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PRospective EnvironMental Impact asSEment (*premise*): a streamlined approach to producing databases for prospective Life Cycle Assessment using Integrated Assessment Models

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Abstract

Prospective Life Cycle Assessment (pLCA) is useful to evaluate the environmental performance of current and emerging technologies in the future. Yet, as energy systems and industries are rapidly shifting towards cleaner means of production, pLCA requires an inventory database that encapsulates the expected changes in technologies and the environment at a given point in time, following specific socio-techno-economic pathways. To this end, this study introduces *premise*, a tool to streamline the generation of prospective inventory databases for pLCA by integrating scenarios generated by Integrated Assessment Models (IAM). More precisely, *premise* applies a number of transformations on energy-intensive activities found in the inventory database ecoinvent according to projections provided by the IAM. Unsurprisingly, the study shows that, within a given socio-economic narrative, the Climate Change mitigation target chosen affects heavily the performance of virtually all activities in the database. This is illustrated by focusing on the effects observed on a few activities, such as systems for direct air capture of CO_2, lithium-ion batteries, electricity and clinker production as well as road transportation, in relation to the applied sector-based transformation and the chosen Climate Change mitigation target. This work also discusses the limitations and challenges faced when coupling IAM and LCA databases and what improvements are to be brought in to further facilitate the development of pLCA.

Highlights

- Prospective LCA can benefit from projections of global models, such as IAMs
- premise streamlines the production of prospective versions of ecoinvent based on IAM scenarios
- Emission and energy efficiencies of major industries are aligned with IAM scenarios

- Stricter GHG mitigation scenarios result in deeper transformations in the LCA database
- However, such scenarios may result in increased LCA impacts other than GHG emissions

Keywords

prospective LCA, IAM, ecoinvent, IMAGE, REMIND

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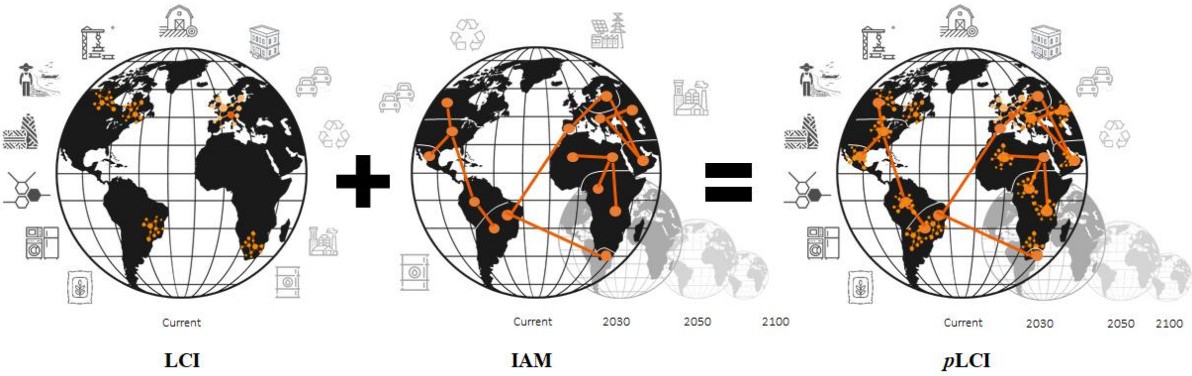
Abbreviations

BEV	Battery electric vehicle	**LNG**	Liquefied natural gas
CCS	Carbon capture and storage	**MGV**	Medium goods vehicle
DACCS	Direct air carbon capture and storage	**NMC**	Lithium nickel manganese cobalt oxide
FCEV	Fuel cell electric vehicle	**NMVOC**	Non-methane Volatile Organic Compounds
GHG	Greenhouse gas	**PM**	Particulate Matter
IAM	Integrated Assessment Model	**pLCA**	Prospective Life Cycle Assessment
ICE	Internal combustion engine	**pLCI**	Prospective Life Cycle Inventory
IMAGE	Integrated Model to Assess the Global Environment	**REMIND**	REgional Model of Investment and Development
LCA	Life Cycle Assessment	**RCP**	Representative Concentration Pathway
LCI	Life Cycle Inventory	**SSP**	Socio-economic pathway
LGV	Large goods vehicle		

Abstract art



1 Introduction

The globalization and digitalization of the economy, as well as the electrification of industry and different means of transport, imply that the environmental footprint of products and services consumed is increasingly dependent on the performance of global supply chains and the energy systems that support them. As energy systems and industrial processes are rapidly changing in the attempt to reduce greenhouse gas emissions, understanding the expected changes in energy supply becomes as important as correctly modeling the product itself for performing Life Cycle Assessment (LCA) and quantifying environmental burdens in a comprehensive way. Furthermore, decision support in environmental and climate policy, for example, usually requires insights into the performance of future technologies. Traditional LCA and its underlying static database is poorly equipped to this end. This gave way to prospective LCA (pLCA), where projections in time are introduced in life cycle inventories [1].

The body of pLCA literature is broad. However, advanced pLCA, in which LCA is informed by prospective energy systems or integrated assessment models, is relatively rare and has only recently gained attention [1]. First exercises linking prospective energy system models and LCA were limited to power generation, residential heating and passenger vehicles. They were used to either quantify the environmental burdens of single future technologies, or environmental impacts on a system level for different transformation pathways until the mid-century. Gibon et al. [2] used the ecoinvent database v.2.2 [3] together with energy scenarios from the International Energy Agency and prospective industry-related inventories from the NEEDS database to generate the "THEMIS" modeling framework - an integrated, prospective hybrid LCA model that covers nine world regions with a time frame of up to 2050. Future performance of power generation technologies and selected industrial activities were integrated in the background LCI database. The THEMIS framework was further developed by Arvesen et al. [4] who presented life cycle coefficients for a wide range of future power generation technologies up to 2050. Pehl et al. [5] built on THEMIS to quantify life cycle-based energy use as well as direct and indirect GHG emissions coefficients for power generation technologies and the global electricity sector up to 2050 according to different scenarios of the integrated assessment model (IAM) REMIND [6]. Finally, Luderer et al. [7] built on THEMIS to combine IAM scenarios with pLCA to explore how alternative technology choices in the power sector compare in terms of non-climate environmental impacts at the system level. Another approach more directly integrating IAM and pLCA models has been proposed in [8–10]. All three studies used projections from the IAM IMAGE [11] to generate prospective Life Cycle Inventory (pLCI) databases and used these to conduct the pLCA of passenger vehicles. The same approach, but with the IAM E3ME-FTT-GENIE [12], was used by Knobloch et al. [13]. They addressed impacts on Climate Change of future passenger vehicles and residential heating systems. Using a similar approach, Rauner et al. [14] quantified the life cycle-based co-benefits of a global coal-exit on human health and ecosystems impacts, this time based on projections from REMIND. The key element of these five studies was a modification of the background LCI database that resulted in pLCI databases reflecting expected developments within the power generation sector.

These previous efforts were valuable as they introduced the idea of enhancing pLCA thanks to the projections of IAM and demonstrated its feasibility. However, as valuable as they were, these works were conducted with the assessment of specific systems in mind, leaving “static” entire pans of industrial activities other than power generation present in the pLCI database. Projecting efficiency gains and market developments within the electricity supply sector encapsulates a large share of the benefits to be expected when the focus is on battery electric cars and heat pumps. But other important sources of environmental damages, such as the production of metals that enter the composition of the chassis, or the cement used to build the road infrastructures, have so far not been addressed. Additionally, the technical implementation of IAM projections in LCI databases showcased in these studies was not designed with large-scale applicability in mind, and would probably not work very well with different IAM or LCI databases.

Building on the work of Beltran and Cox [8,9], this paper presents a tool that follows a streamlined approach to integrating IAM projections into the LCI database ecoinvent [15] to allow for pLCA. More specifically, the tool allows:

- the integration of expected transformations within five major energy-intensive sectors, namely power generation, cement and steel production, freight and passenger road transportation, and supply of conventional and alternative fuels
- applicability across different IAMs
- the export of pLCI databases to different LCA software

With these functionalities, pLCI databases can be generated in a consistent manner across socio-economic pathways and Climate Change mitigation targets produced by one or more IAMs. It also allows for the comparison of pLCI databases following a similar combination of socio-economic pathway and Climate Change mitigation target, but based on solutions of different IAMs. Finally, it allows for consistent and reproducible databases giving similar results regardless of the LCA software used. This contributes to the improvement of the quality of pLCA as practitioners can focus on the foreground modeling of the product system studied.

