offs when including the environmental component in the analysis. Some of the dimensions where choices have to be made are: sectoral coverage (power, heating, transport), temporal and spatial scope (time horizon and region/country/world), temporal and spatial resolution (time steps and number of nodes), life cycle stages (operational vs. "cradle to grave"[2]), qualitative vs. quantitative (the former influenced by subjectivity, while the latter requires more effort), feedback to results (endogenous vs. ex-post analysis) and number and types of impact indicators used to quantify environmental impact (GHG emissions, pollutants externalities, LCA impact indicators, global temperature increase). Therefore, when a model extends in a certain dimension, there is a compromise that is (usually) done in other part of the modeling approach and this creates clusters of studies with a similar methodology. These are:

- Ex-post analysis. These take output from the energy optimization to perform the LCA for specific technologies [58,59], specific sectors (power [46,60,61], heating [62]) or a global level [16], but do so to assess the environmental impact and lack the interaction with other parts of the energy system since there is no feedback to the results. In most of the cases, evaluations are static in time and do not consider the dynamic effect of technology improvements.
- Monetization. When emissions have been considered in the objective function, this has been done through monetization of externalities. The compromise for this set of studies is that the focus has been on air pollutants rather than total emissions and impact across categories. A relatively explored area is power models

[63–72], most of which have built upon the effort done in NEEDS [73] and ExternE, with applications also on a global level [74]. There are also examples of the applications of this approach to energy systems [22,23,75–77], heating [78] and buildings [79]. There are also efforts in the direction of co-benefits of climate change and air pollution [22,23,80]. The clear advantage of this approach is the feedback to the optimization problem and influence on technology mix, while the compromise is uncertainty in the monetization step, that they follow the damage cost approach (as opposed to a detailed pathway analysis which would include dispersion, fate, concentration and vulnerability of the local environment) and the neglect of other impacts (e.g. water, land). There is one case [51] that already includes the monetization of two impact categories (climate change and human health) and not only the pollutants. A variant of this approach is to expand the GHG emissions to life cycle and analyze how it affects the system cost (due to the extra emissions) [80].

- Multi-Objective Optimization. The uncertainty associated to monetizing externalities can be decreased by considering the environmental dimension as a separate objective. This is the approach taken in Multi-Optimization problems [50,81–84]. The compromise is that the focus is on the trade-offs between the objectives (e.g. weighing) with only CO_2 (or GHG) emissions considered and disregarding other impact categories. Even if LCA emissions are used [50,84], this has been only for GHG emissions rather than all the LCA indicators. Similarly, it carries a higher model complexity and evaluations have been limited to power.
- Multi-criteria decision analysis (MCDA). Similar to the above, but also including qualitative aspects, such as risk, resource, social and political drivers. The compromise is that the environmental part is neither considered through representative indicators (e.g. land use, water footprint) [85] nor that the LCA component feeds back to the energy model [13,49]. In this category, there are also studies [48,86,87] that assess the environmental dimension (of the electricity sector), but without including a modeling (optimization) component as part of the study. An advantage of this approach is the wider set of dimensions covered and the holistic policy input including qualitative aspects. A limitation of this type of study is the weight allocation to each objective and how to choose the solution from the Pareto frontier.

From the above review, the two options identified from literature that have been used to endogenize LCA in ESM are monetization and multi-objective optimization. A third approach is to introduce constraints to set maximum impact levels for the various environmental categories. This will ensure achieving a minimum improvement over time. A difficulty arises on the targets to set to ensure an improvement without causing unnecessary additional costs. No example of this approach was found in literature.

2.2. Lessons from similar models to ESM

ESM are partial equilibrium models and do not consider the interaction with macro-economy unless they use the price elasticity of demand [20]. Input-Output are models that capture the economic flows of the society including production, consumption, employment and import/export [57]. The I/O model establishes the relation between processes along specified pathways, while the LCA provides the inventory for each process leading to a hybrid approach called Environmentally Extended Input-Output (EEIO). EEIO allow calculating the impact for entire sectors or for the entire economy rather than focusing on specific processes [88]. The combination of macro-economic models and bottom-up models is relatively common [55,89,90]. However, the combination of EEIO with bottom-up models remains limited to few examples [43,91–94].

Integrated Assessment Models (IAM) are similar to ESM since they can also use cost optimization, can be technology-rich and do not cover

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[2] Cradle to grave refers to emissions in mining, transport, manufacturing (upstream) and disposal and decommissioning.

Table 1
Overview of literature review on Life Cycle Assessment of PtM systems.

Ref.	CO₂ source				Electricity source				Operation mode		Functional unit	Key conclusions
	Power	Biogas	Cement	Air	Wind	PV	EU mix	Threshold	Full	Partial		
[107]	x	x			x	x	x	x	x	x	Produce 1 MJ of CH₄ (LHV)	Global Warming Potential (GWP) of electricity used for PtM has to be lower than 113 gCO₂eq/kWh to be more attractive than fossil gas
[36]	x					x	x	x	x	x	Produce 1 MJ SNG/0.049 kWh electricity	GWP of electricity used for PtM has to be lower than 80 gCO₂eq/kWh to be more attractive than fossil gas for steady state operation and lower than 48 gCO₂eq/kWh for partial load operation
[109]	x	x				x			x		Use 1 MWh of power surplus	CO₂ use only contributes to global warming impact reductions if the CO₂ supply avoids emissions. If CO₂ is used which otherwise would be stored, GHG emissions even increase
[105]	x				x	x	x		x		Satisfy 1 km with CNG/1 kWh of input to electrolysis	PtM effect depends on where the boundaries for the system are defined
[106]¹	x		x	x	x	x	x		x		Produce 1 MJ of CH₄ (HHV)	Use of PV as electricity source can actually lead to a GWP increase compared to conventional gas. Biogenic and atmospheric CO₂ lead to the largest decrease
[110]	x			x		x	x		x		Produce 1 MWh of heat with SNG combustion	Synthetic gas has higher potential impacts than the combustion of conventional Swiss natural gas under all impacts, even with the biogenic carbon origin of emissions
[111]	x						x		x		Produce 1 MJ of CH₄ (LHV)	Using EU electricity mix (560 gCO₂eq/kWh) results in a PtM footprint higher than conventional gas, while the opposite is true when a French mix (100 gCO₂eq/kWh) is used

¹ Concentrated Solar Production, Hydro and electricity surplus were also evaluated as electricity sources.

other impact categories (e.g. toxicity) [95]. The main difference is that existing IAM also cover global carbon cycle, land use, other non-CO₂ GHG, temperature dynamics and a global economy description to assess the marginal welfare costs of emissions [96,97]. The emergence of IAMs was based on the need for representing the dynamics between humans and the environment. Therefore, the extension to LCA is a natural step to cover materials, energy and resources use across different sectors to add to the integrated approach. This gap is also being closed [37,98], but because this type of model is different from energy system models (although both types are engineering, economic and environmental models), a detailed discussion has been left out and the reader is referred to [97].

A lesson from IAM is that there already is a methodology proposed to decompose the LCA coefficients into life cycle stages and energy carriers use by industries [98]. This aids LCA integration to IAM by facilitating data manipulation and consistency in background inventory. The approach has already been applied to scenario modeling for the power sector [99]. An insight from EEIO is that these also have the geographical boundaries and allow quantifying the ratio of direct emissions within the studied region and indirect emissions due to imported materials. Issues EEIO have in common with ESM are dealing with double counting when the level of segregation is not the same in the I/O model and ESM or the lack of standardization to match the processes from ESM to the corresponding I/O sector [91].

2.3. Common issues when combining LCA and ESM

Some of the common issues identified across previous studies [42] are reported below, while the way to tackle them in the current study is described in Section 3.

- Double counting. This issue can arise in three ways. 1. When expanding to LCA, there will be additional energy and material demand for upstream processes (e.g. mining and manufacturing). This demand might already be part of the final demand for the model. Therefore, adding this life cycle demand on top of the final demand could lead to double counting; 2. Some processes use input from another one that is part of the model (e.g. a heat pump using electricity). If the entire LCA is used for all the processes, there would be a double penalty (i.e. electricity would be counted on the production and consumption ends); 3. When using EEIO tables complemented by process-based LCA. For this, only direct and "gate-to-gate" emissions should be used from the process-based, since the indirect ones (e.g. infrastructure, chemicals, materials) are already accounted for in the EEIO framework [94].
- Import, export and emissions target. CO₂ (GHG) targets are usually set for direct emissions within a region. Energy and CO₂ for imported goods and commodities are not included. These can be significant (e.g. 60% of the total emissions for UK in 2050 [91] or more than 50% on a global level [99]), expanding to LCA and including these emissions can have a large effect over the cost (it can double the carbon price for the same target [91]).
- Spatial differentiation [100]. Some of the impacts are global (e.g. global warming), while others are local (e.g. soil pollution) [10]. For the local ones, conditions like population density, susceptibility and weather will affect the dispersion, fate and effect of pollutants. Ecoinvent aims to make a differentiation by country of the impacts. However, it lacks of it for many processes [101] making the use of global values necessary.
- Temporal differentiation [102]. When emissions are monetized, these are usually discounted and traded-off with the rest of the costs. This implies that future impact has less weight than closer one, which is not necessarily applicable to environmental values.
- Biomass emissions. Not all the models cover land use change as part of their scope and the impact for biomass depends directly on assumptions rather than on modeling output.

- Multi-functional (multi-output) processes. This can be an issue when matching processes between LCA and the energy model and allocating the impact. This is dealt by using an energy-based allocation [7,103,104] and using changes in efficiency for changes in the ratio among the streams.
- Future performance of technologies. Some studies consider a learning curve for immature technologies through higher efficiency (and lower fuel consumption or higher output). However, the effect across all the life cycle stages remains highly uncertain.

2.4. LCA of power-to-methane

An overview of the key studies for PtM LCA is shown in Table 1. Some key findings from these literature sources are:

- Synthetic CH_4 from a PtM system shows the highest greenhouse gas emission benefit if biogenic CO_2 sources are used for methanation [105,106] and if the hydrogen used is produced via renewable electricity driven electrolysis [106].
- Higher load hours for PtM will lead to larger greenhouse gas benefit [36].
- The largest contributor to the environmental impact of PtM is the electricity source [36,105,107,108].
- Transport distance of the produced gas has a direct effect on the environmental impact. Longer transport distances require more energy for compression and subsequently higher greenhouse gas emissions [105].
- If the CO_2 used for PtM was supposed to be stored underground, a negative value would be required to make PtM the preferred option) [109].
- If there is power surplus, the best use from an environmental perspective is to satisfy heating demand (power to heat through heat pumps). This is followed by transport (electric cars), direct electricity storage (e.g. batteries) and the last alternative is the conversion to another energy carrier [109].
- Benefit for new technologies will highly depend on the reference processes [107,109].

An area where a trade-off is necessary with the economic dimension is the operating hours. From the economic perspective, these hours should be as high as possible to be able to reduce the CAPEX contribution to the production cost. However, more operating hours mean operating with the electricity from the grid rather than only VRE. Gaps that remain from these studies are:

- Integration of LCA and energy systems modeling. Most of the studies focus only on the electrolysis, methanation and CO_2 capture system with a functional unit of 1 MJ or MWh of output. Nevertheless, the actual effect of the technology will depend on the energy and technologies being displaced, given that with lower environmental impact of the initial system, the lower the benefit for PtM will be. Thus, the interaction with the rest of the energy system for alternative future scenarios has not been explored.
- Single reference comparing all possible PtM pathways. Most of the studies cover specific pathways (e.g. transport [105]) or miss some of the downstream applications for the methane.
- Temporal and spatial differentiation. Consider the different electricity mix for various regions and periods of the year in a single study.
- Expansion to other indicators besides climate change. Most studies focus on CO_2 emissions and climate change. Only [109] and [36] using ReCiPe 1.08 explore 11 and 14 impact categories respectively to estimate the impact of the methane produced. While [110] uses ILCD 2011 to estimate the impact across 9 categories. Using other categories such as land use or water consumption would allow comparing PtM with pumped hydro storage (competing technology

for energy storage) or biomass gasification for power generation (competing technology for balancing the power system).
- Consideration of future efficiencies. Since the largest contribution to PtM LCA is the electricity mix, the technology efficiencies (both electrolysis and methanation) are important. At the same time, electrolysis and methanation are not yet in full commercial scale, there is learning and research that will improve the efficiency (and cost) and this uncertainty should be considered in the LCA.
- CO_2 allocation methodology. When PtM is introduced in the system, the RES fraction will be larger, either because curtailment is reduced or because when the energy is released from the storage is displacing a conventional technology (with a higher environmental impact). A question remains on how to allocate the CO_2 benefit among the different components of the system. This allocation can be based on energy, exergy, economic value, among others. This step would include quantifying the difference with the different indicators.

