



CLEAN ENERGY TRANSITION: REQUIREMENTS, REALITIES, AND CONSEQUENCES

Fatemeh Rostami

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Clean Energy Transition: Requirements, Realities, and Consequences

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**Clean Energy Transition: Requirements, Realities, and
Consequences**

Doctoral Thesis

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SUSCAPE RESEARCH GROUP



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I state that the present study, entitled “**Clean Energy Transition: Requirements, Realities, and Consequences**”, presented by **Fateme Rostami** for the award of the degree of Doctor, has been carried out under my supervision at the Department of Chemical Engineering of this university.

Tarragona, 26th May 2024

Doctoral Thesis Supervisor

Dr. Carlos Pozo Fernandez

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Summary

The production and utilization of fossil fuels have long been criticized for their wide-ranging impacts on various aspects, including environmental degradation, health risks, and social inequities. Conversely, the development of clean energy technologies (CETs) is often hailed as a panacea to solve all these issues, reducing dependence on fossil fuels, mitigating greenhouse gas emissions, promoting diversification of the energy basket, and enhancing energy security. Despite these perceived benefits, there has been no comprehensive evaluation of the requirements and implications associated with the transition to CETs. This thesis seeks to fill that gap by thoroughly examining the requirements and consequences of developing clean energy infrastructures.

Initial apprehensions have surfaced regarding the potential impacts of the transition to clean energy on human rights, land use, and food security. These concerns underscore the need for a balanced and thorough analysis of both the positive and negative effects of clean energy technologies development. With the development of CETs and the emergence of mining as a pivotal sector, we are entering the age of "big shovels." Therefore, significant concerns about sustainable resource utilization, environmental stewardship, and the provision of adequate healthcare are gaining attention to ensure a truly sustainable transition.

Our research objectives include estimating the requirements for the widespread adoption of CETs, assessing our realistic capabilities to develop these technologies, and analyzing the consequences of achieving or failing to meet the projected capacities. This involves a detailed investigation into the socio-economic, environmental, and technical impacts of CETs, as well as the geopolitical ramifications of shifting energy paradigms.

Furthermore, a crucial aspect of this transition is understanding the equitable distribution of its benefits and burdens. It is essential to recognize that a truly inclusive clean energy system must be accessible and beneficial to all, irrespective of nationality, ethnicity, gender, race, age, skin color, or socio-economic status. This thesis aims to provide transparent and accountable information to illuminate the inequalities associated with the transition to clean energy.

In summary, this thesis seeks to contribute to the discourse on clean energy by providing a holistic evaluation of the transition's implications for sustainable development targets. By doing so, we aim to inform policymakers, stakeholders, and the global community about the necessary steps to ensure that the shift towards clean energy is not only technologically and economically feasible but also socially just and inclusive.

Resumen

La producción y utilización de combustibles fósiles han sido durante mucho tiempo objeto de críticas por sus amplios impactos en diversos aspectos, incluida la degradación ambiental, los riesgos para la salud y las inequidades sociales. Por el contrario, el desarrollo de tecnologías de energía limpia (CET, por sus siglas en inglés) suele ser aclamado como una panacea para resolver todos estos problemas, reduciendo la dependencia de los combustibles fósiles, mitigando las emisiones de gases de efecto invernadero, promoviendo la diversificación de la cesta energética y mejorando la seguridad energética. A pesar de estos beneficios percibidos, no ha habido una evaluación exhaustiva de los requisitos e implicaciones asociados con la transición a las CET. Esta tesis busca llenar ese vacío examinando minuciosamente los requisitos y consecuencias del desarrollo de infraestructuras de energía limpia. Han surgido preocupaciones iniciales con respecto a los posibles impactos de la transición a la energía limpia en los derechos humanos, el uso de la tierra y la seguridad alimentaria. Estas preocupaciones subrayan la necesidad de un análisis equilibrado y exhaustivo de los efectos positivos y negativos del desarrollo de tecnologías de energía limpia. Con el desarrollo de las CET y el surgimiento de la minería como un sector pivotal, estamos ingresando en la era de las "grandes palas". Por lo tanto, las preocupaciones significativas sobre la utilización sostenible de los recursos, la administración ambiental y la provisión de atención médica adecuada están ganando atención para asegurar una transición verdaderamente sostenible. Nuestros objetivos de investigación incluyen estimar los requisitos para la adopción generalizada de las CET, evaluar nuestras capacidades realistas para desarrollar estas tecnologías y analizar las consecuencias de lograr o no alcanzar las capacidades proyectadas. Esto implica una investigación detallada sobre los impactos socioeconómicos, ambientales y técnicos de las CET, así como las ramificaciones geopolíticas del cambio de paradigmas energéticos. Además, un aspecto crucial de esta transición es comprender la distribución equitativa de sus beneficios y cargas. Es esencial reconocer que un sistema de energía limpia verdaderamente inclusivo debe ser accesible y beneficioso para todos, independientemente de la nacionalidad, etnia, género, raza, edad, color de piel o situación socioeconómica. Esta tesis tiene como objetivo proporcionar información transparente y responsable para iluminar las desigualdades asociadas con la transición a la energía limpia. En resumen, esta tesis busca contribuir al discurso sobre la energía limpia proporcionando una evaluación holística de las implicaciones de la transición para los objetivos de desarrollo sostenible. Al hacerlo, nuestro objetivo es informar a los formuladores de políticas, partes interesadas y la comunidad global sobre los pasos necesarios para garantizar que el cambio hacia la energía limpia no solo sea tecnológica y económicamente factible, sino también socialmente justo e inclusivo.

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Chapter 1

Introduction

Chapter 1

1. Introduction

1.1 Perspective and motivation

In an era characterized by growing concerns over climate change and environmental degradation, the transition to clean energy technologies (CETs) has emerged as a paramount global imperative [1]. Central to this transition are the minerals that underpin the development and deployment of these technologies, serving as the lifeblood of renewable energy infrastructure [2]. However, the extraction, processing, and supply chain of these minerals present a complex nexus of geopolitical, environmental, and social challenges that demand thorough examination.

This thesis embarks on a journey through interconnected realms crucial for understanding the dynamics of clean energy transitions. It begins by delving into the realm of integrated assessment models (IAMs), which serve as powerful tools for exploring the projected capacities of CETs. IAMs play a crucial role in projecting the capacity of CETs, informing policy decisions, and shaping climate strategies [3]. Yet, they are subject to limitations and criticisms, particularly regarding their ability to capture the complexities of human behavior, technological diffusion, and industrial transformations [4]. This gap between IAM projections and real-world constraints undermines their policy relevance and impedes progress towards climate goals.

Our research aims to bridge this gap by addressing the fundamental dichotomy between IAM projections and real-world dynamics, focusing on materials essential for CETs. Through a thorough analysis, provided in chapter 2, we quantify the tangible challenges associated with material shortages, technological limitations, and the feasibility of achieving ambitious climate targets. Notably, in section 2.3.5, we analyze the deviation from the critical 1.5°C temperature threshold. In this pursuit, the goal is to maximize the achievable capacity of technologies while navigating constraints on materials availability, the limitation overlooked in IAMs. Additionally, we aim to explore the implications of IAMs' limited technological resolution on the reliability of their predictions and propose strategies for enhancing their accuracy and policy relevance. By considering various technological designs, the thesis provides valuable insights into the importance of considering sufficient technological resolution in shaping realistic capacity projections for CETs (see section 2.3.4).

Building upon this foundational understanding, the thesis then shifts its focus to the geopolitics surrounding minerals extraction and their supply chains. This study, acknowledging the necessity of CETs development, aims to address this topic since rushing the development of CETs risks overlooking critical concerns regarding the human rights and sustainable development goals [5], [6]. Our study seeks to address these multifaceted challenges through evidence-based, comprehensive quantitative analysis, provided in chapter 3. By unraveling the intricate interplay between material demand, energy demand, carbon emissions, waste rock, and human health, the study sheds light on the multifaceted challenges inherent in the pursuit of sustainable energy solutions (see section 3.3).

Overall, through a detailed analysis of the global demand for clean energy technologies provided by eight IAMs including 25 scenarios (Table 2 of chapter 6), the requirements and consequences of their development is investigated. Remarkably, the Gini index is employed to measure inequalities among different nations [7], regarding their substantial contributions to material supply or the significant levels of externalities (i.e., energy consumption, Green House Gas (GHG) emissions, resulting waste rock, and human health) they may face (section 7.3).

In its final exploration in chapter 4, the thesis delves into the realm of energy storage technologies, recognizing their indispensable role in balancing energy supply and demand within clean energy systems [8]. Specifically, it examines options such as batteries, or power-to-gas, employing rigorous development analysis techniques to assess their sustainability indicators (section 4.2.2), and market penetration potential (section 4.5.3). We compare the performance of diverse energy storage technologies across economic, environmental, and social dimensions. Employing Data Envelopment Analysis (DEA), we aim to objectively evaluate energy storage technologies, providing quantitative insights for effective decision-making towards a sustainable energy transition. Notably, due to high dependency of DEA on data quality, we do a DEA under uncertainty, as explained in section 1.3.4. By providing a comprehensive evaluation of a wide range of energy storage options, we seek to identify sustainable solutions for meeting future energy needs.

Collectively, these investigations contribute to a nuanced understanding of the complex interrelationships between minerals extraction, CETs, and sustainable development targets. By unraveling the geopolitical, economic, and technological dimensions of clean energy transitions, this thesis endeavors to inform policy decisions, stimulate innovation, and catalyze genuine progress towards a more sustainable future.

In light of these challenges and opportunities, our research aims to address key gaps in the literature related to climate policy, material availability for renewable energy technologies, and energy storage solutions. Specifically, we seek to:

- Investigate the fundamental dichotomy between IAM projections and real-world constraints, particularly concerning critical materials essential for clean energy technologies (chapter 2).
- Assess the impacts of CETs development, considering the implications for mineral supply chains and geopolitical dynamics (chapter 3).
- Evaluate the performance of diverse energy storage technologies across economic, environmental, and social dimensions, using rigorous analytical methods such as data envelopment analysis (chapter 4).

It is worth noting that due to the complexity of the analyses, methodological details are often provided in the supplementary information to ensure transparency and reproducibility. Indeed, while the main body of the thesis, as provided in chapters 2-4, mainly focusing on findings, supplementary information, provided in chapters 5-7, include methodological details and additional insights that contribute to a more comprehensive understanding of the topics at hand.

In the current chapter, our aim is to provide overarching discussions on these critical issues, outlining the methodologies employed and highlighting key findings. However, detailed discussions are reserved for the following chapters, where comprehensive analyses are presented. Having this roadmap in mind, we turn your attention to the next section.

1.2 Research Scope and Objectives

Our research endeavors to delve into the intricate interplay between IAMs and realistically attainable capacity of CETs, aiming to elucidate the challenges and opportunities in achieving ambitious climate targets. By leveraging IAM projections and quantifying the tangible challenges associated with material shortages and technological limitations, we seek to bridge the gap between IAM projections and real-world dynamics.

Additionally, our research aims to address the pressing challenges surrounding material availability for renewable energy technologies, with a focus on the global supply chain dynamics and their implications for energy security and equity. By conducting a comprehensive assessment of the global demand for CETs and quantifying material requirements, we seek to shed light on the disparities and risks inherent in the supply chain.

Finally, we try to advance understanding of energy storage technologies and their role in facilitating grid stability and decarbonization in the transition to renewable energy systems. By conducting a comprehensive evaluation of diverse energy storage options across economic, environmental, and social dimensions, we seek to inform policymakers and stakeholders about the potential of different technologies and support effective decision-making towards a sustainable energy transition.

Specifically, our objectives include:

- Investigating the fundamental dichotomy between IAM projections and real-world constraints, particularly concerning critical materials essential for CETs (chapter 2).
- Translating the capacity demanded for CETs into material requirements, considering the implications for mineral supply chains and geopolitical dynamics (chapter 2).
- Proposing strategies for enhancing the accuracy and policy relevance of IAMs, thereby facilitating informed decision-making, and accelerating the transition to a sustainable energy future (chapter 3).
- Investigating the environmental impacts of materials extraction and processing, including energy requirements, GHG emissions, waste generation, and human health impacts (chapter 3).
- Assessing the inequalities in materials supply and its associated externalities within the supply chain of CETs and identifying strategies for promoting a just and equitable transition to renewable energy (chapter 3).
- Assessing the performance of energy storage technologies, including both fast-response and long-term options, across key sustainability indicators (chapter 4).
- Providing quantitative insights into directions for improvement and offering guidance for technology developers, policymakers, and stakeholders to promote the adoption of sustainable energy storage solutions (chapter 4).

By addressing these research objectives, our study aims to contribute to the development of robust and actionable climate policies, advance global efforts towards a low-carbon, resilient future, and ensure a just and equitable transition to renewable energy for all.

1.3 Methods and Tools

We employ different tools in our analysis including IAMs, mathematical optimization (particularly linear optimization and DEA under uncertainty), as well as Life Cycle Assessment (LCA). Chapters 2-3 and 6-7 utilize IAMs to evaluate the capacity of Clean Energy Technologies (CETs) and perform additional calculations based on these assessments. Optimization techniques are applied to determine the realistically attainable capacity of CETs and the necessary recycling rate for materials (chapters 2 and 6). In chapter 4, we use DEA to compare different energy storage alternatives.

LCA, though subtle, is incorporated across all chapters to support data collection, such as assessing the human health impact of material production, the water or energy required for each energy storage alternative, and the carbon intensity of electricity from the grid mix.

These methods help us gain meaningful insights and draw robust conclusions to support decision-making and policy formulation. Each tool is briefly explained in the following sections, while further details are provided later on in the corresponding chapter (this time, with a larger focus on the particular application).

1.3.1 Integrated Assessment Models

Integrated Assessment Models (IAMs) are tools used by scientists and policymakers to understand complex systems involving the economy, energy, technology, and the environment. They are like big computer programs that simulate how different factors interact with each other over time.

Imagine planning a road trip. Probably considering things like how much gas is necessary, the distance to the destination, the condition of the roads, and maybe even the weather. IAMs work in a similar way but on a much larger scale. These models take into account various factors such as population growth, technological advancements, energy usage, and environmental impacts.

For example, if a government wants to reduce carbon emissions, they can use an IAM to see how different policies, like investing in renewable energy or implementing carbon taxes, might impact the economy, energy markets, and the environment over time.

IAMs serve as comprehensive tools for exploring the complex interactions between human activities, socioeconomic development, and environmental changes [9]. They help researchers and policymakers explore different scenarios and understand how changes in one area might affect others. As presented in Figure 1.1, these models integrate knowledge from various disciplines, including climate science, economics, energy systems, and technology dynamics. Different IAMs scenarios consider a range of variables, including technological advancements, policy interventions, and market dynamics, to provide a robust set of projections [3]. Therefore, IAMs provide valuable insights into long-term climate and energy scenarios, facilitating the evaluation of policy options and their implications. They are pivotal in assessing the long-term impacts of climate policies and strategies aimed at mitigating climate change. Moreover, IAMs are essential tools in the International Panel of Climate Change's (IPCC) Assessment Reports (ARs), underpinning much of the climate modeling and policy analysis presented. Within our study, IAMs are instrumental in projecting the capacity of CETs under different scenarios, which is necessary for the estimation of material demands and the externalities driven with it, including energy consumption, GHG emission, resulting waste rock, and human health.

Specifically, we use projections from eight IAMs, encompassing 25 scenarios, to derive the capacities of various CETs up to the year 2050. These scenarios, provided in Table 2 of chapter 6, are designed to meet the "Below 1.5" and "1.5 low overshoot" temperature targets, aligning with the long-term objective of limiting global warming to 1.5°C by 2100 [3]. Specifically, our analysis covers various CETs, including batteries (both stationery and mobility), Concentrated Solar Power (CSP) systems, electrolyzers, photovoltaic (PV) panels, and wind turbines (see Table 1 of chapter 6).

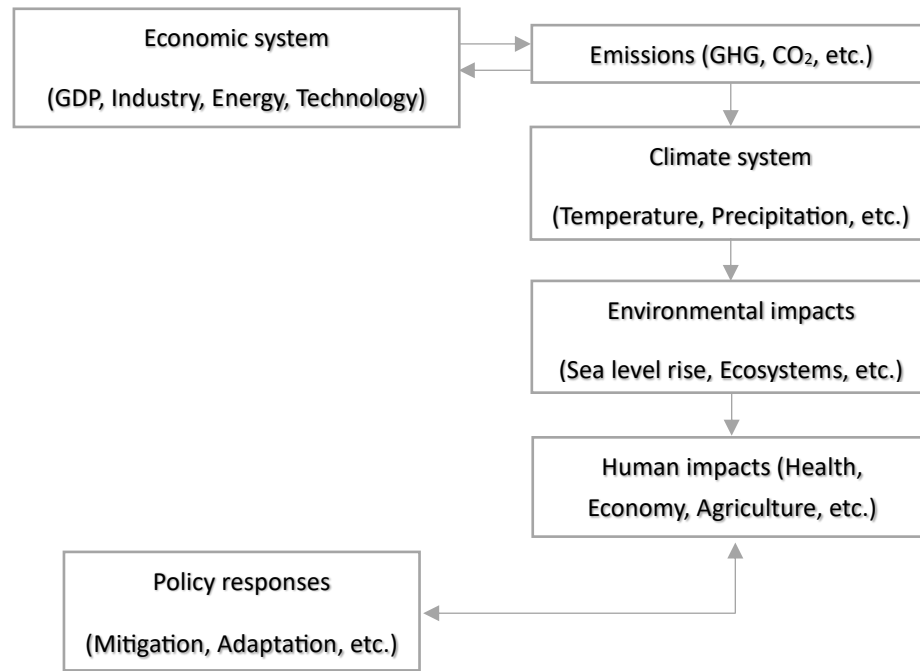


Figure 1.1 Conceptual visualization of IAMs integrated nature.

We collect CET projections from IAMs starting from the earliest available year (2000 or later) up to 2050. While the main results focus on the 2020-2050 period, earlier projections are included to estimate replacements needed after 2020 due to the retirement of technologies installed before 2020. Although projections extend until 2100, we limit our scope to 2050 to mitigate the increasing uncertainty over a longer time frame.

IAMs typically provide overall capacity estimates for a technology (e.g., PV) without detailing individual types (e.g., CdTe, CIGS, CSi). To address this, we use market contribution data for different technology types to estimate the capacity allocated between them. We consider two distinct market contribution trends provided by the German Aerospace Centre: Continued and Technological Change [10]. The Continued trend assumes a smooth evolution of technologies, while the Technological Change trend assumes sudden shifts in technology adoption. These trends are presented in Tables 3-4 of chapter 6.

IAMs capacity projections are compared with estimates from sources such as the International Energy Agency (IEA) [11], [12], [13], and the International Renewable Energy Agency (IRENA) [14]. This comparison helps identify the wide range of projections covered in the study and the robustness of our estimations.

Although not a part of the IAMs, the estimation of materials demand and their associated externalities is based on IAM projections. Therefore, we briefly discuss these points in the following paragraphs.

- Material Demand Estimation

We translate the projected capacities of each technology from the IAM scenarios into material requirements, covering a total of 36 materials (see Table 5 of chapter 6). Given that different technology types have unique material demands, our analysis encompasses a variety of CETs, including

seven battery types, two variants of electrolyzers, three models of PV panels, three types of CSP systems, and six alternative wind turbines (See Table 1 of chapter 2).

Next, we conduct an extensive literature review to compile both current and future raw material intensities for these technology types (e.g., kg of cadmium needed to manufacture a cadmium tellurium PV panel of 1 GW capacity). Material intensity may vary over time due to technological learning curves, so we incorporate both current and future intensity values to enhance the robustness of our findings. This information is available in Tables 6-8 of chapter 5.

We generate 100 scenarios to estimate materials demand by incorporating 25 IAM scenarios for capacity projections, two market contribution trajectories, and two materials intensity projections. For further calculations referred to as externalities, we use the median demand for materials across the 100 scenarios (Table 4 of chapter 7).

- Addressing Externalities

The development of CETs generates externalities, such as driven energy demand, GHG emissions, resulting waste rocks, and human health impacts, described in the following:

- **Energy Consumption Estimation:** We use energy intensity values (e.g., GJ required to produce 1 ton of copper) collected from literature or Ecoinvent database [15], to estimate the energy required for materials extraction and processing (Table 10 of chapter 7). Energy requirements from downstream echelons of the supply (e.g., material transportation or technology manufacturing) are excluded from the analysis.
- **GHG Emissions Estimation:** We use each material's carbon intensity values (e.g., ton of CO₂-equivalent emitted during the production of 1 ton of lithium) to convert material requirements into GHG emissions (Tables 11-12 of chapter 7). Carbon intensities are from literature or Ecoinvent database.
- **Waste Rock Estimation:** We estimate the resulting waste rock using rock-to-metal ratios (e.g., ton of rock extracted to obtain 1 ton of silver). This estimation focuses on 17 minerals, as non-minerals like cement, plastic, or steel do not contribute to waste rock generation (Tables 13-14 of chapter 7). In addition to waste rocks, mineral extraction generates tailings, which are toxic and radioactive in some cases. Hence, we also estimate global cumulative tailings by 2050. The required data for these estimations are from Nassar et al. [16].
- **Human health:** We use the endpoint (H) human health indicator from Recipe 2016 v1.03, as retrieved from Ecoinvent database, to estimate the disability adjusted life years (DALYs) associated with each material's production in each country (Table 16 of chapter 7). For more details, refer to section 1.3.3.
- **Addressing Inequality:** To gauge disparities linked to material supplies and their consequences, we use a type two Gini index estimation [7], to evaluate inequalities in materials supply and its associated externalities among different countries. The formulation of the Gini index used to assess inequalities in materials supply and its externalities can be found in section 7.3.

This framework outlines the comprehensive approach we take to analyze the potential challenges, externalities, and supply chain dynamics associated with CETs. By leveraging IAMs, we provide a robust analysis of the material requirements and supply chain implications, ensuring a thorough understanding of the potential requirements and impacts of the transition to clean energy.

1.3.2 Mathematical optimization

Mathematical programming is a branch of operations research that involves optimizing a specific objective function subject to a set of constraints [17]. It is a powerful tool used in various fields such as economics, engineering, logistics, and management for decision-making and resource allocation. There are several types of mathematical programming, presented by Figure 1.2, each suited to different kinds of problems:

- **Linear Programming (LP):** Linear programming involves optimizing a linear objective function subject to linear constraints. The objective function and the constraints must all be linear equations. LP problems can be solved efficiently using algorithms like Simplex or interior-point methods [17].
- **Nonlinear Programming (NLP):** Nonlinear programming deals with problems where the objective function or at least one of the constraints is nonlinear. These problems are more complex than LP problems and may require specialized algorithms for solution, such as gradient descent, Newton's method, or interior-point methods for nonlinear optimization.
- **Integer Programming (IP):** Integer programming is used when some or all of the decision variables are required to be integers. This is common in situations where the variables represent discrete items, like the number of products to produce or the number of vehicles to use.
- **Mixed-Integer Linear Programming (MILP):** Mixed-integer linear programming is a combination of linear programming and integer programming where some variables are continuous while others are constrained to be integers. Constraints are all linear. MILP problems are solved using branch-and-bound, branch-and-cut, or other advanced algorithms [18].
- **Mixed-Integer Nonlinear Programming (MINLP):** Finally, mixed-integer nonlinear programming can contain integer and continuous variables and, at least, one nonlinear equation. MINLP problems are the most difficult to solve, and are typically addressed with algorithms such as BARON (Branch-And-Reduce Optimization Navigator) or SBB (Simple Branch-and-Bound) [19].

In this thesis, mathematical programming is used in different places. Provided in Section 6.3, two LP models are employed to estimate, respectively, (a) the maximum capacity of CETs that can be achieved taking into account constraints on materials availability, and (b) the minimum material recycling required for the same purpose. Additionally, in section 4.4, we use DEA (which is also an LP model) to compare energy storage options. Therefore, we delve into each of these methodologies in more detail.

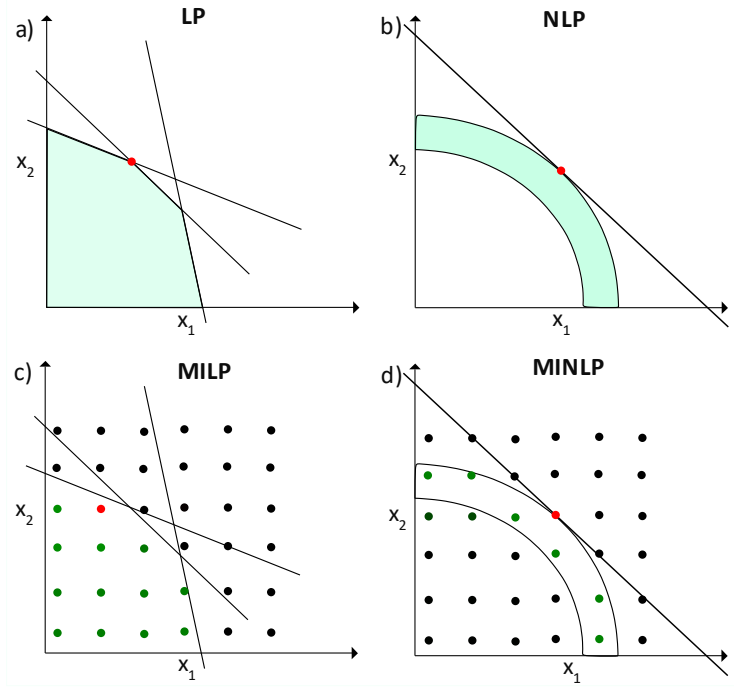


Figure 1.2 Main types of optimization problems in the variable space (x_1 and x_2). In subplots (a) and (b), the green areas represent the feasible regions. In subplots (c) and (d), the green points indicate the feasible regions for integer solutions. The red points mark the hypothetical optimal solutions for each type of problem.