The next section describes the approach used to produce pLCI databases. Its benefits for prospective LCA are illustrated in Section 3 with the example of road construction, battery production, capture of CO_2 from the atmosphere and a few other cases. These examples rely on technologies that will play an important role in deep decarbonization pathways (i.e., cement production, metals extraction and recycling, power generation). They are however energy- and material-intensive, and are expected to undergo rapid development in the next decades.

2 Method

The open-source Python library *premise* builds on the work of Beltran and Cox [8–10] and increases the extent of IAM integration in LCA across multiple models (REMIND, IMAGE and potentially others), versions of the ecoinvent database (from 3.5 to 3.7.1) and industry sectors (i.e., power generation, cement, steel and fuel production, metals recycling). *premise* is currently able to work “out-of-the-box” with IMAGE and REMIND, although extending its ability to work with other IAM would not require significant work. It is worth noting however that the extent to which the integration of a given sector is performed often depends on the information the IAM model can provide. For that reason, *premise* uses data from external sources when not provided by the IAM.

Figure 1 depicts the general workflow to produce a pLCI database. As a Step 1, IAM results are used as inputs together with the LCI database (in this case, ecoinvent). Section 2.1 describes the nature and content of such scenarios. As a Step 2, using the library *wurst* [16], *premise* operates a number of transformations on the LCI database. This step requires the use of additional inventories to represent emerging and future technologies not originally available in the LCI database. This is done by collecting inventories from the literature (e.g., hydrogen and synthetic fuel production, direct air capture, etc.) or by using third-party libraries (e.g., for inventories on novel powertrains for passenger cars and trucks). The end of this second step leads to a modified LCI database for a given year, transformed according to the projections of the IAM scenario chosen. Section 2.2 describes the approach used to operate such transformations. Step 3 consists of exporting the database into a convenient format that common LCA software (i.e., Brightway2, Simapro) accept or as a set of sparse matrix representations that numerical libraries can handle (e.g., in Python or R). A third option consists of producing a "scenario difference file" in order to produce a "superstructure" database to be used by Activity Browser [17] – this option allows to write only one database to disk while being able to explore multiple scenarios – as described in [18]. This step is not the focus of this paper and is not described further. Finally, Steps 4 and 5 consist of producing LCA resource and environmental indicators that feed back to the IAM. These two last steps are not in the scope of this paper, but are discussed briefly in the Discussion section.

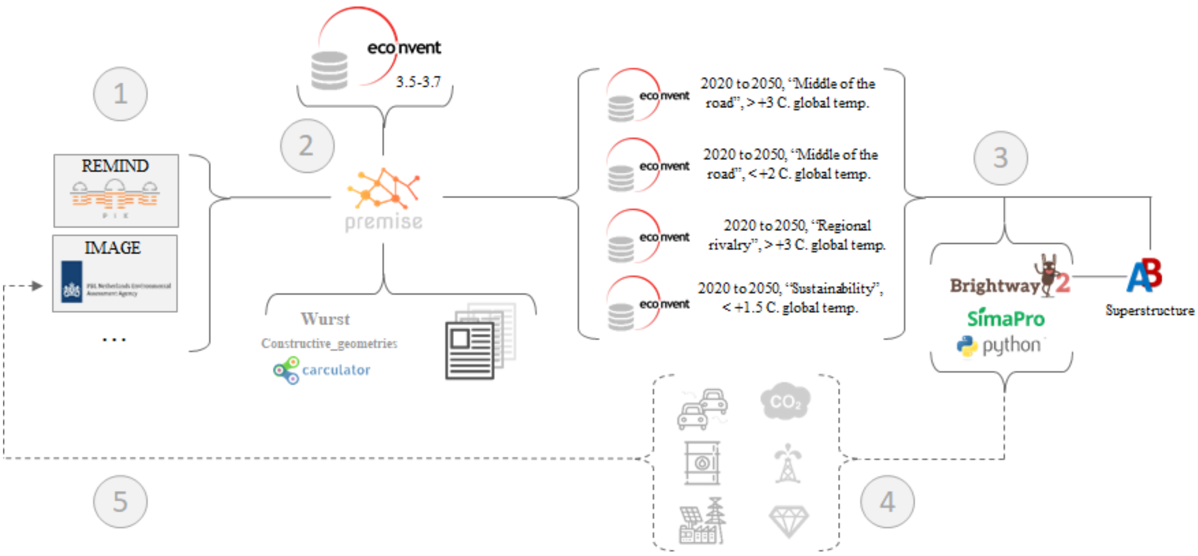


Figure 1 General IAM-LCA coupling workflow

2.1 IAM projections

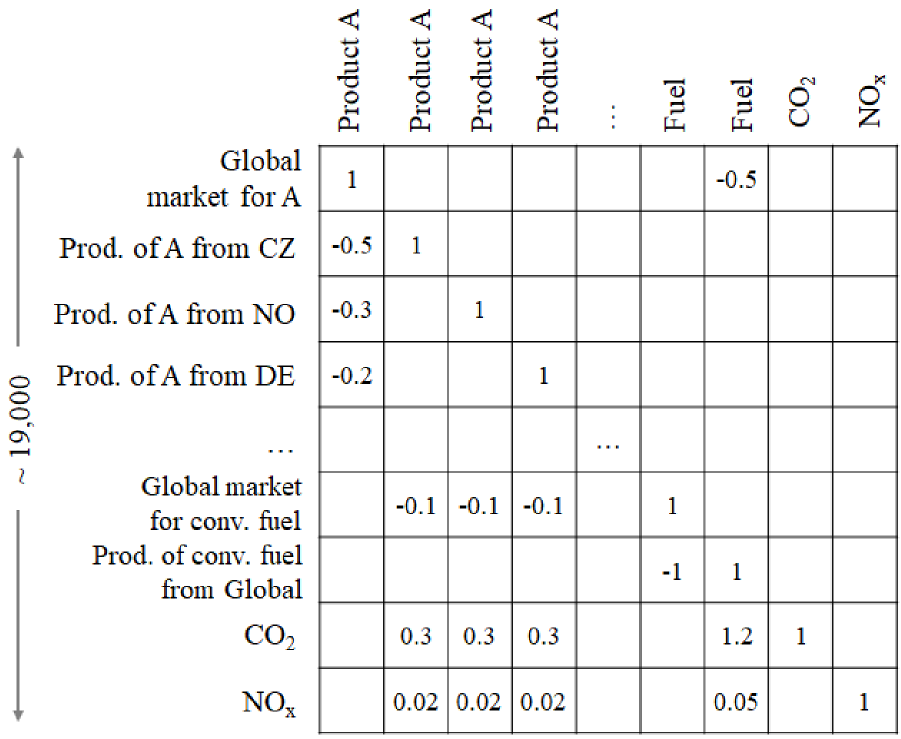
Process-detailed IAMs describe transformation pathways of the interlinked energy-economy-land-climate systems. Process-detailed IAMs are distinct from cost-benefit IAMs in that they represent the energy system and other sources of greenhouse gas emissions as well as mitigation technologies with substantial process detail (e.g., in terms of energy stocks, flows, and conversion technologies). The reader can refer to [19] for a detailed definition of process-based IAMs. Cost-benefit IAMs such as DICE [20] and Fund [21], by contrast, only have a stylized representation of greenhouse gas abatement potential as a function of carbon prices, without representing underlying system changes and their interactions.