From these gaps, the ones addressed within this study are the consideration of the PtM interaction with the rest of the energy system, the temporal and spatial differentiation of the electricity used for PtM, the use of the methane produced for all the applications (captured in JRC-EU-TIMES), the consideration of 18 impact categories and the use of efficiency improvements for both electrolysis and methanation (also captured through JRC-EU-TIMES).

3. Methodology

This section goes through the overall procedure followed, assumptions and solutions to the common issues when integrating LCA into ESM. Further information is provided in Appendix 1.

3.1. Overall procedure

The procedure includes expanding the processes in JRC-EU-TIMES to a full life cycle perspective by considering construction and end-of-life stages and to a broad range of impact categories besides climate change caused by CO_2 emissions. The general framework for the methodology is shown in Fig. 1 followed by a brief explanation of the main steps.

Fig. 1 shows the two main elements of this study: ESM and LCA. ESM have the general structure of resources (with potential and price curves associated) used to satisfy final demand services through primary (e.g. power) or secondary (e.g. heat pumps) conversion processes. Multiple policies can be introduced as constraints. The typical output is the energy balance, cost breakdown and technology mix needed. The information used from JRC-EU-TIMES for the LCA is mainly: (1) static, related to using efficiency, lifetime and capacity factors used to modify the original inventory from the databases and needed to ensure consistency; (2) scenario-dependent (orange box in Fig. 1) that are combined with the life cycle inventory to estimate the environmental impact. In this study, there is no feedback from LCA to the optimization process. The main methodological steps followed are:

(1) Reduce number of processes from JRC-EU-TIMES to facilitate inventory collection (see Section 3.4.1)
(2) Identify entries from the LCA database that are closest to the processes screened (see Section 3.3.2)
(3) Complete LCA data with alternative sources and individual studies from literature review (see Section 3.3.2)
(4) Harmonize data between JRC-EU-TIMES and LCA. This refers to taking TIMES data for efficiency, capacity factor and lifetime and modifying the LCA data, which allows considering the improvement in time and add the dynamic component to LCA
(5) Adjust LCA datasets to avoid double counting (see Section 3.4.2) for upstream emissions that are also part of JRC-EU-TIMES scope
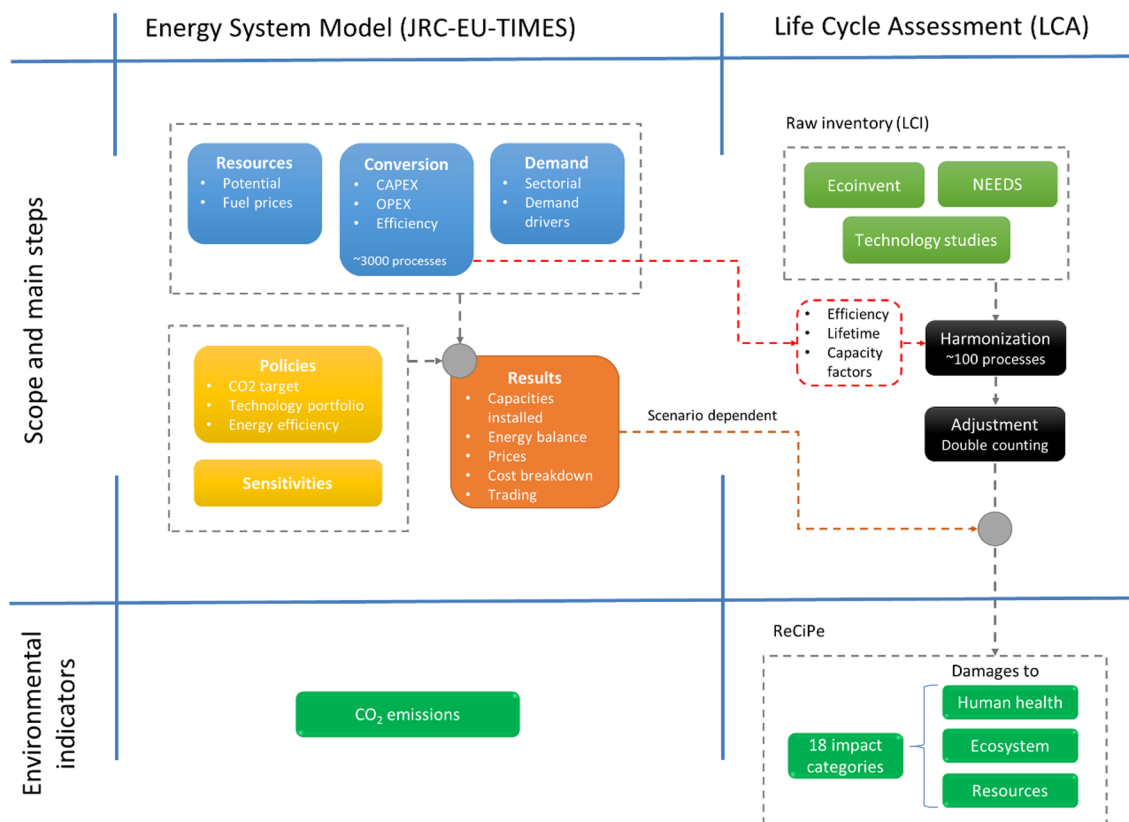(6) Run set of defined scenarios with JRC-EU-TIMES (see Section 4)

Fig. 1. Framework for integrating LCA and energy modeling followed in this study.

(7) Extract activity (production level) and capacity for -selected technologies in Step 1 from JRC-EU-TIMES

(8) Calculate LCA mid-point indicators for each scenario

(9) Understand drivers for changes across indicators and run additional scenarios for confirmation.

3.2. Energy model description

For this study, JRC-EU-TIMES is used [29–32]. This model is an improved version of previous European energy system models developed under several EU funded projects, such as NEEDS [73], RES2020 [112] and REALISEGRID [113]. The current version underwent an extensive validation process in 2013 through the involvement of several external modelers and representatives of several Commission services [29]. Since then, it has been developed further including the development and analysis of Power-to-X pathways [33,114]. The geographical scope is EU28 plus Norway, Switzerland and Iceland (henceforth referred as "EU28+"), with one node per country. Its temporal scope is from 2010 to 2050 (although it can be used beyond this timeframe) with a time resolution of up to one hour. To reduce the calculation time, it uses time slices that represent periods with similar supply and demand patterns. There are 24 time slices for the power sector and 12 for other sectors (4 seasons and 3 periods of the day). It covers 5 sectors (residential, commercial, industry, transport and agriculture). TIMES [115–117] is one of the most widely used energy models [118], this specific version has a EU coverage and will not draw conclusions based on a specific region and because this version is technology rich in both the supply (generation) side, but also on the demand side.

The model uses price elasticities of demand to capture part of the macroeconomic feedback (change in demand as response to price signals), which allows transforming the cost minimization to maximization of societal welfare. Stages of the life cycle that are covered are: mining (energy and emissions for extraction of resources), operational

(e.g. energy efficiency and conversion losses), combustion (heat and power generation or for chemical conversion). Emissions outside EU due to imported goods, materials or commodities is not included as part of the CO_2 target. Coverage of asset cycle does not include construction or decommissioning since their contribution is negligible when compared to the operational and combustion for conventional technologies. The model has been used in the past to assess the role of hydrogen [114] and Power-to-Methane [33].

It includes biomass potentials for woody biomass, agricultural crops, biogas, municipal waste and biosludge. The range for total biomass potential in EU28+ is between 6650 and 21,860 PJ for all categories without considering imports [119]. The model uses technology learning curves with improvement of efficiency over time, which will in turn affect the operational emissions. It covers all the materials demand (e.g. steel, cement, copper, aluminum, see [29] for more detail). This demand is exogenous and it is not affected by endogenous variables (other than through elasticity and prices). The model focuses on CO_2 and does not include other greenhouse gases (CH_4, N_2O). It does not include pollutants (particulate matter, NH_3, SO_2, volatile organic compounds, NO_x). The CO_2 emissions covered are from fuel combustion in the downstream applications, which is ~77% of the total GHG emissions for EU (3390 $MtCO_2$ [120] vs. 4427 $MtCO_{2eq}$ [121] for 2014).

There has been no attempt for multi-criteria optimization (given the model complexity), nor the model output has been used so far for Cost-Benefit Analysis or MCDA. No externalities are included as additional costs and environmental aspect is mainly through constraints to reduce CO_2 emissions and primary energy consumption. Previous versions of the JRC-EU-TIMES model included monetized externalities for the most important emissions and materials [64].

3.3. Life cycle assessment

LCA is an established methodology [8,122]. It covers 4 phases: goal
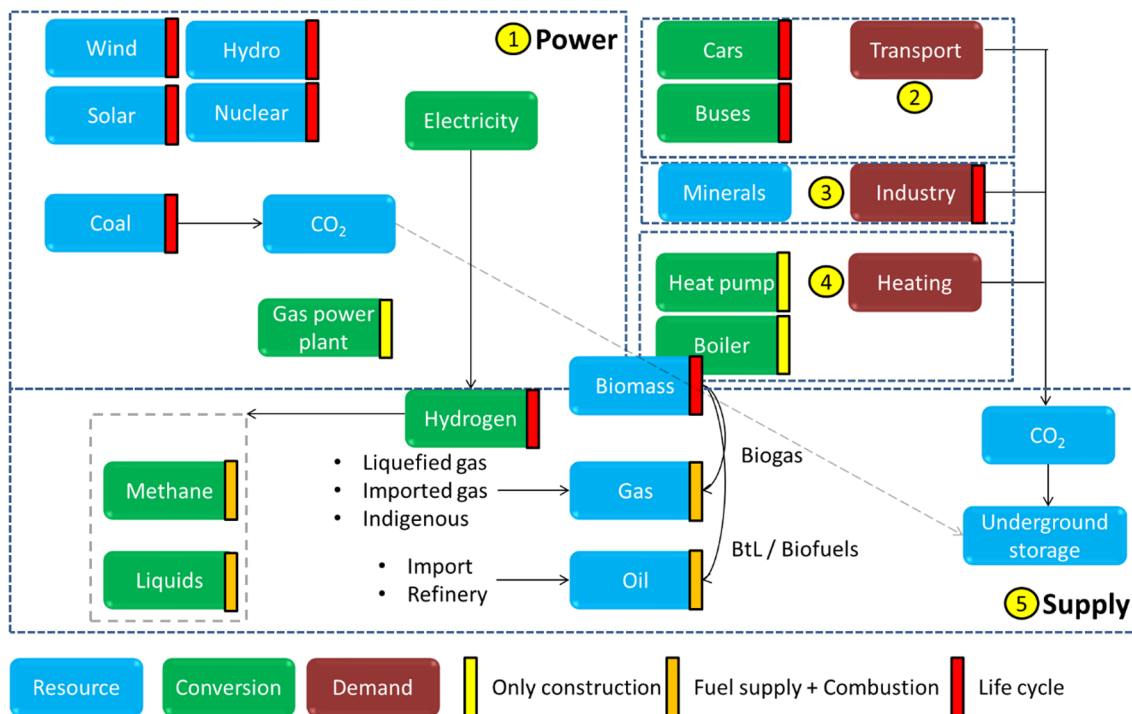
Fig. 2. Boundaries to assess environmental impact of each energy sector (some connections have been omitted for simplification. For example, gas, electricity and hydrogen can be used in almost all downstream applications).

and scope definition, inventory analysis, impact assessment and interpretation. It is based on the input-output (energy, materials and emissions) of every stage of the life cycle.