- Linear programming concept

LP aims to ascertain the optimal solution or outcome based on linear parameters or requirements. Objective function, decision variables, and constraints are the main components of an LP problem. Model M1.1 presents the common formulation of this programming.

$$M1.1: \quad \text{Maximize (or Minimize)} \quad Z = \sum_j c_j x_j \quad (1.1)$$

$$s.t.: \quad a_{ij}x_j \leq b_i \quad \forall i, j \quad (1.2)$$

$$x_j \in R^+ \quad i, j \in N \quad (1.3)$$

The Objective Function (Z) serves as the focal point for optimization, whether it is maximizing or minimizing a particular aspect. For instance, it could represent the capacity of CETs to be maximized. In linear programming, Z is a linear function of decision variables denoted by x_j in model M1.1. These variables shape the outcome, embodying the available choices for the decision-maker. For example, the attainable capacity of various CETs exemplifies a decision variable, with c_j representing the weight or significance assigned to each variable in the objective function.

Constraints, represented by equation (1.2), outline the boundaries or limitations on the decision variables. In linear programming, these constraints also take the form of linear equations or inequalities. Here, a_{ij} denotes the coefficients of the constraints, while b_i represents the constants on the right-hand side. In our case study, a_{ij} could signify the intensity of each material (e.g., tons of copper per GW capacity of photovoltaic panel), whereas b_i might denote the global reserve capacity of materials. Through this formulation, we can gauge the achievable capacity x for each technology j while considering constraints on the availability of material i .

Variables are typically required to be non-negative, as negative quantities often lack practical significance (e.g., negative capacity). For further details, please consult sections 2.3.5 and 6.3.

- **Solving linear programs**

General Algebraic Modeling System (GAMS) is widely used as a tool to solve the different models.

GAMS is a high-level modeling system for mathematical programming problems, including linear programming along with other programming models. It allows to describe the optimization problem using a concise and readable modeling language, and by defining the decision variables, objective function, and constraints in a way that mirrors the mathematical formulation of the problem. At the next step, GAMS translates these formulations into a format that optimization solvers can understand it. It supports various solvers for different types of optimization problems. These solvers use algorithms to find the best solution for the problem based on the objective function provided and the feasible region defined by the constraints; these algorithms include simplex method, interior-point method, branch-and-bound, and branch-and-cut. After the solver has found a solution, GAMS provides the results to the user, who can examine the optimal values of the decision variables, assess the performance of the objective function, and evaluate the satisfaction of constraints.

- **Data envelopment analysis**

Data envelopment analysis (DEA) is a non-parametric linear programming technique designed to evaluate the relative efficiency of a group of comparable entities, the so-called decision-making units (DMUs) [20]. Each DMU transforms multiple inputs into multiple outputs [21]. The primary criterion for higher efficiency is achieving greater outputs while using fewer inputs (Eq. 1.4). However, in scenarios where certain outputs are undesirable (e.g., carbon emissions), minimizing their production is preferable [22].

$$efficiency = \frac{\text{weighted sum of outputs}}{\text{weighted sum of inputs}} \quad (1.4)$$

In our investigation, detailed in chapter 4, we use DEA to assess the effectiveness of diverse energy storage technologies from economic, environmental, and social standpoints [8]. These technologies are conceptualized as DMUs that consume multiple inputs and generate both desired and undesired outputs. Particularly, six performance indicators are selected to cover sustainability dimensions, considering factors such as energy consumption, water use, and global warming potential (GWP), and employment. These sustainability metrics are grouped into three categories (section 4.2.2): input resources consumed, desirable outcomes (e.g., job creation), and undesirable outcomes (e.g., emissions). The values of these indicators are gathered through literature review.

Notably, we first classify energy storage technologies based on their response time and application, ensuring fair comparisons within each class. This classification aids in selecting appropriate indicators for efficiency assessment (Section 4.2.1). The indicators vary between fast-response and long-term storage technologies. The main distinction is that we consider energy density for fast-response technologies due to the importance of size within this category.

DEA functions by examining each DMU independently through a linear programming model. It identifies the most effective performers, termed efficient units. These are non-dominated DMUs, meaning no other DMU achieves greater outputs with equal or fewer inputs. Efficient DMUs collectively establish the 'efficient frontier', which is formed by their convex combination. Subsequently, DEA evaluates the efficiency of non-frontier units (inefficient units) by projecting them onto the efficient frontier, defining a so-called virtual DMU at the intersection. Comparison of an inefficient DMU and the corresponding virtual DMU allows to assign an efficiency score (as given by the distance between them), identify inefficiency sources, and offer tailored recommendations for converting inefficient units into efficient ones [23].

To illustrate DEA concepts, we present Figure 1.3, which applies the CCR (Charnes, Cooper, and Rhodes) and BCC (Banker, Charnes, and Cooper) DEA models to a set of six DMUs (A to F). Under the CCR model, which assumes constant returns to scale, the efficient frontier is represented by a line starting from the origin and passing through the efficient units C and E. In this model, only DMUs C and E are efficient, as they have the highest output-to-input ratios.

In contrast, the BCC model, which assumes variable returns to scale, identifies DMUs A and F as efficient, in addition to DMUs C and E. This forms the reference set due to the model's variable returns to scale property. The frontier formed by these efficient DMUs is referred to as the strongly efficient frontier. Additionally, the efficient frontier includes two segments, represented by grey dotted lines, which extend to infinity parallel to the output and input axes. These segments, formed by the distant efficient DMUs, are known as the weakly efficient frontier.

The inefficient DMUs need to either reduce their input or increase their output to become efficient. The projection of inefficient units onto the efficient frontier can be done in different ways. For instance, an input-oriented DEA model focuses on minimizing inputs while maintaining the current level of outputs. This orientation is particularly useful when the primary objective is to reduce resource consumption, costs, or other inputs. In contrast, an output-oriented DEA model focuses on maximizing outputs while using the current level of inputs. This orientation is useful when the goal is to increase production, service levels, or other outputs [24].

Based on Figure 1.3, DMUs B and D (highlighted in red) are considered inefficient under both models. To determine improvement targets for these inefficient DMUs, they are projected onto the efficient frontier, creating their corresponding virtual DMUs (B' and D'). The BCC model uses radial projections to map the virtual DMUs onto the efficient boundary, with projections being either output-oriented (horizontal) or input-oriented (vertical).

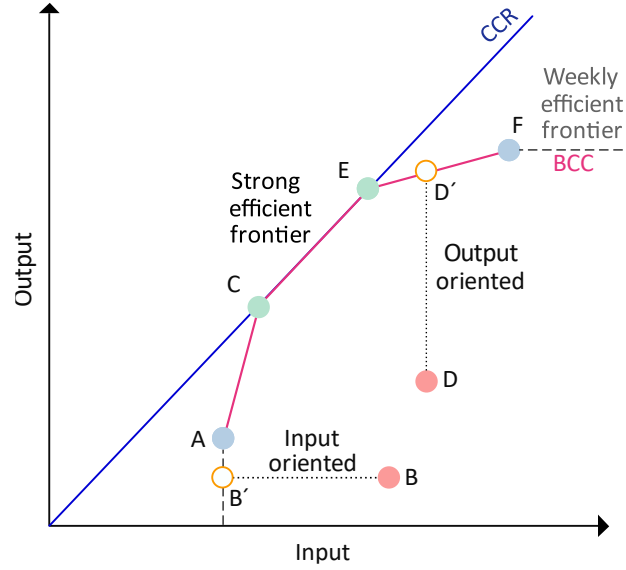


Figure 1.3 Example of a single input, single output DEA with four DMUs. The yellow shading shows the necessary changes in input and/or output for DMU D to become efficient.

Efficiency scores for each DMU are obtained by solving a DEA model, where an efficiency score of 1 indicates efficiency. This approach allows for the comparison of different options, such as energy storage alternatives as our case study. Model M 1.2, presents the common mathematical formulation for an input-oriented DEA, as an example.

M 1.2:

$$\text{Objective: } \theta^* = \min \theta \quad (1.5)$$

$$\text{Subject to: } \sum_{j=1}^n \lambda_j x_{ij} \leq \theta x_{io}, \quad \forall i \quad (1.6)$$

$$\sum_{j=1}^n \lambda_j y_{rj} \leq y_{ro}, \quad \forall r \quad (1.7)$$

$$\lambda_j \geq 0, \quad \forall j \quad (1.8)$$

Here:

- θ is the efficiency score of the DMU under evaluation.
- x_{ij} and y_{rj} are the input i and output r of DMU j .
- x_{io} and y_{ro} are the input i and output r of the DMU being evaluated (i.e., DMU o).
- λ_j is the weight assigned to each DMU j in constructing the efficient frontier.
- n is the total number of DMUs.

Based on this formulation, a DMU is considered efficient if $\theta^*=1$. Otherwise, it is inefficient.

In the traditional DEA model, efficient DMUs receive an efficiency score of 1, meaning they are on the efficient frontier. However, when multiple DMUs are efficient, the basic DEA model does not provide a means to rank them. The super efficiency model, an extension of the basic DEA model, addresses this by allowing efficiency scores greater than 1, thereby providing a mechanism to rank efficient DMUs relative to each other [25]. Since super efficiency provides a measure of how much inputs can be

increased or outputs decreased before a DMU becomes inefficient, it helps in identifying potential areas for further improvement even for those units already deemed efficient [26]. For a detailed explanation of these models refer to section 4.4. Notably, in our study, we use a non-oriented undesired output slack-based model. Additionally, a super-efficiency model is employed to rank efficient DMUs [8]. Both models are implemented and solved using GAMS.

1.3.3 Environmental impact assessment

Environmental Impact Assessment (EIA) is a systematic process for identifying, predicting, and evaluating the potential environmental consequences of proposed projects, policies, or plans. Within our methodology, by conducting comprehensive EIAs associated with the deployment of CETs, including GHG emissions, waste generation, and human health impacts, provided in chapter 3, we aim to inform decision-makers about the environmental trade-offs inherent in clean energy systems.

Among the various methodologies used for environmental impact assessment, LCA has emerged as the leading approach, widely adopted in both private and public environmental decision-making contexts [27], [28]. LCA is a systematic methodology for assessing the environmental impacts associated with all stages of a product's life from cradle to grave (i.e., from raw material extraction through materials processing, manufacture, distribution, use, repair and maintenance, and disposal or recycling) [29], [30]. Figure 1.4 is a brief overview of main steps of each LCA study.

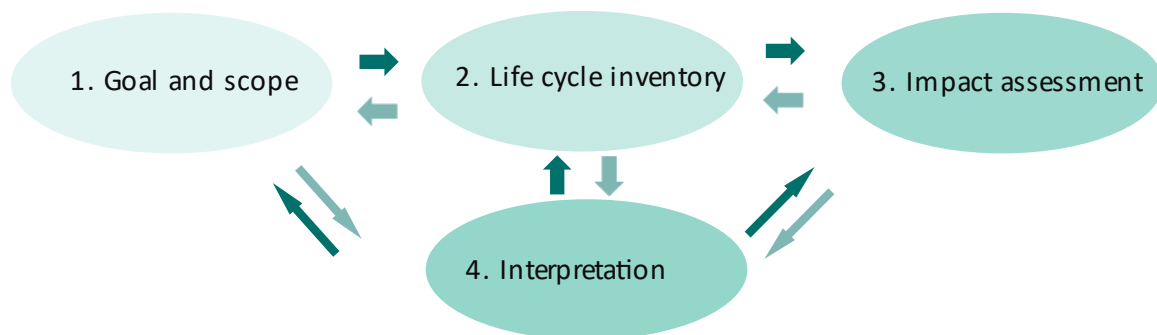


Figure 1.4 Common steps of LCA studies.

- **Goal and Scope Definition:** This initial phase involves defining the objectives of the study, the system boundaries, and the functional unit (the reference unit to which all inputs and outputs are related, for example, GHG emissions per 1kg of each metal produce). It sets the framework for the LCA study, including the depth and breadth of the analysis. There are several other approaches like cradle-to-gate, cradle-to-wheel, and cradle-to-cradle that may be considered as the scope of the analysis.
- **Life Cycle Inventory (LCI) Analysis:** The second phase of the LCA process is the life cycle inventory analysis (LCI). In this phase, all inputs and outputs of the system are compiled, whether measured, estimated, or sourced, and tracked throughout the life cycle. This stage typically involves an iterative process with the scope and goal definition to refine boundaries and allocations. The system is divided into smaller units, with inputs and outputs gathered from various sources. A large amount of data is handled at this stage, leading to variability and uncertainty. The Ecoinvent database, as explained later, is one of the most comprehensive and widely used life cycle inventory databases in the world [15].

- **Life Cycle Impact Assessment (LCIA):** This phase evaluates the potential environmental impacts associated with the LCI data. It involves classifying and characterizing the inventory data into impact categories such as global warming potential, acidification, eutrophication, human toxicity, and resource depletion. Various methodologies can be used to assess these impacts, such as the ReCiPe, TRACI, and CML methods [31]. ReCiPe is known for its comprehensive coverage of environmental impact categories. It includes a wide range of midpoint impact categories, such as climate change, eutrophication, and acidification, as well as endpoint categories like human health, ecosystem quality, and resource depletion.
- **Interpretation:** The final phase involves interpreting the results of the LCI and LCIA in relation to the goals and scope of the study. It identifies significant issues, evaluates the robustness of the results, and provides conclusions, recommendations, and areas for improvement. This phase may also include sensitivity and uncertainty analyses to understand the reliability and accuracy of the results.

Regarding the databases for LCI analysis, the available environmental databases work as repositories of data related to environmental processes, impacts, and resources. They provide valuable information for researchers, policymakers, and businesses to assess the environmental footprint of products, processes, and systems. These databases typically include data on resource use, emissions, energy consumption, and other environmental indicators across various stages of a product's life cycle.

Among these databases, Ecoinvent is one of the most widely used and comprehensive [32]. It provides life cycle inventory data for a wide range of products and processes. It covers a broad spectrum of industries and activities, including agriculture, manufacturing, transportation, energy production, and waste management. Furthermore, Ecoinvent offers data for multiple regions around the world, allowing users to account for regional variations in resource availability, energy sources, and environmental regulations. This enables more accurate assessments of environmental impacts across different geographic contexts.

It plays a critical role in supporting sustainable decision-making by providing comprehensive and reliable data on the environmental performance of products and processes across their life cycles. Its broad coverage, rigorous methodology, and compatibility with LCA tools make it a valuable resource for researchers, businesses, and policymakers aiming to understand and mitigate environmental impacts.

By incorporating LCA into the analysis of CETs, stakeholders can make more informed decisions that balance the need for clean energy with the imperative to minimize environmental impacts associated with their development.

As sustainability becomes a central concern across various industries, the ability to anticipate and address environmental impacts is crucial. Recently, prospective LCA (pLCA) is attracting attentions due to its focus on studying future technological systems and their environmental implications. pLCA must address the dynamic nature of technological advancements, introducing complexities in anticipating long-term environmental impacts. This forward-looking methodology contributes to a more resilient and adaptive approach, ensuring that future innovations align with ecological principles and positively impact global sustainability objectives. It works as a powerful tool for shaping sustainable practices and guiding medium- and long-term decision-making. more on this is available in section 6.4.

In this thesis, LCA is applied across all chapters. In Chapter 2 and its elaboration upon in Chapter 6, we use prospective LCA to estimate the carbon intensity of CETs and their potential substitutes in case of

shortage in their developed capacity (e.g., electric vehicles with trucks). In Chapter 3, further detailed in Chapter 7, LCA is employed to assess the impact of material production on human health, measured by DALYs. In Chapter 4, expanded upon in Chapter 8, we use this methodology to identify the values of key indicators for energy storage technologies and compare them based on these indicators (e.g., including water usage and global warming potential).

1.3.4 Uncertainty analysis

Mathematical optimization models play a crucial role in decision-making processes, but their applicability in practice is often challenged by the presence of uncertainty. These models typically operate under deterministic assumptions, where all parameters are assumed to be perfectly known and constant. However, in reality, there are numerous sources of uncertainty that must be considered to ensure the robustness and practical feasibility of the solutions obtained.

Uncertainties in optimization models can stem from various sources, including variability in input parameters, model simplifications, and inherent randomness in system behavior. For example, when using capacity projections from IAMs, uncertainties stem from the assumptions behind their scenarios; and when employing DEA, the chosen indicators, along with data accuracy, result in variations in our findings. Ignoring these uncertainties can lead to poor decisions and unreliable outcomes. Therefore, we will address each of these uncertainties.

- Uncertainties in CET projections from IAMs

For the sections of our research reliant on IAMs, including chapters 2, 3, 5, and 6, we have extensively incorporated 25 IAM scenarios, covering a broad spectrum of projections. Regarding other variables like materials intensity, technology market share, and the carbon intensity of materials and technologies, we have strived to incorporate all available projections into our analysis, generating 100 scenarios for each material's estimation. Despite this, we acknowledge that the future is naturally uncertain, and our results do not have a 100% certainty.

- Uncertainties in data used in DEA

In our DEA study, we characterize uncertainty associated with the collected data using probability distributions to capture variability and obtain more robust conclusions [8]. As presented in section 4.3, we employ three types of distributions:

- **Uniform Distribution:** Used for parameters where only one value is available in the literature, with uncertainty characterized by an (arbitrary) support of $\pm 10\%$ of the nominal parameter.
- **Triangular Distribution:** Employed for parameters with a range of values available, with limits corresponding to the lowest and highest reported values in the literature, and the mode set to the nominal value.
- **Lognormal Distribution:** Utilized for characterizing uncertainties in GWP based on guidelines from the Ecoinvent database. According to these guidelines, each life cycle inventory entry should follow an individual lognormal distribution, with uncertainty characterized based on the Pedigree Matrix.

The Pedigree Matrix, often used in the context of LCA, is a tool that tracks and assesses the quality of data used in an analysis [33]. It is particularly valuable when dealing with complex systems or processes where multiple data sources are involved. The matrix categorizes data based on its quality and reliability, typically using a grading system or ranking criteria [34]. This allows us to understand the robustness of our data. For further details refer to section 8.3.

After characterizing uncertainty distributions for parameters, we discretize these distributions using Monte Carlo sampling to generate multiple independent scenarios. Monte Carlo sampling is a statistical technique used to simulate and analyze probabilistic systems [21]. The method involves generating a large number of random samples, 100 scenarios in our study, from probability distributions representing the uncertainty in the employed data. These samples are then used to simulate different potential behaviors of the system, allowing us to assess the range of possible outcomes and the likelihood of different scenarios.

Subsequently, the DEA model is solved for each scenario and DMU, resulting in a distribution of efficiency scores that accounts for uncertainty.

The challenges and limitations associated with our studies, as well as our main findings and recommendations for future work, although clear but may not be fully useful to the reader at this step without a thorough review of each study. Therefore, they are presented as a very short and separate chapter. Indeed, chapter 5 serve as a summary for readers after they have completed the main chapters.

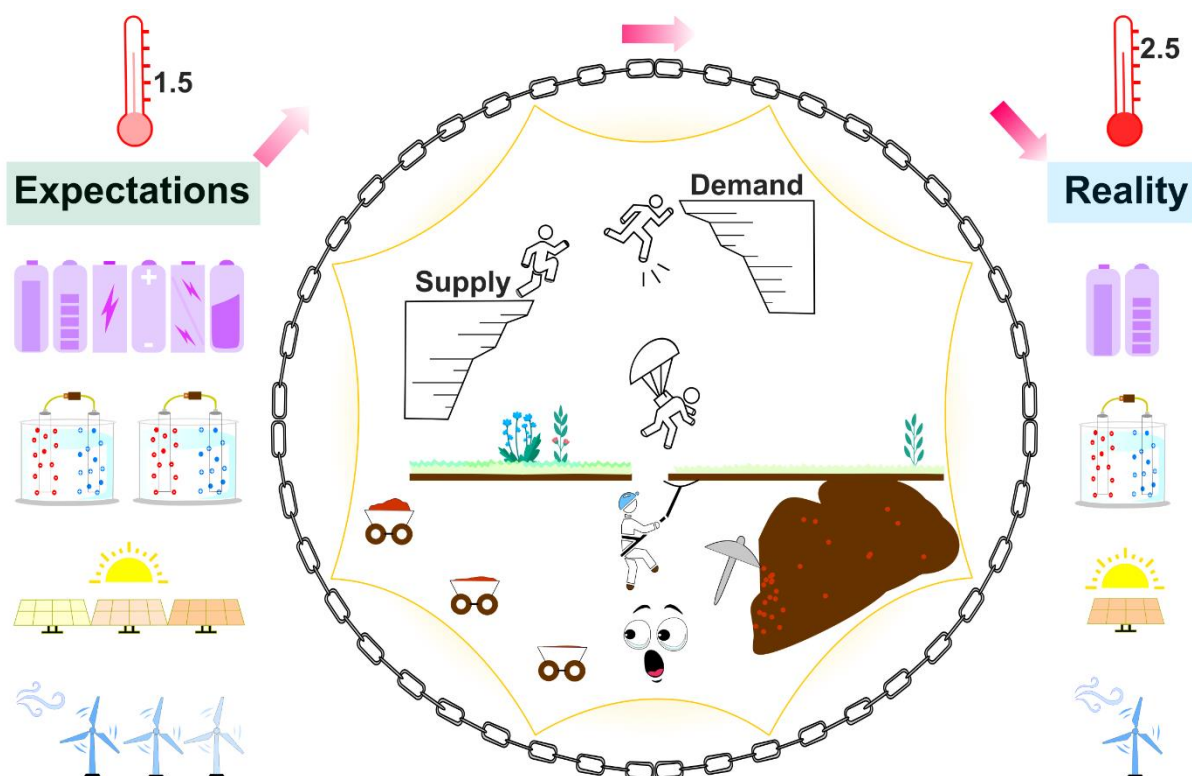
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Chapter 2

Assessing the Realism of Clean Energy Projections



Chapter 2

Assessing the Realism of Clean Energy Projections

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2.1 Introduction

While wealthier individuals may have the means to shield themselves from the effects of global warming, approximately 200 million people would face unprecedented temperature increases, impacting energy security and poverty alleviation policies.^{1,2} Carbon mitigation options look promising for addressing this challenge, yet delays in technology development will render the 1.5°C target unattainable.³ Therefore, a comprehensive understanding of the needs to develop these technologies at the required scale will illuminate the challenges ahead and drive the search for solutions to achieve the targets ambitioned.

Integrated Assessment Models (IAMs) serve as crucial tools in guiding academic discussions and shaping policy strategies in the realm of climate change and mitigation. Their impact transcends academia, influencing policy frameworks and global initiatives dedicated to reducing greenhouse gas (GHG) emissions.⁴ Recognized for their significance, these models are now integral components of the International Panel of Climate Change's (IPCC) assessment reports, which many countries rely on to inform their policymaking efforts.⁵

IAMs use scenario-based inputs to qualitatively project diverse hypothetical futures for natural and human subsystems.^{4,6} In the former subsystem, IAMs include a quantitative representation of a set of Earth-system processes,⁶ while in the latter, these models calculate energy supply and demand to meet simulated human population requirements.⁶ It is this last subsystem that can be seen as the heart of any IAM, with equations describing the assumed behaviours of consumers, producers, and regulators.⁶

Despite their widespread use, IAMs face scrutiny regarding their modelling structures and perceived limitations^{4,6}. In the past, studies underscored the need for IAMs to capture the nuances of human behaviour related to energy consumption, especially in mobility sectors.⁷ Similar studies aiming to infuse socio-technical insights into IAMs reported notable deviations in IAMs projections after including these considerations.⁸ While recognizing IAMs' pivotal role in shaping low-carbon pathways and guiding policymaking, later studies have raised concerns about their political impartiality at the science-policy nexus.⁹ Consequently, attempts have been made to incorporate concepts from international and national public policies into IAM scenarios, aiming to enhance transparency and align pathways with the goals of the Paris Agreement.¹⁰ Koasidis et al. (2023) highlighted that IAMs, with their assumptions of perfect markets and knowledge over a certain future, alone are insufficient

to navigate through multifaceted crises.¹¹ Criticism extends to their depiction of technological diffusion and the underlying transition processes⁴. Real-world complexities influencing technology diffusion rates —such as policy, technology characteristics, infrastructure compatibility, and public acceptance— are inadequately represented in IAMs, if at all.¹² All these often result in overly optimistic projections that neglect challenges inherent in industrial transformations, creating a significant knowledge gap at the science-policy interface.^{13–16} This gap influences policy agendas and undermines the policy relevance of IAMs, ultimately affecting the expected pace and the direction of progress.¹⁷ Such dichotomy is a fundamental challenge that we will elaborate on in the context of critical materials and their impact on our ability to deploy for clean energy technologies (CETs) at the expected rate. To this end, we will take advantage of CET projections that are consistent with the Paris Agreement according to eight prevalent IAMs,¹⁸ and quantify the tangible challenges to achieving them. In essence, these challenges stem from the inability of IAMs to establish a physical link between industrial assets and the materials required to build them.^{4,5} In addition, we will study the impact of the limited technological resolution of IAMs on the reliability of their predictions by exploring the relationship between various technology types and some problematic materials. Finally, considering realistic material supplies, we will estimate attainable CET capacities and translate them into more realistic temperature targets, illustrating a potential way forward for IAMs. Doing these analyses is very necessary since it is a long time that international organizations started warning of soaring costs and potential delays in decarbonization due to mineral shortages, highlighting the entrance into the age of big shovels.¹⁹

Hence, this chapter critically examines IAMs limitations in the context of CETs, shedding light on the fundamental gap between IAM projections and real-world practicalities. Our findings, obtained for 36 materials and based on 25 IAMs scenarios, advocate for a nuanced, integrated approach to bridge this gap and better align IAM insights with the pragmatic imperatives of policymaking.

2.2 Methodology

To assess the feasibility of IAM projections and to identify the effect of constraints not included in IAMs, we aim to evaluate the amount of 36 materials needed to deploy five CETs under “Below 1.5°C” and “low overshoot” temperature targets, both consistent with the Paris Agreement. These include batteries (both mobile and stationary), concentrated solar power (CSP), electrolyzers, photovoltaic (PV) panels, and wind turbines.

We start by determining the annual capacity projected for each of these technologies for 2020-2050, incorporating data from 25 scenarios generated with eight different IAMs (Table S2, chapter 6).²⁰ Hereinafter, whenever we refer to IAMs, we specifically refer to the IAMs and scenarios outlined in Table S2 of chapter 6. Each of these models and scenarios contributes to our comprehensive understanding of potential future trajectories, allowing us to encompass a wide spectrum of possibilities in our analysis. This wide scope is necessary due to the complexity and uncertainty inherent in projecting the capacity of CETs.

