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Integrating planetary boundaries into energy system optimisation models for absolute environmental sustainability assessment: a methodological framework

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ABSTRACT

Transforming energy systems to address climate change must avoid shifting burdens to other planetary boundaries. Yet most energy models still focus primarily on greenhouse gas reduction, often neglecting broader life-cycle impacts on critical Earth-system processes. This narrow scope can unintentionally shift environmental pressures from climate to land, materials, or ecosystems, even in scenarios deemed sustainable. To address this gap, we present a modeling framework that integrates prospective life cycle assessment and planetary boundary metrics into a national energy optimisation model. The framework first integrates life-cycle and planetary-boundary metrics into a multi-objective optimisation model, then uses goal programming to characterise the different trade-offs in environmental impacts, and finally applies interpretable machine learning to streamline the overwhelming set of trade-offs into system archetypes. Applied to a 2045 low-carbon scenario for Belgium as a case study, the approach reveals that all near-optimal pathways can meet the climate target but exceed boundaries for ecotoxicity and particulate matter under the most permissive downscaling principle, indicating that decarbonisation alone is insufficient for absolute sustainability. From the near-optimum space exploration and interpretable machine learning, four distinct system configurations emerge—dominated respectively by electrification, hydrogen, renewable power capacity, or mixed strategies—each achieving similar costs yet distinct environmental trade-offs. Future extensions of this work should incorporate dynamic demand changes, and behavioral adaptations to further align energy systems with absolute sustainability targets.

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Introduction

With seven of the nine Planetary Boundaries (PBs) already exceeded and extreme weather events causing increasing socioeconomic damage, urgent action is required to ensure a livable and sustainable future[1,2]. When looking at the energy transition from a climate change perspective, fossil fuels are the main culprits[3,4]. Yet, when extending to other PBs, the overall energy use has also an impact. Future works will therefore analyse how and which sufficiency scenarios align with absolute sustainability targets. Energy system optimisation models have long supported decision-makers by identifying cost-effective pathways to reduce GreenHouse Gas (GHG) emissions and achieve climate targets[5–7]. However, this carbon-focused perspective often results in burden shifting, where measures that reduce GHG emissions inadvertently increase other environmental pressures, such as land occupation or freshwater use, effectively solving one problem while creating another[8,9]. For instance, a cost-optimal U.S. energy mix compatible with the Paris Agreement's 2°C target would still exceed five PBs, failing to achieve absolute environmental sustainability[10].

This phenomenon, often described as "carbon tunnel vision," highlights the limitations of using GHG emissions as the sole measure of environmental performance[9,11]. Traditional energy planning models were initially developed to phase out fossil fuels and curb global warming, leading to an almost exclusive focus on operational GHG emissions[3,12]. Over time, these models became central tools in energy policy design, yet their carbon-centered scope omits important life cycle stages such as construction, maintenance, and end-of-life[12]. As operational emissions decrease in future systems dominated by low-carbon technologies, these upstream and downstream stages represent an increasing share of total impacts, making a carbon-only view increasingly misleading for strategic planning[13,14].

In parallel, Life Cycle Assessment (LCA) has been widely used to quantify environmental burdens across all life cycle stages and impact categories of processes[15–17]. Specifically, LCA reveals trade-offs between categories such as climate change, freshwater consumption, eutrophication, and resource depletion, thereby helping identify potential impact shifting[18]. However, conventional LCA is a relative method: it compares scenarios to a reference system but does not assess whether a system is

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environmentally sustainable in absolute terms. To address this limitation, the integration of the PBs framework into LCA (PB-LCA) provides a promising solution by introducing absolute thresholds for environmental pressures[2,19]. The PB framework defines nine critical Earth system processes and quantifies safe operating limits for each. Staying within these limits ensures that human activities stays in a state similar to the Holocene, where humanity strives.

Bringing this absolute environmental perspective into energy system optimisation models is promising but challenging. For instance, treating PBs as explicit constraints requires splitting global boundaries across regions and sectors, a process that depends on normative principles of distributive justice and burden sharing[20]. This challenge is even more pronounced when the scope is restricted to a specific sector, such as the energy system, as there is a significant lack of robust data to define the share of environmental impact rightfully attributable to a specific activity across multiple indicators. Moreover, expanding the environmental scope introduces additional complexity: most non-climate indicators lack universally agreed thresholds or transition pathways, and they are expressed in heterogeneous units that complicate their inclusion in mathematical optimisation[18,21]. Applying fixed constraints on indicators can be arbitrary, while aggregating all indicators into a single weighted objective raises issues of transparency and interpretability[22,23]. These challenges have so far limited the application of PB-LCA in energy system modeling to a small number of exploratory studies, and a unified methodology to integrate PB-LCA in energy modeling is currently lacking[14,20].

Another dimension of complexity arises from the dynamic nature of both technologies and background systems during large-scale transformations. While conventional LCA is traditionally a relative comparison tool designed for analysing incremental changes in a static system, its application to the energy transition is gaining ground[15]. However, in this perspective, electricity mixes, industrial processes, and material supply chains are expected to defossilise and evolve, progressively reducing the embedded environmental burdens of future technologies[24,25]. Our framework operationalises this by coupling energy system optimisation with Prospective Life Cycle Assessment (pLCA) through the Premise framework, which "futurizes" background Life Cycle Inventories (LCIs) using projections from Integrated Assessment Models (IAMs) [26]. Accounting for the temporal evolution of upstream systems prevents overestimating long-term environmental impacts and ensures that both the foreground optimisation and background supply chains evolve under synchronized assumptions of defossilisation and technological progress[15].

To fully address these challenges, methodological advances are needed to integrate comprehensive life cycle and PB information into high-resolution energy system optimisation models. Most existing energy models operate at hourly resolution and capture key interactions between energy sectors, demand profiles, and renewable intermittency, but they rarely include life cycle impacts beyond GHGs[27,28]. Conversely, LCA frameworks provide detailed environmental data but lack the system-level optimisation capabilities needed for designing national or regional energy transitions. Bridging these two perspectives is essential to design systems that are not only low-carbon but also environmentally sustainable across multiple impact dimensions[15,29].

Expanding the environmental scope of energy system optimisation thus calls for multi-criteria formulations that can balance cost and environmental performance without relying on arbitrary weighting. Multi-criteria decision analysis, such as linear goal programming with normalisation, offers a way to incorporate several impact indicators within the optimisation objective[30]. Each indicator is minimised according to its relative importance, enabling explicit trade-offs and transparent exploration of competing objectives. As such methods generate a vast set of optimised solutions, interpretable machine learning methods provide powerful tools to analyse large sets of optimised solutions and extract actionable insights[22,31].

In this work, we develop a general methodological framework that integrates LCA and the PB framework into large-scale, whole-energy system optimisation (Figure 1). The approach is illustrated through its application to EnergyScopeTD, a model representing power, heating, mobility, and non-energy demand (i.e., energy products used as feedstocks[32]) at hourly resolution for a given region[27].

Specifically, the Life Cycle Inventory (LCI) for 111 technologies and 28 resources is defined under prospective conditions, converted into impacts on multiple PB indicators, and embedded into the model's optimisation structure. The aggregated impacts are then included in a multi-criteria formulation that jointly minimises system cost and a normalised portfolio of environmental indicators. Then, a range of optimised solutions is generated by exploring the optimisation space. Finally, interpretable machine learning is applied to identify dominant trade-offs and extract key design principles from the set of optimised solutions. By combining the strengths of energy system optimisation, LCA, the PB framework, scenario exploration and interpretable machine learning, this approach enables the design of energy systems that are cost-effective, climate-compatible, and environmentally sustainable within the Earth's safe operating space[14,20,29].

Methods

Environmental impact accounting in energy system models: carbon accounting in EnergyScopeTD

Most energy system models rely on simplified Global Warming Potential (GWP) accounting, typically expressed as CO_2-equivalent emissions associated with energy flows. This conventional practice facilitates comparability with policy-oriented