In the present study, we use the REMIND [22] and IMAGE [11] IAMs as illustrative examples of such process-based IAMs. Both REMIND and IMAGE are among the five IAMs that were used for deriving marker scenarios of the Shared Socio-Economic Pathways [23], and are also prominently featured in past IPCC reports [24,25]. Both IMAGE and REMIND feature substantial detail in the energy sector and energy end uses: on the supply side, they represent a large variety of energy conversion technologies supplying electricity, liquid fuels, hydrogen and other energy carriers. On the demand side, they represent energy services and demands from the transport – refer to [26] for REMIND or [27] for IMAGE --, buildings – refer to [28] for REMIND or [29] for IMAGE -- and industry sectors – refer to [30] for IMAGE -- with considerable detail. Cross-linkages to land use via bioenergy and other land-based mitigation options such as afforestation or abatement of CH_4 and N_2O emissions from land use are represented via direct integration of land use in the IMAGE model [31,32], and via soft-coupling to the MAgPIE land use model [33] in the case of REMIND as demonstrated in [34]. To derive Climate Change mitigation pathways, either constraints of greenhouse gas emissions are imposed (e.g., in terms of cumulative emissions until the end of the century), or the system is subject to greenhouse gas pricing. Other environmental constraints can be considered, such as the area of land available for bioenergy and crop production. REMIND and IMAGE also represent air pollutant emissions [14] and water demands [35,36] by type of power source. A crucial difference between IMAGE and REMIND are assumptions on how the decision-making process is formed. The inter-temporal optimization used in REMIND generally implies perfect foresight by agents taking investment decisions. IMAGE, by contrast, uses recursive-dynamic modeling (i.e., system configurations in each time step are determined sequentially based on the state of the system in the previous time step). In both models, the output includes time series in five or ten-year steps of primary, secondary, final, and useful energy, for each geographical region and by fuel type, technology, or application. The number of regions differs across IAMs (e.g., 12-21 for REMIND, 26 for IMAGE).

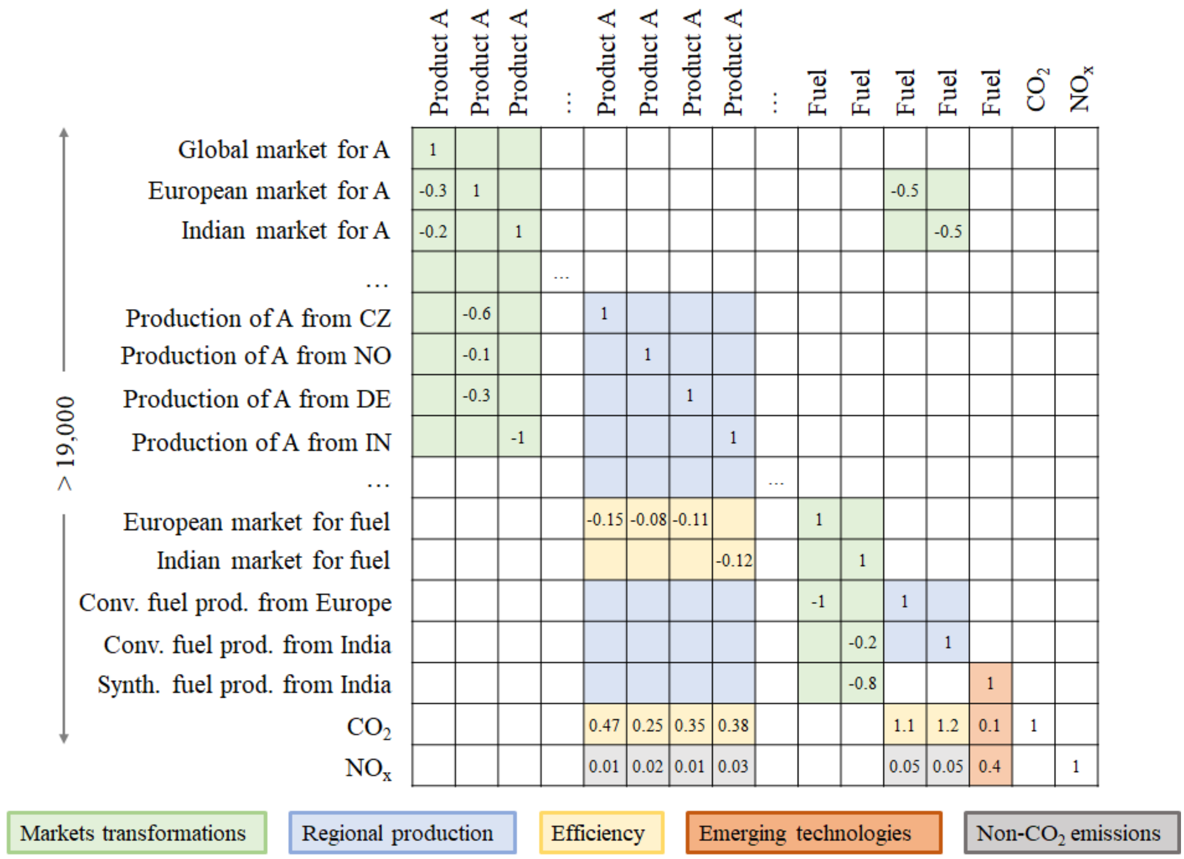
The IAM community has developed the Shared Socio-economic Pathways (SSP) as a means of structuring uncertainty about future socio-economic developments, such as national GDP, education and demographics [37]. In parallel the Representative Concentration Pathways (RCP) have been designed to describe several potential trajectories for atmospheric radiative forcing by 2100, ranging from 1.9 to 8.5 W/m². Combining both frameworks, IAMs make long-term energy and land-use projections that comply with atmospheric radiative forcing targets (given by the RCP) across a set of societal and economic conditions (given by the SSP). The reader may refer to [38] for further details on how RCPs and SSPs relate. This study showcases the integration of IAM solutions in the LCI database using the SSP2 "Middle-of-the-Road" scenario narrative. This narrative describes developments in line with what has been historically observed in the past century. The reader can refer to [39] for additional detail on the SSP2 narrative. Based on this, solutions that comply with the Climate Change mitigation targets RCP 6, 2.6 and 1.9 are presented -- corresponding to a global atmospheric temperature increase by 2100 of above 3.5 degrees C., below 2 degrees C. and 1.5 degrees C., respectively. *premise* also works with IAM solutions considering other scenario narratives and Climate Change mitigation targets.

2.2 Transformations on the LCI database

A number of transformations are operated on the LCI database. An LCI database usually presents itself as a pair of matrices populated with product and emission exchanges between man-made systems (hereafter referred as the "technosphere") and parts of the natural world (hereafter referred as the "biosphere"). A simplified representation of an LCI database is shown in Figure 2.a – where both technosphere and biosphere flows are represented in the same matrix. In this example, Product A (first column) is supplied via the global market for Product A (first row). This market (first column) receives inputs from Czech Republic, Norway and German-based production activities (second to fifth row). These production activities (second to fifth column) respectively require some fuel from the global fuel market and emit some CO_2 as well as NO_x (last two rows). The global fuel market requires some input from a fuel production activity, which itself leads to some emissions. It is of course possible that the fuel production activity requires itself some inputs from the global market for Product A (seventh column, first row). *premise* performs a number of transformations on these matrices to reflect the data granularity and expected changes dictated by the IAM, as shown in Figure 2.b. Markets based on IAM regions are created for certain products (green shaded cells), which receive inputs from production activities located in their respective geographical scope. Production activities based on IAM regions are also created (blue shaded cells), for which a region-specific energy efficiency is applied (yellow shaded cells) -- which also affects CO_2 emissions, if applicable --, as well as a region-specific correction factor for non-CO_2 emissions (grey shaded cells). Finally, some activities for emerging technologies are added should the IAM scenario indicate so (orange shaded cells). Finally, inputs-consuming activities relink to the newly created market activities located in their geographical area.



a) Simplified representation of a LCI database (positive values represent outputs, negative values represent inputs).



b) Simplified representation of transformations operated on the LCI database (positive values represent outputs, negative values represent inputs).

Figure 2 Schematic representation of transformations operated by *premise*

Table 1 shows the type of transformations operated for each sector. The number in each column header refers to the section number where a description of the transformation is found. Not all the sectors in the LCI database undergo the same number of transformations at the moment and some transformations rely on external data.

Table 1 Overview of transformations performed on the LCI database. The reader can refer to the section number indicated for more information.

* transformation that relies on external data

	2.2.1 Regional markets	2.2.2 Temporal markets	2.2.3 Regional production	2.2.4 Efficiency	2.2.5 Emerging technologies*	2.2.6 Non-CO2 emissions*
Electricity	X	X		X	X	X
Road transport	X		X	X	X	X
Cement	X		X	X	X	X
Steel	X		X	X	X	X
Fuel	X		X		X	

2.2.1 Regional markets

Datasets for supplying markets are created for each region of the IAM. These market datasets comprise the inputs of a number of regional production datasets (see Section 2.2.3). Such new markets are created for electricity (for different voltage levels), cement, steel and fuel. After their creation, they are relinked to activities in the database that consume the corresponding commodity and that are located in the same geographical area. As an example, the LCI database contains 12 or 27 region-specific market datasets for low-alloyed steel (depending on the IAM model used), against one “global” market prior to the transformation. These new steel markets contain regional steel production datasets, with the additional distinction between basic oxygen furnace (BOF) and electric furnace (EF) production pathways – only REMIND provides this distinction at the moment. Inversely, for some commodities such as electricity, the number of markets is larger prior to transformation, as the ecoinvent database initially contains a large number of national electricity markets that are removed to give place to fewer but geographically larger regional electricity markets. A slightly different approach is used for road transportation, as instead of markets, region-specific fleet average vehicles (including a representative mix of powertrain technologies) are built and linked back to activities requiring transportation. The correspondence between the geographical areas used by the IAM and those used by ecoinvent is done using *constructive_geometries* [40], a library that uses polygon-based topologies to return ecoinvent areas that intersect with or are included by a given IAM region.