IAMs provide the projected capacities for various technologies in different units, which requires some calculations to obtain capacity values in GW for all of them. In addition, we estimate the replacements needed to compensate for retired facilities and incorporate them into IAM projections. Calculation details are provided in section 6.1 of the Supplementary Information.

IAMs only provide information at the archetypal technology level. However, technology designs can vary in practice, as can material requirements (Table 1). Hence, we focus on two market contribution

scenarios provided by the German Aerospace Center (i.e., Continued and Technological Change) to distribute IAMs' capacity projections among various technology types.²¹ These market scenarios predict how different technology types will contribute to the overall technology market in the following decades.

In the next step, we quantify the material consumption per GW, often referred to as material intensity. We use two material intensity scenarios: one based on current intensities and another that factors in the impact of learning curves.^{21,22} The latter scenario assumes that material intensities decrease over time due to new manufacturing approaches and technological advancements, consequently lessening material requirements.

Combining 25 IAM scenarios with two projections for the market contribution and two trajectories for material intensities (see Table 2), we generate 100 different pathways for the demand for 36 materials used in constructing various CETs. Then, these material demands will be compared with the current material supply infrastructure to critically assess the feasibility of achieving the technology capacities envisioned by the IAMs. For further details on these calculations, refer to section 6.2 of the supplementary information.

Table 1 Clean energy technologies considered and their types.

Technology category	Technology type	Technology full name
Battery	LFP	Lithium Ferro Phosphate
	NCA	Lithium Nickel Cobalt Aluminum
	NMC111	Lithium Nickel Manganese Cobalt (composition Ni/Mn/Co = 1/1/1)
	NMC622	Lithium Nickel Manganese Cobalt (composition Ni/Mn/Co = 6/2/2)
	NMC811	Lithium Nickel Manganese Cobalt (composition Ni/Mn/Co = 8/1/1)
	LiS	Lithium sulfide
	LiO	Lithium oxide
Concentrated solar power	FC	Fresnel collector
	PT	Parabolic trough
	ST	Solar tower
Electrolyzers	Alkaline	Alkaline electrolyzer
	PEM	Proton Exchange Membrane electrolyzer
Photovoltaic panels	C-Si	Crystalline Silicon
	CIGS	Copper Indium Gallium Diselenide
	CdTe	Cadmium-Telluride
Wind turbines	AG	Asynchronous generator
	HTS-DD	High temperature superconductor – direct drive
	SG-E-DD	Synchronous generator – electrically excited – direct drive
	SG-PM-HS	Synchronous generator – permanent magnet – high speed gear
	SG-PM-MS	Synchronous generator – permanent magnet – middle speed gear
	SG-PM-DD	Synchronous generator – permanent magnet – direct drive

Table 2 Classification of materials demand estimations based on IAMs scenarios.

Scenario	Market contribution	Material intensity	Colour/symbol
C_B	Continued	Base	Red
C_L	Continued	Learning	Red (*)
T_B	Technological Change	Base	Blue
T_L	Technological Change	Learning	Blue (*)

Finally, we will approach the problem from the opposite perspective, employing a bottom-up methodology to estimate the capacity of CETs that could be achieved considering current infrastructure and realistic projections for their growth rate. To this end, we formulate an optimization model to meet IAMs projections while considering constraints on materials supply and reserve capacities. Quantifying the disparity between realistic estimates and IAM projections is crucial for different reasons. In the context of IAMs, these calculations will provide a quantitative estimate for the error stemming from insufficient technological resolution and key missing linkages between different sectors in the model. Then, in the context of climate change mitigation, we can estimate the temperature increase stemming from the shortfall in deploying CETs, questioning the ability of IAM projections to achieve timely progress toward the 1.5°C target. In addition, we modify the previous model to investigate the minimum recycling rates needed for materials to meet the CET capacities outlined by the 25 IAMs scenarios. We do this for two market trends, two material intensity forecasts, and three material production rates, generating a total of 300 different results (i.e., 12 variations for each of the 25 IAM scenarios). Further details on these calculations can be found in sections 6.3 and 6.4 of the supplementary information.

2.3 Results and discussion

2.3.1 IAMs envision a rapid increase in the deployment of clean energy

Figure 1 depicts the capacity of CETs added annually between 2020 and 2050 across the eight IAMs and the 25 scenarios considered (Table S2, chapter 6), expressed as the ratio over 2020 values. The figure depicts important variations across scenarios, reflecting the uncertainty in the projected capacity for each technology.²⁰ These variations stem from the different choices each model and scenario make for specific interventions to meet climate goals, including carbon pricing, technology deployment, lifestyle, or coal retirement policies.²⁰ A detailed breakdown of the various scenarios and their underlying assumptions is provided in Section 6.1 of the supplementary information. Note that not all the scenarios include projections of all the technologies assessed (see circles within each panel). Despite existing variations, Fig. 1 illustrates an overall increasing trend in the projected deployment of technologies over time, with some noteworthy exceptions that mainly affect PV and wind. For example, scenarios from the MESSAGE-GLOBIOM model depict rapid growth in PV capacity from 2020 to 2025, followed by either a continuous rise or a constant trend, depending on the scenario. In contrast, some models like IMAGE project a decline in the annual deployment of PV and wind beyond 2040. Overall, according to median estimates, the capacity of PV panels added annually in 2050 is projected to be 10.5 times greater than in 2020, while for wind turbines, it is expected to be about 5 times higher.

The remaining CETs show smaller variations across scenarios. The median capacities added annually for stationary batteries, EV batteries, and CSPs are projected to reach 19, 24, and 37 times those of 2020, respectively. As an exception, the "PEP_1p5C_red_eff" scenario from the "REMIND-MAgPIE 1.7-3.0" model projects battery deployment reaching 104 (stationary) and 139 (EV) times the 2020 values. This scenario is characterized by comprehensive carbon pricing. Similarly, the "IMA15-TOT" scenario from "IMAGE 3.0.1" projects significantly high deployment for CSP (234 times 2020 levels) and electrolyzers (454-fold increase compared to 2030 estimates). This scenario is based on assumptions such as reduced use of CO₂ intensive transportation and rapid adoption of the best available technologies, placing its projections significantly above the median.²⁰

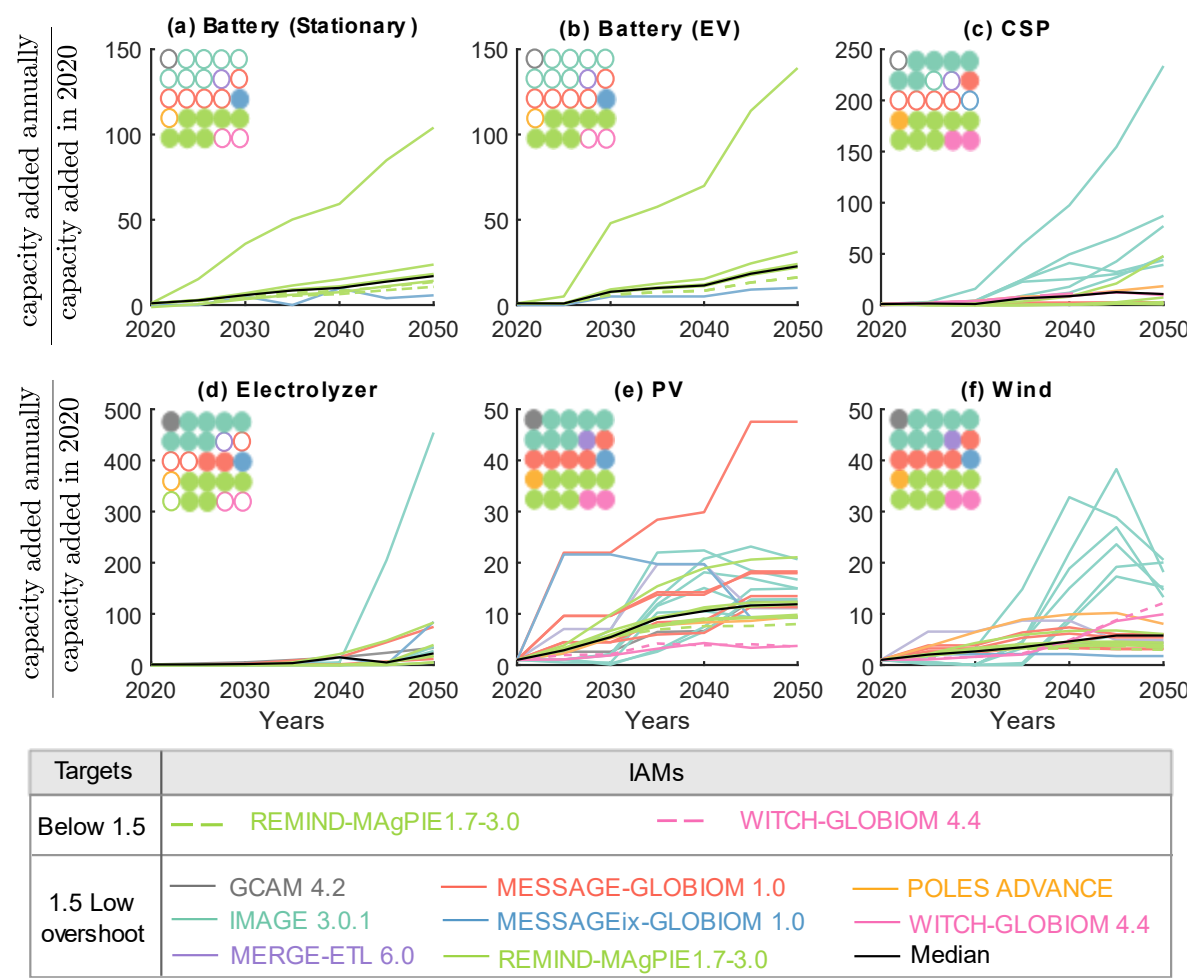


Fig.1 Projections for the capacity of clean energy technologies added annually based on selected IAMs and scenarios (see Table S2, chapter 6). Scenarios represented with dashed lines are compatible with the “Below 1.5” target, while solid lines correspond to scenarios for the “1.5°C low overshoot” target. Capacities for 2020 serve as the baseline for estimating capacity ratios in subsequent years. The only exception are electrolyzers, whose baseline year depends on the scenario (i.e., the first year with non-zero capacity projections is used in each case). Circles in each panel correspond to the different scenarios for each IAM, sorted in the same order as in Table S2 of chapter 6, and using the colour code indicated in the legend. These are used to indicate the scenarios providing capacity projections for the corresponding technology (i.e., those with filled circles). For each technology, the median value is derived by considering its available IAM scenarios. CSP: Concentrated Solar Power, EV: Electric Vehicles, PV: Photovoltaics.

To analyze the impact of these variations, we present Figure 2, illustrating the cumulative capacity developed for these technologies over the present and subsequent decades.

Fig. 2 depicts a rising trend across all scenarios that impact our ability to achieve these forecasts (see later discussion in section 2.3.5). Notably, the application of batteries for EVs, estimated at around 159 TW by 2050, shows the highest cumulative capacity, although this number may vary based on the assumptions for some technical parameters (refer to section 6.1 of the supplementary information). Following this, PV comes in at 41 TW, followed by wind at 12 TW. The remaining options stay below 6 TW by 2050.

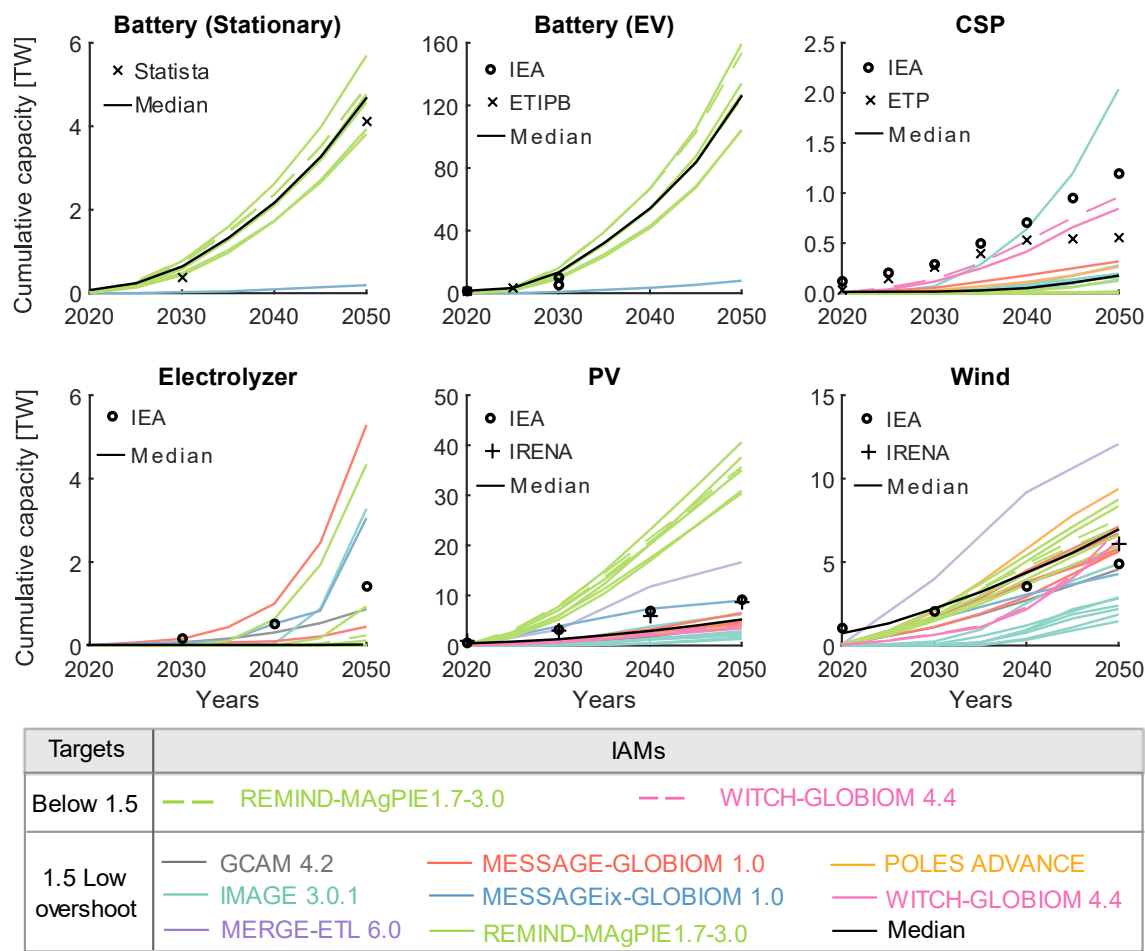


Fig.2 Cumulative projected capacity of clean energy technologies based on selected IAMs and scenarios (Table S2, chapter 6). Markers in each panel represent data from additional sources used for comparison: circles show IEA projections,^{23–25} plus signs denote IRENA data,²⁶ and cross signs correspond either to data from the European Technology and Innovation Platform for Battery (ETIPB),²⁷ from Statista (for stationary batteries projections),²⁸ or from the Energy Technology Perspectives (ETP) (for CSP).²⁹ Black lines present the median of projections.

To provide context, we also compare our estimates with projections from other sources such as the European Technology and Innovation Platform for Battery (ETIPB), the Energy Technology Perspectives (ETP), the International Energy Agency (IEA), the International Renewable Energy Agency (IRENA), and

Statista, all of which focus more specifically on energy-related aspects. We observe that the median among IAM projections allocate smaller capacity to CSPs (169 GW in 2050), electrolyzers (10 GW), and PV panels (5100 GW) compared to estimates from other studies,^{23,26–31} yet the median projections for batteries (4700 GW for stationary and 126 TW for EVs in 2050) and for wind turbines (7000 GW) are consistent with other projections. More importantly, all the projections from other sources fall within the range of IAM scenarios considered in the analysis, highlighting the robustness of our estimations. The only exception are small discrepancies for CSP between 2020 and 2040, which, ultimately, would have little impact in material shortages (see Fig. 5).

In addition, our estimations closely match existing real-world data. For instance, the actual capacity of PV panels added in 2020 was 84 GW,³² close to the average of the values predicted by IAMs (94.5 GW). Similarly, the development of wind turbines is at the range, with the actual 111 GW capacity added in 2020,³² well within the IAM forecasts (i.e., 7-154 GW).

We also note that the share of the total capacity added in 2050 to replace retired facilities is very small, reflecting the modest capacity of clean energy technologies installed during the past decades (Figure S2, chapter 6). However, a challenging decade is expected to start in 2050, when major replacements for batteries, PV panels, and wind turbines are anticipated to commence, given their expected lifetime (i.e., about 15 years for batteries and 30 years for PV panels and wind turbines)^{33,34}.

The timing and magnitude of this surge may vary based on technology quality and durability; aspects necessarily overlooked in already complex IAMs. High-quality materials can extend the durability and lifespan of these technologies, delaying the need for replacements and materials recycling. Furthermore, real-world dynamics involved in developing and replacing retired clean energy technologies are multifaceted, including mine exploration, technological advancements, economic factors, supply chain stability, and operational conditions, making it very complex to accurately estimate the year that each technology is going to be retired.

The challenge caused by technology retirement and replacement could be controlled by developing material recycling facilities, an issue that will be further explored in section 2.3.6.

Hence, even if most IAMs already impose limits on the penetration of technologies, this first analysis is in agreement with the body of literature suggesting that these might be over-optimistic.⁴ The feasibility of attaining envisioned levels in deploying CETs is hard to grasp, and more tangible data on material requirements and supply would be needed for this purpose. The issues starting a call for urgent improvements in permitting, mining, and manufacturing systems. Hence, in the next section, we will translate the projections of installed capacity for these new technologies into material demand to ascertain whether IAMs' estimates are realistically feasible given the current landscape of materials supply and its potential growth.

2.3.2 Materials market dynamics are an obstacle to achieving IAM projections

We next evaluate the annual demand that the development of CETs would impose on 36 distinct materials under each class mentioned in Table 2 for each of the 25 IAM scenarios considered. We start by performing a preliminary analysis to identify those whose supply is expected to be most challenging (see section 6.2.6 for further details), finding an especially concerning situation for the 16 elements depicted in Fig. 3. We will refer to these as problematic materials (results for the remaining materials are provided in Fig. S3 in the supplementary information). We also compare our estimates with the material demands provided by Wang et al.,³⁴ and those reported in the IEA critical mineral data explorer (see Table S16, chapter 6).³⁵

We find that, for all these elements except for cadmium, copper, and praseodymium, the annual demand for the development of CETs alone can potentially exceed their current production for all sectors at some point before 2050 (Fig. 3a). Indeed, the demand-to-production ratio for iridium, tellurium, lithium, indium, cobalt, and terbium could increase up to 143, 49, 17, 8, 6, and 5 respectively. Reaching these figures would require an increase in the production capacity of these materials which seems unattainable for over 30 years. Failure to do so could lead to material shortages and supply chain disruptions, ultimately hindering our progress toward the temperature target defined by the Paris Agreement.

The situation seems less critical for other elements since their median demand does not exceed their current production levels. However, increasing production rates may still be difficult for certain materials like cadmium, gallium, indium, and iridium, as they are byproducts of other elements. This issue is further discussed in the next section.

The crucial point to note here is that IAMs project the total capacity for each archetypal technology, like PV, without distinguishing between different technology types, such as CdTe, CIGS, and CSi panels, irrespective of material assets. This makes it difficult for IAMs to capture factors such as market drivers, innovation, or inertia.³⁶ As each technology type has unique material requirements, allocating capacity to them directly influences the materials needed and the ability to meet the projected capacity. Hence, the demand for some elements is contingent on the market contribution scenario, as illustrated by the red vs blue lines. Take cobalt as an example. The demand for this element would rise in a continued market trend (red lines in Fig. 3) but decrease in scenarios where technological changes replace cobalt-type batteries with cobalt-free alternatives³⁷ (blue lines; further elaborated in section 2.3.4).

This effect is also observed when analysing the demand from CETs alone (i.e., without comparing it with the total production level of each material, Fig. 3b), where we discover many minerals whose annual demand would increase to sky-high levels if the technological change market trends were realised. These include cadmium (whose demand from CETs could be 398 times larger than in 2020), gallium (531), indium (471), lithium (285), nickel (214), selenium (571), and tellurium (396). In the case of cadmium, the demand is primarily driven by CdTe PV panels, which will reach a 24% market contribution by 2050 in the technological change scenario (compared with 5% in the continued market trend). This difference could significantly affect cadmium demand, potentially raising its price and affecting other applications, such as its use in plastic stabilizers and pigments.³⁸ Conversely, the technological change scenario assigns a smaller contribution to C-Si panels, making it a safe bet when considering silver supply limitations.

On the other hand, indium, and tellurium, which have displayed a high supply risk in Fig. 3a, are likely problematic when considering their demand from CETs (Fig. 3b), as this will affect their availability for other sectors and, consequently, their price.

The demand for elements used in electrolyzers, like graphite and iridium, could skyrocket to 2600 and 4000 times their estimated demand in 2020. This happens in IAM scenarios allocating a very minor capacities to this technology initially, followed by a rapid growth. However, considering the median values, which are arguably more likely to occur, the situation for these elements is not as critical.

Overall, some technology types will benefit from particular market scenarios while others may face disadvantages. We acknowledge that modelling detailed markets competing for materials, whose prices vary according to their respective elasticities and demands, might be out of reach of current IAMs. However, even in this case, it should still be possible to simulate distinct market trends, introduced exogenously into the model formulation, similarly to what is done today to limit

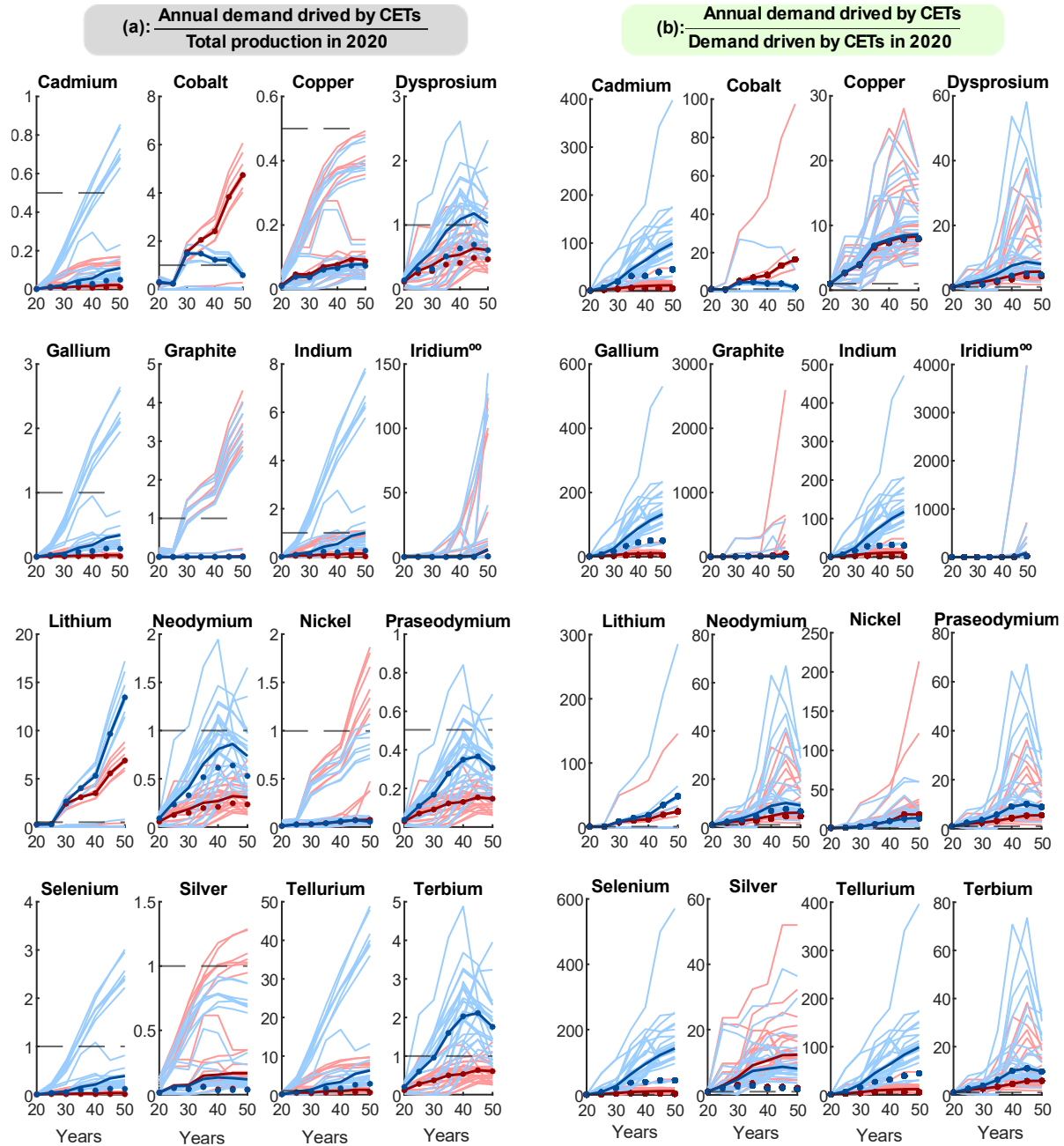


Fig.3 Material demands from clean energy technologies. Panel (a) compares the demand for materials from clean energy technologies with their production rate dedicated to all sectors in 2020. Panel (b) represents materials demand from clean energy technologies compared with their estimated demand in 2020. ^{oo}: Iridium, primarily used in electrolyzers, does not exhibit demand until 2030 and therefore relies on this year or later years, depending on the scenario, as the basis for calculations. Dashed horizontal lines at $y=0.5$ for cadmium, copper, and praseodymium and at $y=1$ for other materials have been included for comparison. Timeframes are indicated as follows: 20: 2020, 30: 2030, 40: 2040, 50: 2050. The results of the continued trend and technological change are distinguished by red and blue colours (see Table 2). In both cases, the median is depicted with a thicker line. The effect of the reductions in material intensities due to learning curves is indicated with star signs, only for median projections. CETs: clean energy technologies.

technology diffusion rates. What is clear is that allocating the capacity of each CET into their various types, while considering material accessibility constraints (market availability), along with material reserve capacities, is vital for achieving the level of technological development required for some temperature targets. Incorporating these pieces of information is essential for any IAM aiming at providing more realistic predictions. In addition, it is imperative to include in IAMs other CETs overlooked here, like fuel cells or electric motors, since their development will increase the demand for critical materials such as dysprosium, neodymium, nickel, and silver.²¹ This inclusion will enable future studies to assess these technologies and anticipate potential challenges more accurately.