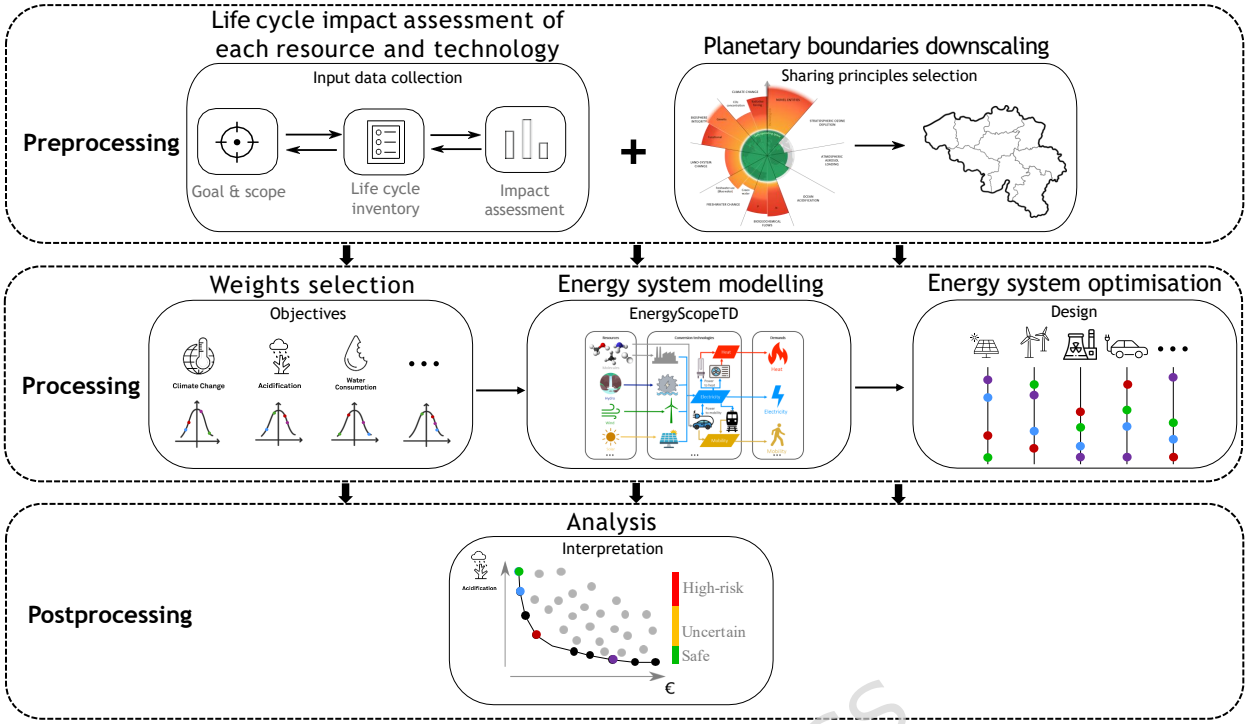


Figure 1. Schematic overview of the integrated modeling framework combining life cycle assessment (LCA) and planetary boundary (PB) analysis with energy system optimisation. The workflow is structured into three stages: preprocessing, processing, and postprocessing. It begins with the preparation of life cycle inventory (LCI) and life cycle impact assessment (LCIA) data for all technologies and resources, alongside the downscaling of PB indicators to the case-study level based on selected sharing principles. These elements are then integrated into the energy system design optimisation model (EnergyScopeTD), where environmental impacts are represented through multiple indicators and combined with economic objectives within a multi-criteria optimisation framework. A range of weight combinations is used to explore trade-offs between cost and environmental objectives, generating a set of optimised solutions rather than a single optimum. The resulting solutions are finally analysed to assess their performance and positioning with respect to PB limits.

assessments from institutions such as the European Commission and the International Energy Agency (IEA), which also focus primarily on CO_2-equivalent metrics[33].

Although this GWP accounting approach is implemented in EnergyScopeTD, the underlying rationale is not specific to this model; it reflects a general modelling practice shared across most energy planning frameworks. In EnergyScopeTD, this carbon-centric perspective is operationalised by evaluating GHG emissions arising from resource extraction or production and from their combustion[27]:

$$GWP_{\text{tot}} = \sum_{j \in \text{TECH}} \frac{GWP_{\text{constr}}(j)}{\text{lifetime}(j)} + \sum_{i \in \text{RES}} GWP_{\text{op}}(i), \tag{1}$$

where the construction emissions $\text{GWP}_{\text{constr}}$ and the operational emissions GWP_{op} are derived from:

$$GWP_{\text{constr}}(j) = gwp_{\text{constr}}(j) \cdot F(j) \quad \forall j \in \text{TECH}, \tag{2}$$

$$GWP_{\text{op}}(i) = \sum_{t \in T} gwp_{\text{op}}(i) \cdot Ft(i,t) \cdot t_{op}(t) \quad \forall i \in \text{RES}, \tag{3}$$

with:

- $i \in \text{RES}$: index over *resources* (e.g., natural gas, diesel, imported electricity);
- $j \in \text{TECH}$: index over *technologies* (e.g., wind turbine, heat pump, gas boiler);

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- $gwp_{constr}(j)$: Specific construction GHG emissions of technology j
- $gwp_{op}(i)$: Specific GHG emissions of resources i
- $F(j)$: installed *capacity* of technology j with respect to its main output, in GW[1];
- $Ft(i,t)$: operation of resource i in period t, in GW;
- $t_{op}(t)$: *duration* of time step t, in hours.

However, although this approach is inspired by life cycle thinking, it remains incomplete when assessed against the four essential phases of LCA[34]. A major limitation lies in the absence of a clearly defined functional unit, which prevents consistent allocation of environmental impacts to energy services. Instead, they are directly associated with resource combustion rather than with the technologies that transform these resources into useful outputs. While such an approach is sufficient to estimate the global warming potential of fossil-based systems, where combustion emissions dominate the life cycle, it becomes inadequate for renewable-based systems, where emissions are largely concentrated in other life cycle phases (e.g., construction) and risks of burden shifting arise.

Moreover, the method is structurally limited by its exclusive focus on combustion-related emissions. It overlooks environmental impacts associated with other key exchanges, such as water use, pollutant emissions, or the environmental pressures linked to infrastructure and material supply chains. These secondary flows are not explicitly represented in the energy system model and cannot be captured through simplified emission accounting based solely on resource flows. As a result, the methodology adopted so far within EnergyScopeTD cannot assess impact categories beyond climate change and therefore fails to provide a comprehensive environmental profile of technologies and resources.

To overcome these shortcomings, a revised methodology is introduced. It builds upon life cycle thinking more systematically and is designed to be applicable beyond EnergyScopeTD, offering a generalised framework for environmental impact assessment in energy system models.

From carbon accounting to life cycle assessment: advancing environmental evaluation in energy planning

The revised methodology addresses the above limitations by adopting a modular cradle-to-cradle LCA structure consistent with the ISO 14040[35]. It introduces a disaggregation of environmental impacts across four distinct stages:

- LCA_{res}: Environmental burdens from resource extraction or production, transformation, and transport (e.g., natural gas, hydrogen, biomass, etc.).
- LCA_{constr}: Emissions and impacts related to the construction and manufacturing of energy technologies and infrastructure (e.g., solar panels, electrolyzers, electric vehicles, etc.).
- LCA_{op}: Impacts from the operation of technologies, including direct emissions (e.g., fuel combustion, electricity use, etc.).
- LCA_{eol}: Emissions and impacts related to the end of life of the technologies (e.g., nuclear dismantling, battery recycling, etc.).

Each component is expressed per unit of service delivered by the technology or resource, ensuring compatibility with LCA standards through the explicit use of functional units (for example, megajoules, kilowatt-hours, or passenger-kilometers). As a result, with this updated formulation, the model accounts for environmental impacts beyond GHG emissions and captures differences in the full life cycle burdens of similar energy carriers or technologies. While construction impacts are physically concentrated at the beginning of a technology's life, they are annualised in Equation 4 to ensure mathematical consistency with the economic optimisation framework, which relies on annualised system costs. Furthermore, when coupled with prospective LCA, this approach remains relevant as it uses background inventories (via the Premise framework) that are updated to reflect the defossilisation of supply chains at the specific time of construction. This ensures that the snapshot at time T accurately represents the system's annual environmental footprint, aligned with the technological reality of that specific instant. The prospective Life Cycle Inventory (pLCI) is generated using Premise (v2.0.0)[26], which transforms the static ecoinvent 3.6 database into scenario-specific future inventories for each target year. This process is based on the SSP2 ("Middle of the Road") socioeconomic pathway, which assumes a continuation of current global development trends. Within this narrative, we selected the REMIND-SSP2-PkBudg1150 scenario, a Paris-aligned pathway designed to limit global warming to 2°C[36]. Compatibility

[1]The main output can differ depending on the end use (e.g. [Mpkm] (millions of passenger-kilometers) for passenger transport, [Mtkm] (millions of ton-kilometers) for freight transport, or [GWh] for storage)

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with the Belgian energy transition case study is ensured through narrative and mathematical consistency. The greenhouse-gas reduction targets imposed in the Belgian optimisation model are derived by applying the annual reduction rates of the European region in the same REMIND scenario to Belgium's 2015 baseline emissions. As a result, both the foreground optimisation model and the background environmental inventories evolve under a coherent set of assumptions regarding climate ambition and technological progress. A more detailed description of the pLCI construction and its integration with the optimisation framework is available in the work of Van den Oever et al[37].

The total environmental impact of the system on an environmental indicator (denoted as LCA_{tot}) is defined as follows:

$$LCA_{tot} = \sum_{i \in RES} LCA_{res}(i) + \sum_{j \in TECH} \frac{LCA_{constr}(j) + LCA_{eol}(j)}{lifetime(j)} + LCA_{op}(j) \quad (4)$$

$$LCA_{res}(i) = \sum_{t \in T} lca_{res}(i) \cdot Ft(i,t) \cdot t_{op}(t) \quad \forall i \in RES \quad (5)$$

$$LCA_{constr}(j) = lca_{constr}(j) \cdot F(j) \quad \forall j \in TECH \quad (6)$$

$$LCA_{eol}(j) = lca_{eol}(j) \cdot F(j) \quad \forall j \in TECH \quad (7)$$

$$LCA_{op}(j) = \sum_{t \in T} lca_{op}(j) \cdot Ft(j,t) \cdot t_{op}(t) \quad \forall j \in TECH \quad (8)$$

LCI data are obtained from the ecoinvent database 3.6 and complemented with data from the literature where necessary. In some cases, several ecoinvent datasets were combined to represent a single resource or technology, using Brightway[38]. The detailed methodology for LCI construction and the interpretation of environmental impact categories beyond climate change are presented in the doctoral thesis of Anne van den Oever[30]. Life cycle impacts are then calculated using Environmental Footprint 3.0[40], enabling a multi-indicator assessment across categories, including, among others, climate change, land use, water scarcity, and resource depletion[15].

The choice was made to limit the analysis to a cradle-to-grave approach rather than a cradle-to-cradle one due to the lack of robust and consistent data regarding the end-of-life treatment of novel energy system technologies (e.g., PV panels, electrolyzers, etc.). End-of-life treatment, such as dismantling and recycling, was included when data were available in the background datasets, for example for nuclear power plants and battery production. For technologies where EoL datasets were not available (e.g., boilers), the EoL phase was neglected. Nevertheless, this omission is expected to result in conservative estimates, as the environmental benefits associated with recycling and material recovery are likely to outweigh the potential burdens of decommissioning and disposal. In future developments, as more reliable data become available, this phase could be conveniently integrated to further enhance the completeness of the assessment.

optimisation methodology in energy system models: extending from cost optimisation to multi-criteria environmental assessment

In its original formulation, the EnergyScopeTD model determines the optimal design and operation of a national or regional energy system over a full target year by solving a Linear Programming (LP) problem. The output of the model is the installed capacity of each technology and its operation in each representative period to meet final energy demands while minimising the total annualised system cost.