3.3.1. Goal and scope definition

The study has been conducted following the standard structure of LCA studies defined in ISO standards 14040/14044 [8,122]. The study has two main goals: 1. To assess the environmental impact across a range of categories for a future EU energy system that achieves 80 to 95% CO_2 reduction by 2050 (vs. 1990) in EU; 2. To assess the environmental impact PtM has in the system and the potential consequence of not having the technology available. The functional unit is not the production of a specific product or commodity, but instead, following a similar approach as [123], is defined as the satisfaction of all the energy and services demand (including residential, commercial, industry, mobility and agriculture) in EU28 by 2050. To facilitate the understanding of the results and identify trends across sectors, the impact has been allocated to sectors. The system boundaries for each sector of the five sectors considered are illustrated in Fig. 2.

CO_2 has a more complex set of sources and sinks [33], but it can come from biogenic sources, air or from any of the sectors. The CO_2 in PtM will eventually be released, leading to biogenic or direct air capture being more attractive CO_2 sources. The use of fossil CO_2 could make sense for the transition phase (e.g. to scale up technology), but should be limited in a low-carbon future. Other sources on non-avoidable CO_2 (e.g. cement) could be considered since they will be emitted anyway regardless of the use or not for PtM. Ultimately however, those CO_2 emissions will also have to be abated (e.g. CCS for the case of cement). Processes for secondary conversion (e.g. heat pumps) have been used for representation, but the complete list of processes can be found in Table SI 1. Most of the CO_2 emissions are accounted for in the "Supply" sector, except for coal, which has the CO_2 emissions in the power sector. The reason for this distinction is that gas and liquid have a network with multiple sources (scenario dependent) that can have a different environmental impact, while coal is assumed to have a single source. For biomass, the impact is allocated to its users since there is no

equivalent network (as in gas or liquid) and each user is linked to a specific type of biomass.

Gaseous fuels can come from natural gas (imported or indigenous), liquefied, biogas, Power-to-Methane [33], while liquid fuels can be imported, product of refineries, synthetic fuels through Fischer-Tropsch or methanol, biofuels or Power-to-Liquid [114]. Depending on this source, the environmental impact of the fuel production stage will be different. At the same time, when the carbon contained in the fuel ultimately comes from air (e.g. biomass or PtX with a biogenic source), the impact for CO_2 emissions during combustion is much lower. To account for this: (1) the combustion emissions have been subtracted in all the processes (e.g. cars or power plants); (2) a gas/liquid supply has been calculated considering the supply mix for each scenario (from JRC-EU-TIMES output) and a representative life cycle entry for each source; (3) assign neutral CO_2 emissions for fuels using biogenic sources (reference biomass potential is 10 EJ/yr, which assumes no land has to be transformed to produce this amount causing no upstream land use change emissions [119]). This approach also includes indirectly the efficiency improvement in time for the various technologies since this would translate into lower fuel consumption seen in the overall fuel balance.

Upstream processes in both the asset cycle (i.e. construction and manufacturing) and the fuel cycle (production/extraction) are included as part of the assessed system in spite of occurring in many cases outside the geographical scope of the demand. In terms of energy consumption, the data includes upstream processes (e.g. mining of resources and raw materials, fuel processing, transport) and downstream processes (operation, transmission, distribution). In terms of materials use, the scope only includes only the construction phase and not the decommissioning and subsequent waste management. The reason for this is that the circular economy strategy, which includes waste treatment and critical materials, is clearly defined for 2030 [124], but it is difficult to assess its evolution to 2050. Since this could introduce more uncertainty and it is not the focus of this study, this stage has been excluded.

3.3.2. Inventory analysis

The Life Cycle Inventory (LCI) phase provides the balance of resources and emissions upon which the assessment will be calculated. For this study, process-based data is used (from Ecoinvent database v3.3) [125], while the relation with upstream and downstream processes is provided by the energy model (e.g. the impact of a gas boiler is not fixed, but dependent on the gas source that comes from JRC-EU-TIMES). Therefore, this overcomes a limitation of process-based LCA by widening the boundaries and a limitation of the EEIO approach by maintaining the technological detail. Allocation at the point of substitution is used. This system model subdivides multi-output activities by physical properties, economic, mass or other properties allocation. By-products of treatment processes are considered to be part of the waste-producing system and are allocated together. Markets in this model include all activities in proportion to their current production volume. This model was called "Allocation, default" in Ecoinvent version 3.01 and 3.1.

As complementary databases for power technologies (e.g. with carbon capture and storage, CCS), NEEDS[3] (New Energy Externalities Development for Sustainability) and CASES[4] (Cost Assessment for Sustainable Energy Systems) were used. An advantage of NEEDS is that it has a wider range of technologies, while a limitation is that only the total life cycle inventory (input-output for entire activity) is provided and no segregation can be done between the construction and the operational components. However, since the database is mostly used for fossil technologies, which have a much larger impact contribution from the operational phase, the need to split the impact in construction and operational phases is less motivated. The dataset also provides fuel consumption, which allows estimating efficiency and modifying accordingly the process LCI to capture the improvement in time.

Other data sources included demo sites in the Store & GO project [126] for methanation and [127] for an alkaline electrolyzer. The RENEW project was used for Biomass-to-Liquid [128,129], as well as for the inventory of the Fischer-Tropsch reactor and downstream processing for Power-to-Liquid [130]. For vehicles, the GREET database from Argonne National Laboratory [131] was used since it is available online and has the complete material requirements for the vehicle and various types of battery. One limitation of Ecoinvent is that the wind turbines available are relatively small size (up to 4.5 MW for onshore and 2 MW for offshore), while already today there are 10-MW turbines available.[5]

The inventories were corrected when possible to account for potential improvements in efficiencies and upstream emissions associated to equipment production (see Section 3.4.3). This also corrects the major material consumption for technologies like wind and solar. However, for biomass no changes in cultivation methods, spatial differentiation of land, land productivity and alike were considered.

3.3.3. Impact assessment

The pollutant emission and resource consumption inventories (i.e. LCI) of the system were translated into impact indicator scores using the life cycle impact assessment (LCIA) methodology ReCiPe 2008 v1.11 [132]. The reasons for this choice are that it combines a framework with midpoint and endpoint indicators; it was the result of combining the strengths of the previous approaches and the harmonization of modeling principles and choices; it also covers a broad range of environmental problems through its 18 midpoint indicators. The perspective used was hierarchical, which is in between the short-term interest of the individualist perspective and the egalitarian one which is more precautionary.

3.4. Simplifications and assumptions

Below is the explanation of how the main issues have been dealt with, while some specific assumptions and remaining limitations have been included in Appendix 1.

3.4.1. Selection of representative technologies

JRC-EU-TIMES covers over 3000 individual processes (including import, mining, duplication for fuels), which represent over 450 technologies. To reduce the effort of the LCA data collection step, the number of technologies has been reduced by:

- Only processes that have significant ($> \sim 1\%$) contribution to CO_2 emissions of their specific sectors across a wide range of (screening) scenarios (over 100 different ones, see [33,114]) were considered. This assumes CO_2 emissions are representative of climate change impact and its relation with other impact categories. This has proven to be the case for urban systems [133] with the lowest correlation for processes that emit toxic substances. However, this is only an approximation and further refinement in this area is needed [134].
- Selection of representative processes. For example, JRC-EU-TIMES has 10 technologies for gas turbines (variations of open cycle, combined cycle and carbon capture for conventional, industrial applications and advanced versions of the technology). These were reduced to only 3 technologies: open cycle (peak contribution), combined cycle and one with carbon capture.
- Fuels simplification. A large part of the residential and commercial heating demand is satisfied with boilers and heat pumps. JRC-EU-TIMES has over 40 different processes to satisfy space heating (variations for air, ground heat pump, combination with water heating, condensing type, position, among others). The overall heating and cooling technologies were narrowed down to 12 entries for LCA data assuming for example that a liquefied petroleum gas boiler has a similar footprint than a natural gas boiler (with respect to impact of the asset cycle). This was done based on the technical similarities and applications.
- Aggregation of value chains. Some industries (e.g. aluminum, chlorine, cement) involve several processing steps until the final product is obtained. Instead of assessing the impact for each of these steps, the entire value chain has been grouped and the impact is related to the material produced.

After this process, the 450 original technologies were reduced to 100 representative entries. The list of processes can be found in Table SI 1.

3.4.2. Double counting

A potential issue is double counting. Two different variations can occur. One is the overlap between material demand for an industry and potential material consumption from the construction stage. The other is the case where the life cycle inventory for one process includes energy flows from processes that are already within the boundaries established in JRC-EU-TIMES. An example of the former is the cement needed for constructing wind turbines and if that demand is already accounted for in the final material demand, it should not be added on top. An example of the latter is electrolysis, which has most of its impact defined by the electricity source [135,136]. Since its electricity demand is already part of the power sector, it is not accounted for in the "supply" sector. An alternative view to the same problem is that either the impact or the (energy/material) demand for upstream processes should be accounted for (see an illustrative example in Appendix 1).

For processes without direct emissions, the contribution for the feed is removed from the process, since the commonly indirect emissions will be covered as direct for other processes included in the model. Furthermore, since the emissions for these processes (without combustion) are only for the asset cycle (i.e. construction), impact is

expressed per unit of installed capacity (rather than energy flow). Expressing the impact in terms of capacity also eliminates the need to harmonize the capacity factors for wind and solar, which will be different for every country and are already implicit in the calculated installed capacity from JRC-EU-TIMES.

3.4.3. Interaction between industry and power sectors

Extending the analysis to a full life cycle perspective, leads to additional demand of energy and materials. This could be fed back to the demand in JRC-EU-TIMES. Nevertheless, this contribution is expected to be small compared to the total demand and the feedback from background processes was not implemented. As an example, from an initial estimate, the consumption (steel and concrete) for wind turbines is between 1 and 2% of the demand for these materials in 2050. Even without considering that more than 90% of steel can be recycled once the turbines are decommissioned [137] and can lead to halving the GHG emissions embodied in the wind turbine [138]. Previous exercises [43] have shown that this contribution is in the order of 0.05–0.5% of the demand. This order of magnitude does not justify the effort of including this demand as endogenous. Furthermore, the original material demand already assumes implicitly the deployment of new technologies [139].

The usually indirect emissions (or background processes) from industry are accounted for as direct emissions from the electricity sector, since electricity and heat demand for industry is included in the model. To account for this, the electricity impact and the fuel supply chain have been subtracted from the industry impact. An advantage of this approach is that demand for both electricity and industry sector come from the same model (i.e. JRC-EU-TIMES) rather than from different models (which could lead to additional inconsistencies [54]). A similar approach to the above has been followed for renewable electricity technologies without direct emissions (i.e. wind and solar) where the electricity impact has been subtracted from the manufacturing stage. See Appendix 2 for the contribution electricity has across impact categories for wind and solar.

For vehicles, GREET database has the material requirements for the vehicle and battery [131]. This allowed making the relation with the industry sector in the model (steel, aluminum, copper and glass) and corresponding reduction in CO_2 emissions depending on the scenario, assuming that the reduction in impact for other categories decreases proportionally to climate change. For plastic and composite materials a reduction of 72 and 85% was assumed for 2050 based on [140]. Considering these reductions, the climate change impact of the vehicles can be reduced by an average of 60%. Aluminum and plastic are the most important materials in conventional vehicles with around 40% of the

impact (only deviating for FCEV, for which their contribution is ~20%). Carbon fiber constitutes 60% of the impact for lightweight vehicles (see Fig. SI 3). Furthermore, the impact for vehicles is computed without accounting the impact of the electricity consumed in the production step. FCEV is still in its early levels of deployment (almost 7200 FCEV at a global level [141]), so the uncertainty in its environmental impact is the highest [142].