On the other hand, we observe that the demand for materials is also influenced by the effects of learning curves, denoted by the star signs in Fig. 3. Cadmium, dysprosium, gallium, indium, neodymium, selenium, silver, and tellurium, serve as prime examples of this phenomenon. However, there are many challenges ahead of attaining these intensity reduction levels.³⁹ Therefore, aside from investments aimed at boosting material production rates, expanding the capacity of both mine and mineral refineries, there is a need for research and development efforts focused on reducing technology dependencies on these challenging materials. Ultimately, IAMs should consider the effect of technological advancements and link them to material constraints to become suitable for modelling future technology capacities.⁵

In this context, material recycling is essential in circumventing supply disruptions and preserving finite resources.⁴⁰ However, previous studies report that, even after employing improved recycling processes, supply may still fall short of demand,⁴¹ an issue further investigated in section 2.3.6.

In any case, the retirement of technologies is expected to occur mainly after 2050, resulting in a market of obsolete technologies that can be used for materials recycling. Before 2050, materials replacement remains an option (Table S20, chapter 6), provided it does not compromise technology performance, an issue necessitating thorough examination. For example, sulphur dioxide is a potential alternative to selenium dioxide, yet it exhibits comparatively lower energy efficiency. Additionally, bismuth, calcium, lead, phosphorus, selenium, and sulphur are among the elements viable for replacing tellurium in numerous free-machining steels, but often result in decreased efficiency or altered product characteristics. Similarly, graphene has been engineered as a substitute for indium tin oxide electrodes in solar cell technology.³⁸ However, improper material incorporation in PV panels would lead to reduced efficiency, thus resulting in more units and increased land requirements to achieve the same service.

Currently, most IAMs overlook the explicit representation of material cycles, ignoring how materials move through the stages of production, use, and disposal.⁵ Omitting such information makes them myopic to additional constraints that may limit mitigation trajectories in practice. Considering the level of aggregation of industrial activities in IAMs, we acknowledge the challenge of representing complex industrial networks for material production, manufacturing, and recycling. However, we also claim the need to improve the link between mitigation trajectories and underground realities. Hence, as a first step towards further evolving IAMs, we advocate considering at least different technology types and linking them to the availability of materials through the corresponding material intensities and learning curves. This simple modification would add little mathematical complexity while adding a new layer of constraints to obtain more realistic estimates.

2.3.3 Additional challenges are foreseen for coproducts

Elements sometimes coexist within rock formations, resulting in what is known as a “guest element”, acquired as a byproduct during the extraction of the so-called primary or “host” element.^{38, 42} An illustrative instance is the worldwide production of iridium, 98% of which is obtained as a byproduct of platinum extraction.⁴² Sourcing guest elements in large quantities could potentially be problematic as they have limited, if any, dedicated extraction activities today.

In this section, we examine the demand for host elements necessitated by CETs and use it to derive the amount of the corresponding guest elements that would be generated as byproducts in the process. Then, we use these values as benchmarks (i.e., denominator) to compare the specific demand for guest elements originating from CETs (numerator). For materials that this ratio lies above one, shortages could be experienced unless additional actions are implemented. Further details on the calculations are provided in section 6.2.5.

As shown in Fig. 4, based on the median values, the annual demand for all elements except for gallium and silver may exceed their annual production as byproducts. This suggests that, in certain cases, larger quantities of their host elements might need to be extracted to meet the required demand for the guest element.

For cadmium, gallium, and indium, scenarios based on the technological change market contribution (blue lines) present a more challenging situation owing to the higher share of CdTe and CIGS PV panels in the market. Specifically, when considering the median values, the market contribution plays a decisive role for indium.

The continued market scenario seems effective in addressing these elements, yet it might not suit all materials. For example, it resolves the issue of indium supply by reducing contributions from CIGS and CdTe panels, yet the increased penetration of CSi PV panels would result in a higher demand for other problematic elements like silver (Fig. 3). This challenge is somewhat alleviated when considering the effect of learning curves, as indicated by the star signs. This highlights the importance of investing in material-related research when advancing CETs, particularly concerning these elements.

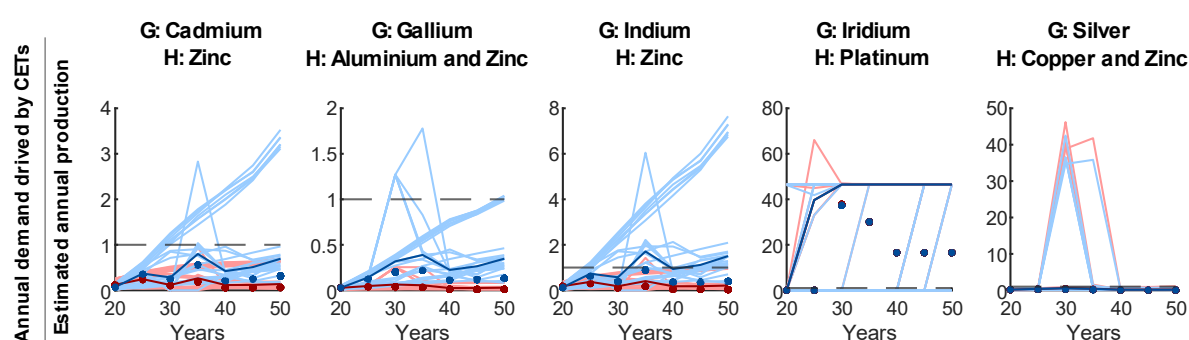


Fig.4 Ratio between the annual demand for guest elements and their potential production as byproducts. We have included a horizontal dashed line at $y=1$ to aid comparison. In most of the IAMs scenarios, there is almost no demand value for iridium and platinum before 2030, as the development of their host technology, electrolyzers, commences mainly after 2030. Timeframes are indicated as 20: 2020, 30: 2030, 40: 2040, and 50: 2050. The results of the continued trend and technological change are distinguished by red and blue colours (see Table 2). In both cases, the median is depicted with a thicker line. The effect of the reductions in material intensities due to learning curves is indicated with star signs, only for median projections. CETs: clean energy technologies.

In the case of iridium, its median demand would rapidly surge to 46.5 times the annual production that could be obtained from its host element (platinum). Fortunately, reducing iridium intensity seems attainable thanks to a recent breakthrough by Torrero et al., who developed an advanced catalyst with a ten-fold reduction in iridium loading.⁴³ Nevertheless, even with these improvements, iridium demand would escalate to 16.5 times the amount that can be produced as a byproduct. An alternative solution could involve replacing iridium in platinum-iridium alloys with elements such as tungsten, nickel, ruthenium, osmium, copper, gold, rhodium, or palladium. However, this substitution might alter the resulting alloy's electrical resistance and thermal expansion coefficients.⁴⁴

Challenges related to other guest elements like cadmium, gallium, or indium are generally less significant than iridium. The same conclusion could be reached for silver based on median values, yet challenges may arise between 2025 and 2040 if the development of wind turbines and, in turn, the demand for zinc (host) is small.

On the other hand, we note that other sectors also require host elements, which could potentially lead to an increased production of guest elements. For instance, 75% of the global copper supply caters to non-energy sectors.³⁰ In this context, surpluses of host or guest elements could impact their pricing and the associated CETs. For instance, while zinc is not problematic, it attracts attention because it is linked with cadmium, gallium, indium, and silver. Consequently, its production rate and price are interlinked with and influenced by the supply of its guest elements and their prices.

Capturing all these connections, which could ultimately affect the market shares of the different technology types, would be very challenging for IAMs unless they are linked to more detailed sector-specific partial equilibrium models.^{45,46} Integrating these models into current IAMs, where industrial sectors are highly aggregated, will necessitate time. As a compromise solution in the interim, IAMs could incorporate constraints on materials supply, considering specific bonds between guest and host elements. This represents an opportunity for IAM developers since models that link technology types with constraints on materials supply can capture the effect of various market contribution scenarios more effectively. Again, this highlights the importance of considering technology types and modelling the supply of, at least, key problematic elements to ensure that IAMs can offer a more realistic representation of the range of actions available to combat climate change.

2.3.4 Increasing technological resolution in IAMs is imperative

We next dig further into the intricate connections between various CET types and problematic materials so as to evaluate the consequences of potential material shortages in developing specific designs (Fig. 5). Ribbons in the figure symbolize the connections between the materials and their corresponding technology hosts based on material intensity values for 2020. All these materials, except for cobalt, copper, praseodymium, graphite, lithium, and nickel, are expected to exhibit a reduction in their material intensity over the decades due to learning curves, which could benefit technology development (please refer to Fig. S4 to visualize the effect of learning curves on technologies available in the 2050 market). We note that not all the 36 materials studied (Table S5, chapter 6) are included in Fig. 5. Instead, we focus only on problematic materials outlined in Fig. 3.

Considering the right-hand side of the figure, it becomes evident that all types of PV panels heavily rely on problematic materials, which raises concerns about our capacity to develop this technology at the expected rate. The situation is particularly concerning for CIGS panels, which demand three problematic elements: indium, whose annual production should increase by up to 8-fold over the next three decades (Fig. 3a), as well as gallium and selenium, both signalling a potential price increase

owing to additional demand from competing sectors (Fig. 3b). Consequently, developers might opt to prioritize the development of CSi and even CdTe types to mitigate the potential scarcity or price increase in elements associated with CIGS panels. However, this shift could also threaten the supply of silver. Based on Fig. 3a, the demand-to-supply ratio for silver could slightly exceed one, while Fig. 3b shows that the demand from CETs could rise up to 53 times that of 2020. This indicates that, while such a shift may be feasible, it would have higher costs for CSi panels and may also affect CSPs development. Specifically, all types of CSPs show a high dependency on silver, while ST-type CSPs also require nickel, primarily used by the electrolyzers.

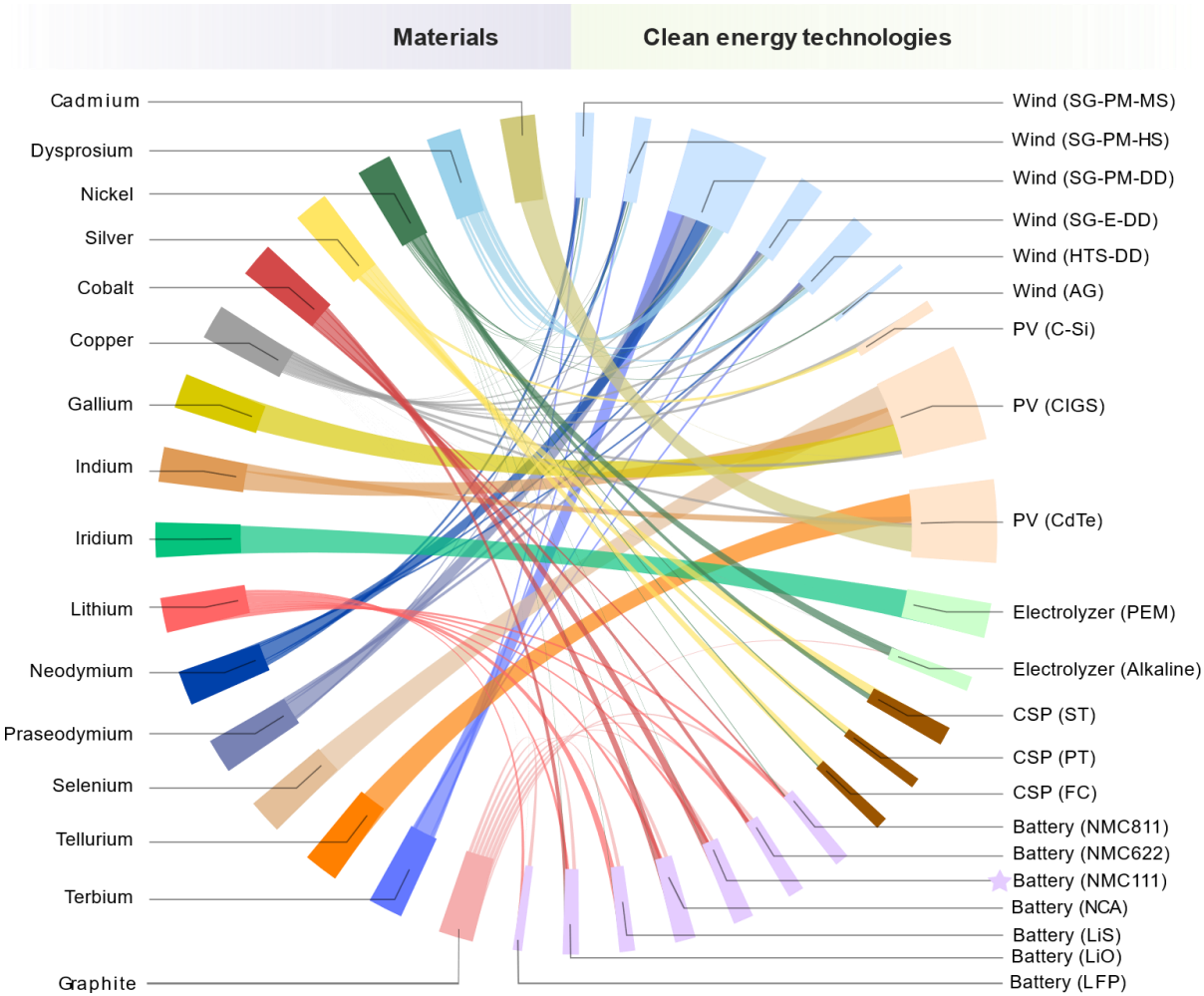


Fig.5 Links between materials (left-hand side) and clean energy technologies (right-hand side), based on material intensity values in 2020. The width of the ribbons is proportional to material intensity values. Technologies that will disappear by 2050 according to both market contribution scenarios are distinguished by a star. Material intensity values have been normalized to ensure visibility (see section 6.2.7 of the supplementary information). For clarity, technology types are enclosed in brackets, with the corresponding acronyms found in Table 1.

Most IAMs model investments in technologies based on the economic performance of competing alternatives considering perfectly functioning markets.^{6,12} This approach often reflects first-best policies, providing valuable optimal scenarios for benchmarking.¹² However, these models may not encompass all real-world complexities. Real-life policy and consumer choices do not always align with purely economic rationality.⁴ While attempting to incorporate these aspects into models, including IAMs, may seem ambitious, establishing a direct link between technology assets and the specific amounts and types of materials required for their construction appears more straightforward. This approach, although still not perfect, would allow IAMs to immediately discard infeasible situations with marginal modelling and computational effort.

For instance, our calculations suggest that if the focus shifts to CdTe panels, it will further strain the supply of cadmium and tellurium. As shown in Fig. 3, tellurium is among the most problematic elements due to its production rate and potential price increase, while cadmium is a byproduct showing signs of price surges due to its rapidly increasing demand. Therefore, an IAM including some constraints on the availability of materials might opt for CSi panels. Ideally, IAMs should also include the effect of technological advancements on material intensities, as they can draw a significantly different picture of the landscape of CETs (Fig. S4).

All these issues are not exclusive to PV panels. Similarly, wind turbines, especially the SG-PM-DD turbine type, will face challenges in their development. Even considering the new technology types that may appear in the market (Figure S4, chapter 6), all types have a link with some of these problematic materials. Their main obstacles are rare earth elements, which include dysprosium, neodymium, praseodymium, and terbium. These elements are crucial components in the permanent magnets of wind turbines.²² While alternative options exist, rare earth elements are considered irreplaceable due to their superior performance.⁴⁷ According to the technological change market, by 2050, the focus will shift to any wind turbine type rather than SG-PM-DD due to its dependency on praseodymium. Although praseodymium's demand-to-production ratio never exceeds 0.8 (Fig. 3a), its potential price increase could be the critical point (Fig. 3b).

The situation is also critical for PEM electrolyzers due to their reliance on iridium and, consequently, on platinum (iridium's host element). Alkaline electrolyzer development faces challenges given its dependency on nickel and graphite. However, if both technologies eventually achieve the intensity values targeted in their learning curves, PEM electrolyzers may gain an advantage over alkaline electrolyzers (Fig. S4), enabling them to lead the market. Hence, the consideration in any model of material availability and material intensities, varying over time, could result in different market trends compared to those externally defined. On the other hand, IAMs opting for the simulation of exogenous market shares could spot whether these are attainable if the IAM accounts for material flows, as advocated here.

Cobalt, nickel, copper, graphite, and lithium pose challenges for battery development. Among them, copper is also in demand for PV and wind technologies, and nickel is needed by CSPs and electrolyzers as well. All these elements are experiencing significant demand increases, potentially leading to competition with other applications and affecting battery costs. Lithium, which is more demanded from LiS battery types³³ (not relevant in 2020; see Figure S4, chapter 6), is also identified as an element requiring a substantial increase in its production (Fig. 3). Technology learning curves do not greatly impact different battery types. Still, the disappearance of NMC111 and the introduction of new battery types like LiS and LiO into the market would influence the demand for materials, particularly for cobalt and lithium. However, a different trajectory for the development of batteries in particular, and CETs in general, might arise due to shortages in material availability or sudden price surges within

this sector. Additionally, including explicit projections for EVs and their battery requirements in IAMs would be beneficial for future studies, enhancing their comprehensiveness and accuracy.

All these factors can profoundly affect adopting the associated types of CETs, which are inherently intertwined with the materials sector. Consequently, fluctuations in material supply pose a tangible barrier to realizing the projected capacities envisioned by IAMs, which, today, are myopic to these material flows, technology types, and their market shares.

2.3.5 Introducing material flows into IAMs to obtain more realistic solutions

In previous sections, we highlighted the limitations preventing IAMs from providing reliable projections. In this section, we illustrate a straightforward method to enhance these models. Departing from their capacity projections, we employ a bottom-up approach to evaluate the realistic deployment capacity of CETs. This evaluation considers (a) material availability constraints and (b) different technology types. This will allow us to identify the designs with the lowest dependence on critical materials and quantify the gap between realistic estimates and the projections outlined by IAMs.

To attain these objectives, we have developed an optimization model that places constraints on the availability of the 36 materials assessed in this study. These constraints serve two purposes. Firstly, they limit the demand for each material based on the reserves assessed in 2020, which is crucial for minerals like cobalt, indium, selenium, silver, and tellurium, for which the demand may exceed reserve capacity (Fig. S5). Secondly, they constrain the share of any material dedicated to advancing CETs based on 2020 levels. This simulates the situation where other sectors demanding these materials grow proportional to the clean energy sector. Note that we do not integrate these constraints directly into IAM formulations; instead, we build a separate model that takes advantage of the capacity for CETs projected by IAM.

Acknowledging that future pathways might not necessarily follow the pattern of past transitions, we project the production rate of the different materials in coming years based on historical trends, which depicts an average annual growth of metal mining of 2.7% since the 1970s.⁴⁸ We also conduct a sensitivity analysis by varying this increase between 0.7% and 4.7% (i.e., historical trend $\pm$ 2%); we will refer to these as the pessimistic and optimistic scenarios.

Regarding technological resolution, our model covers 21 technology types across five technology archetypes (Table 1). Each technology type has specific material requirements, which may vary over time depending on the trends followed by material intensity (i.e., base vs learning), ultimately affecting material demands.

The aim of the model is to mathematically demonstrate whether IAM projections for CETs are achievable considering the aforementioned constraints in material availability and supply. To this end, we estimate the capacity of a given technology archetype (e.g., PV) by combining the individual capacities that can be developed for the corresponding technology types (i.e., C-Si, CIGS and CdTe panels) according to the materials available, and minimize the disparities compared to IAM projections. As an example, we try to meet the PV capacity projected from IAMs by developing any type of PV panels. We perform this analysis across the 25 IAM scenarios, considering three different materials production rates and two materials intensity trends. The outcome is a range of potential capacity shortages, illustrated in Fig. 6(a), as well as the preferred technology types based on materials availability considerations, as presented in Fig. 6(b). Refer to section 6.3 in the supplementary material for more details on the model.

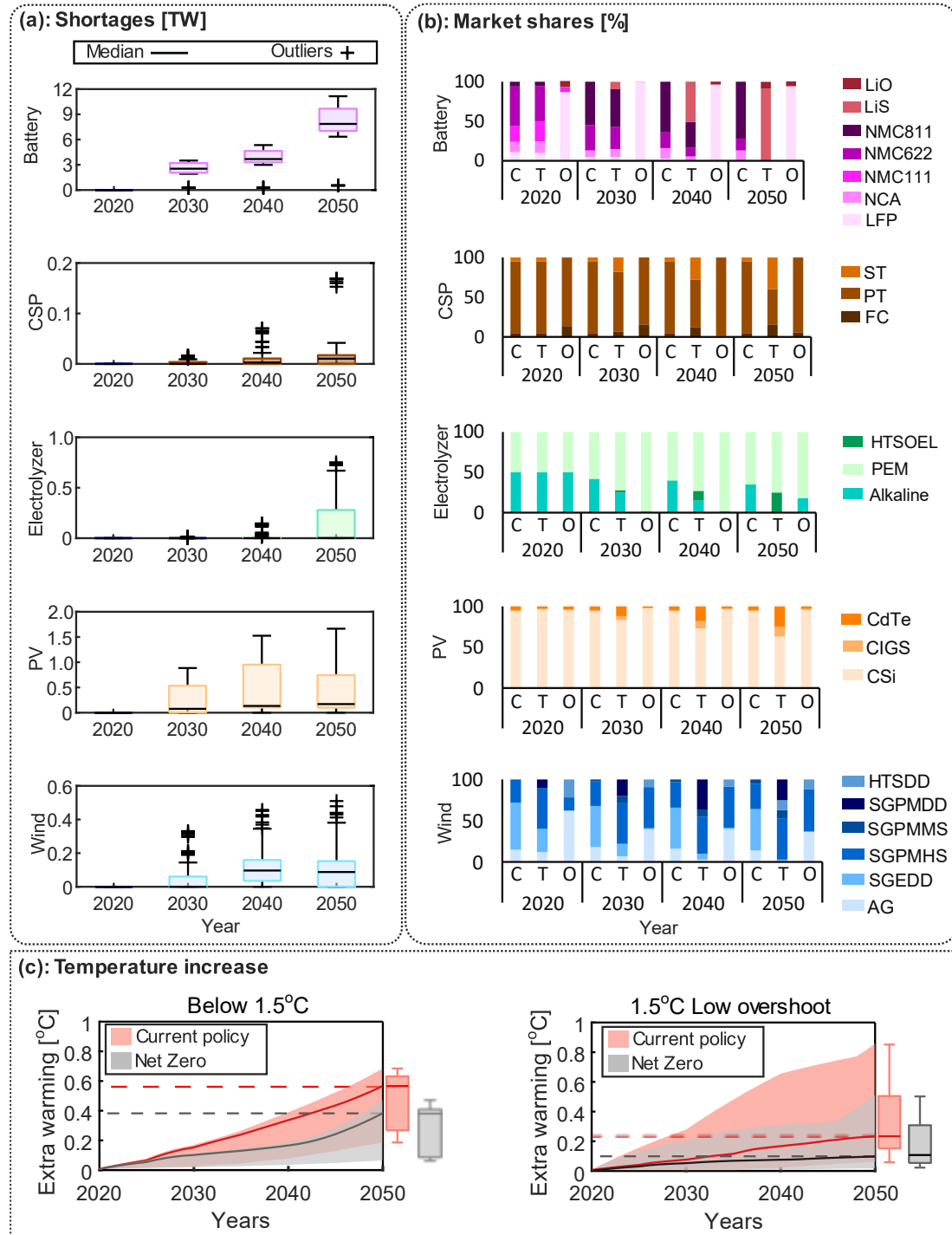


Fig.6 Assessment of shortage capacities in clean energy technologies development. (a): Shortage in developed capacity of clean energy technologies for each year obtained from the optimization model. The shortage bar in each instance represents the disparity between the technology's optimized capacity and IAMs' projections. Error bars represent the variability in shortage capacity depending on the potential fluctuations in materials production rates and their intensity; (b): Market share of different technology types based on a continued trend (C), technological change trend (T), and the optimization model (O); (c): Extra warming due to the shortages in the capacity of CETs based on carbon intensity values under the Current Policy (CP) and the Net Zero (NZ) scenarios. The solid line inside each curve corresponds to the median value obtained from six sets of the results (i.e., three material production rates and two different material intensity trajectories) for each of the 25 IAM scenarios.

Fig. 6a offers a comprehensive overview of the outcomes for each of the five technology archetypes assessed, unveiling varying challenges. Our model indicates that, while each technology faces potential shortages, achieving projected capacities for electrolyzers may be feasible based on median values. However, it is important to note that if material supply grows according to our pessimistic estimates, electrolyzer capacity could decrease significantly (e.g., a 752 GW shortfall), primarily due to iridium unavailability. This decline would represent a 99% shortfall compared to the projections from MESSAGEix-GLOBIOM 1.0 (Fig. S6), which anticipated a high development rate and cumulative capacity for electrolyzers, particularly after 2045 (Figs. 1-2). Similarly, potential shortages of copper and neodymium would prevent us from reaching IAM projections for wind turbines, with a median shortage of around 88GW or 54% lower capacity by 2050. These would be even higher for scenarios projecting simultaneous increased wind and PV capacity such as CD-LINKS_NPi2020_400 based on WITCH-GLOBIOM 4.4 (435 GW shortage in wind capacity in 2050, see Fig. S6).