The cost function C_{tot} is defined as the sum of:

- the annualised investment cost of each technology (C_{inv}),
- the operation and maintenance cost of technologies (C_{maint}),
- the operating cost of resources (C_{op}).

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$$\min \boldsymbol{C}_{\text{tot}} = \sum_{j \in TECH} (\tau(j)\boldsymbol{C}_{\text{inv}}(j) + \boldsymbol{C}_{\text{maint}}(j)) + \sum_{i \in RES} \boldsymbol{C}_{\text{op}}(i) \tag{1}$$

$$\text{s.t.} \quad \tau(j) = \frac{i_{\text{rate}}(i_{\text{rate}}+1)^{\text{lifetime}(j)}}{(i_{\text{rate}}+1)^{\text{lifetime}(j)} - 1} \quad \forall j \in TECH \tag{2}$$

$$\boldsymbol{C}_{\text{inv}}(j) = c_{\text{inv}}(j)\boldsymbol{F}(j) \quad \forall j \in TECH \tag{3}$$

$$\boldsymbol{C}_{\text{maint}}(j) = c_{\text{maint}}(j)\boldsymbol{F}(j) \quad \forall j \in TECH \tag{4}$$

$$\boldsymbol{C}_{\text{op}}(i) = \sum_{t \in T \mid \{h,td\} \in T_H_TD(t)} \boldsymbol{c}_{\text{op}}(i)\boldsymbol{F_t}(i,h,td)\, t_{\text{op}}(h,td) \quad \forall i \in RES \tag{5}$$

Here, the annualisation factor $\tau(j)$ in Equation 2 is computed from the interest rate i_{rate} and the lifetime of technology j. The total investment and maintenance costs in Equation 3 and Equation 4 are obtained by multiplying specific costs by the installed capacity $\boldsymbol{F}(j)$. The total operating cost of resources in Equation 5 is computed as the sum of the quantities consumed in each period, multiplied by their specific operating costs $\boldsymbol{c}_{\text{op}}(i)$ and the period duration $t_{\text{op}}(h,td)$. Summation over the set T_H_TD is equivalent to summing over the 8760 hours of the year.

The optimisation is constrained by a set of linear relationships that ensure the internal consistency and feasibility of the energy system. For each energy carrier and representative time slice, the total supply from all technologies must equal the corresponding end-use demand. Installed capacities and utilisation factors are limited by technical characteristics and resource availabilities. Additional policy and technical bounds are also imposed, including upper limits on GHG emissions, restrictions on nuclear capacity, minimum renewable energy share targets, and constraints on fuel imports.

Environmental performance in the original EnergyScopeTD is addressed through a single GHG constraint, using an LCA approach from cradle to grave. For climate change, the indicator is the global warming potential (GWP), expressed in $ktCO_2$-eq/year:

$$\text{GWP}_{\text{tot}} \leq \text{GWP}_{\text{max}} \tag{9}$$

Advances in life cycle impact assessment (LCIA) enable the use of a broad set of normalised indicators, such as those defined by the *Environmental Footprint (EF)* method, which includes midpoint categories like acidification (mol H^+ eq), freshwater ecotoxicity (CTUe), resource depletion (kg Sb eq), and 13 others[40]. Integrating these indicators directly into the model's objective space requires moving beyond fixed constraints and adopting a genuinely multi-objective optimisation structure.

To preserve the computational advantages of linear programming while integrating multiple objectives, we implement a goal programming (GP) approach[41].

$$\min Z = \sum_{i=1}^{n} w_i \cdot (d_i^+ + d_i^-) \tag{10}$$

subject to:

$$f_i(x) + d_i^- - d_i^+ = G_i \quad \forall i \in \{1, \ldots, n\} \tag{11}$$

$$d_i^+, d_i^- \geq 0 \quad \forall i \tag{12}$$

where $f_i(x)$ denotes the computed value of environmental footprint (EF) indicator i as a function of decision variables x, G_i is the target value, and w_i is a weight reflecting its relative importance. In this work, they are not fixed a priori but are systematically sampled to avoid subjective bias and to explore a wide range of trade-offs; their definition and sampling procedure are detailed in the Section "Scenario generation and decision-making using interpretable machine learning".

In our implementation, the set of indicators f_i includes the total cost and several environmental impacts derived from LCA. Each target G_i is set to the minimum value obtained through a prior single-objective optimisation of the corresponding indicator, which represents an idealized performance baseline. Consequently, the negative deviations d_i^- are always zero in any feasible solution, as no solution can outperform the known minimum. The optimisation thus simplifies to:

$$\min Z = \sum_{i=1}^{n} w_i \cdot d_i^+ \tag{13}$$

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This asymmetric GP formulation penalises only underperformance relative to the ideal, without rewarding overperformance. Such an approach aligns with a precautionary principle: exceeding safe thresholds is undesirable, while exceeding best-case performance yields limited additional value.

However, this formulation inherits a central limitation of LCA: the absence of a universal reference scale to interpret the magnitude of impacts. Units such as mol H^+ eq (acidification), CTUe (ecotoxicity), or kg Sb eq (resource use) are often abstract and lack intuitive meaning, making it difficult to judge whether a given value represents an acceptable level of environmental pressure. This reinforces the importance of normalisation for comparability, but also highlights that normalisation alone does not address the deeper challenge of linking model outputs to absolute sustainability targets.

normalisation methodology in multi-objective optimisation: from conventional comparability to planetary boundaries alignment

A crucial prerequisite for meaningful GP optimisation is the normalisation of all indicators to a common, dimensionless scale. LCA impact indicators are expressed in heterogeneous units, such as kg CO_2-eq for climate change, CTUe for ecotoxicity, or kg Sb eq for resource depletion, and often differ by several orders of magnitude. Without normalisation, the numerical magnitude of each criterion would dominate over the assigned weight w_i, undermining the intended prioritisation between criteria. Classical normalisation approaches, such as the min–max scaling[42], address this issue by expressing each criterion relative to its best and worst achievable values. However, such methods remain purely mathematical: they equalise indicators without considering their environmental significance. Categories already beyond safe limits receive the same weight as those still within sustainable ranges, potentially leading to solutions that are optimal in a relative sense but misaligned with absolute ecological thresholds.

To overcome this limitation, we adopt a revised normalisation scheme anchored in the PB framework, where each life-cycle impact is expressed relative to its corresponding global PB threshold. This approach aligns environmental impact assessment with scientifically defined planetary limits, ensuring that energy transitions operate within global ecological boundaries. Specifically, the threshold values used for normalisation, summarised in Table 1, are obtained directly from the research of Sala et al.[43]. Their work established a quantitative bridge between the Environmental Footprint (EF 3.0) indicators and Planetary Boundary control variables by translating global biophysical limits into LCIA-based PBs. These thresholds were derived by applying conversion factors to existing carrying capacity frameworks, ensuring that the limits are fully aligned with the specific characterisation models and elementary flows of the EF method.

$$f_i^{\text{norm}} = \frac{f_i}{PB_i}, \tag{14}$$

where f_i is the total life cycle impact of category i, and PB_i is its PB at the global scale. This yields a dimensionless measure of the relative pressure exerted on each Earth-system process, ensuring direct comparability and a science-based prioritisation among impact categories. The threshold values summarised in Table 1 represent the annual global safe operating space for each impact category, operationalised as allowable environmental pressures per year (e.g., kg CO2-eq/year or Tg N/year). This one-year time dimension is fully consistent with the temporal scope of EnergyScopeTD, which optimises the energy system's design and operation over a target year of 8,760 hours. Consequently, the normalisation step directly compares the system's total annual life-cycle pressure against the Earth's annual regenerative or absorptive capacity.

Compared to conventional scaling, this approach offers two advantages: (i) normalisation is anchored in absolute ecological limits rather than arbitrary optimisation bounds, and (ii) impact categories nearing or exceeding their PB are automatically prioritised in the optimisation. Building on Sala's work, this PB-aligned normalisation goes beyond the relative improvements highlighted by classical methods and instead provides a direct assessment of the absolute environmental acceptability of each design. The following table summarises the PB thresholds and their corresponding EF-based equivalents used in this study.

However, although impacts are now expressed relative to the PBs, which provides a clearer view of how significant the system's environmental pressures are, this normalisation alone does not determine whether the system can be considered sustainable in an absolute sense. PBs are defined at the global scale, while any studied system, be it a national energy system or a specific technology, represents only one contributor among many to those global impacts.

Therefore, to evaluate whether a system operates within its "fair share" of the safe operating space, it is necessary to allocate a portion of the global environmental budget to it. This allocation relies on so-called sharing principles, which define how the global limits are distributed across countries, sectors, or actors. The challenge lies precisely in the definition of what is "fair": different principles lead to markedly different conclusions[45]. For instance, equal per capita allocation, grandfathering based on historical responsibility, or economic-based approaches (e.g., proportional to GDP) each reflect distinct ethical and political standpoints.