2.2.2 Temporal markets

Additional markets are created to answer specific modeling needs when an electricity-consuming service or product is to operate over a long period. In such cases, “temporal” markets that contain time-weighted average electricity mixes are also available for different periods (i.e., 10, 20, 30, 40 and 50 years). This can be useful for modeling the life cycle use phase of battery electric vehicles or buildings, which typically have an extended lifetime.

2.2.3 Regional production

Region-specific production datasets are created for a number of commodities. They are either built as copies of existing datasets (e.g., clinker production), or created entirely (e.g., transport by passenger car). A number of adjustments are made for these production datasets to be as region-specific as possible. Notably, some of their inputs (e.g., electricity, fuel, transport) are relinked to supplying markets located within their new geographical scope, and their energy efficiency as well as emissions of substances other than CO_2 are adjusted according to projections for the said region – see Section 2.2.4 and 2.2.6. For road transportation, region and year-specific fleet average passenger car and truck transport datasets are created based on fleet projections from EDGE-T [26]. These regional production datasets provide inputs to their respective regional market datasets, as explained in the above Section 2.2.2.

2.2.4 Efficiency

Power generation, cement, steel, and road transportation activities have their energy efficiency adjusted according to the IAM year and narrative chosen. More precisely, *premise* calculates an improvement factor in a given sector relative to 2020 and applies it to the energy inputs of the corresponding activities in the LCI database. Based on the new efficiency of the dataset, fuel-related CO_2 emissions are also updated. For renewable systems, such as photovoltaic power systems, the efficiency is defined as the area of panel needed per kilowatt of peak power installed.

2.2.5 Emerging technologies

A number of technologies are not originally available in the LCI database. Inventories from the literature are used for modeling CCS infrastructure and operation datasets for power generation [41], steelmaking, cement [42] and natural gas, biogas and biomass-based hydrogen production [43,44]. Capture and storage of CO_2 is applied to power generation, cement and steel production datasets, if indicated by the IAM scenario. In such cases, the emission of CO_2 is reduced and infrastructure and energy requirements for capture and subsequent underground storage are added, including potential leakage during capture and storage. Additional inventories are also imported to represent blue [43,44], green [45] and grey [46] hydrogen production pathways, biomass-based [47] and synthetic fuels production – Fischer-Tropsch [48] and methanol-based [49,50] – and direct air capture of CO_2 [51]. Finally, inventories for passenger cars and heavy and medium-duty trucks with novel powertrains (i.e., electric, hybrid and fuel cell) are also added. Here, the datasets are created by the libraries *carculator* [52] and *carculator_truck* [53].

2.2.6 Non-CO_2 emissions

The adjustment of non-CO_2 emissions is, along with the addition of inventories for emerging technologies, a type of transformation that does not rely on IAM outputs at the moment. The air emissions model GAINS [54] provides time-series on the evolution of non-CO_2 emissions for each scenario narrative and industrial sector. Such projections are used to update the emission of CO, SO_2, NO_x, NH_3 and VOCs for combustion-based power generation, cement and steel production datasets -- emissions of PM are not updated at the moment. For road transportation datasets (passenger cars and medium- and heavy-duty trucks), two mechanisms reduce exhaust and non-exhaust emissions: the progressive hybridization of conventional ICE powertrains, as well as their increasing substitution by battery and fuel cell electric vehicles in the regional fleet.

As the following results section will show, the transformations described above may lead to remarkable changes in the database, more even so as a few key activities provide inputs to virtually all other activities.

3 Results

Section 3.1 starts with presenting the effect of the different Climate Change mitigation targets relative to the original LCI database, as transformations are being applied. With Section 3.2, the focus is then set on the effect of such transformations on a few specific activities in the database across years. Finally, Section 3.3 compares the GHG emissions of a specific activity for a same Climate Change mitigation target and year between IAMs.

3.1 The influence of Climate Change mitigation targets on energy- and material-intensive product systems

Using the IAM model REMIND, Figure 3 illustrates the normalized effect of transformations applied to the LCI database considering three Climate Change mitigation targets for the year 2050: RCP 6.0, RCP 2.6 and RCP 1.9. Four subplots are shown to distinguish the effect of the transformation applied: (1) the electricity sector only, (2) the electricity and steel sectors (3), the electricity, steel and cement sectors, and (4) all sectors, including fuel markets, passenger cars and medium and heavy-duty trucks. An LCA has been performed on the database activities to obtain their unitary GHG emissions using the impact assessment method (IPCC 2013 GWP100a). Market, treatment and land use activities are excluded to avoid double-counting in the cumulative sum. The horizontal axis shows the number of activities included in the cumulative sum. The database transformations are normalized by the cumulative GHG emissions of the reference database ecoinvent 3.7.1, for which the sum is denoted by ‘1’ (or 100%). This allows comparing the carbon intensity of the database across sector transformations. Updating the *Electricity sector (1)* with variables given by the RCP 1.9 scenario in 2050 results in a sum of cumulative GHG emissions 63% lower than that of the ecoinvent 3.7.1 database. Note that the jumps in Figure 3 are caused by a few activities that have a large carbon footprint, such as the construction of port facilities, hydropower plants as well as airports, respectively.

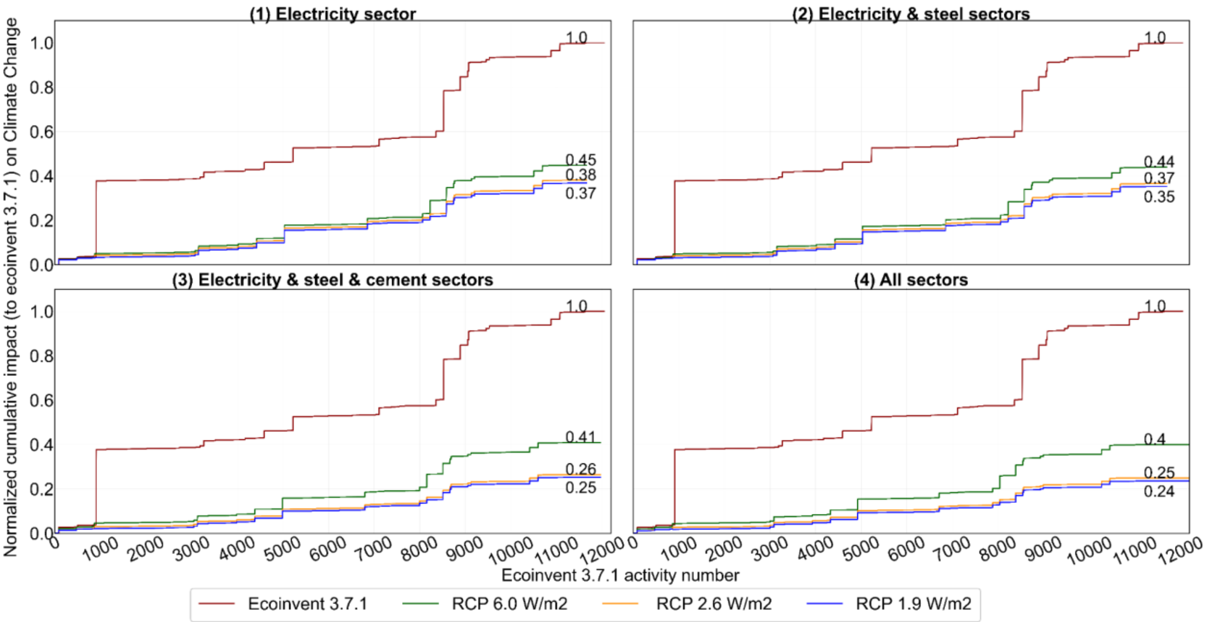


Figure 3 Cumulative sum of GHG emissions across activities in ecoinvent, for several Climate Change mitigation targets, in 2050, using the IAM REMIND

Figure 3 also indicates modifications on the electricity sector as having the largest influence on the cumulative sum of GHG emissions of the database. The relative change in the sum of GHG emissions following transformations on other sectors is usually within the range of 10%. However, specific sector integrations can have a significant impact for individual activities or specific sector-related product systems. Interestingly, the choice in terms of Climate Change mitigation targets also has a large influence on the results. While the scenario using the Climate Change mitigation target RCP 6.0 reduces the sum of GHG emissions of the database by 60% in 2050, the more stringent scenario using RCP 1.9 leads to a reduction of 76% that same year. It is worth noting that although the relative difference in results between scenarios using RCP 2.6 and 1.9 may appear negligible in 2050, it is more pronounced in earlier years. This is explained by the fact that while a similar efficiency and carbon intensity level is reached in both scenarios by 2050, significant Climate Change mitigation measures (such as CCS) are engaged in the RCP 1.9 scenario as soon as 2035.