The median shortfall is less pronounced for CSP (10.4 GW in 2050). However, under a pessimistic situation, we could lose the entire 169 GW projected for this technology in the IMA15-TOT scenario from IMAGE 3.0.1 model. It is worth noting that this scenario envisions the most rapid escalation in annual installed capacity of the CSPs and the highest cumulative installed capacity by 2050 (Figs. 1-2). Even more profound challenges arise when meeting IAM projections for batteries and PV panels. Focusing solely on mobility batteries, our estimates indicate a consistent shortfall, reaching up to 11.1 TW or 94% of the capacity estimated based on the REMIND-MAgPIE 1.7-3.0 for this technology in 2050 (Fig S6). Median values also reveal remarkable shortages that start this decade. This underscores the critical need for mineral production rates to outpace the 4.7% annual increase assumed here for the optimistic scenario, or for a substantial allocation of minerals to develop CETs to meet battery projections. Shortages are also apparent for PV panels when compared with ambitious projections of REMIND-MAgPIE 1.7-3.0, reaching up to 1.6 TW or 94% in 2050, mainly due to the limited availability of copper. Similar challenges are observed for gallium, graphite, indium, selenium, silicon, and tellurium, whose supply would be completely exhausted in certain years. These results reveal that including constraints on materials availability would increase the accuracy of IAM projections. Either expectations for rate of these technologies development will have to be scaled back, or rate of material production will have to be scaled up, or both.

While a brief surge in annual mineral production may be feasible for a limited period, sustaining such high rates for about three decades poses significant challenges. This becomes crucial, especially if we aim to shield other economic sectors from the repercussions of the rapid development of clean energy technologies. In the backdrop of COP28, where some countries aim to triple global renewable power generation capacity by 2030,⁴⁹ a reevaluation of IAM capacity projections is imperative. We suggest that these projections should consider material availability, an issue not perceived as problematic in the past but demonstrated to be essential here.

Considering the present and future landscape of materials supply, certain technology types emerge as the most reliable bets for deploying clean energy (Fig. 6b). These include LFP batteries, PT CSPs, PEM electrolyzers, CSi PV panels, as well as AG and SG-PM-HS wind turbines. These technologies exhibit increased capacity in our optimization model compared to continued and technological change market contributions. Indeed, we already anticipated potential shortages in the developed capacity of PV panels and a heightened focus on CSi panels in sections 2.3.2-2.3.4. In addition, by running our model and failing to meet IAM projections, we mathematically demonstrated that the two (or any other) market trend scenarios are, by definition, infeasible when considering IAM projections.

In any case, it is important to note that under a free-market scenario where developers and customers might opt for technology types different from those selected by our model, disparities from IAM capacity projections may exceed our estimations. Hence, we underscore the importance of factoring in specific technology types in IAM capacity projections for each archetypal technology.

Similarly, here, we adopted a conservative approach whereby the availability of guest elements was not based on the production of their host elements but only limited by the growth in their supply. This is equivalent to assuming that dedicated extractions could take place if needed.

Notably, technological innovation and reductions in material intensities hold promise in alleviating potential shortages in technology development, yet competition among different technologies for the same materials may lead to unintended consequences. For instance, reductions in material intensities could result in additional 23 GW of PV panels in 2050. However, this would bring a decrease of 11 GW in the capacity for wind turbines owing to the reduced availability of materials like aluminium, copper, and nickel, also used in PV panels.

While our analysis is limited to CETs, it is important to note that material constraints will inevitably impact other aspects of any IAM into which they would be introduced. As an illustrative example, the capacity projected for PV by the GENeSYS-MOD model under no climate assessment target is nearly three times the median capacity projected across the 25 scenarios in our study, while its projection for wind aligns closely with the upper bound of the projection ranges in Figure 2.²⁰ Indeed, some models anticipate cost reductions for CETs based on technological advancements and, in consequence, they assign significant capacity to these technologies, independent of climate considerations. Therefore, we expect a more realistic depiction of future scenarios by incorporating these constraints into any IAMs. Adding material constraints will not only impact the deployment of CETs but also other aspects connected with the various sectors within each model. These impacts may vary depending on the model and scenario used, as each model depicts reality differently.

While we recognize that our assumptions may not perfectly align with reality, they do offer an upper bound on the actual availability of materials and, consequently, CETs. For instance, our model implicitly assumes free global flow of raw materials, while the global trade landscape is far from friction-free, and geopolitical tensions and transportation requirements would further affect the availability of materials and technology costs. For instance, the value chains of PV panels rely on minerals like copper and aluminium, typically sourced from China and Africa, assembled in developing Asian economies, and distributed worldwide.⁵⁰ This emphasizes the importance of addressing regional supply constraints and associated challenges in future studies.

Establishing a direct link between industrial assets and required materials represents a pragmatic starting point to address material supply chain complexities and technology development challenges. Despite its limitations, this approach lays the groundwork for more comprehensive solutions that target the root causes of optimistic projections.

On the other hand, any shortfall in the capacity developed for CETs would directly impact our ability to achieve the 1.5°C target of the Paris Agreement. To illustrate this, we estimate the greenhouse gas (GHG) emissions that would not be avoided due to shortages in the capacities projected for various technologies and translate them into the corresponding temperature raise. This is achieved by compensating shortages in CETs (compared with IAM projections) with equivalent services (e.g., electricity or transportation) offered by fossil fuel-based options (e.g., grid electricity or diesel cars). We exclude electrolyzers from this analysis, assuming that the hydrogen they produce would be used in chemistry (instead of energy) applications.

Arguably, the carbon intensity of these alternative options will vary over time, reason why we employ prospective life cycle assessment,⁵¹ to calculate their associated GHG emissions between 2020 and 2050. Acknowledging that the technology trajectories obtained with our optimization model do not correspond to any specific IAM scenario, we use two conflicting scenarios to estimate the carbon intensities of these alternative services. On the one hand, the Current Policy (CP) scenario considers the second Shared Socio-economic Pathway (SSP2) and a Representative Concentration Pathway with a radiative forcing level of 3.4 (RCP3.4), allowing global warming to exceed 2°C. This scenario would provide an upper bound on carbon emissions, reflecting a situation where a slow decarbonization results in failing to meet the Paris Agreement. This is arguably consistent with scenarios for which our model discerns significant shortages in CETs. On the other hand, the Net Zero (NZ) scenario aligns with SSP1 and RCP 1.9, prioritizing the deployment of CETs and other measures to limit global warming to 1.5°C. Thus, NZ serves as a lower bound for the carbon footprint of the alternative services, and thus, is better aligned with scenarios with minor shortages of CETs. Acknowledging the uncertainty associated with both estimates, we opted to assess the 25 IAM scenarios analysed with the two carbon intensities, avoiding the need to arbitrarily match each of the 25 IAM scenarios considered with one of the two carbon intensity trajectories (i.e., CP vs NZ). This approach results a wide range of estimates that better covers all potential realization of uncertainties. Further details can be found in section 6.4 of the supplementary information.

Fig. 6c illustrates the additional warming for the different cases analysed. CET shortages in scenarios consistent with the "Below 1.5" temperature target could result in a median temperature raise of additional 0.38°C (0.06-0.46°C) under NZ. The situation would be even worse under CP, where the median extra warming would reach 0.56°C (0.18-0.68°C), underscoring the urgency of decarbonizing the electricity grid and the mobility sector by embracing renewables or options like biofuels.⁵²

The situation is slightly milder for scenarios consistent with the "low overshoot" target, where shortages in CETs would translate into additional 0.10°C (0.01-0.50°C) under NZ. Still, the temperature could raise by additional 0.85°C in the most pessimistic estimations. It is important to note that the values provided for these scenarios should be further increased by 0.10°C to reflect the overshoot.⁵³ These findings resonate with previous observations that IAMs can sometimes offer overly optimistic trajectories for climate change mitigation. In this case, the optimism stems from a lack of technological resolution together with information regarding the material flows, essential for constructing clean energy assets. Adding these two pieces of information into IAMs, while moderately simple, could dramatically change the outcome of these models, as demonstrated by these calculations.

2.3.6 Could material recycling be the solution?

Arguably, recycling retired technologies can significantly impact material availability, mitigating the shortages and supply chain disruptions anticipated in the previous sections. It can also reduce the need for long-distance transport of materials, making them available in regions lacking the corresponding natural assets.

Motivated by these factors, we next estimate the minimum recycling rates that would be required for each material to meet the CET projections from IAMs. To accomplish this task, we employ a second optimization model, similar to the one described in the preceding section, where we integrate recycling as an option to increase material supply. We run our model 12 times for each of the 25 IAM scenarios, each considering a different combination of the two market trends, the two material intensity projections, and the three annual production rates for each material. This entails a total of

300 (i.e., 25×12) estimates for each material. Further details about the model are outlined in section 6.3 of the supplementary information.

Results are presented in Fig. 7, where we illustrate the recycling rates required as a percentage of the annual production of each material. If available, current recycling rate are also depicted for comparison. Materials excluded from this figure demonstrate an almost negligible need for recycling. Comparison between existing recycling rates and the median values depicted in Figure 7 underscores the urgent necessity for increasing recycling rates, particularly for lithium (escalating from 1% to 325%), iridium (rising from 17% to 64%), and terbium (elevating from 1% to 12%), but also for silicon, dysprosium, and graphite (all within 0.2%-2.2%). For materials like lithium, this would imply recycling more material than produced annually (i.e., the median recycling required in 2050 equals 325% its annual production rate in the same year). Hence, achieving these numbers would require the annual dismantling of obsolete devices from several years, a strategy that cannot be maintained forever. In addition, the current recovery of precious metals from electronic waste primarily involves smelting and leaching, resulting in prolonged purification processes and adverse environmental impacts.⁵⁴ Moreover, with the exception of copper and manganese, the remaining materials show a probability that the current recycling rate is insufficient and needs to be increased. This underscores the necessity for further research on minerals recycling and additional investments to establish recycling units. Both endeavours require significant time, emphasizing the urgency to commence and prioritize them.

2.3.7 Limitations and uncovered issues

Before concluding the findings, we turn our attention to the main limitations and issues uncovered in this study:

1. The projections of technology capacities, market contributions, and material intensities used in our estimations are all dynamic parameters subject to change over time. This inherent variability introduces uncertainty into the conclusions, which could be mitigated by revisiting estimates as newer data become available.
2. Our estimates for the capacity of each technology that could be deployed based on material availability (section 2.3.5) rely on the assumption of a friction-free market. This assessment could be enhanced by considering the regional availability of each material, the corresponding transportation requirements, socio-economic factors, and environmental constraints to provide a more accurate representation of real-world practicalities.
3. The discovery of new technological designs using alternative materials, material substitution, and recycling practices are factors that can significantly impact material demands in practice. Incorporating these considerations could enhance the accuracy of projections for material demands.
4. Beyond the scope of the technologies evaluated in this study, the demand for other technologies (e.g., electric motors, fuel cells) will also influence material markets. Recognizing and accounting for these broader technological spectrums is essential for a more comprehensive understanding of material market dynamics.
5. Finally, we note that the replacement of obsolete CET facilities results in a minor contribution on material demands in our analysis, owing to the temporal scope we consider. However, these might play an important role from 2050 onwards, the magnitude of which will depend on the lifespan eventually achieved by the different technologies.

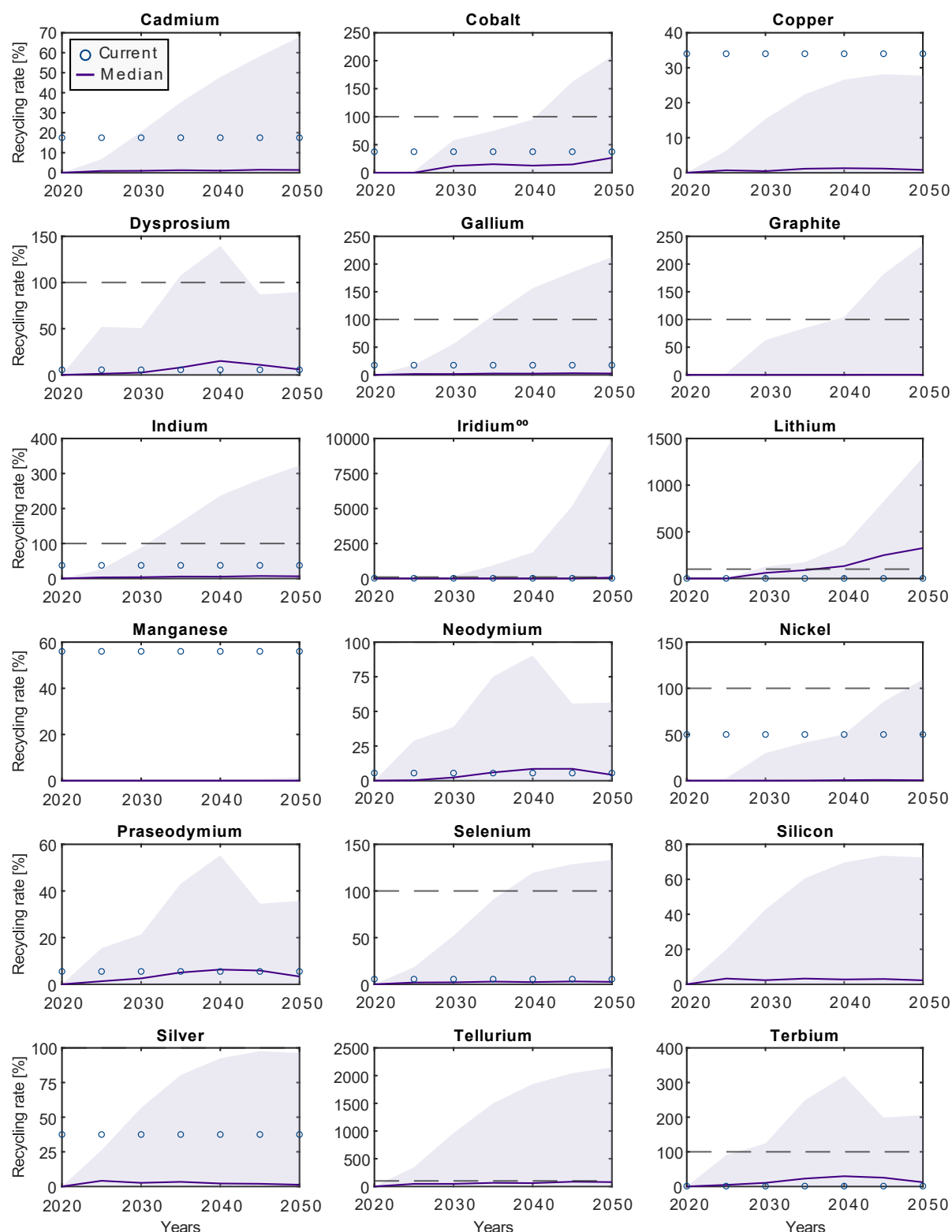


Fig.7 Material recycling rates required to meet IAM capacity projections. The area presents the range resulting by considering 12 sets of results (i.e., three production rates, two market contribution trends, and two material intensity projections) for each of the 25 IAM scenarios. The purple line denotes the median recycling rate required for each material to meet AIM projections. The circles represent the current recycling rates (Table S12, chapter 6). For graphite, silicon, and tellurium current recycling data is not available. Materials not depicted in this figure do not show any need for recycling, based on the scenarios analysed.

2.4 Conclusions

In this contribution, we critically discuss the plausibility of scenarios developed from essential yet imperfect IAMs, in the context of clean energy technologies and the associated critical materials. We base our assessment on 25 scenarios consistent with the Paris Agreement, sourced from eight different IAMs.

We find that IAMs foresee a steep surge in the annual deployment rate of clean energy technologies. Trying to achieve these projections would exert immense pressure on material supply chains over the next three decades, increasing today's demand from clean energy technologies by up to 571 (for selenium) and current production levels by up to 143 (for iridium). This information, omitted from IAM formulations, is evidence of how optimistic their estimates are since it is hard to believe that the required mining, refining, and manufacturing levels can be achieved in less than 30 years.

Also absent from IAMs, we observe that the expected market contribution of the different technology types (e.g., diverse types of PV panels) and the anticipated change in material intensities over time strongly impact material demand trajectories. For instance, assuming a technological change market trend, rare earth elements such as dysprosium, neodymium, and terbium look prone to material shortages, compromising the manufacture of SG-PM-DD wind turbines. This trend would also put elements such as tellurium, lithium, indium, and selenium at risk and, ultimately, might hamper the development of CdTe PV panels and LiS batteries, among others.

In the realm of IAMs, technological investments serve as a pivotal mechanism to decide among various technologies based on their capital and operational costs, but at a much lower resolution regarding technology types. In addition, IAMs predict technology capacities, ignoring materials availability, which is analogous to forecasting bioenergy potentials neglecting the amount of land that can be used for biomass cultivation. Moreover, while IAMs predominantly focus on the cost-effectiveness of technology deployment, it is arguable that consumers or policy choices might not follow economically rational patterns. This delineation in rationality underscores the complexity of IAMs and the necessity for a more comprehensive integration of real-world market frictions and decision-making dynamics to enhance their predictive accuracy and applicability within the broader economic landscape.

Arguably, to do science-based policymaking, the tools providing the pieces of evidence need to be fit for purpose. In this case, IAMs could be improved by integrating bottom-up energy technology models with top-down aggregated economic equilibrium models. Alternatively, tailored constraints in IAMs could be informed based on dedicated models for specific sectors.

As a first step towards more sophisticated efforts, we underscore the profound impact that slight adjustments can exert on the projected capacities of clean energy within IAMs. Specifically, we evaluated the feasibility of achieving the capacity projections from IAMs by employing a bottom-up approach considering material availability constraints and a higher technological resolution. Results underscored significant shortages in the capacity developed annually for batteries (0-11.1 TW) and PV panels (0-1.6 TW), questioning our capacity to achieve the projections envisioned by the ambitious IAMs. Replacing this lack of clean energy with conventional alternatives to provide the same services, we find that the cumulative additional emitted carbon by 2050 would be about 279-530 Gt CO₂-eq, which translates into additional 0.06-0.95°C above the targeted 1.5°C. Material recycling could certainly help in bridging these gaps, yet our estimations suggest that current recycling rates for materials are insufficient and need to be increased. In some cases, like lithium, the required recycling rate exceeds its annual production. Hence, incorporating material availability constraints and technological diversity into IAMs offers an opportunity to enhance their predictive accuracy at the cost of marginal mathematical complexity.

In addition to helping provide better advice to policymakers, this opens new research avenues in other scientific fields. For instance, while our calculations offer a more realistic estimation compared to those obtained solely from IAMs, they remain a dramatic simplification of reality, overlooking market elasticities, other environmental issues such as water consumption and dust spreading of mining activities, land use change, and social aspects like miners and farmers rights, among others. This suggests further refinement and frequent updates as newer data become available to provide realistic and timely projections in an evolving landscape. In conclusion, IAMs require continuous improvements to align their predictions more closely with real-world complexities. This alignment could better reflect the dynamic realities of material availability within the clean energy sector, greatly enhancing the relevance of IAMs in the scientific and political spheres.

Author Contributions

Fateme Rostami: conceptualization, data curation, formal analysis, investigation, methodology, software, validation, visualization, writing – original draft, writing – reviewing and editing. **Piera Patrizio:** conceptualization, data curation, methodology. **Laureano Jimenez:** funding acquisition, reviewing, resources, supervision. **Carlos Pozo:** conceptualization, formal analysis, funding acquisition, investigation, methodology, resources, software, supervision, visualization, writing – reviewing and editing. **Niall Mac Dowell:** conceptualization, formal analysis, methodology, reviewing and editing, supervision, validation.

Conflicts of interest

There are no conflicts to declare.

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2.5 References

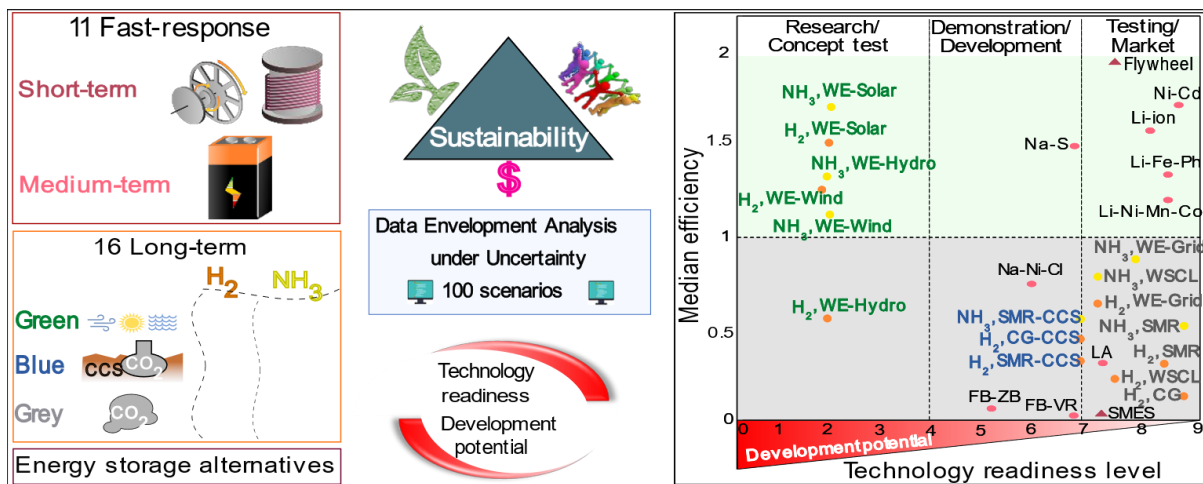
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Chapter 4

Comparative sustainability study of energy storage technologies using data envelopment analysis



Chapter 4

Comparative sustainability study of energy storage technologies using data envelopment analysis

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4.1 Introduction

Electricity is among the cornerstones for most economic activities and human living conditions [1]. Electricity systems link generators with consumers through transmission and distribution grids. Traditionally, secure electricity systems were designed based on key technical parameters such as stability, flexibility, resilience, adequacy, and robustness [2]. This, among other factors, led to the widespread deployment of dispatchable technologies such as those based on fossil fuels or nuclear energy [3]. More recently, environmental concerns have pushed the adoption of various clean and renewable electricity production technologies [4]. However, while conventional generation technologies can easily adapt to the inherent fluctuating demand, renewable sources like solar and wind are intermittent, unpredictable, and uncertain, therefore compromising the system capacity to match supply with demand [5].

One of the most promising solutions to rapidly meet the electricity demand when the supply comes from non-dispatchable sources is energy storage [6, 7]. Electricity storage technologies convert the electricity to storable forms, store it, and reconvert it to be released in the network when needed [8]. Electricity storage can improve the electricity grid's reliability, efficiency, safety, security, and stability [9, 10] while bringing down the cost of electricity supply [11] through the reduction of the number and duration of costly electrical interruptions [12]. In a context where global power generation with renewable technologies is expected to rise from 25% in 2020 to 86% in 2050 [11], it is not surprising that energy storage is deemed key to achieving the energy sector's decarbonization [13].

Energy storage technologies can be classified according to their functions, the storage duration, and the form of stored energy [14], with no single technology performing well in all situations [9]. For instance, large-scale mechanical energy storage options can shift a large volume of electricity from

one time to another, while batteries are rapidly responding to a signal [11]. Thus, a myriad of energy storage technologies with different characteristics are and will be needed to provide service in different applications [14].

To facilitate the development and deployment of energy storage technologies, these must satisfy economic, environmental, and technical targets [5]. For instance, the European Association for Storage of Energy, in their 2017 roadmap, suggested that storage technologies should aim to achieve a levelized cost of stored energy lower than the levelized cost of energy appointed to other flexibility options such as grid upgrades or flexible generators [15]. Meanwhile, the 2030-plan for stationary energy storage systems aims at the cost of ≤ 0.05 €/kWh, cycle, in addition to achieving 10000 cycles durability and 20 years lifetime [16]. Further cost reductions besides technical and/or environmental improvements could make these technologies even more attractive. Therefore, gathering quantified and updated information about energy storage technologies is one of the first tasks needed to pave the way for their development and widespread application.

Several works have compared energy storage technologies based only on economic, technical [17], or environmental aspects [18]. For instance, Koochi-Fayegh et al. compared the performance of fast-response storage technologies in frequency regulation applications based on their energy and power density, cycle efficiency, lifetime, and capital costs [19]. A review concerning the life cycle cost of energy storage technologies was presented by Zakeri and Syri [20], including elements such as capital, operational, maintenance, and replacement costs. They concluded that the power conversion system and the energy storage unit section strongly affect an energy storage system's technical and economic performance [20].

On the other hand, some works shifted the focus from economic and technical considerations to the environmental implications of storage technologies. In this context, a cradle-to-gate life cycle assessment (LCA) study of vanadium redox flow batteries and zinc-cerium batteries illustrated that the electrolyte production process contributes significantly to most impact categories [21]. A similar conclusion was reported for lead-acid, lithium-manganese, and lithium-iron-phosphate batteries [22]. Very few studies considered environmental aspects and other sustainability dimensions simultaneously, and in case they did, it was limited to only one or a few storage technologies. Stougie et al. employed a multi-dimensional life cycle assessment for analyzing the sustainability of five different energy storage units considering economic and environmental criteria, in addition to each technology's total cumulative exergy loss [23]. Another multi-objective optimization was reported by Li et al. to select energy storage systems. They used economic and environmental objectives and technical constraints, finding flow batteries and hydrogen energy storage as the optimal solutions for emerging distributed energy systems [24]. Kapila et al. compared energy, life cycle greenhouse gas emissions, and costs for large-scale mechanical energy storage systems. Their results revealed that the unit's energy consumption (i.e., amount and energy source) is more relevant than the construction material considering greenhouse gas emissions from a life-cycle perspective [25].

Going beyond previous research, this chapter aims to provide a comprehensive assessment of a wide range of energy storage technologies (11 fast-response and 16 long-term storage options) considering a total of six key performance indicators that allow covering the three sustainability dimensions concurrently (i.e., economic, environmental, and social perspectives). To ensure a fair comparison, technologies are first classified into two clusters according to their response time. In addition, we analyze for the first time the sustainability performance of ammonia as an energy storage material. We include the operation phase of storage technologies within the scope of our work, thus advancing previous research in both depth and breadth.