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EF impact category	Unit	PB	PB/cap
Climate change	kg CO_2 eq	6.81E+12	9.85E+02
Ozone depletion	kg CFC-11 eq	5.39E+08	7.80E-02
Eutrophication, marine	kg N eq	2.01E+11	2.90E+01
Eutrophication, freshwater	kg P eq	5.81E+09	8.40E-01
Eutrophication, terrestrial	mole N eq	6.13E+12	8.87E+02
Acidification	mole H^+ eq	1.00E+12	1.45E+02
Land use	kg soil loss	1.27E+13	1.84E+03
Water use	m^3 world eq	1.82E+14	2.63E+04
Particulate matter	Disease incidence	5.16E+05	7.47E-05
Photochemical ozone formation (HH)	kg NMVOC eq	4.07E+11	5.88E+01
Human toxicity, cancer	CTUh	9.62E+05	1.39E-04
Human toxicity, non-cancer	CTUh	4.10E+06	5.93E-04
Ecotoxicity, freshwater	CTUe	1.31E+14	1.90E+04
Ionising radiation	kg U235 eq	5.27E+14	7.62E+04
Resource use, fossil	MJ	2.24E+14	3.24E+04
Resource use, minerals	kg	2.19E+08	3.18E-02

Table 1. Planetary boundaries (PBs) expressed using the EF metrics associated with each impact category, enabling comparison with the LCIA results reported in the latest JRC report (2023): *Consumption Footprint and Domestic Footprint: Assessing the environmental impacts of EU consumption and production*[44].

Scenario generation and decision-making using interpretable machine learning

Following Equation 13, weights must be assigned to each LCA metric in the objective function to construct the objective vector. These weights represent the relative importance of minimising each variable, and therefore strongly influence the results. However, setting weights is inherently subjective; assigning higher importance to one indicator over another depends on user preferences and value judgments.

To avoid fixed subjective weighting, we adopt a stochastic sampling approach based on the Dirichlet distribution[46] to generate a large set of possible weight combinations. Each weight vector is drawn from a Dirichlet distribution with concentration parameters $\alpha = 0.5$ for all indicators, ensuring that all weights are non-negative and sum to one. This choice of α promotes sparsity in the sampled weights, meaning that individual optimisation runs tend to emphasize one or a few indicators while still allowing balanced combinations. A total of 1000 weight vectors are generated, each defining a distinct optimisation problem. This feature is particularly valuable in the LCA context, as it systematically explores situations where decision-making is driven by the minimisation of a single environmental pressure (e.g., land use) as well as cases where impacts are jointly minimised. The resulting set of weighting schemes thus enables the generation of a comprehensive Pareto front of near-optimal energy system configurations that reflect a wide range of implicit environmental priorities, without imposing a single, fixed subjective weighting scheme a priori.

When applying these weighting schemes, however, it is necessary to ensure that the resulting solutions remain economically meaningful. Without a cost constraint, the optimisation could identify low-impact solutions that are prohibitively expensive and therefore unrealistic. To prevent this, we constrain total system costs relative to the optimal solution. In this approach, the cost is minimised once to establish the mathematical optimum, after which it is reformulated as a constraint with a slack allowance. This ensures that all solutions remain close to cost-optimality while still exploring different environmental trade-offs. Formally, let C^*_{tot} denote the optimal total annualised system cost obtained from the primary optimisation. We then impose the following constraint in subsequent runs:

$$C_{\text{tot}}(x) \leq C^*_{\text{tot}}(1+\delta), \tag{15}$$

where $\delta \geq 0$ is a slack factor that defines the permissible deviation from the optimal cost.

The resulting space of optimised solutions, one for each distinct LCA weighting scheme, can quickly become overwhelming and difficult for decision-makers to interpret. Each solution may imply very different design directions: for instance, one solution might emphasize wind-heavy infrastructure while another leans toward solar or bioenergy, even though both are within the cost tolerance limit[47].

To streamline this large set of solutions into actionable insights, interpretable machine learning is employed[48]. Rather than treating each optimised design as an isolated outcome, this approach uncovers the patterns that explain why different solutions emerge. It highlights which design choices consistently appear across many scenarios and which ones shift depending on how environmental priorities are weighted. In doing so, interpretable machine learning helps transform a complex and potentially

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overwhelming solution space into clear and actionable insights.

The framework developed by Baader et al.[31] is applied to systematically analyse the large set of optimised energy-system designs and identify a small number of interpretable archetypes. First, the 1000 optimisation runs are represented in terms of a selected subset of system-design variables that capture the main differences between configurations. In this study, these variables include renewable hydrogen imports, synthetic methanation, hydrogen electrolysis, battery-electric vehicles, hydrogen fuel-cell trucks, low-temperature heat pumps, high-temperature electrification, offshore wind power, geothermal power, and PV power. Before analysis, all variables are normalised to unit scale.

Second, the solutions are grouped into k clusters using the k-means algorithm. These cluster labels provide an initial grouping of similar system configurations. The number of clusters is selected using the elbow method, which indicates that four clusters provide a suitable balance between capturing the main structure of the near-optimal solution space and preserving interpretability.

Third, a supervised machine-learning model based on the Classification and Regression Trees (CART) algorithm[49], implemented in *scikit-learn 1.3.0*[50], is trained using the normalised decision variables as input features and the cluster labels as target classes. The decision tree recursively identifies threshold values on the decision variables that best separate the clusters, thereby translating the original clustering into a compact set of hierarchical and interpretable decision rules.

To avoid overfitting and maintain interpretability, the complexity of the tree is restricted by balancing predictive performance against structural simplicity. Following Baader et al.[31], this trade-off is assessed using coverage and interpretability scores. The coverage score measures the proportion of solutions consistently assigned to the corresponding archetype, while the interpretability score reflects the complexity of the tree in terms of the number of distinct variables used. In addition, k-fold cross-validation is performed to assess classification robustness on data not used during training. The final number of archetypes and the depth of the tree are selected as a compromise between faithful representation of the near-optimal solution space and ease of interpretation.

Method pipeline and application to the case study

The framework is applied to Belgium's national energy planning, using the complete reference dataset for technology performance, costs, efficiencies, and energy demand from Limpens et al.[28]. The application follows a structured sequence designed to first establish a feasible space of solutions, then assess environmental performance against PBs, then identify the critical indicators to be included in the multi-criteria optimisation, and finally apply clustering and decision tree analysis to identify coherent energy system archetypes that capture the dominant trade-offs between environmental objectives.

In the first step, we determine the cost-optimal configuration of the Belgian energy system under a national CO_2 emission constraint. The $CO_{2,eq}$ limit is set to 20 Mt in 2045. This value follows the national decarbonisation trajectory developed by van den Oever[39] in a normative scenario. This trajectory is derived by applying the annual GHG reduction percentages of the European REMIND SSP2-PkBudg1150 pathway proportionally to Belgium's 2015 baseline emissions by 2045, reflecting a decarbonisation pace aligned with European targets.

The remaining emissions in 2050, which cannot be fully eliminated through structural changes in the energy system, will require the deployment of carbon capture and removal technologies. This need is explicitly highlighted in the European Union's most recent 2040 climate target communication, which stresses that achieving the final percentages of decarbonisation will depend on a substantial scale-up of carbon capture, utilisation and storage (CCUS) and carbon dioxide removal (CDR) solutions[51]. Although this constraint is policy-based rather than derived directly from the PBs framework, it provides an environmentally consistent reference for the case study.

Once the least-cost solution is obtained, a cost-tolerance slack δ is introduced to define the feasible near-optimal space. A 30% slack is adopted, consistent with common practice in near-optimal energy system exploration[47,52]. This choice reflects the intention to remain aligned with current policy contexts, where economic optimality remains a dominant decision criterion, and to rely on well-established benchmark settings. At the same time, it enables the demonstration that substantial environmental trade-offs already emerge within this economically plausible solution space. As the primary objective of this study is to demonstrate the relevance and robustness of the proposed methodological framework, anchoring the analysis in such familiar conditions ensures both interpretability and comparability of the results.

In the second step, we systematically investigate this feasible space to characterise the attainable range of environmental performance. Each life-cycle impact category is optimised individually, one at a time, to identify its minimum achievable value while satisfying the cost and CO_2 emission constraints. This process defines the lower and upper limits of all LCA impact indicators, effectively mapping the boundaries of the optimisation space. These results represent the optimal environmental performance that the system can achieve for each impact category, given the imposed economic and climatic constraints.

The third step evaluates how these minimum-impact solutions perform relative to PBs. Because PBs are defined at the global scale, they must be downscaled to derive national-level limits for comparison. In this framework, we deliberately avoid a fixed sectoral allocation, such as a specific share for the energy sector, as legitimate sector-specific budgets for most non-climate

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indicators remain currently unknown. Instead, the system's performance is benchmarked directly against the total Belgian national budget. To define this national safe operating space, two allocation principles are applied to downscale the global boundaries. The egalitarian principle distributes boundaries equally on a per capita basis, while the utilitarian principle allocates them proportionally to national GDP. This dual approach provides an indicative range of national "fair-share" limits, allowing for an assessment of the portion of the total national environmental budget required by the energy system under different transition scenarios.

Finally, indicators whose worst-achievable values in the feasible space still exceed their nationalized PBs are identified as critical. These critical indicators are selected for inclusion in the second stage of the method, where they are explicitly considered in the goal-programming formulation. In this stage, we perform 1000 optimisation runs, each based on a different combination of weighting factors randomly drawn from a Dirichlet distribution. This systematic sampling explores the full spectrum of trade-offs between cost and environmental performance. The large set of resulting solutions is then analysed using interpretable machine learning techniques, specifically, clustering and decision tree analysis, to identify recurring patterns and group similar system configurations. The resulting archetypes reveal coherent energy system designs that embody distinct trade-offs between environmental indicators, providing a transparent view of the dominant strategies that emerge within the near-optimal solution space.