Figure 4 illustrates the GHG emissions associated with the construction of one meter of a road, full width, normalized by its lifetime (one meter-year from the dataset ‘road construction’, for the region “Rest of the World”) for four different years – 2020, 2030, 2040 and 2050 – across the three different Climate Change mitigation targets. Again, the four subplots present different transformations of specific sectors as explained in the previous paragraphs. The bar plots also show the contribution of different components in the total GHG emissions of a meter-year of road.

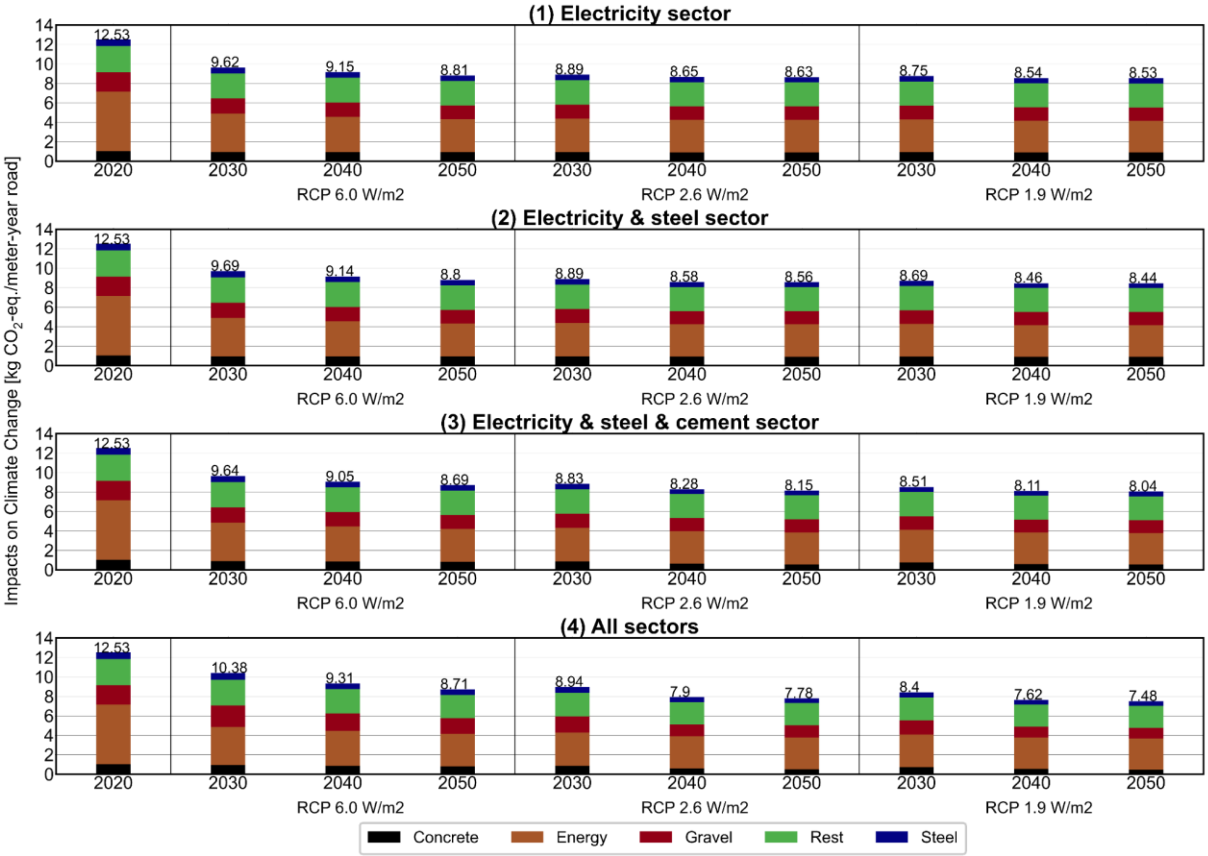


Figure 4 GHG emission for the construction of one meter-year of road sector transformations, for different years and Climate Change mitigation targets

The reference (static) GHG emissions for the construction of 1 meter-year of road is 12.5 kg CO_2-eq. in 2020. The results indicate transformations on the electric sector having, here again, the largest influence. This is mainly due to lower GHG emissions associated with power supply, because the electricity sector is increasingly fed by renewable energy plants. Also, total GHG emissions reduce significantly over time: a reduction of 32% in 2050 compared to 2020 is observed using the Climate Change mitigation target RCP 1.9. The influence of the integration of the remaining sectors is not negligible for road construction activities. The transformations applied on the cement sector lead to an additional ~5% GHG emissions reduction using RCP 1.9 compared to the integration of the electricity and steel sectors only. This is mainly due to three mechanisms: the utilization of cement in concrete with a lower clinker content, an improved clinker kiln efficiency as well as the capture of both process and fuel CO_2 emissions. In this particular case, the road construction dataset “Rest of the World” is supplied by a variety of concrete suppliers, which are themselves supplied by a variety of cement and clinker suppliers. Therefore it is difficult to attribute the exact gains in CO_2 emissions reduction across the above-mentioned mechanisms and regions. But overall, between 2020 and 2050 in the RCP 1.9 scenario, the clinker-to-cement ratio drops for all regions by 13% on average (they start at different levels across regions), the fuel efficiency of the kiln increases from between 30 to 50% depending on the region, and the rate of carbon capture ranges between 65 and 75% by then. The integration of all sectors in 2050 using RCP 1.9 leads to an 12% GHG emissions reduction (compared to integrating transformations associated to the electricity sector only). Interestingly, not all sector transformations lead to a reduction in GHG emissions. For example, in the RCP 6 scenario, the transformations of the electricity, steel and cement sectors reduce the overall GHG emissions as expected, while the transformation of the road transport sector increases them. More specifically, the transformation of the transport sector increases GHG emissions from the "Gravel" supply. This is explained by the gravel being transported by a less performant fleet average heavy-duty vehicle than initially modeled in the reference database. This is the case when a part of the fleet is electrified and supplied with electricity that is not decarbonized enough.

Figure 5 illustrates the life-cycle GHG emissions for the capture of 1 ton CO_2 from ambient air with its subsequent storage -- *i.e.*, direct air carbon capture and storage (DACCS) – using waste heat and grid electricity as energy sources to operate the process, as described in [51]. Two subplots and database transformations are considered; (1) transformations of the electricity sector only, and (2) transformations of all sectors, as this specific product system is very energy-intensive. A negative Climate Change impact on the vertical axis indicates the net permanent removal of CO_2 from the atmosphere -- i.e., the amount of CO_2 sequestered to which various GHG emissions that result from the life cycle of the DACCS system are subtracted. The secondary vertical axis shows the corresponding CO_2 removal efficiency. Six geographical regions are included – Japan, Latin America, Europe, the United States, China and India - to show the region-specific Climate Change impacts of DACCS deployment.