Comparing options in terms of multiple sustainability indicators is a challenging task calling for multicriteria decision-making methods. Among available tools, we resort to Data Envelopment Analysis (DEA) [26] because it can combine multiple indicators into a single score, avoiding defining subjective weights between the indicators. The uncertainty associated with the data used for the analysis is considered to draw robust and reliable conclusions.

In the past, DEA has been widely used to investigate and compare engineering systems for the energy sector, such as nuclear energy [27], thermal powerplants [28], power industries [29], energy-consuming equipment [30], renewable energy production [31-37], and the electricity mix in European countries [26]. Nevertheless, to the best of the authors' knowledge, there is only one previous work on applying DEA to benchmark energy storage technologies. It compares pumped hydro storage, compressed air energy storage, lead-acid battery, and lithium-ion battery using sustainability indicators and employing DEA, reporting lithium-ion battery as the most efficient case [38].

The analysis carried out first-grade technologies within each cluster as either efficient or inefficient, providing evidence to support policies promoting the most appealing technologies to underpin the sustainability transition. For inefficient technologies, quantitative guidelines regarding directions and targets for improvement are provided. This valuable information will be key for technology developers to push their designs to the frontier of the best-performing options available in the market.

As will be further detailed later in the manuscript, the results obtained suggest that flywheel, nickel-cadmium, lithium-ion, and sodium-sulfur batteries are the preferred options as the fast-response technologies, while green ammonia from water electrolysis powered by solar energy is ranked first between long-term storage options. Other efficient options for the later cluster are green hydrogen from solar and wind.

The remaining of this chapter is structured as follows. The methodology applied for the multicriteria assessment of energy storage technologies is described in section 4.2, while the results are presented and discussed in section 4.3. Finally, the conclusions drawn on how these results can be used for effective policymaking are presented in section 4.4.

4.2 Methodological approach

In this contribution, we use DEA to compare the performance of energy storage technologies through the lens of sustainability (i.e., economic, environmental, and social perspectives). DEA is a linear programming method that allows measuring the relative efficiency of a set of homogenous entities (called Decision-Making Units, DMUs) in transforming one or several input(s) into one or several output(s) [39]. Producing more outputs using fewer inputs is the general criterion for higher efficiency (see Eq.1 [40]), yet if some outputs are undesirable (e.g., carbon emissions), producing lower amounts of them is desired [41].

$$\text{efficiency} = \frac{\text{weighted sum of outputs}}{\text{weighted sum of inputs}} \quad (1)$$

In the context of this contribution, we model energy storage technologies as DMUs consuming m inputs and producing s_1 desired outputs and s_2 undesired outputs. The value of inputs and outputs for each DMU are obtained from different sustainability indicators, which are classified in these three categories depending on whether they are resources “consumed” by the technology (i.e., inputs, e.g., water), beneficial outputs from the process (i.e., desirable outputs, e.g., the creation of new job opportunities) or outputs that are not desired (i.e., undesirable outputs, e.g., polluting emissions to

air). The DMUs considered are presented in section 4.2.1, while details on inputs and outputs are provided in section 4.2.2.

With input and output values at hand, an efficiency score will be obtained for every DMU by solving a DEA model for each of them. The model will return an efficiency score of 1 if the DMU is efficient, that is, if and only if there is no other DMU with lower or equal levels of inputs and undesirable outputs while simultaneously achieving greater or equal output levels.

Note that, in DEA, the efficiency score is given by a weighted (i.e., linear) combination of indicators, which is a common approach also used in other multicriteria decision-making methods and algorithms and in environmental impact metrics such as the EcoIndicator99 [42]. This approach is not always underpinned by a physical interpretation but is still useful for estimating technological options' relative ranking. In addition, the use of DEA avoids the need to define these weights in advance, thus preventing a subjective bias in the assessment of the different technological options. This is equivalent to implicitly assuming that all the inputs, desired outputs, and undesired outputs are equally important. The case where a higher weight is assigned to environmental indicators is later analysed in Appendix A.1. Specifically, we use a unit-invariant model that makes it possible to combine different indicators without their units altering the final efficiency score obtained [43]. Further, the monetized analysis, presented in Appendix A.2, translates all the indicators to their monetary values before combining them.

4.2.1 DMU modelling

Storage technologies can be classified based on the duration and frequency of power supply, and each class has its particular characteristics and applications [44]. To prevent unfair comparisons across classes, technologies are grouped into fast-response (including short- and medium-term storage technologies) and long-term (Figure 1), considering their response time. H_2 produced using coal gasification is considered in our study, while NH_3 produced from such H_2 is discarded due to the lack of reliable data. Except for it, all the other considered alternatives are the same for H_2 and NH_3 .

Fast-response technologies show response times ranging between a few seconds to a few hours, reason why these technologies are typically used for voltage stabilization, frequency control, peak shaving, load leveling, and daily storage. They should be able to offer several cycles during a day and, therefore, the number of cycles during their lifetime and their power and energy density are very relevant aspects [2]. This cluster includes two short- and nine medium-term technologies. Flywheel and super magnetic energy storage (SMES) are short-term storage technologies, while vanadium redox flow battery (FB-VR), zinc-bromine flow battery (FB-ZB), lead-acid (LA), lithium-ion, lithium-Ferro-phosphate (Li-Fe-Ph), lithium-nickel-manganese-cobalt (Li-Ni-Mn-Co), sodium-nickel-chloride (Na-Ni-Cl), sodium-sulfide (Na-S), and nickel-cadmium (Ni-Cd) batteries are the options considered as medium-term energy storage technologies. There are various types of lithium-ion, redox flow, and sodium batteries with different battery characteristics regarding the materials used for the electrolytes and electrodes. For instance, a graphite-based anode, a cathode made using a lithium metal oxide (e.g. Li-Fe-Ph, Li-Ni-Mn-Co, etc.), and an electrolyte are the main components of a lithium-ion battery [9]. Significant research efforts are taking place to identify the material combination leading to the best battery characteristics in each case.

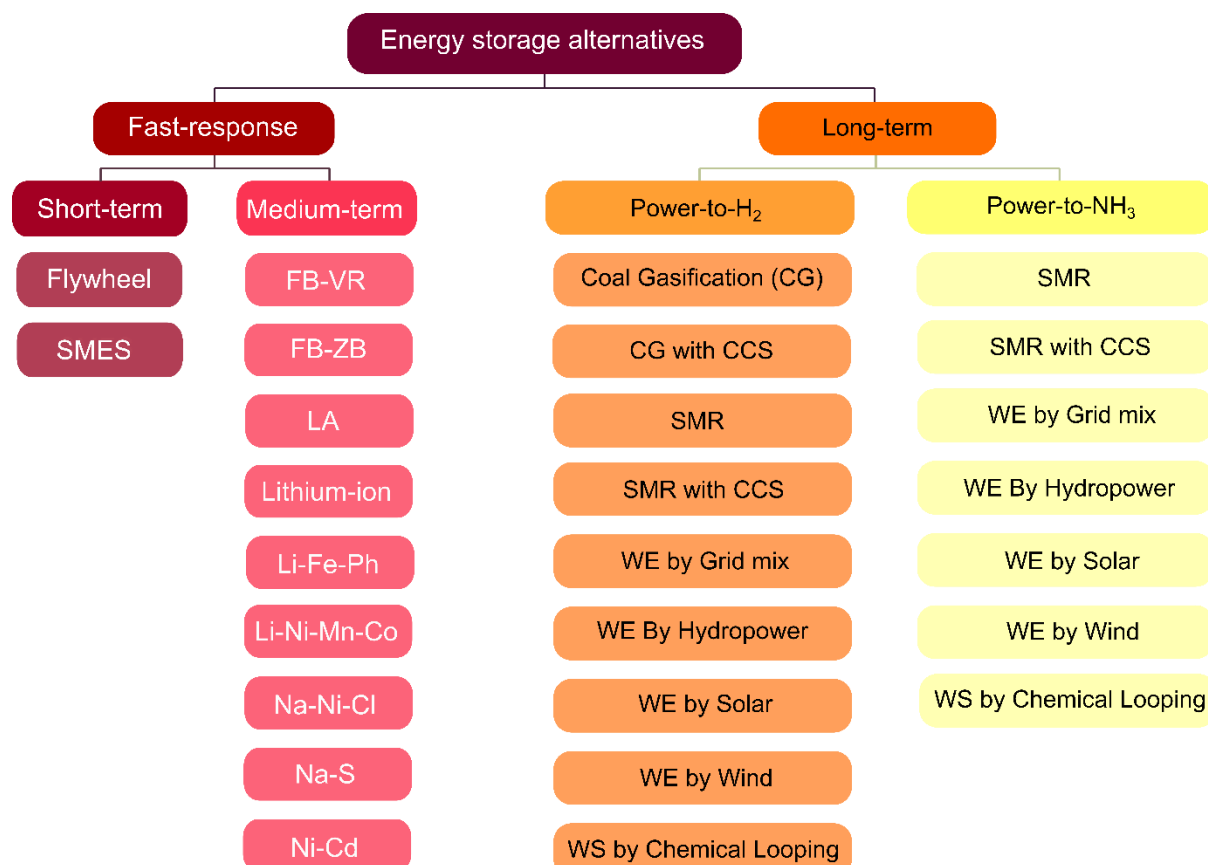


Figure 1. Classification of the energy storage technologies (or DMUs under the concept of DEA) considered. SMES: Super Magnetic Energy Storage, FB: Flow Battery, VR: Vanadium Redox, ZB: Zinc-Bromine, LA: Lead-Acid, Li-Fe-Ph: Lithium-Ferro-Phosphate, Li-Ni-Mn-Co: Lithium-Nickel-Manganese-Cobalt, Na-Ni-Cl: Sodium-Nickel-Chloride, Na-S: Sodium-Sulfur, Ni-Cd: Nickel-Cadmium, CCS: Carbon Capture and Storage, SMR: Steam Methane Reforming, WE: Water Electrolysis, WS: Water Splitting

All these DMUs are entirely based on data found in the literature (see supplementary information, section 8.2). Pumped hydro storage and compressed air energy storage are two medium-term storage technologies not considered in this study since they are large-scale storage options and including them in the analysis could lead to unfair comparison.

On the other hand, long-term storage alternatives are usually used for dark-calm control during the no sun-no wind weeks in cold regions, prioritizing a low self-discharge rate. Since they have a very high energy density and acceptable reliability for long-term applications, they have strategic importance. We consider a total of 16 long-term energy storage alternatives (i.e., DMUs under the concept of DEA) for long-term storage, which result from combining two energy carriers (namely H_2 and NH_3) with the different production processes (e.g., hydrogen obtained from steam methane reforming with carbon capture or without it). Data for these DMUs is not readily available in the literature, so we modeled them as follows.

Hydrogen can be obtained using a variety of fossil fuels and renewable energy sources, which will result, in turn, in multiple DMUs (e.g., H_2 from coal gasification, H_2 from water electrolysis using solar energy, etc.). Renewable (or green) hydrogen is produced from water electrolysis powered by renewable energy sources. Blue hydrogen refers to the hydrogen produced using fossil fuels and a carbon capture and storage (CCS) unit used to capture carbon emissions [45]. The carbon captured

during this process can be used in applications like enhanced oil recovery [46] or valuable chemical production [47]. Hydrogen produced using fossil fuels without capturing the associated carbon emissions is called grey hydrogen (Figure 2) [45]. The hydrogen produced can be used as a standalone energy storage alternative or as raw material for ammonia production. For the former, three conversion steps are required. First, hydrogen is compressed using a reciprocating compressor with ~90% efficiency. Then, the compressed gas is stored with 98% efficiency. Finally, hydrogen can be reconverted back to electricity using different alternatives: an open cycle gas turbine with 35% efficiency, a combined cycle process with 60% electricity generation efficiency [48], or a fuel cell with about 20-50% efficiency [49]. Intending to capture all these nuances, we assume the widest range (i.e., 20-60% conversion efficiency) and use its average as the nominal case; this results in 40% efficiency for this final step. Therefore, the overall conversion efficiency of 35% is obtained for hydrogen (i.e., 90%98%40%).

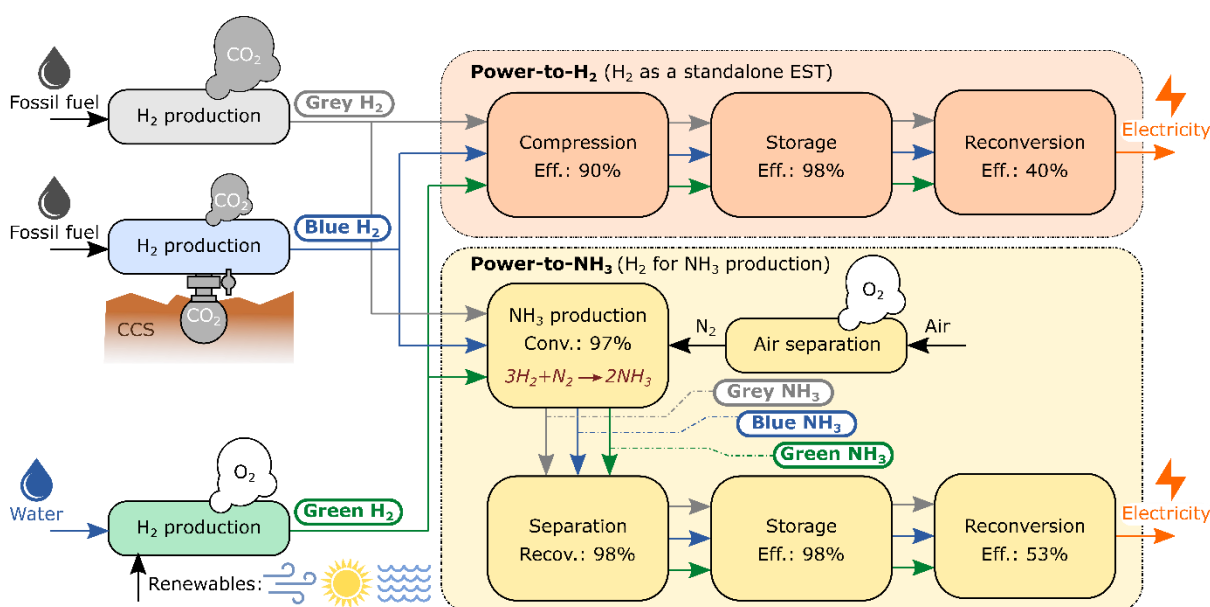


Figure 2. Flow diagrams for H₂ and NH₃ production. Grey H₂/NH₃: H₂ or NH₃ produced using fossil fuels, Blue H₂/NH₃: H₂ or NH₃ produced using fossil fuels and the emitted carbon captured by CCS, Green H₂/NH₃: H₂ or NH₃ produced using renewable energy sources.

In case hydrogen is used as a raw material to produce ammonia through the Haber-Bosch process [50], several DMUs with similar color codes as for hydrogen (i.e., blue, green, and grey ammonia) will result, depending on the energy source and hydrogen production process. Converting hydrogen to ammonia requires an additional air separation unit to obtain N₂ from the air, in addition to the other process units included in a typical Haber-Bosch process, such as separation equipment [51]. Based on experimental studies, 22 kg/s NH₃ are produced using 4 kg/s H₂ [50]. According to the reaction's stoichiometry, 22.67 kg ammonia can be achieved using 4 kg H₂. Therefore, we consider a conversion of 97% (22/22.67) for this step. This value is consistent with other studies reporting conversions above >90% [52] or even 98% [53]. Ammonia is then separated from the remaining reactants with a recovery of 97% (>95% [52]). Ammonia storage efficiency is the same as hydrogen, while different options arise for converting ammonia into electricity. For instance, one can use fuel cells at efficiencies varying

between 37% [54] and 54% [55], while a solid oxide fuel cell-gas turbine combined cycle of ammonia can achieve efficiencies of 68% [56]. For the sake of simplicity, we consider the average of the widest range based on the reported data (i.e., 37%-68%), which is 53% for the efficiency of the ammonia reconversion step. Therefore, the overall efficiency of storing and transforming ammonia to electricity is about 52% (i.e., 98%*53%).

Independent DEAs will be carried for each cluster, where different inputs and outputs will also be assessed (i.e., gravimetric energy density will be assessed for fast-response technologies, but not for long-term energy storage alternatives). The specific list of inputs and outputs (desired and undesired) included in each analysis is described in detail in the next section. Note that some of these technologies can be used for different purposes (e.g., flywheel for power quality control and distributed generation support), potentially achieving different performance (i.e., indicator values) in each case [20]. For simplicity, we assume only a certain value based on their more common application (e.g., power quality control in the case of flywheels). The explicit consideration of the uncertainty associated with the data is expected to cover all the potential inaccuracies stemming from the different modelling choices and assumptions, leading to robust conclusions (see section 4.2.4).

4.2.2 Inputs and outputs

A total of six performance indicators are selected to cover the three sustainability dimensions. These indicators are classified as inputs and desired or undesired outputs of the DMUs in each cluster, as reported in Figure 3. The only difference between the indicators considered in the two clusters is that the gravimetric energy density (GJ/kg) is used for fast-response technologies and not for the long-term. The reason is that size is a crucial factor for fast-response technologies, which are many times used for portable applications [7], while it is not so determinant for long-term options.

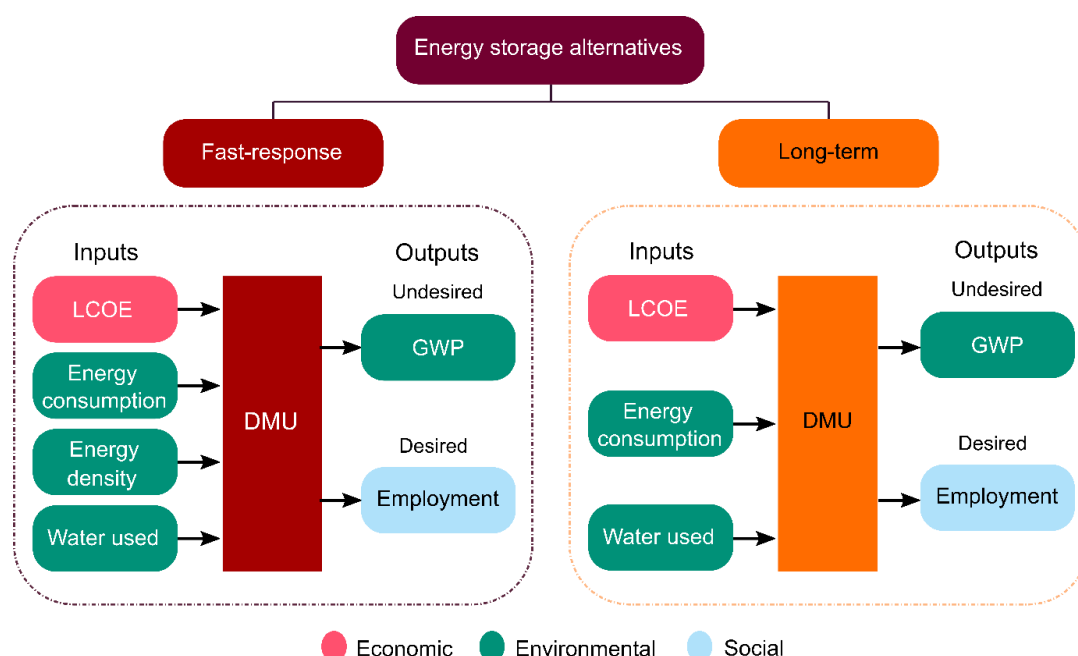


Figure 3. Diagram of DMUs for each of the clusters: fast-response and long-term storage systems. LCOE: Levelized cost of energy. GWP: Global warming potential. In practice, the inverse of energy density (expressed in kg/GJ) is used instead of the normal indicator to align with the input concept of “the less, the better”.

Data for fast-response technologies are mainly gathered from literature, using the average value among available data where more than one reference is available for a certain indicator. Data gaps are filled based on average values of similar technologies (e.g., the LCOE reported for Li-ion is used for Li-Fe-Ph). All the indicators in this cluster are downscaled to unitary values through their division by the amount of energy delivered during the lifetime of technology, e.g., they are expressed per GJ of energy delivered (see supplementary information, section 8.1.1 for details on the calculation of the delivered energy for fast-response technologies). Note that these values indirectly consider factors such as dedicated lifespans, number of cycles, energy capacities, round-trip efficiency, and depth of discharge.

For long-term storage alternatives, hydrogen data are collected from the relevant literature, with missing data replaced by the average values of similar options (e.g., water consumption for hydrogen production using coal gasification is considered the same as steam methane reformation (SMR), since both are based on fossil fuels process). Likewise, ammonia data are collected from the relevant literature. Missing data for ammonia based DMUs is sometimes estimated from hydrogen (e.g., cost of ammonia = cost of hydrogen + their typical cost difference). Data can be estimated per kg of NH_3 considering the reaction stoichiometry and the efficiency of the different conversion steps. In addition, data of a typical carbon-capturing unit is used to estimate the energy consumption of hydrogen and ammonia production with CCS. In this cluster, indicators are divided by the amount of energy delivered by 1 kg gas, as estimated using the gravimetric energy density of the gas and the efficiency of the gas-to-power processes (i.e., compression, separation, storage, and reconversion). Details are provided in the supplementary information, section 8.1.2. These values are implicitly affected by indirect factors such as the lifespan of the facilities involved in these processes (e.g., 10000 working hours equivalent to five years lifespan for the equipment used in hydrogen production based on water electrolysis using wind energy [57]).

All the data collected, their references, and the assumptions considered to estimate the missing data are reported in detail in section 8.2 of supplementary information. The following subsections briefly explain the indicators considered (further details provided in the supplementary information, section 8.2), while the final values used in our investigations are reported in Tables 1-2.

4.2.2.1 Economic indicators

The Levelized cost of energy (LCOE) is used here to capture the economic dimension, similar to other works [58]. Typically, the LCOE considers all relevant initial, variable, and end-of-life costs [59]. We source the LCOE directly from the literature for fast-response technologies, although values used neglect end-of-life costs due to the unavailability of data [20]. In the case of long-term storage options, the LCOE is obtained from the cost of producing 1 kg of gas using each of the production routes considered.

4.2.2.2 Environmental indicators

Four environmental indicators (three in the case of the long-term cluster) are considered in the analysis. Acknowledging all impact categories are important, we focus on energy consumption, energy density, water consumption, and global warming potential (GWP) since data on other indicators such as ecotoxicity or human health were not found for all the technologies considered. Regarding their use in DEA, environmental indicators are classified as follows: energy consumption, the inverse value of energy density, and water use are considered inputs, while GWP is deemed an undesired output.

Note that energy consumption is not an impact *per se*, yet it is included here to capture other potential direct and indirect impacts associated with generating any energy carrier. Energy is required to manufacture storage units, operate them (in some cases), and is also fed for storage; therefore, the total energy consumption aggregates these three contributions.

For fast-response storage technologies, the energy consumption for manufacturing is retrieved mainly from techno-economic studies of the different technologies, while their operational energy is considered zero, and the energy fed for storage is calculated based on typical usage as reported in the supplementary information, section 8.2. For long-term storage alternatives, the energy required to produce 1 kg gas is used as their total energy consumption.

The energy density is also used as an environmental indicator as a higher gravimetric density will result in lower material use and subsequent environmental impacts [60]. Since all the indicators are expressed per GJ, its reciprocal value (1/energy density) is used.

Water use stems mainly from the manufacturing stage for fast-response technologies and is collected from techno-environmental studies. The operational water consumed to produce 1kg of gas is used for long-term energy storage options.

The global warming potential (i.e., CO₂-eq emissions) is quantified using Life Cycle Assessment (LCA), a standardized tool for evaluating environmental impacts incurred during all life stages of a product [22, 61]. The CO₂-eq emissions for fast-response technologies are usually provided per capacity of the storage unit. Likewise, for long-term storage, the CO₂-eq emissions are related to the production of 1 kg gas. Additional calculations necessary to obtain the global warming potential per GJ of delivered energy are reported in section 8.2 of the supplementary information.

4.2.2.3 Social indicators

Employment, energy security, health, public acceptability, and safety are the most widely used indicators of the energy sector [58]. Despite this, only direct employment is used in this study as data for the remaining indicators were missing for all or most technologies [62].

In the context of DEA, labor could arguably be considered either as a desired output with positive social effects or as an input for the construction or operation tasks. Without loss of generality, we here adopt the former approach because the energy sector is a promising source of new job opportunities worldwide.

4.2.2.4 Summary

The final indicator values used for each DMU in the corresponding DEAs are presented in Tables 1-2.

Table 1. Input and output indicators for fast-response technologies. LCOE: Levelized cost of energy, GWP: Global warming potential. FTEJ: Full Time Equivalent Jobs.

Storage options	Inputs				Undesired output	Desired output
	LCOE (€)	Energy (GJ)	1/Energy density (kg/GJ)	Water (m ³)	GWP (CO ₂ -eq emissions)	Employ (FTEJ)
Flywheels	163.89	1.39	5291.0	1.8	44.2	2.68·10 ⁻⁴
SMES	102.50	1.74	101010.1	1.2	115.5	3.35·10 ⁻⁴
FB-VR	98.61	1.40	12345.7	2.9·10 ⁻³	8.9	1.72·10 ⁻⁴
FB-ZB	59.44	1.58	4830.9	2.9·10 ⁻³	12.1	2.11·10 ⁻⁴
LA	90.28	1.64	6944.4	2.0·10 ⁻³	20.0	9.14·10 ⁻⁴
Li-ion	172.92	1.40	1111.1	0.5·10 ⁻³	3.0	13.19·10 ⁻⁴
Li-Fe-Ph	172.92	1.54	1111.1	0.5·10 ⁻³	14.3	14.06·10 ⁻⁴
Li-Ni-Mn-Co	172.92	1.40	1111.1	0.5·10 ⁻³	11.8	13.15·10 ⁻⁴
Na-Ni-Cl	97.22	1.45	2314.8	4.8·10 ⁻³	18.2	9.80·10 ⁻⁴
Na-S	68.06	1.41	1388.9	1.8·10 ⁻³	0.2	3.06·10 ⁻⁴
Ni-Cd	117.36	1.51	1763.7	0.2·10 ⁻³	2.8	22.86·10 ⁻⁴
Average	119.65	1.50	12656.62	276.3·10 ⁻³	22.8	8.65·10 ⁻⁴
Std. deviation	43.43	0.12	29507.67	626.8·10 ⁻³	33.0	6.8·10 ⁻⁴

Table 2. Input and output indicators for long-term energy storage alternatives. LCOE: Levelized cost of energy, GWP: Global warming potential. FTEJ: Full Time Equivalent Jobs.