Results

Reference scenario

The cost-optimal solution for 2045 under the GHG emission constraint serves as a reference for assessing future scenarios and explore the near optimum solutions. At this cost optimum, Belgium's energy system maximises the use of local renewable resources, notably wind, solar, and biomass, while deploying nuclear energy up to the limits set by national policies (Figure 2). Since domestic renewable capacity is insufficient to meet total demand, the system relies on importing electrofuels, such as hydrogen, methanol, and ammonia, alongside electricity imports to close the gap. Seasonal intermittency is managed through

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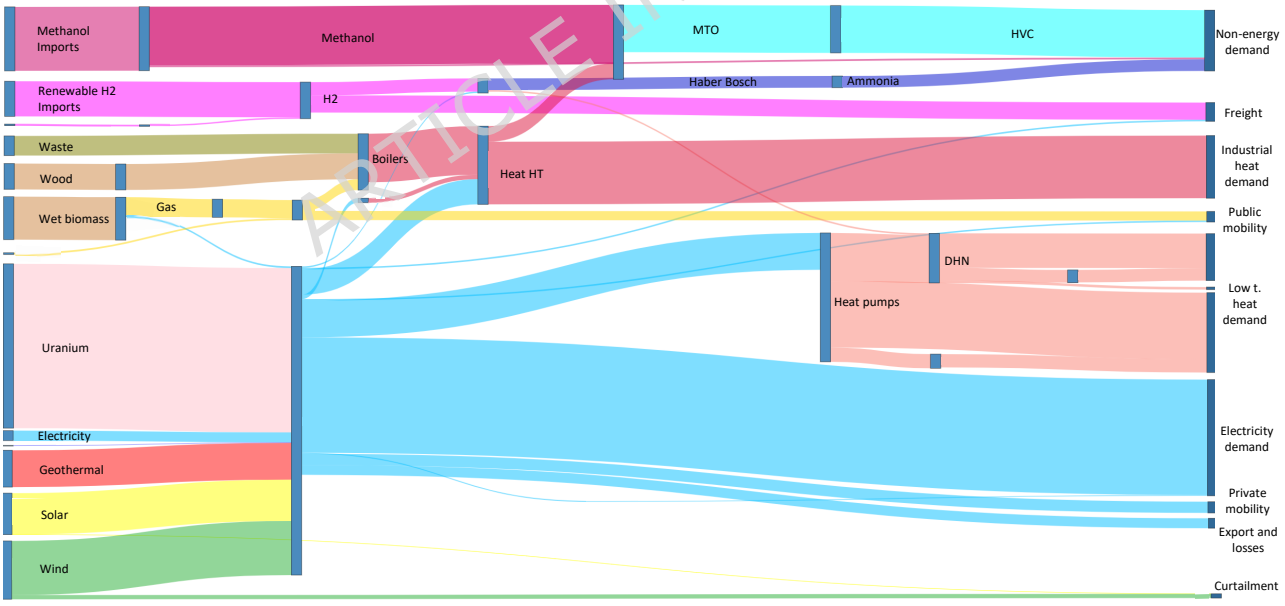


Figure 2. Energy flows in the reference scenario representing the cost-optimum Belgian energy system in 2045, with a climate target of 20 $MtCO_{2,eq}$. The left-hand side gathers all the resources, while the right-hand side represents final energy consumption. In between are the conversion technologies. Abbreviations: import (imp), production (prod), storage (sto), high-value chemicals (HVC), curtailment (Curt.), district heating networks (DHN), hydrogen (H_2), heat pump (HP), high temperature (HT), low temperature (LT), industrial (ind), decentralized (Dec), private and public mobility (Mob priv and Mob public), and exports and losses (Exp & Loss).

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extensive use of heat pumps with thermal storage, district heating, and demand-side flexibility, particularly through optimised electric vehicle charging. At this cost-optimal configuration, the total system cost amounts to approximately 40 billion EUR in 2045, covering all investment, operation, and import expenditures. The solution meets the national CO_2 reduction target, limiting total CO_2-equivalent emissions to 20 $MtCO_{2,eq}$. For reference, the 2015 system exhibited a 5%/95% split between construction and operation emissions. Under the 20 $MtCO_2$ cap, this balance shifts to 33%/66%, and at 10 $MtCO_2$ it reaches 23%/77%, consistent with expected trends as operational emissions decrease [12].

Solution space of the case study

Environmental indicators

The second step explores the near-optimal cost space to identify how environmental impacts can be reduced at the expense of a higher total system cost. This exploration reveals a broad and diverse set of feasible designs that exhibit trade-offs among LCA indicators (Figure 3). The boundaries of this space are determined by optimising each indicator individually, assigning full weight to one impact category at a time, which defines the attainable limits of environmental performance within the imposed cost and GHG constraints.

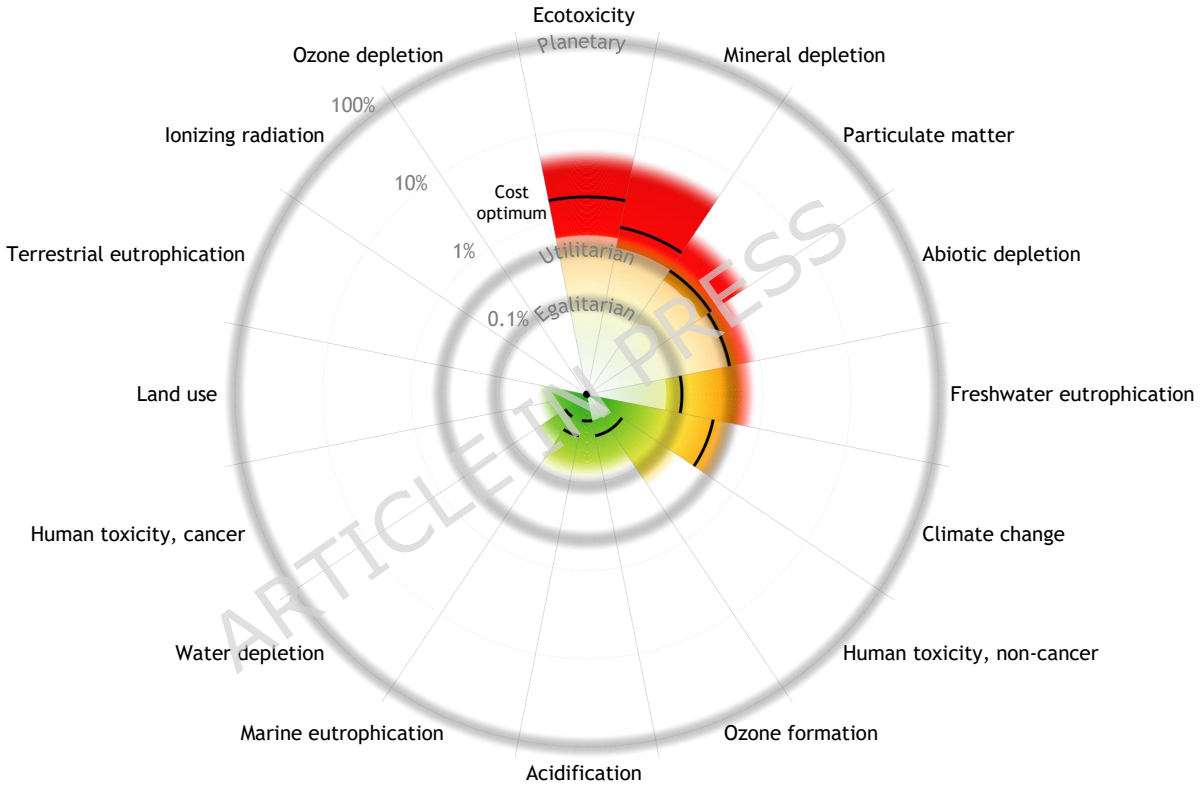


Figure 3. Each LCA indicator obtained from energy system designs satisfying the constraint of 20 Mt $CO_{2,eq}$ emissions in 2045, aligned with the work of Van den Oever[39], and a total system cost below 130% of the optimal-cost solution can vary within a solution space represented by the strongly colored areas. The indicator values corresponding to the optimal-cost solution are shown as black lines. Three boundaries are displayed to facilitate interpretation: moving from the center outward, the first corresponds to the egalitarian sharing principle, the second to the utilitarian sharing principle, and the outermost boundary represents the total PB (at 100%), as reported in Table 1. The radial format is intentionally chosen to remain consistent with the standard visualization commonly used in the planetary boundaries literature[2], allowing direct interpretation in terms of relative pressure and exceedance across multiple indicators. Because PB thresholds and associated risks remain uncertain, the benchmark boundaries are shown as blurred bands rather than sharp limits.

Five indicators are critical at their highest attainable values within the feasible space: ecotoxicity, mineral depletion, particulate matter emissions, abiotic depletion, and freshwater eutrophication (Figure 3). This aligns with the indicators commonly used in the literature to assess systemic ecological and human health risks, which include, among others, climate change, freshwater eutrophication and particulate matter formation[15]. The criticality of these results is evaluated against limits derived from two distinct burden-sharing principles: an egalitarian (per-capita) principle and a GDP-based (utilitarian) principle.

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Both are normative by nature, and comparing them provides an indicative range of how sustainability conclusions vary with underlying fairness assumptions. These results are presented under both allocation approaches for transparency, acknowledging that a comprehensive assessment of burden sharing would require a dedicated, multidisciplinary analysis integrating ethical, political, and socio-economic perspectives. Yet, this framework enables an indicative assessment of the system's sustainability in a global context, while acknowledging that it represents only one possible interpretation among others.

It is also important to distinguish between indicators that are directly tied to PBs and those that primarily affect the sustainability of human activities. Ecotoxicity and freshwater eutrophication have direct consequences on ecosystems and biodiversity, making them integral to planetary-scale stability. In contrast, mineral depletion and abiotic depletion affects resource availability for human activities without disrupting fundamental Earth system processes, and particulate matter emissions pose a significant threat to human health but do not strongly interfere with global ecological cycles. This distinction is crucial for guiding policy and technological choices.