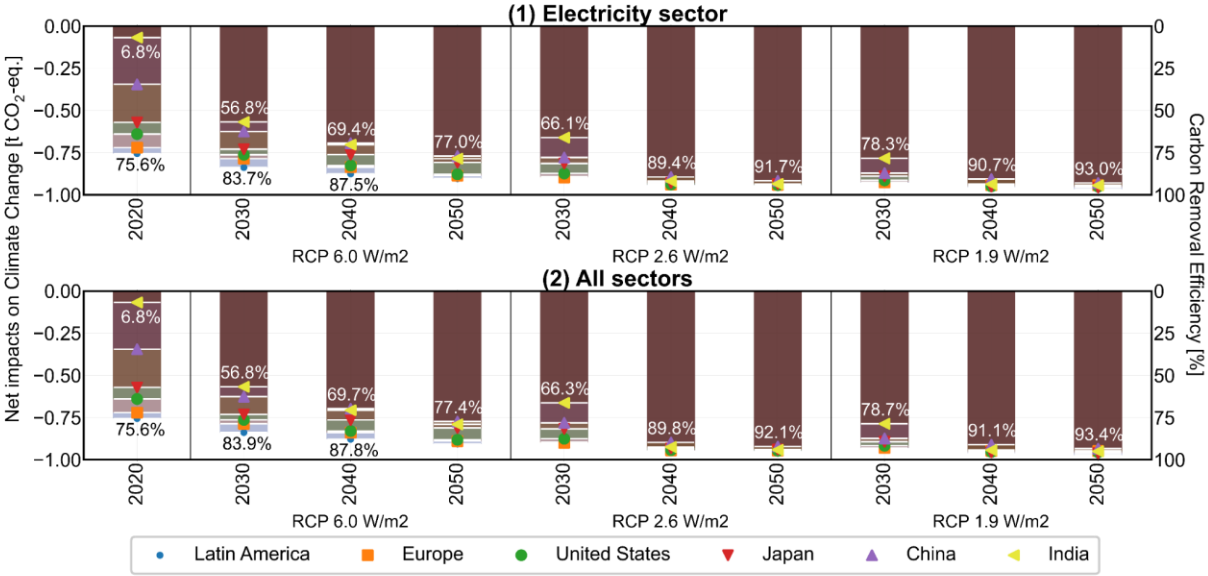


Figure 5 Net GHG emissions for the capture and storage of 1 ton of CO_2 from the atmosphere, using DACCS, for different IAM regions, years and Climate Change mitigation targets

The comparison between the upper and lower panels of Figure 5 indicates very small differences between the transformations of (1) the electricity sector and of (2) all sectors, on the Climate Change impacts of DACCS deployment (i.e., less than 0.5% of the total carbon removal efficiency in all instances). The life cycle Climate Change impacts of DACCS are largely driven by the GHG-intensity of energy sources needed for CO_2 capture; a substantial amount of grid electricity is for example required for grid-coupled DACCS systems [51]. DACCS deployment in geographical regions with GHG-intensive electricity supply and the integration of the electricity sector of a specific IAM scenario have an important influence on the total Climate Change Impacts (or carbon removal efficiency). The most stringent Climate Change mitigation scenario RCP 1.9 has, for example, a minimum carbon removal efficiency of 93% in 2050 - mainly due to the decarbonization of the electricity sector - against 77% for the RCP 6 scenario, leaving room for variation across geographical regions. Regions with a GHG-intensive electricity supply (*e.g.*, India and China) exhibit very low carbon removal efficiencies - as low as 7% in 2020 - compared to regions with a cleaner electricity supply, such as Latin America and Europe. First, this implies that grid-coupled DACCS systems are only suitable in geographical regions with clean electricity supply. Second, more ambitious climate policies will increase the carbon removal efficiency of grid-coupled DACCS. Both findings are in line with the work of Terlouw et al. [51].

Another case study is presented in the Supplementary Information (SI) and shows the GHG emissions for production of 1 kg of NMC battery cell. This case study is chosen to demonstrate the importance of integrating metal recycling as well as the integration of other sub-sectors such as heat supply at a later stage of software development of *premise*.

3.2 Convergence and divergence of results between IAMs

Figure 6 illustrates the relative change in Climate Change impacts - normalized to the reference database ecoinvent 3.7.1 - with respect to four activities; (1) clinker production (in the United States), (2) medium voltage electricity supply (global average), (3) low-alloyed steel production (global average) and (4) transportation with a light duty vehicle (European fleet average). The analysis uses the three Climate Change mitigation scenarios as used previously to compare results from IMAGE (green lines) to those of REMIND (red lines) from 2020 to 2050.

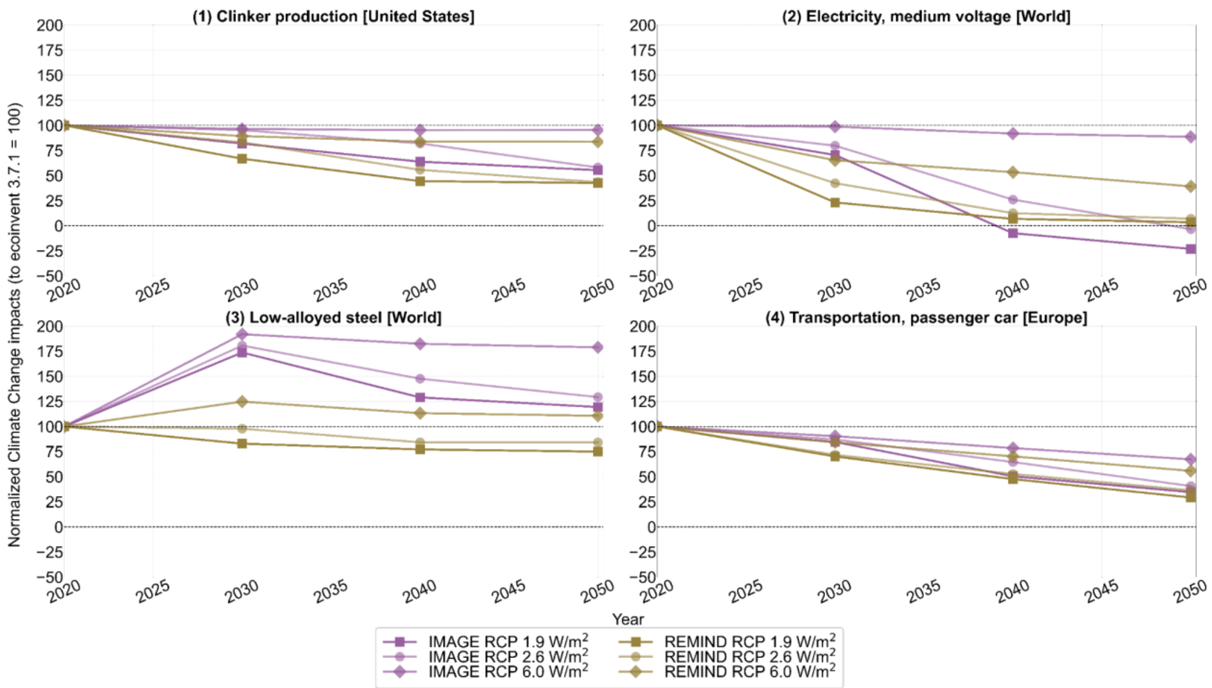


Figure 6 Relative change in GHG emissions for different products and services compared to 2020, across years and Climate Change mitigation targets, for REMIND and IMAGE, all sectorial transformations considered

Regarding emissions levels in 2050 using the RCP 6 scenario, REMIND and IMAGE roughly agree in respect to clinker production and passenger car transportation, but much less so in regard to electricity production and production of low alloyed steel. The divergence regarding steel production between REMIND and IMAGE is explained by the fact that regional shares of secondary steel production are not provided by IMAGE at the moment. Hence, all the steel is supplied by a BOF process, which is significantly different from what is considered in REMIND and the reference database. For the production of global average electricity, which is a market that consists of a production volume-weighted electricity mix from the different IAM regions, the difference is explained by the extent to which renewable sources of energy are used in RCP 6: they represent 60% of the production mix that year in REMIND, against 21% in IMAGE. It is worth noting that neither REMIND nor IMAGE consider the use of CCS in any sectors for that Climate Change mitigation target. Looking at the RCP 1.9 scenario, there is a general agreement on emissions levels with the exception once again for electricity, for which a 25% difference is observed (-100% change for REMIND, against -125% change for IMAGE). The respective global production mixes chosen by the IAM models that year differ: while REMIND relies extensively on renewable sources of energy (90%, when summing hydropower, photovoltaic and wind power), IMAGE relies comparatively more on combustion-based technologies (56%), as well as renewables and nuclear power representing 31% and 11%, respectively. CCS is applied to 64% of the electricity production involving a combustion process, 20% of which is applied on biomass-based power generation, leading to net negative GHG emissions.