3.5. Consequential analysis for PtM

The information used from JRC-EU-TIMES output to estimate the PtM impact is: (1) electricity mix; (2) CO_2 source and (3) impact for steel, cement and copper. The electricity mix largely defines the environmental impact of PtM in cases where electrolysis is used for hydrogen production [36,105,107,108]. Output from JRC-EU-TIMES has the electricity mix differentiated by: (1) scenario; (2) country and (3) time slice. The model covers 31 regions and 12 time slices (372 combinations for each scenario). Specifically for the power sector, each time slice is further sub-divided in a period of pure VRE surplus and one where the rest of the technologies can contribute to satisfy demand. For the construction component, the total impact by country and scenario is calculated and allocated by time slice proportional to the length of each one [29]. The CO_2 used for methanation comes mainly from biomass (either gasification for hydrogen or Biomass-to-Liquid – BtL – [33]). Therefore, it is considered that the CO_2 emissions upon combustion of the synthetic gas are neutral and for this consequential analysis the upstream emissions for biomass production and collection are outside the boundaries. This is different for natural gas, where the CO_2 from the end use will be positive.

4. Scenario definition

Six scenarios were analyzed and divided in two sets (see full description in Table 2). One set (first four scenarios in Table 2) is meant to analyze how the indicators change across alternative low carbon futures by varying parameters that have a widespread impact over the system. The other set (last two scenarios in Table 2) varies parameters that will have a more specific effect over PtM. From previous studies [33], the variables having the largest impact over the system are the CO_2 reduction target and limitations for CO_2 underground storage, while for PtM it is a higher process efficiency (leading to heat recovery) and direct technology subsidy combined with a low Capex and higher Variable Renewable Energy (VRE) potential that leads to a larger need for flexibility in power.

These are technical scenarios which consist of using ranges and

Table 2
Description and reasoning for scenarios explored.

Name	Description	Justification
80	80% CO_2 reduction[1] vs. 1990 by 2050 [143]	Target is an intermediate point between ambitious targets (ultimately leading to zero emissions) and current energy system, which will allow identifying trends and critical technologies
80_NoCCS	Same as above, but without possibility of CO_2 storage	CO_2 is not widely spread and could face political and social resistance that prevent its deployment
95	95% CO_2 reduction vs. 1990 by 2050	Allows evaluating changes for deeper decarbonization and identifying the areas with the largest impact in high renewable scenarios
95_NoCCS	Same as above, but without possibility of CO_2 storage	Similar reasoning as above with the extra information of different CO_2 storage effect with lower carbon scenarios
95_Optimistic	Same as above, but with additional system and technology drivers that favor PtM deployment[2]	This establishes an upper bound for PtM capacity and its environmental impact and will allow identifying its effect over the rest of the system, also when making the comparison with a less constrained scenario (e.g. 95_NoCCS)
95_Optimistic_NoPtM	Same as above, but PtM is not part of the technology portfolio	This quantifies the regret cost in terms of environmental impact for not developing the technology. It is the maximum penalty that can be incurred since it has the largest PtM capacity

[1] As mentioned in Section 3.4 this target does not cover background processes for imports, construction and decommissioning.
[2] Low (75 €/kW) Capex (only for methanation), low biomass potential (7 EJ/yr), high gas price (almost 20 €/GJ by 2050), high cost for the electricity network, high PtM efficiency (> 85% including heat recovery), high electrolyzer performance (400 €/kW and 86% efficiency), low PtL performance, SOEC possible and high LMG efficiency in ships, see [33] for more details.
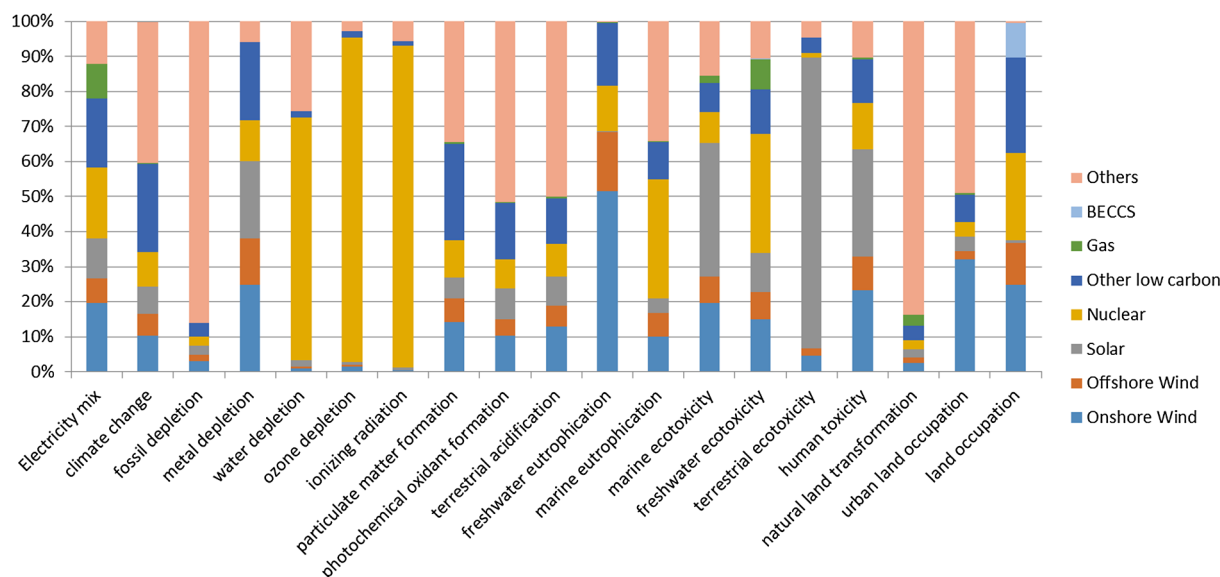
Fig. 3. Impact for the power sector by category and technology in the *80* Scenario (EU28 +).

different values for the input, but not making complete storylines to represent the future [144–146]. The scenarios analyzed in this study are both normative and exploratory [147,148]. Normative since the technologies chosen will reach the CO_2 target constraint, but exploratory in terms of what the choices are to reach this target with different technologies available. These constitute the quantitative part of a scenario analysis. The relation between the input used and dynamics between technical, political, economic, social drivers that could lead to such conditions has not been done.

5. Results

The results are divided in two main sections describing the environmental impacts across categories for the various scenarios and sectors in 2050 (Section 5.1); and the environmental impact of Power-to-Methane compared to natural gas and impact of not having the technology available (Section 5.2).

5.1. Environmental impact from the energy system

This section starts by analyzing the contribution of the each sector (power in 5.1.1 and other sectors in 5.1.2), then comparing across scenarios (5.1.3) and then quantifying the indirect emissions added by LCA and putting them in perspective with the direct emissions from JRC-EU-TIMES (5.1.4).

5.1.1. Environmental impact from the power sector

The least ambitious scenario (and closest to current system) is the scenario with 80% CO_2 reduction. The relative contribution by impact category and technology group for the power system is shown in Fig. 3.

For gas-based technologies, only the contribution of the construction component is accounted for in the power sector since the operational emissions are part of the "supply" sector (see Section 3.3.1). For all the other technologies, the operational emissions are included. For climate change, almost 40% of the impact is due to coal. In spite of being used in combination with CCS, its emissions are still relatively high (~100 gCO_{2eq}/kWh). It produces almost 600 TWh of electricity (see Fig. SI 4), leading to 60 $MtCO_2$ produced. This is still optimistic since CO_2 emissions from coal with CCS can be twice as high [149,150]. Two main reasons for still having coal in the mix by 2050 are: (1) this scenario has CCS, which allows reducing the net CO_2 emissions; (2) the price ratio between gas and coal. In case coal is either banned or more

expensive, it would be mostly replaced by gas and the operational emissions would be displaced from the power to the "supply" sector (see Fig. SI 5 for the impact profile without coal). In spite of the large capacities for wind and solar (630 and 520 GW respectively), their combined contribution is only 25% of the total CO_2 emissions from the power sector. The rest of the climate change impact is due to hydropower (15%) and geothermal (< 5%). The total emissions from the power sector are ~135 $MtCO_{2eq}$/yr, considering the high electrification rate that leads to a total production of 5200 TWh, it results in specific CO_2 emissions for the electricity of ~24 gCO_2/kWh. To put these numbers in perspective, the CO_2 target of 80% reduction, translates into total (for the entire system) CO_2 emissions of 914 $MtCO_{2eq}$/yr. The CO_2 emissions from combustion in the power (and heat) production were reported to be over 1000 $MtCO_{2eq}$ in 2016.[6] Considering the total gross electricity production was 3250 TWh for the same year,[7] the average EU emissions are ~310 gCO_{2eq}/kWh.

The two largest contributors to water consumption are nuclear and coal (with CCS). These consume on average 3.1 and 2.2 m^3/MWh of water respectively (data from Ecoinvent). This is in agreement with literature [151], where the range for 6 different studies was 1.9–5.0 m^3/MWh for nuclear (wet tower and excluding the "high" from [152]), while IGCC (integrated gasification combined cycle) with carbon capture had a range 2.2–2.6 m^3/MWh. Among other renewable technologies, geothermal and CSP have a relatively high water consumption (1.9 m^3/MWh for enhanced geothermal system with dry cooling and 3.8 m^3/MWh for CSP with cooling tower). However, since their relative contribution to power generation is small (125 and 0 TWh respectively for this scenario), the impact over the total water footprint for the system is small. The largest technologies in terms of capacities are wind and solar (1150 GW combined), but since their water footprint is relatively small (< 0.01 m^3/MWh for wind [152,153] and ~0.1 m^3/MWh for solar [154]), they represent less than 4% of the total footprint. The average for the entire power system is 0.8 m^3/MWh.

For land occupation, hydropower is the largest contributor (25%), along with onshore wind (25%). In spite of being less than 4% of the electricity production, biomass gasification combined with CCS contributes with almost 10% of the land impact (using wood). This is considering an impact of 1100–1400 m^2/GWh for onshore wind (sum of
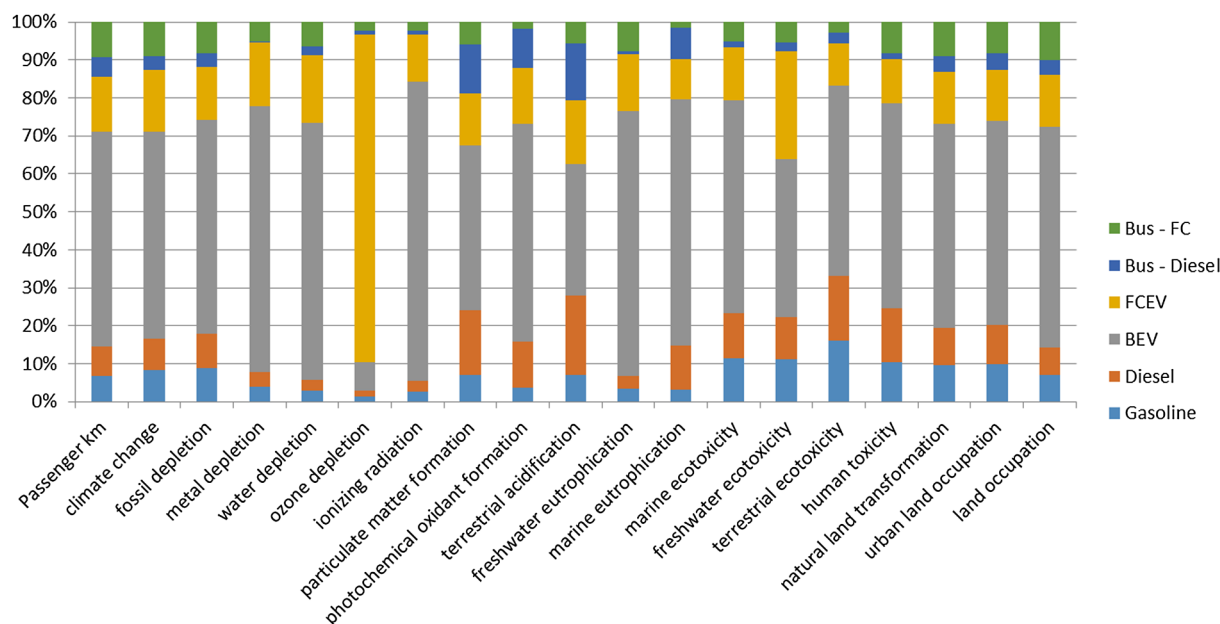

Fig. 4. Impact for the transport sector by category and powertrain in the *80* Scenario (EU28 +, only manufacturing).

natural land and urban land occupation), 500–800 m²/GWh for off-shore wind and 600–2100 m²/GWh (depending on size and run-of-river vs. lake) for hydropower. These numbers are within the range from literature, where wind has 1100–2100 m²/GWh and hydropower has 151–4100 m²/GWh according to [95], while [155] reports 2090–3230 m²/GWh for wind in Germany and Denmark and up to 25000 m²/GWh for generic hydropower (although in US). At the same time, the order of magnitude for the production process of biomass is in the order of 360,000–700,000 m²/GWh [155] (145,000 m²/GWh considered in this study), which explains its high contribution to this impact category in spite of the relatively small contribution to total production. Based on the electricity mix, the average for the power sector is ~1300 m²/GWh. Using the electricity production of 5700 TWh, the land transformed is ~7400 km², which is less than 0.2% of the total land available in EU (4.42 million km²).