To explain the LCA indicator reduction potential shown in Figure 3, the correlation between the selected LCA indicators is assessed for the attained solution space (Figure 4). The correlation matrix shows that climate change is negatively correlated with non-climate indicators: most strongly with particulate matter ($r = -0.35$), and more weakly with freshwater eutrophication ($r = -0.21$) and ecotoxicity ($r = -0.09$). In contrast, a small positive correlation exists between climate change and abiotic depletion ($r = 0.23$). The non-climate indicators—particulate matter, ecotoxicity, freshwater eutrophication, mineral depletion, and abiotic depletion—are all positively correlated (except for a minor negative correlation between abiotic depletion and ecotoxicity), indicating that these impacts tend to increase or decrease together. In particular, strong correlations exist between freshwater eutrophication and mineral depletion ($r = 0.70$), and between freshwater eutrophication and particulate matter ($r = 0.73$). Consequently, within the attained solution space, shifting the design focus away from climate change tends to increase the impacts on non-climate environmental indicators simultaneously.

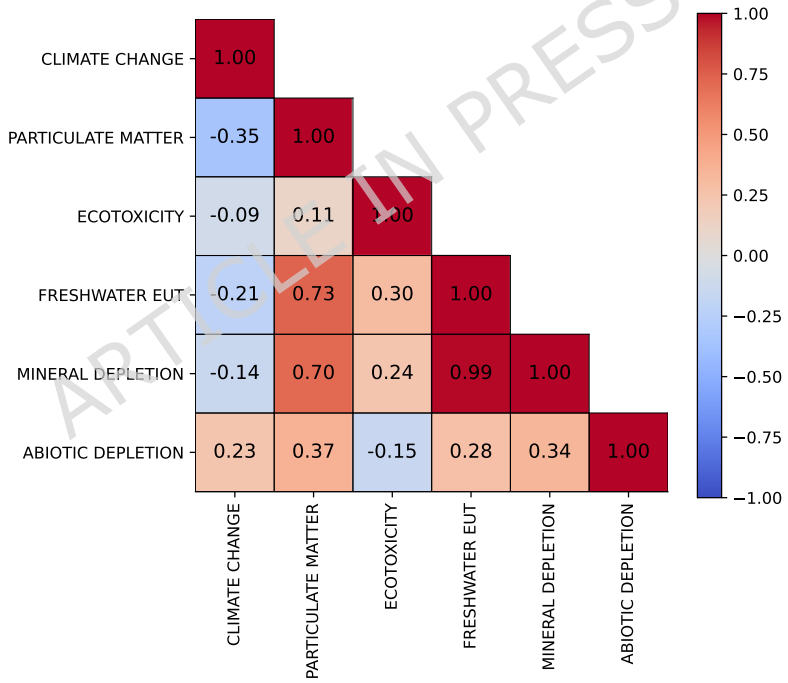
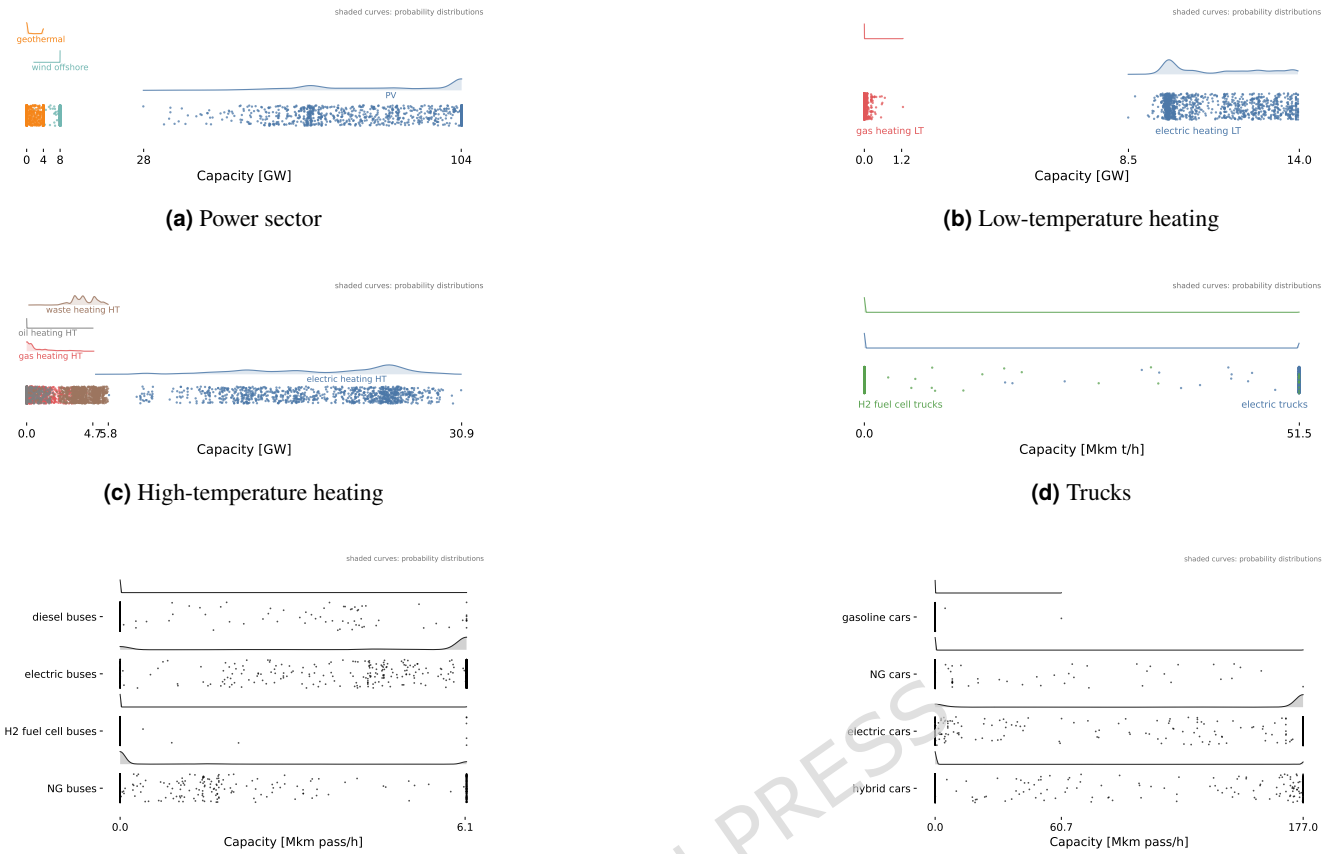


Figure 4. Correlation matrix of the attained solution space, showing the relationships between climate change, particulate matter, ecotoxicity, freshwater eutrophication, mineral depletion and abiotic depletion. Climate change correlates negatively with non-climate indicators, indicating a trade-off when reducing greenhouse gas emissions. In contrast, the non-climate indicators exhibit positive correlations, with strong associations among mineral depletion, particulate matter, and freshwater eutrophication, illustrating that these impacts tend to increase or decrease together within the explored design space.

Investment decisions

Figure 5 shows the selection of technology capacities across the near-optimal solution space, reflecting the diversity of investment choices consistent with the cost and CO_2 emission constraint. The results reveal that a large set of diverse technology portfolios can be attained within the cost slack to reduce the impact on the various LCA indicators considered.

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(a) Power sector

(b) Low-temperature heating

(c) High-temperature heating

(d) Trucks

(e) Buses

(f) Passenger cars

Figure 5. Distributions and strip plots of selected technology capacities across the near-optimal solution space. The distributions above each strip plot summarize the frequency and spread of the corresponding capacity values. In the power sector, solar PV exhibits wide variability, offshore wind is almost always deployed at its maximum capacity, and geothermal is either unused or installed at its full potential. Low-temperature heating is dominated by electric heat pumps, while gas-based options appear only in a minority of solutions. High-temperature heating shows greater diversity, with both electric and fuel-based technologies represented across the solution set. In the mobility sector, electric and hybrid passenger cars dominate, while gasoline- and natural-gas-powered vehicles appear only sparsely. Bus technologies vary substantially; electric-, hydrogen-, gas-, and diesel-powered options each serve as the sole technology in part of the solution space. Freight transport shows a split between electric and hydrogen trucks, with electric trucks selected more frequently.

In the power sector (Figure 5a), solar PV investments vary widely between 28 GW_p and 104 GW_p. The solutions for offshore wind illustrate that it is nearly always selected at maximum capacity, while geothermal capacity is either excluded or installed at its maximum potential (4 GW for geothermal power, 8 GW for offshore wind power). In contrast, nuclear and onshore wind are always deployed at their upper bounds, leaving no diversity in these investment decisions. Low-temperature heating (Figure 5b) is dominated by electric heat pumps, while gas-based heating appears only in a subset of solutions—typically below 0.7 GW. High-temperature heating (Figure 5c) exhibits greater diversity, with total installed capacities for direct electrification ranging from 4 GW to 30 GW. Electric and gas-based options appear in most configurations, while waste-fueled boilers (up to 5.8 GW) and oil-fueled boilers (up to 1.9 GW) persist in part of the feasible space. In the mobility sector, electric and hybrid passenger cars dominate most configurations (Figure 5f) and are often selected as the sole technology. Gasoline and natural gas vehicles occupy smaller shares, appearing in only a few solutions and never fully satisfying private mobility demand. For buses (Figure 5e), four main technologies emerge across the solution set (electric-, hydrogen-, gas-, and diesel-powered), each serving as the exclusive option in some configurations. In freight transport (Figure 5d), either electric or hydrogen trucks are deployed, with electric trucks more frequently selected as the preferred technology. Diesel trucks are not selected in any of the near-optimal solutions under the imposed CO_2 constraint.

To assess how variations within the decision space influence LCA indicators, we generated a correlation matrix between technology deployment and environmental impacts (Figure 6). The results show that hydrogen from biomass and biomethanation

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are strongly and negatively correlated with climate change impacts, confirming that these technologies are the main pathways used to further reduce emissions below the 20 $MtCO_2eq$ target. However, biomethanation correlates positively with particulate matter, indicating environmental trade-offs associated with its large-scale deployment. Geothermal power, although cost-effective, exhibits strong positive correlations with ecotoxicity, while PV capacity is expanded primarily in configurations targeting lower ecotoxicity.