Storage options	Inputs			Undesired outputs	Desired output
	LCOE (€)	Energy (GJ)	Water (m ³)	GWP (CO ₂ -eq emissions)	Employ (FTEJ)
H ₂ , CG	124.82	5.52	2.74	2392.7	1.12·10 ⁻³
H ₂ , CG-CCS	261.81	9.72	2.74	103.2	2.34·10 ⁻³
H ₂ , SMR	139.79	5.52	2.74	1611.2	1.25·10 ⁻³
H ₂ , SMR-CCS	234.25	8.27	2.74	110.2	2.10·10 ⁻³
H ₂ , WE-Grid mix	650.67	5.52	2.74	4170.0	5.82·10 ⁻³
H ₂ , WE-Hydropower	918.86	5.52	1.31	175.0	8.22·10 ⁻³
H ₂ , WE-Solar	1949.45	5.52	1.31	699.9	17.44·10 ⁻³
H ₂ , WE-Wind	1080.48	5.52	1.31	87.5	9.67·10 ⁻³
H ₂ , WSCL	134.72	5.52	4.61	210.0	1.20·10 ⁻³
NH ₃ , SMR	279.64	5.42	0.46	554.15	2.50·10 ⁻³
NH ₃ , SMR-CCS	301.57	5.80	0.46	346.35	2.70·10 ⁻³
NH ₃ , WE-Grid mix	635.02	5.42	0.46	512.61	5.67·10 ⁻³
NH ₃ , WE-Hydropower	821.84	5.42	0.29	69.45	7.36·10 ⁻³
NH ₃ , WE-Solar	1539.72	5.42	0.30	233.40	13.77·10 ⁻³
NH ₃ , WE-Wind	934.56	5.42	0.30	90.65	8.36·10 ⁻³
NH ₃ , WSCL	275.98	5.42	0.30	68.27	2.50·10 ⁻³
Average	642.70	5.93	1.55	714.65	5.75·10 ⁻³
Std. deviation	539.83	1.23	1.33	1122.36	4.83·10 ⁻³

4.3 Data uncertainty

As already discussed, the value of specific indicators may vary within a certain range due to simplifications and the diversity of alternatives available for some storage options, sometimes affected by regional differences. We characterize the uncertainty associated with each input and output using uncertainty distributions to consider this variability and obtain more robust conclusions. This implicitly assumes that the propagation of uncertainties associated with the individual factors needed to compute a particular indicator falls within the uncertainty considered for the final value of the indicator itself.

Specifically, three types of distributions are used as follows. For parameters where we could find only one value in the literature (i.e., no range of values is available), uncertainty is characterized based on a uniform distribution with support of $\pm 10\%$ of the nominal parameter. This is the case of water use and feed energy during the lifetime of technologies (see Tables B3, B6, and B7 of chapter 8).

For parameters with a range of values available, we select triangular distributions whose limits correspond to the lowest and highest data reported in the literature for the indicator and its mode to the nominal value (i.e., the average among all values in the literature). The indicators belonging to this group are LCOE, energy consumption, energy density, and employment. Note that for each of these indicators, there are a few DMUs for which we have only a single value rather than a range for them. For these cases, $\pm 10\%$ of the nominal parameter is used to estimate a range following a triangular distribution.

Uncertainties on GWP are characterized following the guidelines from the Ecoinvent database [63]. According to this, each life cycle inventory entry (e.g., methane emissions, carbon dioxide emissions, etc.) used to compute the final life cycle impact (e.g., global warming potential) is assumed to follow an individual lognormal distribution whose uncertainty is characterized based on the so-called Pedigree Matrix [63]. This matrix assigns scores to different data quality categories for each dataset, which are later translated into the corresponding standard deviation (σ). These categories are reliability, completeness, temporal correlation, geographical correlation, and future technical correlation [64].

For simplicity, we assume that the standard deviation of the life cycle impact can be characterized based only on the most significant stressor among life cycle entries (i.e., CO₂ emission in the case of the GWP). This simplification, previously used elsewhere [65], avoids characterizing uncertainty distributions for hundreds of life cycle entries that would contribute very little to the variability in the final impact. Further details on this approach are provided in the supplementary information, section 8.3.

After characterizing all the uncertain distributions for the different parameters, these distributions are discretized using Monte Carlo sampling to generate 100 independent scenarios for each indicator. Finally, a DEA model is solved for each scenario and DMU, following the approach in Ewertowska et al. [40]. It results in 100 different efficiency scores for each DMU (one for each scenario), which will be reported in results as error bars over efficiency scores. The next section provides the details on the DEA model used.

4.4 DEA model

With the values of the different indicators, we can finally use DEA to estimate the efficiency score of each DMU in each scenario. Without loss of generality, the non-oriented undesired output slack-based

model (Un-Outputs SBM) is used in this study (M1, where variables are represented in italics, while parameters appear in normal font) [66].

$$\begin{aligned}
 \tau^* = \min t - \frac{1}{m} \sum_{i=1}^m \frac{S_i^-}{x_{io}} \\
 s. t. \quad 1 = t + \frac{1}{s_1 + s_2} \left(\sum_{r=1}^{s_1} \frac{S_r^g}{y_{ro}^g} + \sum_{r=1}^{s_2} \frac{S_r^b}{y_{ro}^b} \right) \\
 x_0 t = X\Lambda + S^- \\
 y_0^g t = Y^g \Lambda - S^g \\
 y_0^b t = Y^b \Lambda + S^b \\
 S^- \geq 0, \quad S^g \geq 0, \quad S^b \geq 0, \quad \Lambda \geq 0, \quad t > 0.
 \end{aligned} \tag{M1}$$

Here, T^* is the efficiency score of DMU o under evaluation, with the $*$ superscript denoting the optimal value of the variable, that is, the value the variable takes in the optimal solution to the corresponding problem. Variable t is the Charnes-Cooper linear transformation coefficient, necessary to transform the original nonlinear undesired output SBM model into a linear model like M1 (see Li et al. for more details [66]). Also, m , s_1 , and s_2 stand for the number of the inputs, the number of desired outputs, and the number of undesired outputs, respectively. In all cases, subscript i refers to inputs, while subscript r refers to outputs. Variables S_i^- , S_r^g , and S_r^b correspond to the slacks in inputs, desirable (good), and undesirable (bad) outputs. In this model, slack variables quantify the distance from each DMU to the efficient frontier. This will be further discussed in the next paragraph. Similarly, x_{io} , y_{ro}^g , and y_{ro}^b refer to the input, the desired output, and the undesired output of DMU o , respectively. X is the matrix of inputs ($X = [x_1, x_2, \dots, x_n]$), while Y^g and Y^b are the analogous matrices for desired ($Y^g = [y_1^g, y_2^g, \dots, y_n^g]$) and undesired outputs ($Y^b = [y_1^b, y_2^b, \dots, y_n^b]$). Finally, Λ reports the weights with which efficient DMUs are combined to constitute the virtual DMU of the DMU assessed. Therefore, elements of Λ with non-zero values correspond to efficient DMUs belonging to the reference set of the DMU assessed. The concept of virtual DMU is further explained in the next paragraph.

According to model M1, a DMU is efficient ($T^*=1$) when all the slack variables are zero for all the inputs and outputs ($S_i^- = 0$, $S_r^g = 0$, $S_r^b = 0$, $\forall i, r$). Efficient DMUs are linearly combined to form the so-called efficient frontier. Conversely, if $T^* < 1$, the DMU is inefficient, and at least one of the slacks (S_i^- , S_r^g , S_r^b) has a strictly positive value. In this case, the exact efficiency score (T^*) depends on the distance to a reference point on the frontier. The reference point is constructed by combining the efficient DMUs that are closer to the inefficient DMU under evaluation. Therefore, the reference point presents an efficient-equivalent version of the inefficient DMU assessed; this point is the so-called virtual DMU. Slack variables provide the distance from the inefficient DMU to its virtual DMU. SBM models are non-radial in the sense that they handle input(s) and output(s) without imposing proportional changes for them [67] (i.e., slacks can freely take any value independently from each other). Note that slack values can guide improvement efforts (i.e., the required decrease in inputs and undesired outputs and the required increase in the desired outputs). For more clarification, see Figure 4 of Zurano-Cervelló et al. [26].

Model M1 assumes that the ratio of outputs to inputs does not depend on the inputs' level. This assumption is known as constant returns-to-scale (CRS) in DEA literature [26]. The use of CRS is consistent with the use of normalized data (i.e., per GJ), as explained in section 4.2.2.

One well-known limitation of DEA models is that efficient DMUs cannot be further discriminated, thus preventing the obtention of a ranking that might help decision-making purposes [68]. To overcome this, a super-efficiency model that allows the efficiency score to be higher than one is used for efficient DMUs [41]. In a super-efficiency model, the DMU to be evaluated is removed from the set of candidate DMUs that can form the efficient frontier, thus, measuring the distance from this DMU to the frontier created with the remaining ones [68, 69]. The undesired output slack-based super-efficiency DEA model (M2) is selected in this study. The mathematical formulation for the fractional form of this model is as follows, although we use the linear form in our investigations. Additional details on the model and how to transform it to a linear-equivalent version can be found elsewhere [66, 70, 71].

$$\begin{aligned} \delta^* = \min & \frac{1 + \frac{1}{m} \sum_{i=1}^m \frac{S_i}{x_{io}}}{1 - \frac{1}{s_1 + s_2} \left(\sum_{r=1}^{s_1} \frac{S_r^g}{y_{ro}^g} + \sum_{r=1}^{s_2} \frac{S_r^b}{y_{ro}^b} \right)} \quad (M2) \\ \text{s. t.} \quad & x_o \geq \sum_{j=1, \neq 0}^n \lambda_j x_j - S \\ & y_o^g \leq \sum_{j=1, \neq 0}^n \lambda_j y_j^g + S^g \\ & y_o^b \geq \sum_{j=1, \neq 0}^n \lambda_j y_j^b - S^b \\ & 1 - \frac{1}{s_1 + s_2} \left(\sum_{r=1}^{s_1} \frac{S_r^g}{y_{ro}^g} + \sum_{r=1}^{s_2} \frac{S_r^b}{y_{ro}^b} \right) \geq \varepsilon \\ & \lambda, S, S^g, S^b \geq 0 \end{aligned}$$

Here, δ^* is the super efficiency score of DMU o under evaluation, with the * superscript denoting the value the variable takes in the optimal solution to the corresponding problem (i.e., the optimal value of the variable). Note that, since this model is used to rank the efficient DMUs, the super efficiency score is always greater than or equal to one ($\delta^* \geq 1$). The highest value of δ^* corresponds to the first ranked DMU among those under evaluation. Also, λ is the intensity vector that reports the weights of efficient DMUs in constructing the corresponding virtual DMU, ε is the non-Archimedean infinitely small value that forces the denominator to be positive even after the growth of undesirable output(s). All other symbols are the same as in M1 [70]. Note that, in this model, the slack values can be understood as a safe margin of changes for input(s) and output(s) in the sense that the DMU assessed can afford worsening its performance by these quantities while remaining efficient. Therefore, slacks are proportional to the stability level of the efficient condition of the DMU (i.e., the higher the super-efficiency slacks, the more likely it is the DMU will remain efficient). Therefore, safe margins hint at sustainability indicators that the efficient technology relies on to be deemed efficient. In addition, these margins provide a safe room for technology development, quantifying affordable downgrades in key performance indicators that may arise due to the enhancement of other features of the technology.

Models M1 and M2 need to be solved for each DMU and scenario, providing 100 (super)-efficiency scores for each DMU.

4.5 Results and discussion

The results obtained for fast-response technologies are reported in section 4.3.1, while the results for long-term options are presented in section 4.3.2. Safe margins of change are also reported for efficient DMUs, providing insight into why a particular technology is efficient. In addition, improvement targets are presented for inefficient DMUs, offering guidelines for technology developers to enhance their performance. Further, section 4.3.3 discusses DEA results in the context of the technology readiness level (TRL) of the different technologies, providing insight into the future of the energy storage systems market. Finally, section 4.3.4 incorporates the stakeholders' concerns for technology section.

4.5.1 Fast-response technologies

Figure 4 depicts the efficiency scores distribution obtained by solving models M1 and M2 for each DMU in the fast-response cluster for 100 scenarios. Each of these scenarios corresponds to a particular realization of the uncertain parameters, obtained by applying Monte Carlo sampling to the associated uncertain distributions. As a result, instead of having a single efficiency score for each DMU, 100 values are obtained, i.e., one for each scenario. The lowest efficiency score obtained for each DMU corresponds to its worst scenario, while its highest efficiency score represents its best scenario. The efficiency scores obtained for the remaining scenarios are distributed between these extreme values. This distribution is depicted using a violin plot, where wider violin sections correspond to efficiency scores with a higher probability of occurrence (i.e., the DMU achieves this efficiency score in more scenarios). Technologies whose violins are wholly located in the efficient area have obtained an efficiency score greater than or equal to one in all the scenarios and, therefore, have a 100% probability of being efficient according to our data (e.g., Ni-Cd and Na-S). Note that the violin plots in this figure have been truncated to report the minimum and maximum efficiency obtained for each technology; meanwhile, the median efficiency is presented using a black dashed line inside the plots, and the lower (first) and upper (third) quartiles are shown with dot lines inside the plots. The percentage next to each violin provides the probability of each technology being efficient. For instance, a 70% probability means that among the 100 scenarios discretized using Monte Carlo sampling, the technology is efficient in 70 scenarios and inefficient in the remaining 30.

Flywheel is the most efficient option among fast-response technologies, with an efficiency score of 2 in 99% of the scenarios (inefficient only in one scenario). Flywheel is a short-term technology with high power density [44] and cheap power cost [20], despite having a more challenging energy density and energy cost (the fourth highest LCOE in this group, see Table B1 of chapter 8). Therefore, according to these results, the flywheel should be the technology of choice, especially for applications such as power quality control, where power is more important than energy. Indeed, the flywheel is suitable for frequent and rapid charge-discharge cycles that are required in a short time horizon, as otherwise, its long cyclability and high self-discharge might hamper its performance [5, 10].

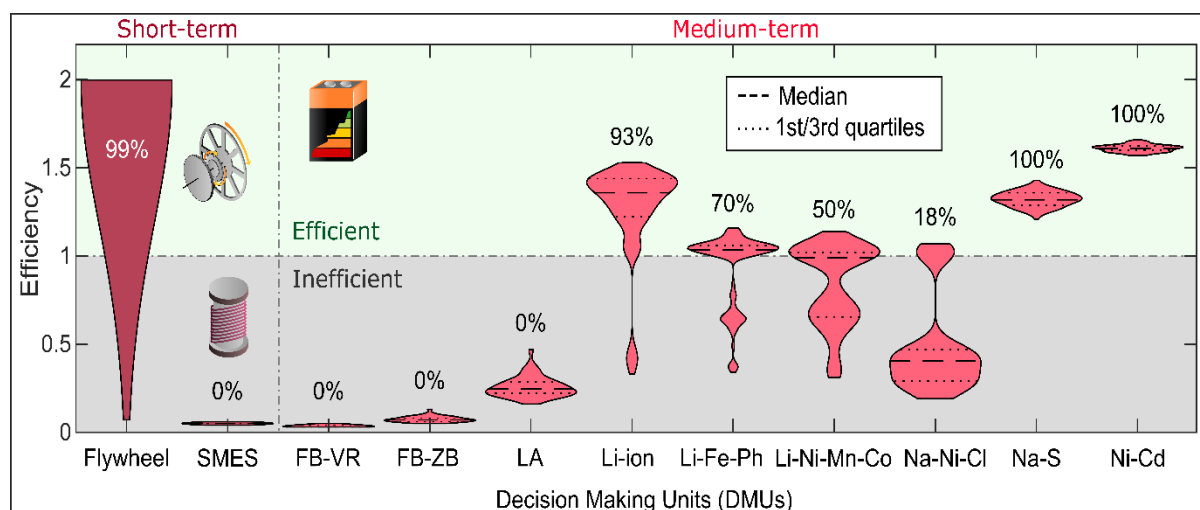


Figure 4. Distribution of efficiency scores for fast-response energy storage technologies under uncertainty. Short-term technologies: Flywheel, SMES; Medium-Term: rest of the technologies. Grey region: inefficient, Light green region: efficient. Median efficiency: dashed line inside the plots. 1st (lower) and 3rd (upper) quartiles: dot lines inside the plots. Changes in the plot's width: distribution of the data standing for the corresponding efficiency. Percentages next to violins: number of efficiency scores that are equal to or more than 1 (i.e., probability of being efficient).

Ni-Cd, Li-ion, and Na-S batteries stand at the second to fourth positions with median efficiency scores of 1.61, 1.36, and 1.32, respectively. As shown in Fig.4, all types of lithium-ion batteries are found more efficient than a lead-acid battery, consistent with previous findings [38]. In the case of Ni-Cd batteries, it is worth noting that cadmium is the by-product of zinc production processes (3 kg Cd/ton Zn), which suggests that the amount of cadmium production might be inflexible. Cadmium is a limited and valuable resource that is also dangerous for human health. Hence, its safe application needs extra caution [72]. Other factors attracting attention towards this battery include its high strength, good performance at low temperatures, and fast-charging capacity [10, 73]. Conversely, sodium batteries take advantage of this low-cost and non-toxic material with high recyclability potential, making these batteries a promising candidate for high power applications [44, 74]. Nonetheless, technical features such as low conductivity, volume expansion of cathode, and corrosion of their anode by the electrolyte need some improvements [75].

Other Li-ion battery types such as Li-Fe-Ph and Li-Ni-Mn-Co have a certain chance of being efficient (70% and 50%, respectively). Still, there are scenarios where their performance can drop down to 0.34 and 0.31, respectively. Overall, lithium batteries, widely used in electric vehicles [76], reveal an acceptable performance regarding the sustainability indicators considered in this study, with median efficiency scores between 0.99 and 1.36. Using them in electric vehicles means exposing them to hit in the event of an accident. Therefore, the explosion danger of these batteries, mainly caused by the elevated temperatures, needs to be solved [77, 78]. One promising solution for this issue is to endow separators with thermal shutdown functions in their structure [77]. Nonetheless, their widespread use should be cautioned until more environmental studies investigate their impact on human toxicity and other environmental categories.

FB-ZB, SMES, and FB-VR with median efficiency scores below 0.07, 0.05, and 0.03 are by far the most inefficient technologies.

Note that the variability of the efficiency scores of the SMES, FB-VR, FB-ZB, LA, Na-S, and Ni-Cd is small, which suggests that their obtained efficiencies are reliable. Conversely, technologies such as Li-ion, Li-Fe-Ph, Li-Ni-Mn-Co, and Na-Ni-Cl show significant changes depending on the scenario, to the point of affecting their classification as efficient (green-shaded background in Figure 4) or inefficient (i.e., dark-shadowed region). For instance, while the flywheel is inefficient only in one scenario, Ni-Cd and Na-S are always efficient. FB-VR, SMES, FB-ZB, and LA have no chance to be efficient (efficiency scores always lower than 1), while Li-ion, Li-Fe-Ph, Li-Ni-Mn-Co, and Na-Ni-Cl may be efficient or inefficient. Within this last group, Li-ion, with a 93% probability of being efficient, is always more efficient than the other three and, therefore, should be the preferred choice. Indeed, comparing the probability of Li-ion and Na-S batteries of being efficient, we find that Na-S is deemed efficient in all the scenarios, while there is a small probability (7%) that Li-ion batteries show an inefficient performance, reaching efficiency scores as low as 0.33 in the most pessimistic estimates. Despite this, Li-ion achieves a higher median efficiency score (1.36 vs. 1.32) and a higher maximum efficiency score (1.53 vs. 1.43), suggesting that Li-ion can perform better than Na-S batteries in the most optimistic scenarios. A risk-taker policy/investor may be inclined towards Li-ion batteries, capable of achieving better performance. In contrast, a risk-averse policy/investor will bet on Na-S, as there is “no risk” of it being a non-competitive technology. Likewise, Li-Fe-Ph (70% chance to be efficient) shows a better performance than Li-Ni-Mn-Co and Na-Ni-Cl in each of the scenarios, which suggests that it can be the selected alternative in case of storage technology with high energy density or low water consumption is needed (see Tables B5 and B6 of chapter 8). Similarly, Li-Ni-Mn-Co is more efficient than Na-Ni-Cl, with the former showing a 50% probability of being efficient, while this is only 18% for the latter. All this is, of course, besides other considerations not explicitly assessed in our DEA (e.g., Li-ion technology is already well developed [79], and is more accessible).

Figure 5 shows the safe margin of change for the fast-response technologies deemed efficient in at least one scenario, with the values depicted corresponding to the average safe margins among the 100 scenarios. These margins represent the maximum percentage of change that can be introduced *ceteris paribus* to the current value of the indicators (added for inputs and deducted for outputs) before the DMU stops being efficient.

The simultaneous analysis of Figure 4 and Figure 5 indicates that the more efficient a technology is (i.e., a higher super-efficiency score), the higher its safe margin. Flywheel, the first-ranked technology among fast-response options, has a 198% safe margin on its employment. Similarly, Ni-Cd and Na-S batteries also reveal safe margins on employment of about 122% and 64.5%. This suggests that the top three technologies in this cluster are mainly selected because of their relatively higher job creation ability. The deployment of these technologies may be challenging in regions with a high wage rate, affecting their LCOE. In this case, automation may help overcome the lack of skilled laborers or their high wages.

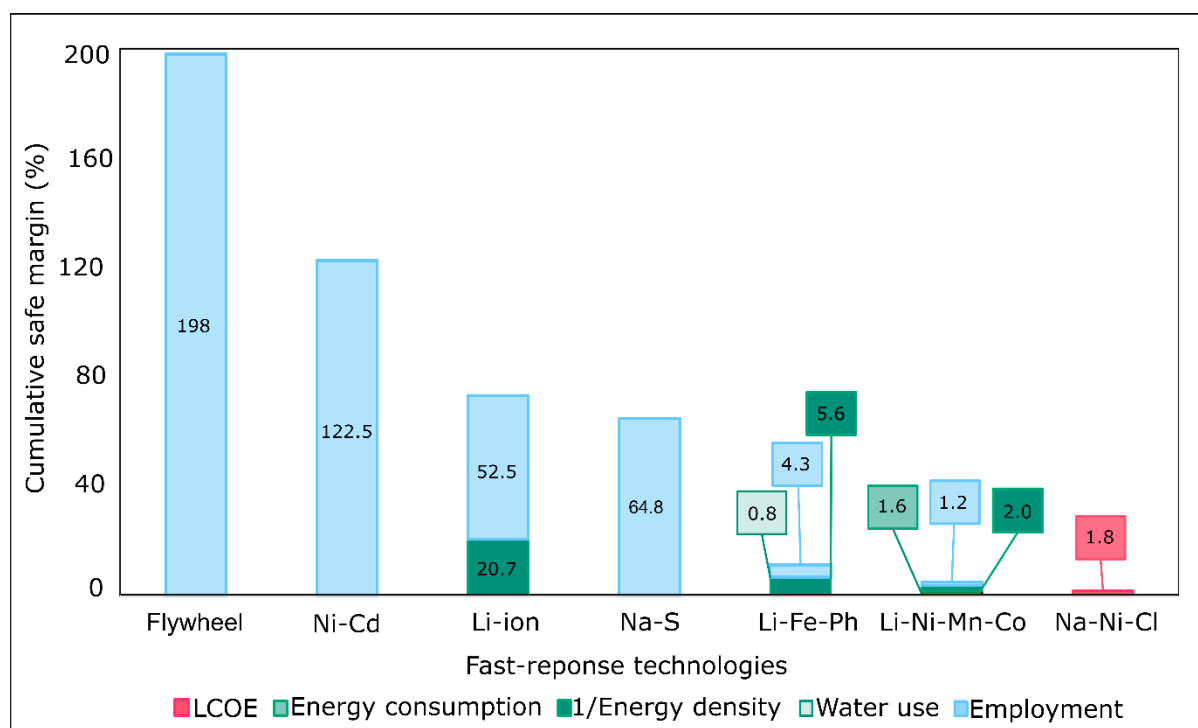


Figure 5. The safe margin of change for efficient fast-response energy storage technologies under uncertainty (%). Employment (desire output): allowed reduction, Rest of the indicators (inputs): allowed increase. LCOE: Levelized cost of energy

Li-ion also relies on its appealing performance on employment (52.5% safe margin), yet it also counts with the contribution of energy density (20.7% safe margin) to ensure its efficient status. Note that 1/energy density is used here as an input, which means that the safe margin of 20.7% in the indicator translates into an equivalent 82.8% that can be afforded in its real energy density (from 0.9 MJ/kg to 0.75 MJ/kg).

Following the same pattern, Li-Fe-Ph and Li-Ni-Mn-Co show safe margins on employment and 1/energy density. Yet, Li-Ni-Mn-Co could afford a marginal increase of 1.56% in its energy consumption, while the LCOE of Na-Ni-Cl could slightly worsen (no more than 1.79%), making it the only technology of this cluster with such a cost advantage.

We next turn our attention to inefficient technologies, for which improvement targets provide the minimum changes (i.e., reductions for input and undesired output and increments for desired outputs) required to make them efficient. Figure 6 presents the average improvement targets for inefficient fast-response technologies across the 100 scenarios, including technologies that are only inefficient in some scenarios. In this latter case, the average is calculated over the 100 scenarios. For DMUs with improvement targets on more than one indicator, changing only one of the indicators will not be sufficient to make the DMU efficient. Note that, although improvement targets are reported for all the indicators used, some of them might not be controllable directly due to design features, production factors, or other constraints [80]. Hence, technology developers can use a different model orientation if improvements in some particular directions are preferred.



Figure 6. Improvement targets for inefficient technologies of fast-response energy storage cluster under uncertainty (%). All the indicators: demanded reduction. LCOE: Levelized cost of energy. GWP: Global warming potential.