For human toxicity, the benefit for PV and wind is much lower than the benefit in climate change [134]. The impact for a Si-based panel on a roof can be within 10% of a natural gas plant with CCS [47]. Given the large installed capacities these two technologies have, they constitute almost two thirds of the human toxicity impact, while only representing around one third of the electricity mix. Similarly, solar represents the largest contributor to terrestrial ecotoxicity mainly due to the metal emissions during the manufacturing stage of the panels.

5.1.2. Environmental impact from other sectors

For heating and transport, only the construction component is taken into account. For heating, in case it is satisfied with gaseous and liquid fuels, the upstream impact considers the production route (see Section 3.3.1) and in case it is satisfied with electricity is accounted for in that sector (see Section 3.4.2). For transport, it considers the impact reduction by scenario for the materials that are included in JRC-EU-TIMES (e.g. steel, cement, aluminum, among others; see Table SI 3 for the list of industries and CO₂ emission reduction by scenario). Fig. 4 shows the impact by powertrain and category in the *80* scenario, while Fig. SI 3 has the material contribution for each powertrain with and without feedback from the industries in JRC-EU-TIMES and Fig. SI 6 has the corresponding figure for the heating sector.

The impact due to so-called "zero emission vehicles" (BEV and FCEV) is between 70 and 90% of the total for most of the impact categories, which is expected since they constitute 75% of the fleet (see Fig. SI 7) and the impact only compares the manufacturing stage. FCEV

impact across categories is similar to their share of the transport demand. There is potential for impact reduction as the efficiency of the manufacturing process (especially the fuel cell) improves [142]. The production of steel, aluminum, copper and glass, which are the ones with endogenous feedback from the industry sector constitute around 35–50% of the manufacturing impact. Plastic and rubber, which constitute around 40% of the impact, also see their effect reduced by 2050 with the factors from [140]. Therefore, the impact reduction for the manufacturing stage is ~60% to reach 15–29 gCO₂/km for most powertrains. The contribution from the battery and fuel cell to BEV and FCEV is between 7 and 11% of the total (reduced) impact (depending on the size).

For the heating sector, most of the contribution is due to the biomass-based processes (furnaces and boilers with wood pellets). In spite of their relatively small contribution to the total heat demand (between 3 and 5% for the scenarios analyzed), their contribution for most of the impact categories is more than 60–70% (see Fig. SI 6). The main reason is that for these processes, there is no "supply" sector and the upstream impact due to biomass production is considered directly in the process where it is consumed, while the impact for heat pumps or gas boilers does not include the electricity production (power sector) or the gas production and combustion (supply sector). Because of the combination of these two effects (low biomass contribution and only construction for other technologies), the share of the heating sector (compared to the total for the system) is less than 0.1–0.2% for most of the impact categories.

For the industry sector (see Fig. SI 8 for breakdown by impact category and type of industry), the reduction in emissions can be clustered in 3 main groups. First, the impact CCS has, since this scenario has this possibility. This is used for part of the steel demand, achieving 65% reduction in emissions when using it in combination with top-gas recycling in the blast furnace. For cement, CCS allows achieving almost 80% CO₂ reduction (although with a high energy penalty of 3.4–4 GJ/tCO₂ captured [156,157]). Ammonia already has a stream with a high CO₂ concentration and this CO₂ is already used today for urea production (115 MtCO₂ at a global level [158]). Second, the reductions caused by the use of hydrogen from electrolysis. This is mainly relevant for steel (35% of the steel demand shifts to direct reduction in the *80* scenario), but can also help to reduce the emissions from aluminum. Third, energy efficiency leads to smaller fuel input for heat and power generation, while electrifying as much as possible each industry.
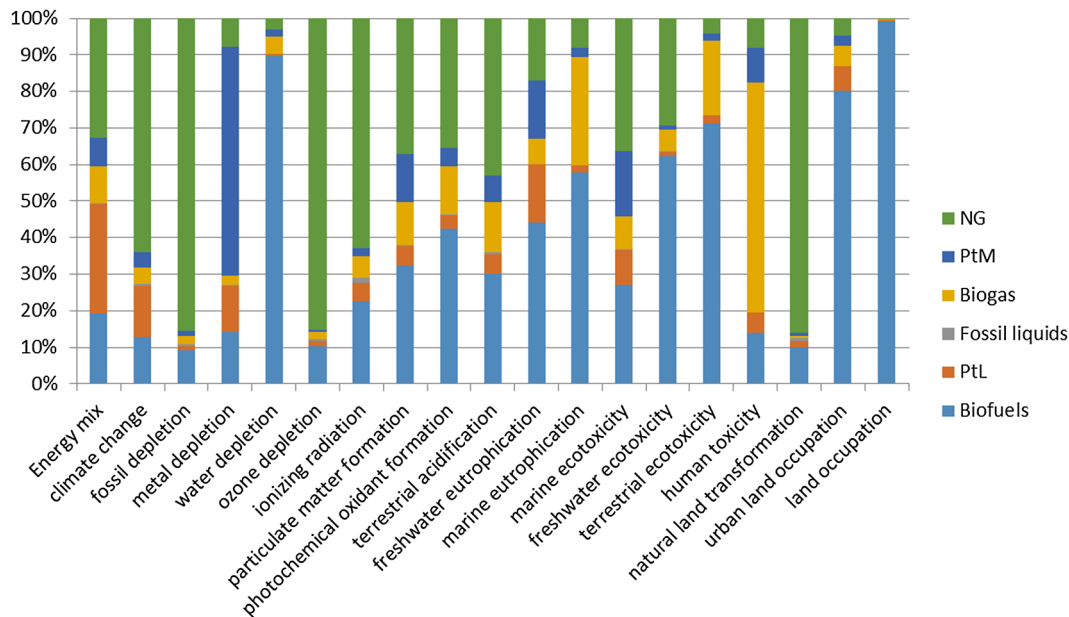
Fig. 5. Impact for the supply sector by category and source in the *95 No CCS* Scenario (EU28+, including upstream production and combustion).

The supply sector is constituted by the different gas and liquid sources (see Section 3.3.1) and biomass use for sectors other than power. Fig. 5 shows the impact breakdown by each of these activities across categories for the *95 No CCS* scenario. This scenario was chosen since it has a balance between the least fossil-based fuels and the highest (since it is the most restricted) biomass use. In less restricted scenarios (e.g. *80* or *95*), the fossil-based fuels are higher and dominate most of the categories (which is already the case for some categories in *95 No CCS* scenario).

Natural gas production has the largest impact for fossil depletion (this scenario has less than 1% of fossil-derived liquids since most of them have been replaced by BtL/PtL) and ozone depletion. Fig. 5 has the contribution by activity, but this needs to be put in perspective with other sectors (see Section 5.1.3) since for example in ionizing radiation gas production has the highest impact, but this is relatively small when compared to the impact of nuclear in the power sector.

5.1.3. Impact variation across future scenarios

From the economic perspective, adding constraints to the system leads to fewer choices to achieve the CO_2 emission reduction target and hence a more expensive system with a higher marginal CO_2 price [114]. The LCA analysis allows establishing if a similar trend occurs from the environmental perspective. Fig. 6 shows the ratio by impact category for the energy system with progressive restrictions in technology portfolio (CCS) and CO_2 reduction. Noting that only the capture component has been considered (CO_2 transport and storage are not included), assuming that similar to the economic impact [159], the largest share is due to the capture step.

The color scale in Fig. 6 is assigned with the highest impact within a specific sector. For example, looking at climate change in the total impact, the two scenarios with 80% CO_2 emission reductions are darker red than the other four scenarios, which have 95% CO_2 emission reduction. A similar trend is observed for the individual sectors, except for power, where the *Optimistic – No PtG* has the highest impact. This is due to the higher installed capacity (and associated construction impact) needed to replace gas capacity in power (further explained in 5.2.3). For power, most of the highest impact (i.e. red) is in the *95 No CCS* scenario. This is expected since this scenario has the double constraint of ambitious CO_2 target without a key technology such as CCS. This requires a higher electrification rate and more hydrogen through electrolysis, which results in larger installed capacities and therefore

higher environmental impact for most categories. For ionizing radiation in power, the impact is relatively the same across scenarios, since it is mainly defined by nuclear which remains at a similar level than today for all scenarios. Terrestrial ecotoxicity is dominated by solar (since combustion is not part of this sector) and this nearly increases by a factor 6 in the *95 No CCS* scenario to reach 50% of the total impact the system has in this category.

Industry and transport are the most expensive (i.e. higher marginal CO_2 price) sectors to decarbonize. This means they emit most of the allowed emissions from the target. Impact for the first 11 categories in Fig. 6 can be 30–70% lower in a scenario with 95% CO_2 emission reduction compared to a scenario with 80% mainly through the larger fraction of steel that shifts to direct reduction with hydrogen. This is different for the toxicity categories that actually show a higher impact as the CO_2 emissions decrease. This is in agreement with previous studies [134] that show that carbon footprint has the weakest correlation with toxicity categories. Transport is the worst for the *80* scenario. However, the impact for the other scenarios remains within 5% for most categories, since only the manufacturing step is considered in this sector (see Table SI 4).

For 80% CO_2 emission reduction, most of the impact is dominated by the "Supply" sector (see Fig. SI 9). This is expected since this scenario still has significant fossil gas and liquid demand and in spite of the lower specific impact, the net impact is higher due to the larger energy flows. As the system becomes more restricted (either CCS or CO_2 target), the same fossil fuel supply cannot be sustained and the contribution from this sector to the total of the system decreases (i.e. see in Fig. 6 how the shade for the supply sector changes from red closer to green). This enables a reduction of 75% for freshwater ecotoxicity and fossil depletion for the change from *80* to *95 No CCS*. A lower reduction in impact (20–40%) occurs across the ozone depletion, particulate matter formation, photochemical oxidant formation and terrestrial acidification categories. Overall, the scenarios with 80% CO_2 reduction have the highest impact, while for 95% CO_2 reduction there are trade-offs across impact categories.