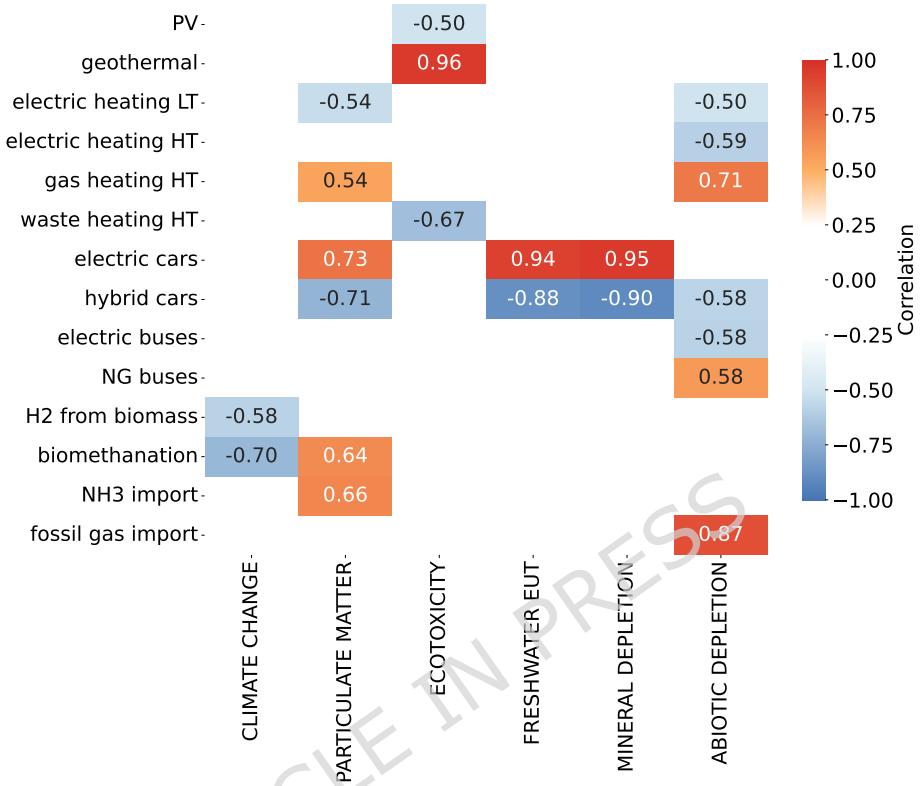


Figure 6. Correlation matrix between technology deployment and environmental impact indicators. Biomethanation is strongly and negatively correlated with climate change impacts, indicating its key role in achieving the 20 $MtCO_2eq$ target, but it increases particulate matter. PV deployment mitigates ecotoxicity, while geothermal power correlates positively with ecotoxicity. Electric vehicles reduce emissions but worsen water-related and particulate impacts, whereas hybrid cars alleviate these effects. Renewable ammonia imports contribute to decarbonisation, yet increase particulate matter. Correlations reflect trade-offs within the decision space rather than isolated technology performance. Cells with absolute correlation values below 0.5 are masked for clarity.

Electric cars are widely deployed to achieve the CO_2 target in a cost-optimal configuration, but are strongly and positively correlated with mineral depletion, particulate matter, and freshwater eutrophication. In near-cost-optimal solutions, the deployment of hybrid cars as a substitute helps reduce these impacts, highlighting a trade-off between cost efficiency and environmental co-benefits.

Abiotic depletion is driven mainly by fossil gas consumption and by deploying fossil-gas technologies in heating (gas boilers in high-temperature industry) and mobility (CNG buses in public transport). In configurations where abiotic depletion is minimised, electric alternatives are deployed in low-temperature heating (heat pumps), high-temperature heating (direct electrification), private mobility (hybrid cars), and public mobility (electric buses).

Finally, renewable ammonia imports, while providing a low-carbon energy carrier to meet demand, are positively correlated with particulate matter, reflecting the environmental burden of their production or import pathways.

It is important to note that these correlations represent relationships within the decision space rather than the isolated environmental performance of each technology. For example, while geothermal power generally reduces CO_2 emissions, this effect does not appear in the matrix because it often substitutes PV rather than fossil generation in the set of solutions generated. In such cases, both technologies already contribute to decarbonisation, and the correlation reflects trade-offs among low-carbon options rather than their absolute mitigation potential.

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System archetypes

The previous section shows that a broad range of configurations can achieve the carbon emission reduction target within a 30% cost tolerance, although these configurations differ in their performance across other LCA indicators. Because this wide range of options can overwhelm decision-makers, we applied clustering and decision tree analysis to organize the solutions into a few interpretable and actionable decisions.

The resulting decision tree identifies four main system archetypes (Figure 7). The first split occurs along the share of battery-electric vehicles (BEVs) in private mobility. When BEVs account for less than 40% of private transport demand (71 Mkm pass/h), a set of compensatory decisions emerges to still meet the CO_2 target within the total cost tolerance: a full deployment of offshore wind (8 GW), a strong expansion of PV (median at 90 GW), and extensive electrification of both low- and high-temperature heat. In this configuration, the energy system avoids renewable hydrogen imports, thereby reducing vulnerability to import disruptions. Instead, local hydrogen production is prioritised, with subsequent conversion into methane via synthetic methanation using the surplus renewable electricity from high PV and offshore wind deployment. This cluster shows the highest impacts on climate change, with most configurations approaching the GHG emission constraint. However, it achieves the lowest impacts across the other indicators, particulate matter formation, ecotoxicity, freshwater eutrophication, mineral depletion and abiotic depletion. This pattern aligns with the correlation matrix between decisions and impacts (Figure 6), which shows a positive correlation between BEV deployment and non-climate LCA impacts, while PV and low-temperature electrification correlate negatively with those indicators.

Conversely, when BEVs cover at least 40% of private mobility demand, three distinct system archetypes emerge. The first appears when geothermal power exceeds 2.2 GW. This cluster is characterised by lower heating electrification, reduced reliance on renewable hydrogen imports and local production, and lower PV capacity, compensated by higher geothermal deployment. It yields the highest impacts on ecotoxicity, consistent with the observed correlation between geothermal generation and ecotoxicity in Figure 6.

When geothermal power deployment is limited ($\leq$2.2 GW), two additional archetypes arise depending on the degree of local hydrogen production (electrolysis capacity above or below 4.1 GW). In the high-hydrogen archetype, extensive local hydrogen production is paired with large-scale synthetic methanation to convert the additional hydrogen into methane. PV and offshore wind are fully utilised, while electrification of both low- and high-temperature heating are strongly favored. Mobility is also strongly electrified, no hydrogen trucks are deployed in most configurations. Renewable hydrogen imports are excluded entirely, making this a fully domestic, local electricity production system. This configuration minimises climate change impacts, with limited variation across other indicators.

In contrast, when local hydrogen production is limited, the system exhibits more flexibility in PV deployment, high-temperature electrification, renewable hydrogen imports, and hydrogen trucks. While overall LCA impacts are similar to the high-hydrogen case, the broader decision flexibility results in wider ranges across impact indicators.

Discussion

Applying the framework to the case study reveals several concrete insights. Even under near-optimal configurations within a 30% cost tolerance, persistent trade-offs remain across environmental dimensions. All feasible pathways respect the imposed climate target but still exceed other PBs, indicating that focusing on defossilisation alone in energy system optimisation models does not ensure absolute sustainability. The ensemble of diverse, near-optimal solutions for the Belgian energy mix demonstrates that multiple designs, rather than a single optimum, can achieve similar costs and emissions.

Exploring the near-optimal solution space reveals a wide degree of flexibility in system design. Onshore wind consistently appears at its upper technical limit across all solutions, confirming it as a no-regret option, while solar PV, offshore wind, renewable hydrogen (domestic production and imports), and electrification options in transport exhibit substantial variability, highlighting strong substitution potential across the system. In this first study, restricting the analysis to a cost-based near-optimal space is intentional, as the primary objective is to introduce and validate the proposed methodological framework under a familiar economic benchmark. This ensures transparency and comparability with existing energy system studies. Broader explorations relaxing the cost constraint or explicitly integrating externalities are left for future work, where the focus will shift towards fully sustainability-constrained solution spaces.

The decision tree distilled this diversity into four main system archetypes that capture the dominant structural choices of the energy transition. These archetypes show that by excluding hydrogen imports, limiting the deployment of battery-electric vehicles, and prioritising large-scale offshore wind, the CO_2 target can be achieved while substantially reducing impacts on particulate matter, ecotoxicity, freshwater eutrophication, mineral depletion and abiotic depletion. Notably, two archetypes exclude renewable hydrogen imports entirely, indicating that viable configurations exist without reliance on external energy carriers. Such dependence can pose a vulnerability by exposing the system to supply-chain disruptions, price volatility, and geopolitical risks, factors that undermine the resilience of a decarbonised energy system[53].