While both electricity mixes are part of a solution that tries to satisfy the same Climate Change mitigation target, the effect on indicators other than Climate Change can differ. This is what Figure 7 indicates, using midpoint indicators from the impact assessment method ILCD 2018: the evolution over time of several midpoint indicators are shown for that same low voltage global electricity supply in the RCP 1.9 scenario. In both models, the reduction of GHG emissions comes with the increase of other midpoint indicators such as agricultural and urban land occupation as well as water and metal depletion and emissions of ionizing radiation. The increase in land occupation is however more pronounced in IMAGE because of the extensive use of biomass-based power generation -- 13% of the gross production mix. A note of warning: as the integration of land use dynamics and biomass markets between the IAM model and the LCI database is not yet complete, the biomass (i.e., wood chips) comes exclusively from the conversion of natural forests to energy crop plantations on the LCI side at the moment, while in the IAMs bioenergy is largely provided from agricultural residues and land-use is subject to economic and biophysical constraints [31,55]. Once that integration is available in *premise*, the land occupation-related indicators will probably reduce significantly. The increase in metals use comes mostly from rare earths and precious metals used by renewable plants such as wind turbines -- 40% of the gross production mix in REMIND -- and electricity network infrastructures for high and medium-voltage electricity transformation and transmission. The share of electricity coming from low voltage (e.g., photovoltaic panels) as opposed to medium and high voltage plays a role here. The use of water is dominated by hydropower in both mixes, but the difference comes from the additional supply of electricity from nuclear power plants for cooling purposes. Nuclear-based electricity is more present in IMAGE than in REMIND in this scenario. It also explains increased emissions of ionizing radiation. More comprehensive results - regarding the comparison between REMIND and IMAGE - can be found in Appendix B of the SI. Such feedback could prove useful to the future development of IAMs.

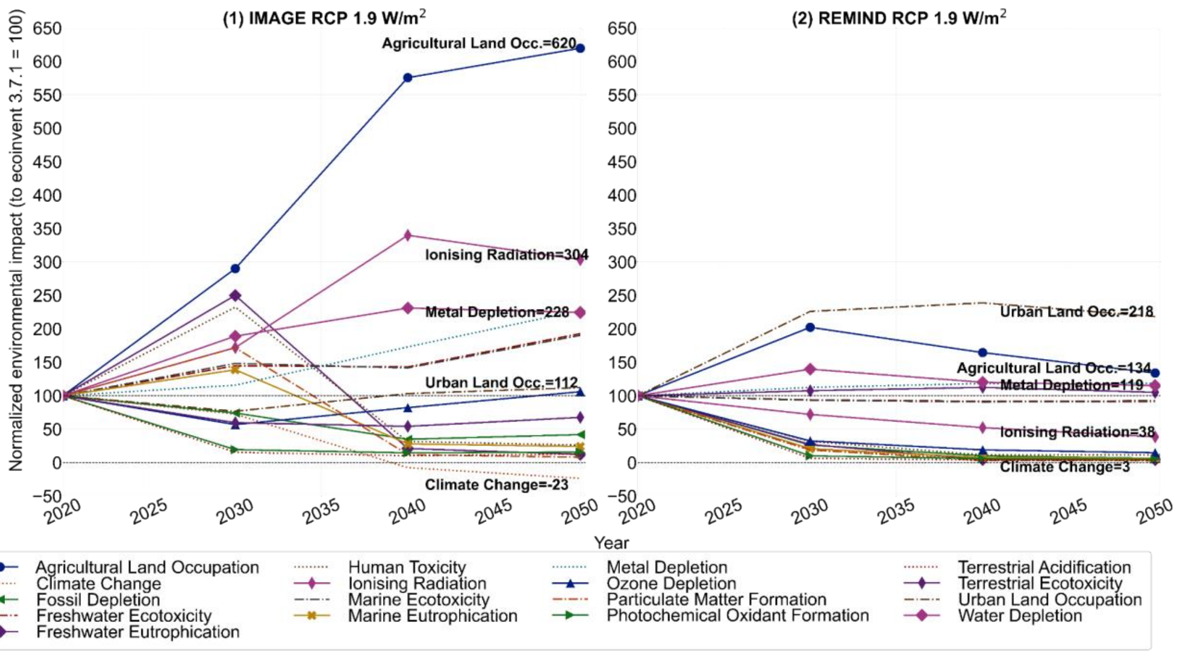


Figure 7 Relative change to 2020 for several midpoint indicators for the provision of low voltage electricity, global average, across years, for the RCP 1.9 Climate Change mitigation target, for IMAGE (left) and REMIND (right).

4 Discussion

4.1 Limitations

The largest challenge in coupling IAMs and LCA is the potential mismatch between the modeled technologies in IAM and the available life-cycle inventories. In order to reduce the computational complexity, IAMs group similar technologies and assign generic properties to them based on historical information. They also cluster regions spatially based on their location and socio-economic properties. Life-cycle inventories have no computational constraints and strive to be as detailed and differentiated between technologies and geographic scopes as possible. The discrepancy in data granularity might lead to semantic ambiguity, where an IAM process could have one or multiple corresponding activities with unspecified shares in the LCI database. A typical example would be the lack of a distinction based on grades for steel products in the IAM, while such distinction has a significant importance in terms of material and energy inventory in the LCI database. It could also lead to semantic mismatch, for example if the region “Europe” has a different geographical definition for the IAM and for the LCI database. While these discrepancies cannot be alleviated completely without altering the resolution of the IAM and/or the LCI database, it is possible to minimize their impact through a proper understanding and a correct interpretation of the data on both sides.

Also, for some transformations, *premise* relies at the moment on external data sources, such as the GAINS model for projections on non-CO2 emissions reduction, but also on inventories from the LCA literature for various emerging technologies. This can potentially introduce some inconsistencies.

Finally, there is also a temporal constraint: while IAMs provide projections up to 2100-2150, it seems difficult to extend reliably the coupling between IAM and LCA beyond 2050-2060. While the LCI database can accommodate incremental shifts in efficiency, which is what *premise* does, it cannot anticipate potentially disruptive shifts in technologies (e.g., nuclear fusion).

4.2 Integrating IAM projections into LCA: a means to a larger goal?

The results have shown the effects of integrating IAM projections into the LCI database, by contrasting results calculated with the static ecoinvent database v3.7.1 to those derived from the coupling. Unlike a scenario-based pLCA relying on independent assumptions, the use of the IAMs provides a coherent narrative, balancing the global perspective with the regional singularities. The benefits for IAMs are equally unequivocal: through the LCA coupling, it is possible to quantify impacts of indicators that are not directly modeled in the IAM, such as impacts on human health and ecosystems, land use or metal depletion. Hence, without affecting the computational complexity of the IAMs or straying away from the objective of system decarbonization, it is possible to quantify the environmental side effects of different scenarios. Ultimately, it is possible to feed the LCA impacts back into the IAMs, for instance by monetizing them and recalculating the cost-optimal solution in an iterative process, or by introducing additional constraints. Either way, this has the potential to provide a holistic approach to the system transformation, anticipate resource bottlenecks, and swiftly adjust the solution according to them.

4.3 Next steps

Being open source, the *premise* library is under continuous development, with new features expected in the short and mid-term. The addition of new sectors -- heat supply but also extraction, refining and recycling of metals, supply of biomass, and negative CO_2 emission technologies -- will expand its functionality. Also, the dominance of renewable energy sources in the electricity mixes projected highlights the necessity to improve inventories of renewable energy plants, such as photovoltaic panels and wind turbines, but also their efficiency and load factor, which are only rudimentarily represented in ecoinvent. At the moment, *premise* only adjusts the efficiency of photovoltaic panels by modifying the surface of panel needed per kilowatt of peak power capacity installed. But ultimately, parametrized models such as those developed in [56,57] and [58] will be needed to create region and year-specific inventories.

Furthermore, new collaborations with other IAMs are sought after in order to develop an interface to additional models. Also, substantial efforts are channeled into improved reporting. Ultimately, a fully-detailed report should be generated with each pLCI database produced, to indicate all the changes made as well as the boundary conditions behind the scenario narrative and Climate Change mitigation target used by the IAM.

Finally yet importantly, the user-friendliness would increase considerably when the planned graphical user interface is completed, allowing non-Python users to generate their own pLCI databases.