Previous studies [149] have shown that there may be an increase in other environmental impacts when the climate change impact is reduced with CCS. This would mean that in scenarios without CCS, these impacts would be smaller. This is the case for most categories, which have 5–10% lower impacts in the *No CCS* variations, with the exception of freshwater and marine eutrophication for which indicator scores
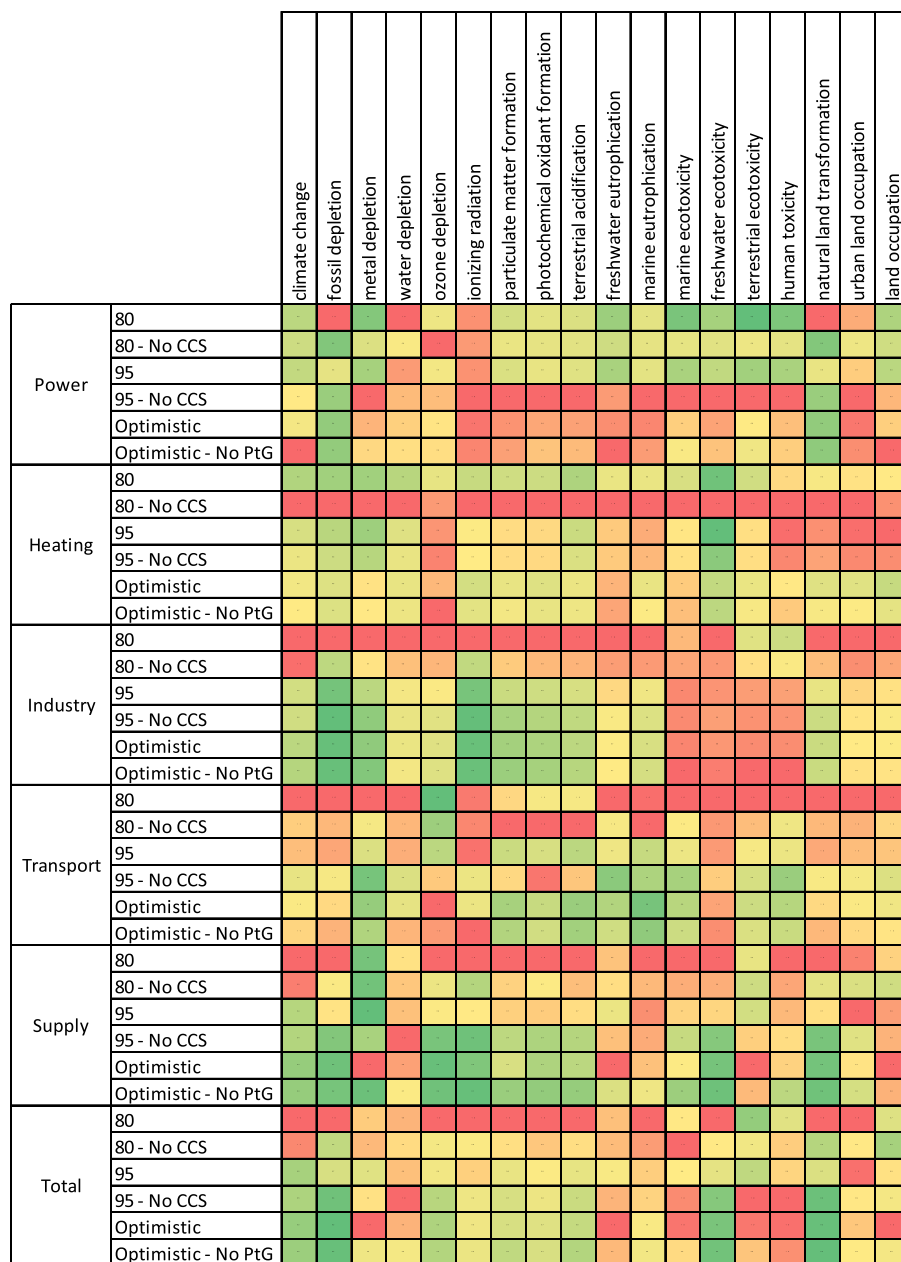
*Red means highest impact in the respective sector across scenarios, while green is the lowest. Relative weights are assigned by impact category.

Fig. 6. Impact ratio by category and sectors across scenarios. *Red means highest impact in the respective sector across scenarios, while green is the lowest. Relative weights are assigned by impact category.

remain the same. The toxicity impact categories show higher impact when CCS is possible is not possible. Particularly terrestrial ecotoxicity can be 50–80% higher in the *No CCS* variation, mainly driven by the larger electrification, wind and solar capacity and associated mineral production.

5.1.4. Direct and indirect CO_2 emissions

This sub-section aims to quantify the additional (indirect) emissions that are not part of the CO_2 target implemented in JRC-EU-TIMES (which is in line with the current accounting and target setting). These are related to either upstream activities (for fuel or asset) or emissions that are outside the EU geographical boundaries and therefore currently not included in the EU CO_2 target. Fig. 7 shows the contribution by activity sector for the main scenarios, while Table SI 5 has the corresponding values.

The direct emissions mostly originate from the "Combustion"

category (in Fig. 7) minus the CO_2 that is stored underground. These (yellow dots in Fig. 7) closely resemble the CO_2 targets of 914 MtCO$_2$ for 80% reduction and 293 MtCO$_2$ for 95% reduction. The advantage of the combustion category is that the accounting is done upstream, where the gas and liquid are produced and considering the different sources, rather than downstream in all the specific gas and liquid uses. This has the advantage of not correcting the emissions from all the equipment downstream (depending on the fraction of renewable gases) and that this gas and liquid consumption already considers the efficiencies of the downstream equipment. For the *95 No CCS* scenario, part of the CO_2 is not fully renewable (see Fig. SI 11). Around 25% of the CO_2 used comes from gas used for power generation, while only around 20% of this gas is supplied by PtM. Therefore, most of the gas (for this scenario) comes from non-renewable sources and it is affecting the combustion emissions.

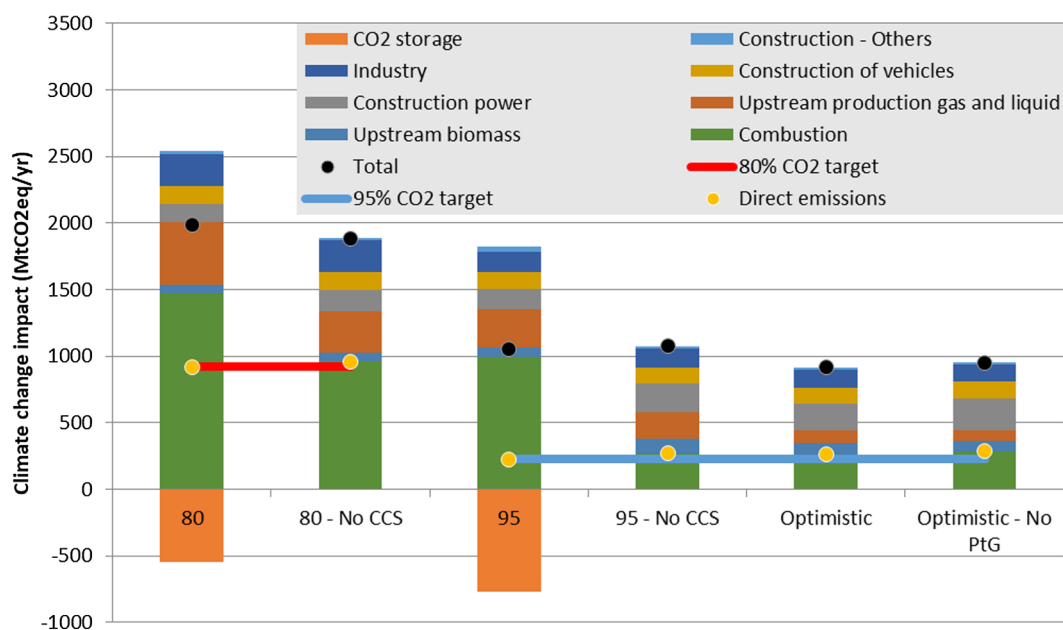The largest contributor to indirect emissions in the 80% CO_2

Fig. 7. Climate change impacts and breakdown by activity sector for all scenarios (see Appendix 4 for values).

reduction scenarios is upstream production of biomass, gas and liquid (see Fig. SI 10 for further breakdown of these two categories). Between 67 and 75% of this impact is in turn just for the gas production (for these two scenarios). These are highly dependent on the gas source and methane leakage associated. One entry with high impact (Slovakia - SK) and one entry with intermediate (50% of SK) impact were chosen as representative of the spectrum of gas sources. This represents emissions of 280–360 $MtCO_2$ (which is already 30–40% of the CO_2 target). Similarly, the *80* scenario has biomass combined with CCS, which compensates for positive emissions in the transport sector (harder to decarbonize), resulting in upstream emissions for the fossil liquids production of almost 100 $MtCO_2$. This decreases to 25 $MtCO_2$ with no CCS possible since the amount of fossil liquids used decreases (partially replaced by PtL, see [114] for a more detailed discussion). Contribution from both fossil gas and liquid production reduces drastically for scenarios with 95% CO_2 reduction and no CCS, since there is not enough CO_2 allowance for fossil fuels and they cannot be compensated by CCS. For these, the upstream emissions are only 30–85 $MtCO_2$ related to the minimum gas use in the system. In contrast, upstream emissions for biomass have an opposite trend. As the system becomes more restricted, the biomass use is closer to its potential and emissions increase from 65 $MtCO_2$ in the 80% reduction scenarios to up to 100 $MtCO_2$ for the *95 No CCS* scenario.

For industry, the remaining impact is mostly for mining and production of minerals, chemical conversion, metals and materials use. Considering that the impact for the different industries has the same trend as the CO_2 emissions (which come from JRC-EU-TIMES), the total impact for industry is reduced to 245 $MtCO_2$ in the 80% CO_2 reduction scenarios and to 125–145 $MtCO_2$ in the 95% CO_2 reduction scenarios. This is already subtracting the impact for electricity (see Section 3.4.3). The original impact for the same set of industries is equivalent to 410 $MtCO_2$ when no correction is introduced. The emissions from construction of power plants has the opposite trend (increases with stricter targets) since most of the leftover emissions comes from wind and solar. Production from these resources increases with lower CO_2 target resulting in CO_2 emissions from 135 to 155 $MtCO_2$ for 80% CO_2 reduction and 210 $MtCO_2$ for *95 No CCS*.

Accounting for these indirect emissions results in total climate change impacts twice higher than the CO_2 target for 80% CO_2 reduction, while it is close to four times the target for the 95% CO_2 reduction scenarios. These additional emissions can be explained by 3 clusters of

sources: (1) Coverage of other GHGs, especially methane in gas production; (2) Mining and upstream processing in industries not covered in JRC-EU-TIMES, e.g. materials used for vehicles production; and (3) emissions from construction and manufacturing.

A couple of previous studies have also quantified the indirect emissions, mostly from the power sector. In reference [92], the ratio of indirect to direct emissions was found around 2 to 1 for a scenario that only optimized the direct emissions. The additional cost for mitigating indirect emissions as well was 5.2% absolute cost increase compared to a scenario with mitigation of only the direct emissions. In [91], there was also a 2:1 ratio when optimizing direct emissions only. This increased to almost 5:1 when the direct CO_2 emissions were kept fixed at a level that would allow reaching the CO_2 target counting the indirect emissions. In [43], the indirect emissions from power are quantified as 10% of the direct emissions. All of these studies were for 80% CO_2 emission reduction by 2050. This is expected to be worse for more stringent targets as shown in the present study where a ratio of 4:1 was found for 95% CO_2 reduction.

5.2. Environmental impact of PtM

5.2.1. CO_2 emissions allowance for electricity input

Most of the PtM impact is defined by the electricity mix used upstream. Examples of the variability across time slices and effect over environmental impact of hydrogen is discussed in Appendix 5. This section estimates the maximum climate change impacts the electricity mix can have in order for PtM to be better than natural gas. Fig. 8 shows the breakdown of PtM process contributors to climate change taking Germany in the *95 No CCS* scenario as example.