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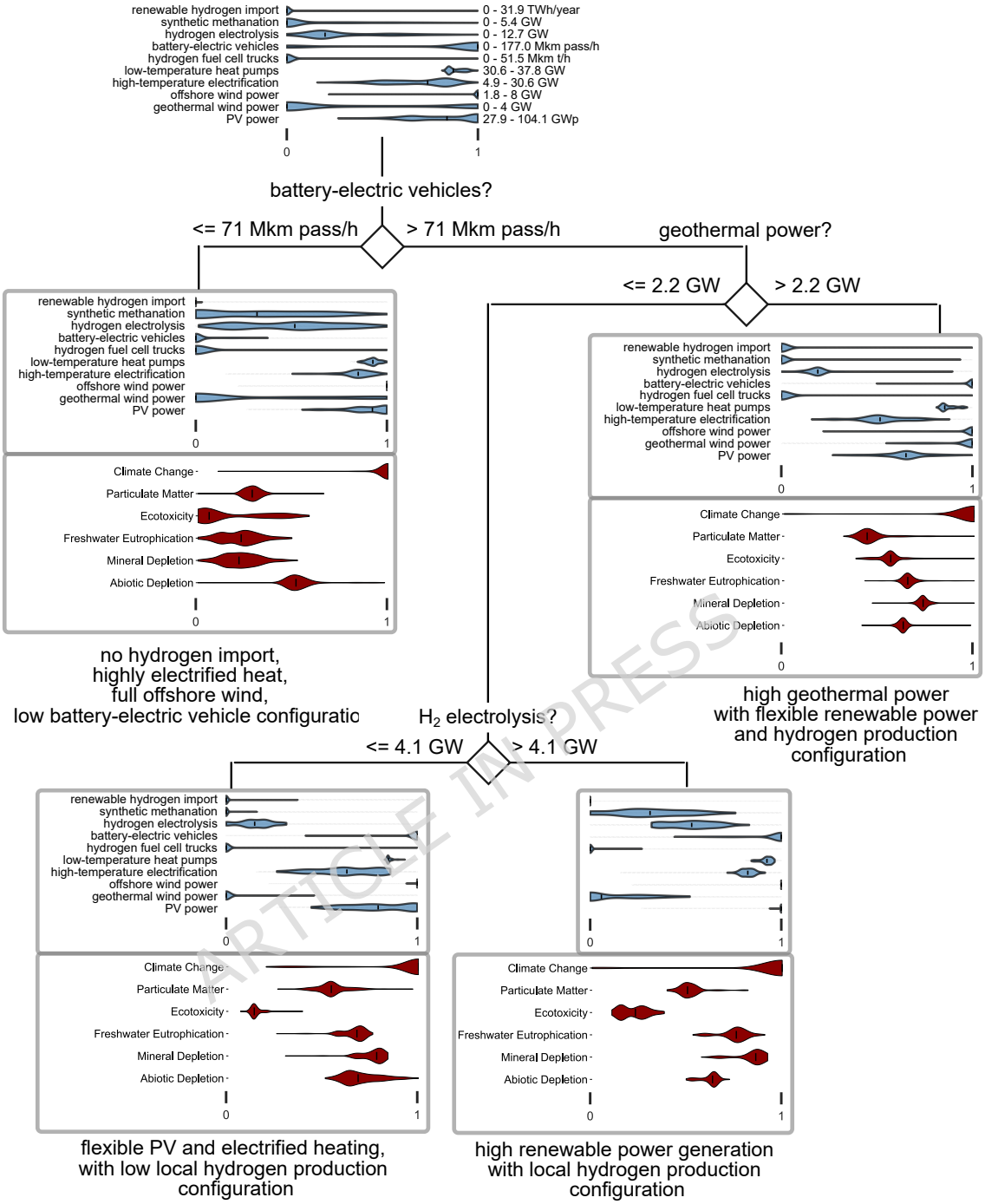


Figure 7. Decision tree of system configuration archetypes identified through clustering analysis. The first split separates cases with low battery-electric vehicle (BEV) penetration (<40%) from those with higher BEV shares. Low-BEV systems rely on full offshore wind and extensive PV deployment, combined with high electrification of heating, and achieve the lowest non-climate LCA impacts but the highest climate change impact. When BEV deployment exceeds 40%, three distinct archetypes emerge: geothermal-oriented systems (>2.2 GW) with lower electrification and higher ecotoxicity; hydrogen-focused systems with extensive local hydrogen production and synthetic methanation, showing little variation in indicators; and limited local hydrogen production, partial reliance on renewable hydrogen imports, and wider variability across environmental impacts.

Notably, across all configurations, private mobility emerges as a central design driver of the energy transition, with the electrification of transport, particularly through battery-electric vehicles, playing a decisive role in shaping system composition and cost. This observation is consistent with previous findings by Limpens, who identified that investments required in

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mobility represents almost two third of the total investment required during the transition[54]. While electric vehicles are often framed as a cornerstone of decarbonisation, the results here underline that this technology also carries significant material and energetic implications. The scale of energy and resource flows required by widespread electric mobility introduces additional sustainability pressures, corroborating insights from material-based and life-cycle analyses[55]. This highlights the importance of complementing technology-focused transition strategies with demand-side approaches, exploring alternative mobility pathways that move beyond the continued expansion of private car ownership, particularly in segments dominated by large and resource-intensive vehicles such as SUVs.

This diversity of options provides important insight for policy design: it shows that there is genuine flexibility in how the transition can unfold, but that this flexibility comes with clear conditional trade-offs. Choosing not to pursue one direction necessarily requires reinforcing others. For example, limiting the role of imported hydrogen implies stronger electrification of transport and heating, while a preference for lower electrification demands greater reliance on renewable fuels or firm generation such as geothermal power. At the same time, the analysis indicates that none of the trade-offs explored so far are sufficient to remain within all planetary boundaries simultaneously, suggesting that technological substitution alone may not be enough. This highlights the need to investigate sufficiency-oriented pathways and demand reduction strategies alongside supply-side transformations. Hence, the analysis therefore makes explicit the consequences of strategic preferences and societal choices: several routes to sustainability exist, but each demands a coherent and internally consistent set of complementary measures to remain within environmental and economic limits. Sustainable transitions therefore require internally consistent pathways, where strategic choices about electrification, fuel imports, or firm generation are made with clear understanding of how each decision constrains the available options in other parts of the system[56].

Despite these advances, several limitations shape the interpretation of our results. First, PB limits were implemented as global normalisation references without formal downscaling to the national level; therefore, no information is provided on the exceedance of the boundaries, suggesting the need for future work on national PB allocation[57]. This choice reflects a conservative approach aimed at limiting uncertainty, as the methodology is already in place but robust downscaling remains constrained by data availability. This limitation is further exacerbated when focusing on a restricted case study such as the energy system, for which even fewer reliable estimates exist to determine the share of environmental impacts attributable to a specific sector across different indicators. Second, the integrated LCA excluded most end-of-life stages due to data scarcity, leading to a conservative bias. End-of-life treatment was included when available in background datasets, but omitted for some technologies lacking robust data, which likely leads to an underestimation of potential recycling benefits. Moreover, although the Premise framework[26] was used to develop prospective life cycle inventories for the technologies, some underlying ecoinvent datasets may still rely on outdated assumptions about waste treatment. Therefore, the life cycle of key technologies must be thoroughly checked and updated as more accurate recycling and disposal data become available[58]. Third, the model treats energy service demand as exogenous and fixed, omitting potential demand reductions or behavioral changes. Demand-side strategies could strongly complement supply-side measures; for example, global low-energy-demand scenarios show that deep emission cuts become far more achievable under reduced demand[59]. Future extensions should thus incorporate dynamic demand trajectories and circular-economy processes to fully capture the interplay of technology, consumption, and sustainability.

However, even in its current state, the framework provides a systematic approach to evaluate energy transitions within PBs. It offers a foundation for integrating absolute sustainability principles into real-world energy planning and policy design.

Conclusion

This paper presented an integrated framework that embeds prospective LCA and PB concepts directly within a national energy system optimisation model. The approach allows simultaneous consideration of cost, greenhouse gas mitigation, and multiple environmental pressures within a single decision space. By combining PB-aligned normalisation, multi-objective goal programming, and interpretable machine learning, the framework identifies transparent trade-offs and policy-relevant design configurations.

Three methodological elements underpin the generality of the framework. First, PB-based normalisation translates heterogeneous impact categories into a general, science-based scale, enabling consistent aggregation and comparison between LCA indicators. Second, the goal-programming formulation with a relaxed cost objective generates a spectrum of near-optimal solutions, exposing the shape of the vast solution space and avoiding dominance by a single weighting scheme. Third, interpretable machine learning condenses a large ensemble of model runs into a small set of decision rules, improving transparency and facilitating communication with policymakers and stakeholders. These features collectively enhance both the analytical rigor and interpretability of integrating PB-based LCA in energy system optimisation models, qualities often absent from complex, high-dimensional energy system optimisation studies.

Applied to a case study for the energy planning of Belgium in 2045, the results show that achieving the national climate target is feasible across a broad design space. Within the feasible space, several near-optimal pathways emerge. Onshore wind consistently appears as a "no-regret" technology, while the balance among offshore wind, solar PV, hydrogen, and electrified

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heat supply remains flexible. Decision-tree analysis highlights that most clusters primarily differ in their mobility strategies. While electric vehicles are generally selected as a preferred option in decarbonisation scenarios, the analysis reveals that their large-scale deployment may induce higher pressures on certain PBs compared to alternative mobility pathways. These findings suggest that future policy design should consider trade-offs beyond greenhouse gas emissions to ensure a truly sustainable transition.

In conclusion, energy planning within the planetary safe operating space requires optimising for cost and multiple environmental limits simultaneously, then selecting a consistent pathway that reflects societal preferences and risk tolerances. Multiple routes remain technically feasible, but none are free of trade-offs. Importantly, the results show that no trade-off explored so far enables compliance with all planetary boundaries simultaneously, highlighting the limits of purely technological optimisation approaches. This makes the exploration of sufficiency scenarios and demand reduction strategies a necessary next step. The central challenge for policy is therefore not finding a single least-cost solution, but rather choosing among competing, near-optimal futures with explicit awareness of the burdens each entails. By integrating PB-informed LCA with energy system optimisation, this framework provides the analytical structure needed to make those choices transparent, evidence-based, and consistent with the biophysical limits of the planet.

Data availability

The data and materials are available from the corresponding author upon reasonable request.

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Author contributions

N.G. conceptualized the initial ideas; N.G., D.C., M.K and A. V.d.O. designed the research; N.G. and D.C. developed the code and performed simulations; N.G., D.C. and M.K. analysed the results; N.G. and D.C. wrote the first draft of the manuscript; H.J. and F.C. reviewed the manuscript and supervised the work.

Competing interests

The authors declare no competing interests.

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