5 Conclusion

As commitments to curb emissions of greenhouse gases accelerate, rapid transformations are expected in energy systems and industries. This makes prospective LCA useful to assess the environmental performance of quickly developing, but also emerging or yet-to-be-developed technologies. This study shows that it is possible to streamline the production of comprehensive pLCI databases in order to facilitate the development and increase the quality of pLCA studies. It also shows that the scenario narrative chosen as well as the selected IAM and its specific way of achieving Climate Change mitigation goals can have significant effects on the LCI database (and thereby any foreground model that relies on it). There is therefore some critical uncertainty in any LCA study using such databases, as the decarbonization pathway and the actual technological breakthroughs are unknown. However, *premise* allows to have a broad idea on the effect such uncertainty can have on the LCI database as producing a multitude of scenario-specific databases is made easy.

CRediT author statement

Romain Sacchi: Methodology, Software, Writing - Original Draft, **Alois Dirnaichner**: Methodology, Software, **Christopher L. Mutel**: Methodology, Software, **Christian Bauer**: Supervision, Writing - Review & Editing, **Brian L. Cox**: Conceptualization, Writing - Review & Editing, **Vassilis Daioglou**: Writing - Review & Editing, **Tom Terlouw**: Software, Visualization, **Kais Siala**: Writing - Review & Editing, **Gunnar Luderer**: Supervision, Writing - Review & Editing

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Data availability

The tool presented in this study as well as its source code are available in the following repository:

https://github.com/romainsacchi/premise

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PRospective EnvironMental Impact asSEment (*premise*): a streamlined approach to producing databases for prospective Life Cycle Assessment using Integrated Assessment Models

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Supplementary Information

Contents

A. Battery case study

Figure A.1 illustrates the Climate Change impacts for the production of a 1 kg lithium nickel manganese cobalt oxide (NMC) battery cell. Four assessment years are considered - 2020, 2030, 2040 and 2050 – as well as three IAM scenarios are included from the REMIND model: RCP 6.0, RCP 2.6 and RCP 1.9. Again, the four subplots present different integrations of specific sectors as explained in the previous paragraph(s). The bar plots show a contribution analysis in addition, to show the Climate Change impact for NMC battery cells components, such as the anode, cathode and the electrolyte.

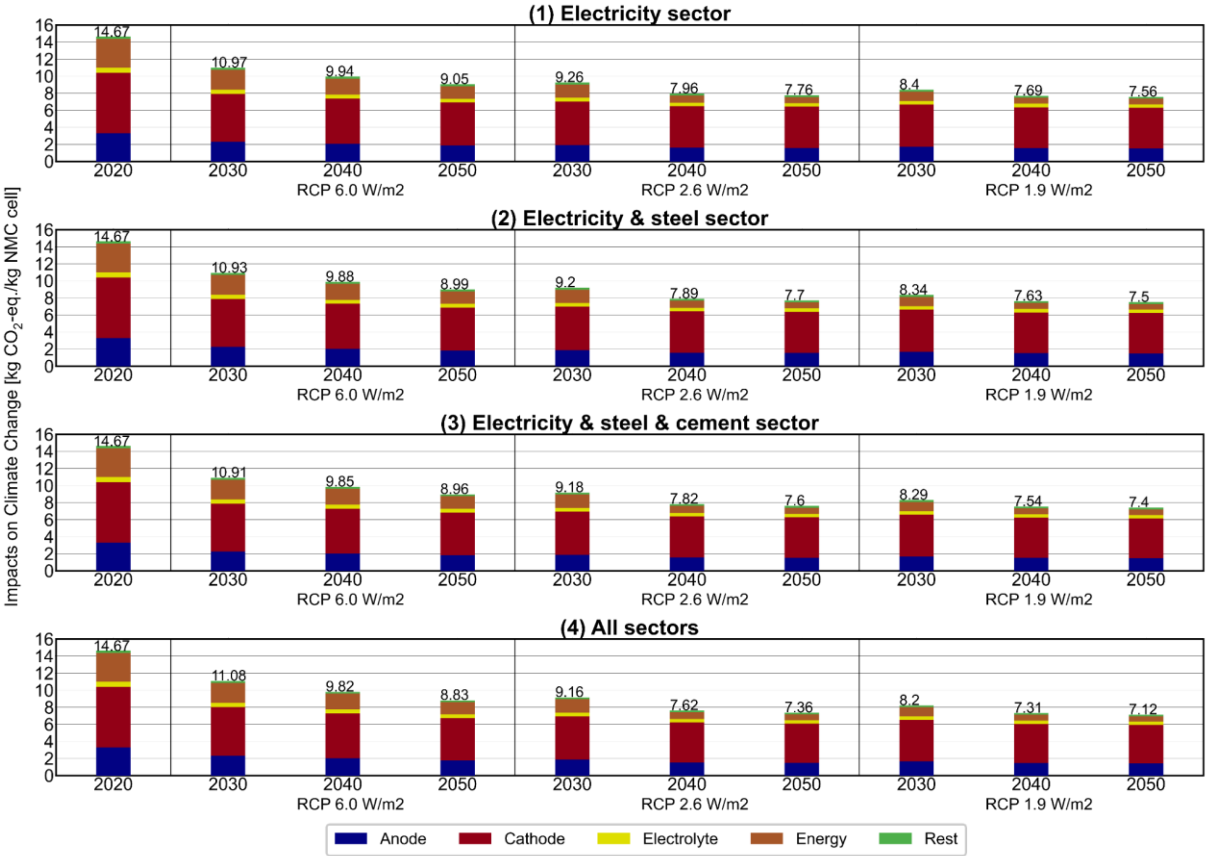

Figure A.1 GHG emission for the production of 1 kg NMC battery cell, considering different years and Climate Change mitigation targets

The results demonstrate the biggest influence for the integration of the electricity sector. The reference (static) Climate Change impact for the production of 1 kg NMC battery cell is 14.7 kg CO_2-eq. in 2020. The prospective integration of the electricity sector results in a decreasing impact on Climate Change, mainly due to lower GHG emissions generated from energy requirements, because the electricity sector is increasingly dominated by renewable electricity generators. Further, the Climate Change impact is significantly different between prospective IAM scenarios. The update of the electricity sector in combination with the application of an optimistic climate scenario - for example RCP 1.9 in 2050 - exhibits 7.6 kg CO_2-eq. per kg NMC battery cell, *i.e.* a GHG reduction of ~48%. The influence of the integration of all other sectors in prospective databases is rather small for NMC battery cell production. The integration of all sectors – for the same IAM scenario in 2050 – generates 7.1 kg CO_2-eq. per kg NMC battery cell, *i.e.* a GHG reduction of ~52%. On the contrary, the integration of all sectors - applying the more conservative RCP 6 scenario - exhibits a significantly smaller reduction on Climate Change; a GHG reduction of ~40% in 2050 compared to 2020.

The improvement of the foreground system of the NMC battery cell is not considered in this assessment, and therefore it can be expected that the (future) environmental impacts of NMC battery cell production could be further reduced due to increased recycling rates and improved energy density of batteries.

B. Table - comparison IMAGE vs. REMIND

Table B.1 Comparison of midpoint LCIA indicators for 1kWh from the global low voltage electricity market for 2020, 2030, 2040 and 2050, normalized by the results for 2020 (index 100)

	IMAGE				**REMIND**			
RCP 1.9 W/m²	**2020**	**2030**	**2040**	**2050**	**2020**	**2030**	**2040**	**2050**
Freshwater Ecotoxicity	100	145	143	193	100	94	92	92
Human Toxicity	100	232	32	26	100	32	12	11
Marine Ecotoxicity	100	148	142	190	100	93	91	91
Terrestrial Ecotoxicity	100	60	54	68	100	108	113	105
Metal Depletion	100	116	173	228	100	113	118	119
Agricultural Land Occupation	100	290	576	620	100	202	165	134
Fossil Depletion	100	74	35	42	100	26	10	7
Freshwater Eutrophication	100	250	21	12	100	27	5	5
Ionising Radiation	100	172	340	304	100	72	52	38
Marine Eutrophication	100	139	28	24	100	21	8	7

Ozone Depletion	100	57	82	106	100	33	19	15
Particulate Matter Formation	100	172	12	8	100	19	3	3
Photochemical Oxidant Formation	100	19	15	16	100	10	6	5
Terrestrial Acidification	100	16	10	13	100	6	4	3
Urban Land Occupation	100	77	103	112	100	226	239	218
Water Depletion	100	189	231	225	100	140	120	115
Climate Change	100	73	-7	-23	100	18	6	3