Fig. 8 uses an electricity footprint of 25 gCO_{2eq}/kWh representative of a wind (1–40 gCO_{2eq}/kWh [26]) and PV (10–190 gCO_{2eq}/kWh [26]) mix. The actual mix by time slice is available and discussed in Fig. SI 12. Using this mix, the impact for PtM is 13.3 gCO_{2eq}/MJ. Natural gas is between 58 and 85 gCO_{2eq}/MJ,[8] where the source of variability is mainly the upstream emissions. Conventional gas production can have methane leaks in the upstream system (i.e. at the well site and gas processing) equivalent to 0.2–2.0% of the gas production [160]. The

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[8] Range for 22 entries included in Ecoinvent ("natural gas, high pressure// [XX] market for natural gas, high pressure", where "XX" is the region).
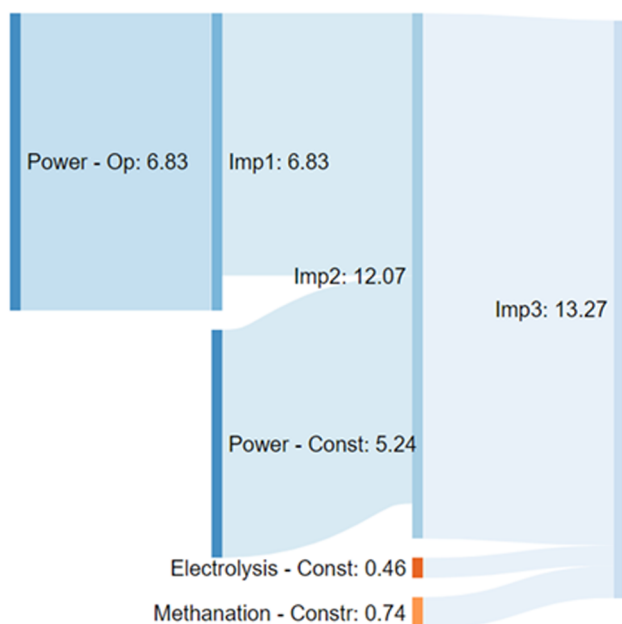
Fig. 8. Breakdown of the climate change impact for synthetic methane from PtM (all numbers in gCO_{2eq}/MJ) in Germany for the *95 No CCS* scenario. "Imp" 1 to 3 are just sub-totals of the impact with the overall one corresponding to "Imp3"

minimum impact PtM can have is the equipment contribution ($0.7 \, gCO_{2eq}$/MJ from methanation and $0.5 \, gCO_{2eq}$/MJ from electrolysis). This leaves $57–84 \, gCO_{2eq}$/MJ that can be emitted in the electricity production stage. This translates to $122.6–180.9 \, gCO_{2eq}$/kWh (considering a 60% efficiency from electricity to methane [34]). Downstream emissions (storage, long-distance transport and distribution to local customers) can be 0.4–2.5% of the gas production. Nevertheless, these emissions will be the same for both synthetic and natural gas.

The above calculation assumes that PtM does not incur in positive CO_2 emissions upon combustion. To fulfill this condition, CO_2 should come from biogenic sources or air. For the *80 No CCS* and *95 No CCS* scenarios, 91 and 94% of the CO_2 comes from biomass. However, when the carbon used for PtM results in positive GHG emissions, the allowance should be estimated only considering the upstream emissions from natural gas (since the GHG emissions will be positive for both natural gas and PtM). This is the case for the Optimistic scenario where 10% of the CO_2 is from fossil fuels use for combined heat and power and another 17% from industry. This happens because the multiple incentives in the *Optimistic* scenario that promote PtM make it cheaper to use this fossil CO_2 compared to the option of not using the CO_2. Subtracting the CO_2 emissions from combustion, the upstream emissions for natural gas are $3–30 \, gCO_{2eq}$/MJ. Subtracting the fixed emissions from the PtM equipment, leaves an allowance of $3.8–62.2 \, gCO_{2eq}$/kWh.

When looking at the electricity impact for each country across the main scenarios (see Fig. SI 16), all the countries are below the maximum allowable impact of $122.6–180.9 \, gCO_{2eq}$/kWh. All the countries are also below the least stringent value of $62.2 \, gCO_{2eq}$/kWh when the part of the CO_2 does not come from biogenic sources. However, all the countries are also above the minimum of $-6.2 \, gCO_{2eq}$/kWh since PtM is attractive when CCS is not possible and this in turn prevents the electricity impact to be negative. In scenarios with CCS, the electricity impact is on average lower, given that some countries have some (5–10%) contribution from biomass and its negative emissions, the average for the grid can be $-40 \, gCO_{2eq}$/kWh for the countries with the highest biomass share. Therefore, either high upstream emissions from natural gas production are needed for production of synthetic methane to be equivalent or the CO_2 used for PtM needs to come from biogenic

sources. The latter conclusion is in line with [106].

To put these numbers in perspective, previous studies are used. In [36], the allowance for electricity impact was estimated at $80 \, gCO_{2eq}$/kWh. For that case, only the upstream process (without combustion) was used since the CO_2 was assumed to come from a coal power plant. The system boundaries in that study also included the electricity produced from the power plant providing the CO_2 and this constituted most (85%) of the emissions in the reference process. The allowance became $120 \, gCO_{2eq}$/kWh when credit for by-products (e.g. steam) was used and nearly $-20 \, gCO_{2eq}$/kWh when PtM was compared to a reference where the CO_2 was assumed to be stored (instead of used). In [107], the electricity impact was estimated at $73–113 \, gCO_{2eq}$/kWh, which was only achieved when the CO_2 was considered as a waste product (emitted if not used for PtM). When this is not the case and direct emissions (as well as the energy consumption from separation) need to be allocated to PtM, then the allowance becomes negative.

5.2.2. PtM comparison with natural gas across impact categories

For impact categories other than climate change, three dimensions are analyzed: (1) variability by time slice; (2) contribution of steps in the PtM value chain; (3) comparison with natural gas. The daily and seasonal variability can be found in Appendix 5 (for both electricity and methane). It follows the same pattern as hydrogen, where the time slice with the highest impact is the winter peak. Average impact (considering time slice length) for most categories is around a third of the winter peak. The environmental impact of the synthetic methane produced during the nights, highly depends on the technologies covering the gap from solar. Depending on the country, this can be hydro, nuclear, gas, biomass or geothermal. Considering that it is not only about marginal unit of production (that defines the impact), but also about the energy balance (much lower production overnight), the production of synthetic methane decreases drastically by night, so it will reduce its contribution to the total impact. The contributions of each step in the synthetic methane value chain, as well as the comparison of the total impact with natural gas are shown in Fig. 9.

PtM has similar or lower impact than natural gas for 10 out of 18 categories. For most of these categories, the major contribution is the electricity consumption in the electrolyzer. For climate change, even though the *95 No CCS* scenario has average emissions of less than 20 gCO_2/kWh for the electricity, its contribution is almost 90% of the total impact for PtM. This is due to a relatively small impact from the construction of the electrolyzer and methanation plant, which makes the electricity share larger. Electrolysis equipment does contribute up to 40% in some categories given that the high renewable contribution to the electricity mix reduces this share of the total impact.

The worst performing categories for PtM are: (1) metal depletion; (2) water depletion; (3) ionizing radiation and (4) terrestrial, marine and human toxicity. PtM metal depletion is more than 10 times higher than natural gas, given that a share of the construction of upstream electricity production is allocated to the PtM plant. The sole purpose of constructing these plants is to satisfy PtM demand and hence their impact is directly allocated to PtM. At the same time, natural gas production is relatively efficient and simple (a well vs. a chemical plant for PtM). The same effect justifies the higher PtM impact in land related categories (these represent an inventory of land occupation rather than impact) and toxicity categories. Water depletion is also expected to be higher since that is the main source of hydrogen for electrolysis, while natural gas production requires limited water use. Fig. 9 shows the entire water consumption of the electrolyzer. However, this impact could be halved by treating the water produced by PtM and recycling it as feed to the electrolyzer. Ionizing radiation is higher for PtM due to the nuclear share of the electricity consumed. Fig. 9 has the average for all countries with a corresponding 10% share of nuclear in the *95 No CCS* scenario. For the toxicity related categories, it should be noted that uncertainty is high and a large difference could still mean that PtM and NG have similar impacts.
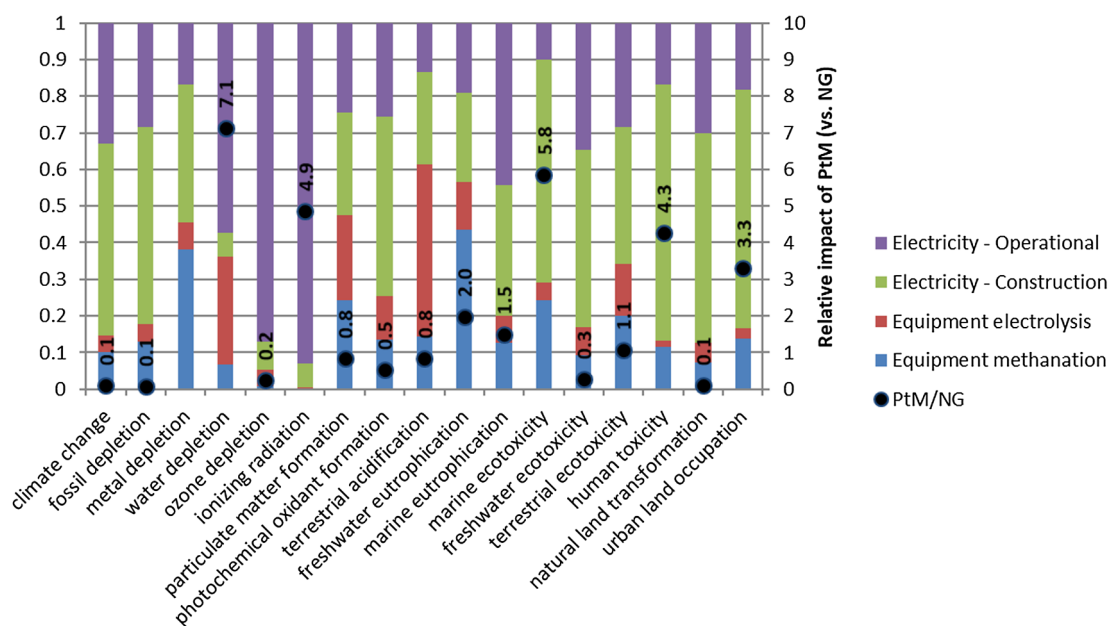
Fig. 9. Breakdown by individual steps of PtM environmental impact across categories (left axis) and comparison with natural gas (right axis) in the *95 No CCS* scenario (average electricity for all countries). *Note:* PtM/NG impact ratio for metal depletion is 16.3 for terrestrial ecotoxicity, omitted for readability of the rest of categories.

Hitherto, a limited number of studies has assessed the environmental impact of PtM for categories other than climate change. In [36], PtM was more attractive than natural gas only in climate change and fossil depletion. For marine eutrophication, particulate matter formation, terrestrial acidification and photochemical oxidant formation, the impact for both was comparable. For the rest (8 categories), the PtM impact was higher including 3 categories with an impact ratio over 100. One category where the current study differs is in natural land transformation. The higher land occupation for PtM is spread across three categories related to land, resulting in a higher overall PtM impact, while in [36] land was expressed in a single category. Another study [109] also assessed the impact for other categories. It compared the potential uses of 1 MWh of surplus VRE electricity covering electricity storage and Power-to-X. For freshwater and marine eutrophication, human toxicity, particulate matter formation and terrestrial acidification, PtM had a similar effect than natural gas, while for mineral resource depletion PtM performed better. Similar results were obtained in [110]. Higher (than NG) PtM impacts were obtained for ionizing radiation, particulate matter, acidification freshwater and terrestrial eutrophication with a lower impact for climate change and ozone depletion.

For some categories, PtM impact can be higher than NG, but if the original NG was already small in comparison to the total impact of the system, then an impact increase by PtM would have less relevance. The total PtM impact is expressed as a fraction of the total system impact to understand its contribution (see Fig. SI 19). For 7 (out of 18) categories, PtM impact is relatively small (less than 3%). Most of the impact across categories is dominated by the electricity input, which covers both construction and operational components. So for example, fossil depletion is mainly defined by fossil use for power generation (through combined heat and power and for the winter peak and some nights). Similarly, metal depletion is dominated by the construction of upstream power plants just to supply the electricity for the electrolyzers and subsequently to methanation. The PtM equipment itself (electrolyzer and methanation) has limited impact across categories, except for water consumption and terrestrial acidification that are driven by the water consumption for electrolysis (the latter could be halved by recycling the water produced by PtM).

The relative PtM impact also reaches a significant share (10% or

more) for 6 of the categories for the *Optimistic* scenario. This is to be expected since almost 75% of the gas demand is satisfied by PtM in this scenario. The other factor contributing to making PtM impact larger is that the rest of the system is also decarbonizing to achieve the overall 80 to 95% CO_2 reduction target, so PtM relative contribution increases since the total is also smaller.

5.2.3. Environmental impact of not developing PtM

Currently PtM has not been deployed on large commercial scale. There is the risk that it does not go beyond the "valley of death" [161] typical of technologies in development. This sub-section assesses the consequence of not having PtM in the technology portfolio. The approach was to establish the upper bound for this impact by using the *Optimistic* scenario where PtM capacity is the largest compared with the same scenario and boundary conditions, but without PtM. This *Optimistic* scenario has all the drivers in favor of PtM (see Table 2), resulting in an installed capacity (for methanation) of almost 670 GW. It satisfies almost 75% of the gas demand. This gas demand is largely reduced to around 7 EJ/yr (compared to 18 EJ/yr in 2015), where the largest demands are power (~2 EJ/yr), marine transport (~1.5 EJ/yr) and industry (~1.5 EJ/yr). This requires investments in the order of 8 bln€/yr by 2050.

In case the technology is not available in such favorable conditions, more expensive options are chosen throughout the system. 1 EJ/yr of biomass is diverted from BtL (i.e. transport) to heating, where it replaces the heat recovered from PtM (since the *Optimistic* scenario assumes a higher efficiency through heat recovery) through centralized gasification and district heating. Biogas is partially (0.2 EJ/yr) diverted from heat generation industry to power to cover part of the gap left by PtM. There is a lower gas demand for power generation (1.1 EJ/yr) and VRE resources with lower capacity factors are chosen for power generation to compensate for the lower gas-based generation. 70 $MtCO_2$ from direct air capture are needed and used for PtL. CO_2 use for PtL increases from 60 Mt/yr to 225 Mt/yr to be able to use the biogenic CO_2 to satisfy transport demand. This displaces fossil fuels and allows the equivalent CO_2 emissions from gas combustion, which now comes mainly (75%) from Norway. Based on this, total gas demand reduces from 8.7 EJ/yr to 5.5 EJ/yr. These changes make the removal of those last CO_2 molecules 15% more expensive. However, the total discounted
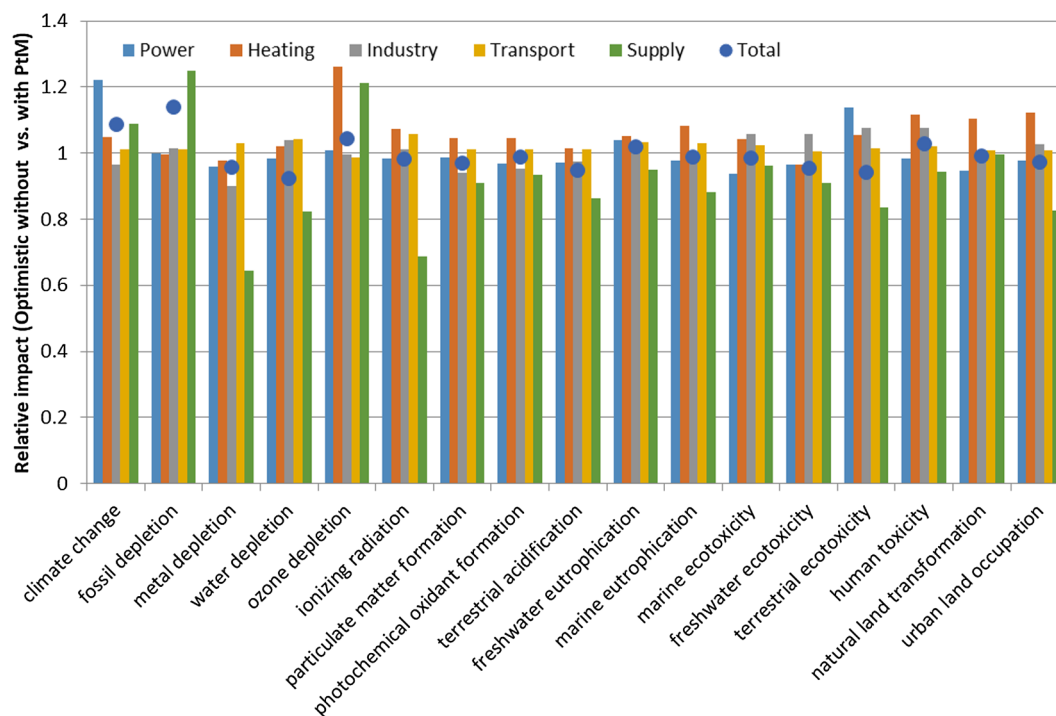
Fig. 10. Impact ratios by LCA category of the *Optimistic* scenario with PtM over *Optimistic* scenario without PtM.

cost for the system is only 1.2% higher. The corresponding changes in the environmental impact are presented in Fig. 10.

The main change without PtM is that a larger installed capacity (and corresponding construction emissions) is needed in the power sector to replace PtM contribution. This results in 20% higher impact for climate change without PtM. This negative impact is attenuated by the relatively small contribution (less than 5%) gas has in the overall electricity mix. At the same time, power is only 25% of the overall impact for the system (see Fig. SI 20). 50% of the impact comes from the "Supply" sector, where the increase in emissions due to upstream gas production is compensated by lower combustion emissions from liquid fuels resulting in the same total emissions. The fossil-based liquids are further displaced by PtL given that (1) the CO_2 budget is now needed for natural gas; (2) PtL is the only CO_2 sink left (neither CO_2 storage nor CO_2 use in PtM are possible in this scenario). Biomass is not used anymore for hydrogen production and replaced instead by electrolysis. Therefore, the scenario without PtM has a climate change impact just over 4% higher than the same scenario with PtM, mainly due to the higher construction of the additional power generation.

When looking at other categories, the main changes come from the different gas and liquid balances. For fossil depletion, natural gas replaces part (considering that gas demand is lower when there is no PtM) of the PtM gap, which increases fossil depletion. However, that is partially compensated by PtL displacing part of the fossil-based liquids. Even considering this, the impact for the "Supply" sector is 15% higher upon PtM absence which translates into 9% higher for the entire system. In the eutrophication and toxicity categories, the change is mainly associated to the lower impact that natural gas has in these categories (compared to PtM), resulting in slightly (~5%) lower impact for the system without PtM. Metal depletion is overall 20% lower for the scenario without PtM. This change is driven by the "Supply" sector, where the 670 GW of PtM are not present anymore combined with 200 GW less of electrolysis. This is replaced by only 285 GW of additional PtL capacity. Therefore, one reason for the large difference is the equivalent difference in capacities and materials needed for construction, as well as the level of detail in the inventory data used. While the methanation step uses data from the Store&GO project [126], which

seems to introduce a higher construction penalty (see Fig. 8), while PtL uses data from the RENEW project [128,129] and carries a small penalty (when using impact per unit of energy produced). No studies assessing systems designed with and without PtM (to consider replacing technologies) were found in existing literature, hence precluding any benchmark of these findings.

6. Conclusions

This study has evaluated future scenarios for an energy system that reaches 80 to 95% CO_2 reduction by 2050 in line with the EU decarbonization strategy. The main contribution of this research to EU policy (and other countries that apply the same methodology) is the use of a framework that combines economic and environmental aspects to low-carbon scenarios and thus, expanding the usually unidimensional character of analyses and allowing to provide insights for policy-making based on a more holistic approach still based on quantitative results. This avoids achieving lower costs at the expense of deterioration of environmental impact or focusing only on climate change. For this, an energy system model, based on cost optimization (JRC-EU-TIMES) has been used to evaluate the different pathways. Ex-post analysis of the output using life cycle assessment has allowed to expand the environmental impact to 18 midpoint categories using ReCiPe methodology. Conclusions are drawn on two aspects: (1) for the entire system; (2) with emphasis on PtM.

For the entire system, indirect GHG emissions can be as large as direct ones for 80% CO_2 reduction targets, while they can be up to three times as large for 95% CO_2 reduction. Up to 50% of these extra emissions are associated to the upstream production of fossil fuels that are left in the 80% CO_2 reduction scenario, while these are more evenly distributed across sectors for a 95% CO_2 reduction including the manufacture of vehicles, construction of power plants and remaining emissions from the industry sector. This is even considering significant improvement in time for industry and corresponding impact for materials during the construction phase. The potential policy impact for EU is that currently, part of these emissions is not covered in the CO_2 target. This could mean lower actual reductions when accounted for,

especially for low carbon targets.

This research has also contributed to understanding the trends in other impact categories besides climate change. Impact across categories does improve as the CO_2 target decreases, but to a smaller extent. A change from 80 to 95% CO_2 reduction can translate into improvements of up to 30% in other categories. A large share of the impact is defined by the mix of fuel sources. The use of Power-to-X technologies presents a clear opportunity to decrease the climate change impact, but it can be detrimental in other categories such as metal depletion, eutrophication or toxicity-related impacts. The sector with the next largest impact across categories is power, where the largest impacts are due to the construction of wind turbines and solar panels. These contribute up to 75% of the electricity production in scenarios without CO_2 storage since additional power is needed to produce hydrogen through electrolysis. Impact for the transport sector had limited changes across the scenarios evaluated since it is mainly defined by the fuel choice accounted for upstream.

For PtM, the contribution from construction of the plants was found to be 4.3 gCO_{2eq}/kWh (1.2 gCO_{2eq}/MJ) of CH_4. Considering that the impact associated to natural gas production can be between 10 and 108 gCO_{2eq}/kWh (3–30 gCO_{2eq}/MJ), the allowable electricity footprint is 3.8–62.2 gCO_{2eq}/kWh for PtM to be more attractive than natural gas production. When adding combustion emissions from natural gas, this allowance increases to 122.6–180.9 gCO_{2eq}/kWh, as long as the CO_2 used for PtM comes ultimately from air (biogenic or direct air capture). In the low carbon scenarios analyzed, all the countries were below 50 gCO_{2eq}/kWh (on average for the entire year). PtM has similar or lower impact than natural gas for 10 out of 18 categories. For most of these categories, the major contribution is due to the electricity consumption in the electrolyzer. The electrolyzer does contribute up to 40% in some categories (water depletion and terrestrial acidification) given its large (compared to the total system) water use. This impact can be halved by using the water produced by PtM back in electrolysis. The worst performing categories for PtM (compared to natural gas) are: (1) metal depletion; (2) water depletion; (3) ionizing radiation and (4) terrestrial, marine and human toxicity.

The impact of not having the technology was assessed in a scenario where all the drivers (co-occurrence of 9 parameters in JRC-EU-TIMES in favor of PtM) are in favor of the technology. PtM reaches 670 GW of installed capacity across EU providing around 75% of the gas demand. This establishes the upper bound for the environmental impact. Upon its absence, climate change impacts become worse by ~4% and fossil depletion by 9% (since it is partially replaced by natural gas). In contrast, there is an improvement for most of the other categories mainly associated to the absent impact of the construction of methanation (and associated upstream equipment) facilities.

Among the limitations of this work are the ex-post nature of the analysis and the lack of feedback to the optimization results. The level of technological detail for life cycle data in industry was not at the same level as the ESM. Factors like waste use, recycling rates and circular economy were not explicitly included as part of the analysis, but are expected to play a large role in the path to a low carbon system. The level of detail for Power-to-Liquid inventory needs to be improved as new demo sites or plants are constructed. LCA and ESM integration is largely beneficial for both methods. It can benefit from standardization, having a centralized database to use as reference for common processes in ESM, criteria for matching technologies with ESM and alternatives to handle the data. The analysis is still based on quantitative aspects and qualitative aspects such as society, politics, risks that would make the analysis more holistic could be part of future work.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

Appendix A. Supplementary material

Supplementary data to this article can be found online at https://doi.org/10.1016/j.apenergy.2019.114160.

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