We detect an urgent need to improve the performance of SMES in most of the categories: it requires more than 80% reduction in its LCOE and energy consumption, while even more demanding changes (>90%) are required in its energy density, water use, and GWP. Recalling that the sustainability indicators used in this study correspond to unitary values expressed per GJ of delivered energy, the results obtained can be explained by a very low net delivered energy of SMES compared with its nominal value. Acknowledging that most storage technologies have certain losses, these are dramatic for SMES, which, undoubtedly, makes it necessary to control the amount of energy wasted before attempting to achieve the performance levels requested by DEA. In a SMES, the superconducting coil is cryogenically cooled to avoid loss of stored energy [7]. Making coils out of superconducting materials like mercury and vanadium can decrease resistance and the need for cooling. Submerging the coil in liquid helium can also contribute to keeping it cold, avoiding losses, and gaining the superconducting advantage [14]. Note that these modifications might also affect the economic performance of SMES, which is already critical with an operational cost ten times higher than for batteries [11].

The two flow batteries evaluated, FB-VR and FB-ZB, need about a 90% reduction on their input indicators and their GWP to become efficient. Although they need considerable improvements in all the categories, these batteries are still at the early stages of their development (technology readiness level 6 out of 9 [79]), therefore, such changes may not be out of reach for them. It seems that a

remarkable rise in the efficiency score of these batteries can be achieved by a better understanding of their construction that could help to improve their currently low energy density [81, 82]. Currently, the unclear reaction mechanisms and electrolyte performance are barriers to their improvements [9]. In this context, the application of finite element simulations could guide the construction of their electrode structure, providing information about the dimension of channels in electrode fibres and the path of electrolyte flow while helping to understand the reactions mechanisms better [83]. The application of 3D nanostructures as electrocatalysts is also useful to increase the catalytic activity (that affects the polarization resistance and energy loss [84]) and the cycling stability of flow batteries, which are necessary factors to make these batteries viable at the commercial level [85]. Still, poor cycling [9], corrosivity of electrolytes, and the environmental pollution associated with flow batteries also need significant improvements [86]. Today, the cycling of redox flow batteries is limited by the sluggish anode redox chemistry [87]. Regarding FB-VR, the number of operational cycles during their lifetime is expected to rise from about 12000 cycles [14, 20] to 50000 cycles by 2030 [88]. This *ceteris paribus* change would increase their delivered energy during its lifetime by 428.4% and decrease, in turn, the value of their energy consumption by 3.8% (i.e., 76.7% reduction in manufacturing energy consumption, while the feed-in energy to charge the technology will not change), and its GWP by 85.2%. This battery's targeted improvement for energy consumption and GWP is 92.0% and 97.8%, respectively (see Figure 6 for improvement targets). Hence, rising the number of cycles is very helpful but still not enough to reach the improvements targeted. Acknowledging that a significant part of the battery value depends on the raw materials used in its structure [89], essential developments in material science are required to guarantee the achievement of such targets. For instance, ammonium-based electrolytes [90], and low-cost non-corrosive advanced ion-conducting membranes are the most promising solutions to solve the cyclability issue and the stability and environmental concerns associated with flow batteries [91]. In addition, employing nonaqueous electrolytes solves the corrosivity problems and is more environmentally friendly [92]. Also, application of organic redox-active species can significantly reduce the cost of flow batteries in the future [93]. It seems that, the development of low-cost membranes, increasing the power density, and rising the life cycle would help these technologies to improve their performance significantly [81, 94].

Two other technologies need significant improvements to become efficient. The first is LA, with improvement targets above 40% for LCOE, energy consumption, and energy density and above 90% for water use and GWP. The second one is Na-Ni-Cl, with targets around 20% on LCOE and energy density, 40% on energy consumption, and more than 70% on water use and GWP. These two technologies ranked second and third expensive between the batteries based on the cost of their storage section, while their operational cost is lower than most of the batteries. Therefore, decreasing the cost of the storage section will lead to a significant improvement in their LCOE [20]. In the absence of practical methods to decrease the cost of the storage section, raising their lifetime and life cycle, which currently is not interesting for LA, will lead to delivering more energy during their lifetime and consequently a lower LCOE [10]. On the other hand, their energy consumption can be decreased by improving the power stack materials manufacturing, the plant balance, and the power control system, which are the steps with the highest energy consumption [95]. Also, the economy of scale can be to the benefit of their environmental impacts. For instance, the GWP per GJ of an 8 MW lead-acid battery is much lower than a 2 MW one [96]. Certainly, recycling battery materials will decrease their associated environmental impacts and increase material availability [59]. This observation is underpinned by studies reporting that the impacts of recycling are lower than the impacts of producing fresh materials [95]. Currently, lead-acid is the only battery with a very good recycling

operation procedure, and a high percentage of recycled lead is usable in the production of new batteries [72]. Also, its good performance in different temperature ranges makes it a potential candidate for operations with fluctuating temperatures [10].

Two batteries have a remarkable chance to be efficient, Li-Fe-Ph and Li-Ni-Mn-Co, with average improvement targets of 8.54% and 13.51%, respectively. To this end, they should decrease their GWP (23 and 35%, respectively). Like the lead-acid battery, this group of batteries can gain from the economy of scale to decrease their GWP. Recycling operations exist for lithium-ion batteries (not economical) [97], but these are not well established yet and need further attention. For instance, in the case of their cathode, the material used, its morphology, and microstructure affect the recycling process and production of hazardous pollutions [98]. High nickel-metal carbons and spinels Li-rich Mn are recommended for the cathode to improve the battery capacity and operating voltage. At the same time, graphite containing silicon oxides attract attention for the application on the anode side [89]. On the other hand, the LCOE of these batteries requires improvements beyond 5% for Li-Fe-Ph and beyond 9% for Li-Ni-Mn-Co. Regarding the fast and broad research concerning these batteries' characteristics and costs, the cost reduction deemed is not far to achieve [15]. Layered lithium-rich low-cost cathode materials are the most attractive option for this purpose [99]. In addition, controlling other indicators, such as water use, will be necessary. Battery manufacturing processes should be highlighted to control water consumption since these processes contribute more in their material consumption than operation and end-of-life processes [100]. Furthermore, Li-ion needs to obtain safety and environmental certificates to solve the legal issues that ban its extensive application [88]. The latest development suggests that its safety can be improved by using a physical separator between electrodes, which provides a reliable bridge for ion transport [101]. Their frequent charging needs and long charging time are other issues that need to be solved [9, 10].

Finally, flywheel and Li-ion are almost always efficient, translating into very small improvement targets (always below 5.5%). These could be achieved by the targeted choice of material [100], of course, so as not to worsen other aspects (e.g., self-discharge, lifetime, charging time, etc.).

The estimated improvement target for employment is always zero for all the technologies, the reason why it is not depicted in Figure 5.

4.5.2 Long-term energy storage options

Figure 7 presents the efficiency scores for long-term energy storage alternatives. Like Figure 4, violin plots have been truncated to report each alternative's minimum and maximum efficiency. Median efficiencies are presented using a black dashed line inside the plots, while the lower (first) and upper (third) quartiles are shown with dot lines inside the plots. The percentage next to each violin provides the probability of each technology being efficient. For clarification of the used colors for hydrogen and nitrogen underneath the x-axis labels, see Figure 2.

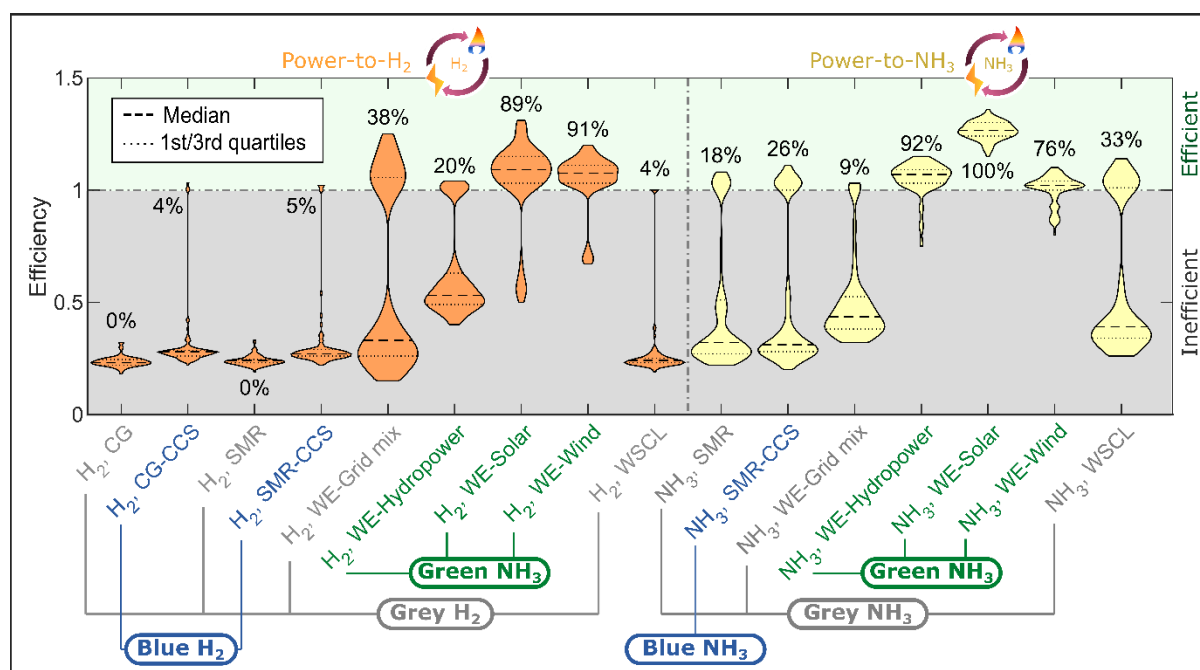


Figure 7. Distribution of efficiency scores for long-term energy storage options under uncertainty. The colors for hydrogen and nitrogen are indicated underneath the x-axis labels. Grey region: inefficient, Light green region: efficient. Median efficiency: dashed line inside the plots. 1st (lower) and 3rd (upper) quartiles: dot lines inside the plots. Changes in the plot's width: distribution of the data standing for the corresponding efficiency. Percentages next to violins: number of efficiency scores that are equal to or more than 1 (i.e., probability of being efficient).

As shown in Figure 7, green ammonia from solar energy is the only long-term storage option that is always efficient, achieving a median efficiency of 1.265. This efficiency score is mainly due to this technology's high employment and low water consumption (Table B7 and B11 of chapter 8). Green hydrogen produced with solar energy and then the one produced with wind energy are the next two alternatives, with median efficiency scores of 1.09 and 1.08, respectively. The former takes advantage of its low energy consumption, while the latter offers important employment opportunities. Green ammonia from hydropower and wind energy are ranked fourth and fifth, with median efficiencies of 1.07 and 1.02, respectively. These results reveal that the top five long-term storage alternatives relate to water electrolysis using renewable energies (i.e., green hydrogen and ammonia). Although green hydrogen and ammonia are still very expensive compared with grey and even blue ones, it is expected that future cost reduction of renewable energy sources will help them to become the cheapest options [45]. As will be further discussed later, other options like green hydrogen using hydropower, ammonia produced by water electrolysis using grid mix energy, and ammonia produced by chemical looping processes have a certain chance of being efficient despite displaying median efficiencies below one: 0.53, 0.44, and 0.39, respectively. Moving to any of the remaining eight long-term storage options results in a dramatic decrease in the median efficiency score, below 0.33 in all the cases. It means that these technologies are, in principle, inferior to the other eight when assessed based on the economic, environmental, and social indicators we considered. Between these alternatives, grey hydrogen does not have any chance of being efficient, regardless of the technology employed in its manufacturing (max efficiency of 0.33 for coal gasification and 0.32 for SMR). In addition to their high GWP, their high energy and water consumption also exacerbate their situation. Therefore, they need remarkable improvements to be comparative with other options in the market.

Among the five alternatives that are efficient in all or most of the scenarios, two are related to hydrogen and three to ammonia, and all of them use renewable energy. It means that only 22% of hydrogen alternatives can be deemed efficient, while 43% of ammonia-based options are found efficient in at least some scenarios. Compared to hydrogen, ammonia is safer and generally needs lower space for storage due to its higher volumetric density [102]. However, developments like applying complex hydride materials can help store hydrogen safely and efficiently [103].

Green hydrogen or ammonia have better performance than their grey alternatives, even between inefficient options. Despite this, grey alternatives still are widely used owing to the higher reliability of fossil fuels and the possibility of gas production with higher capacity. Maybe in the form of policies, extra efforts seem necessary to move to cleaner sources [104].

Employing a CCS unit is essential for processes that use fossil fuels to control CO₂ emissions, although we did not find this to cause a fundamental change in their efficiency scores. Indeed, the maximum difference in efficiency scores of production units (hydrogen or ammonia) with and without CCS is approximately 0.05 (based on the median). This happens because when a CCS unit is used, the reduction of GWP comes at the cost of increasing LCOE and energy consumption. Hopefully, reducing the cost of electricity generation using cleaner sources besides other technical improvements will increase the contribution of more sustainable gas production methods such as green hydrogen and ammonia. For instance, projections indicate that, in 2030, the cost of ammonia production using renewable sources will be lower than its production using methane reforming [105].

In terms of the variability of the efficiency scores, we find that green ammonia from solar energy is always efficient. The next green alternatives based on water electrolysis are ammonia from hydropower, hydrogen from wind, and hydrogen from solar, showing 92%, 91%, and 89% probability of performing better than the remaining alternatives in each scenario. Among the other options, green ammonia from wind (NH₃, WE-Wind) and hydrogen relying on the grid for water electrolysis (H₂, WE-Grid mix) have a 76% and 38% probability of being efficient. Other options like ammonia produced using water splitting by chemical looping (NH₃, WSCL), ammonia produced by steam methane reformation and using carbon capture and storage (NH₃, SMR-CCS), hydrogen produced by water electrolysis powered by hydropower energy (H₂, WE-Hydropower), ammonia produced by steam methane reformation (NH₃, SMR), ammonia produced by water electrolysis powered by grid mix (NH₃, WE-Grid mix), hydrogen by steam methane reformation using CCS (H₂, SMR-CCS), hydrogen from coal gasification using CCS (H₂, CG-CCS), and hydrogen produced using water splitting by chemical looping (H₂, WSCL) have smaller probabilities of being efficient (33%-4%), which suggests these technologies are among the best performance alternatives only in some particular contexts. For instance, green ammonia based on wind energy might be particularly suitable for regions with strong and constant winds and without reliable solar energy potentials. Meanwhile, grey hydrogen production options such as coal gasification (H₂, CG) and steam methane reforming (H₂, SMR) are inefficient in all the scenarios. Even blue hydrogen alternatives such as hydrogen production based on the coal gasification with CCS (H₂, CG-CCS) and hydrogen production based on the SMR and with CCS (H₂, SMR-CCS) only have a small chance to be efficient (less than 5%). This suggests they might still be viable alternatives for some niche applications, although less likely than the alternatives previously discussed. Overall, green processes are preferred over blue and grey due to their higher efficiency according to the indicators employed in this contribution.

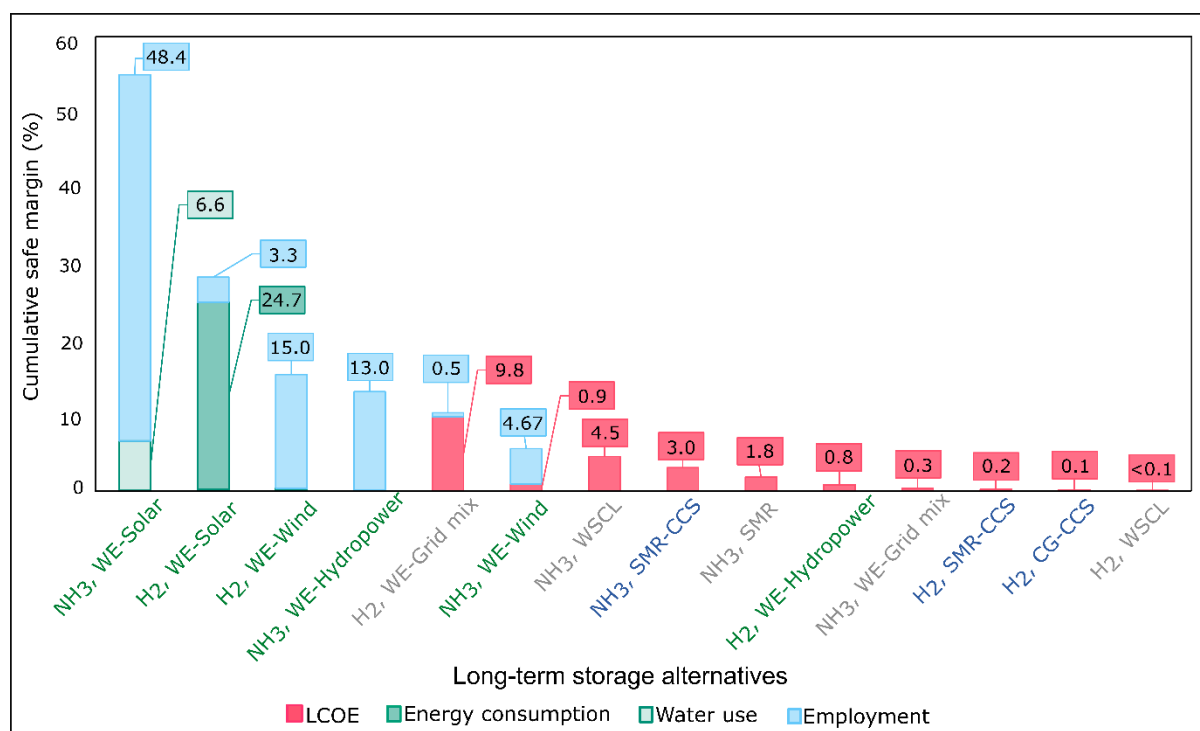


Figure 8. The safe margin of change for efficient long-term energy storage alternatives under uncertainty (%). Employment (desire output): allowed reduction, Rest of the indicators (inputs): allowed increase. The colors for hydrogen and nitrogen are indicated underneath the x-axis labels. LCOE: Levelized cost of energy.

Comparing hydrogen use as a standalone energy storage option with ammonia obtained from the same hydrogen, we can see that ammonia has better performance almost always. The only exception is when wind energy is used for water electrolysis. In this case, the median efficiency of hydrogen is 0.055 higher than for ammonia. Therefore, converting hydrogen to ammonia is recommended if the ultimate goal is to have a long-term energy storage alternative.

We next investigate why some technologies are efficient. To this end, we plot the safe margins of change for alternatives that are efficient at least in one scenario (see Figure 8). Overall, efficient alternatives have safe margins only on one or two of their indicators at most, while the rest should remain at equal or better values to retain their efficient condition. The case that attracts the most attention is the 48.3% safe margin on employment that is related to ammonia produced using water electrolysis by solar energy (NH₃, WE-Solar). Supposing that technological innovations and automation decrease labor needs for this alternative as it moves from 5 to higher technology readiness levels [106, 107], the next storage options in terms of their efficiency scores could be explored as alternatives. Note that, in this case, the safe margin on employment is also high for the third and the fourth most efficient options, hydrogen produced by water electrolysis powered by wind (H₂, WE-Wind) and ammonia produced by water electrolysis powered by hydropower (NH₃, WE-Hydropower), with values of 15% and 12.9%, respectively. However, the second standing alternative, (H₂, WE-Solar), can also afford to increase its low energy consumption by 24.7%, while (H₂, WE-Grid mix) could raise its LCOE by 9.7%, if deemed necessary for introducing additional innovations affecting other features. In addition, about 4.53%, 3.04%, and 1.79% rise in LCOE is allowed for (NH₃, WSCL), (NH₃, SMR-CCS), and (NH₃, SMR), respectively, which highlights the economic competitiveness of the chemical looping

method compared to other options for energy production. For the rest of the alternatives, the safe margin is only obtained on LCOE and is lower than 1%. These are the alternatives that have a slight chance to be efficient.

Improvement targets are next computed for alternatives that are inefficient in at least one scenario (see Figure 9). As in Figure 6, the values depicted correspond to perceptual changes concerning the current value of the indicators, calculated as the average of all 100 scenarios.

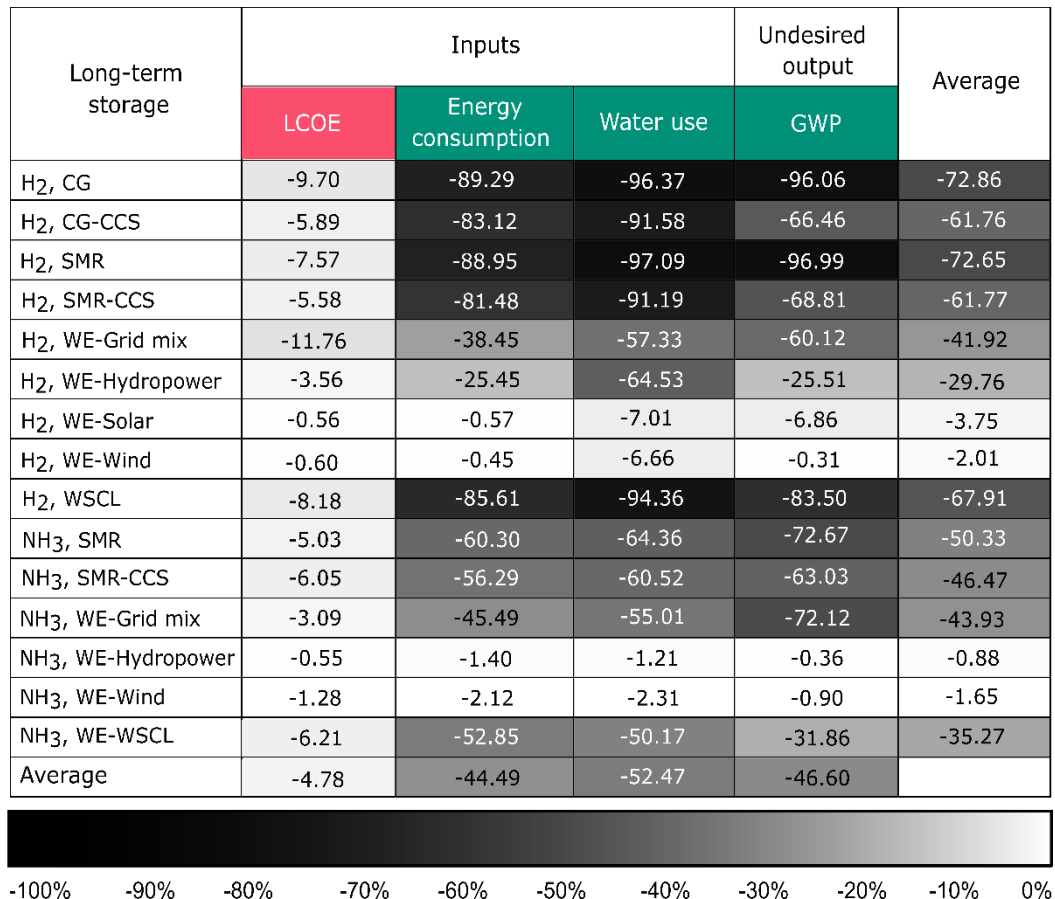


Figure 9. Improvement targets for inefficient technologies of long-term energy storage cluster under uncertainty (%). All the indicators: demanded reduction. GWP: Global warming potential.

Figure 9 reveals that the minimum reduction required in LCOE is 0.6% and is related to (H₂, WE-Wind), which could be naturally achieved by falling costs of renewable energies, including wind. Meanwhile, the maximum reduction in LCOE is 11.76% for (H₂, WE-Grid mix). The rest of the options are demanded LCOE reductions within this range, but generally lower for ammonia than for hydrogen. Note that the cost of producing 1 kg hydrogen is more than producing 1 kg ammonia [108]. Also, since converting the gas to electricity using a fuel cell is more expensive than gas turbines [20], using gas turbines rather than fuel cells can help control the LCOE for hydrogen. In addition, the cost of storing the gas generated changes from 130 €/kWh for above-ground storage to 3.7 €/kWh for underground storage [20]. Therefore, the DMUs needing to reduce their LCOE, can move to underground gas storage to help reach their target, provided this option is socially and politically accepted in the region.

The highest reduction required in energy consumption is about 90% related to grey and blue hydrogen, followed by WSCL. The current pilot efforts for CCS systems consume significant amounts of energy, but new technologies are being investigated that could bring the energy demand down [109]. For green hydrogen and ammonia, the reduction required in energy consumption is meager, and (H₂, WE-Wind) with 0.45% demanded reduction in energy consumption is the last and the best one in this indicator. It is worth noting that there is considerable heat waste in the gas production reactors [50], and heat integration can improve their performance.

Regarding water use, the situation presents a similar pattern to energy consumption but with different values, ranging from 1.21% for (NH₃, WE-Hydropower) to 97.09% for (H₂, SMR).

Almost all the investigated long-term storage options need to decrease their GWP. Between the inefficient DMUs, changes requested start at 0.31% for (H₂, WE-Wind) and climb until 96.99% related to (H₂, SMR). Using CCS, CO₂ emissions can be controlled, but as already discussed, the contribution of CCS does not seem very effective in improving the efficiency score of DMUs (only 0.05), as CCS worsens the performance in energy consumption and LCOE. Despite this, a CCS unit is necessary for ammonia production since the existence of CO₂ in the reactor can affect the hydrogen and nitrogen reaction catalyst [110]. The improvement target obtained for employment of all the long-term storage options is zero and, therefore, not represented in Figure 9.

4.5.3 Future market and development trajectory of energy storage options

A technology may look much more appealing than the other technologies in a comparative analysis such as DEA regarding the considered indicators. Despite this, not all energy storage technologies will successfully access the energy market [106]. The technology readiness level (TRL) of each technology allows us to assess the maturity and its level of expected changes in the future [88]. When TRL is low, and the technology is still in its research or concept stage, it is highly uncertain whether the technology will be able to be implemented or not [79]. If it succeeds, its development potential will be high at first. Still, as it gets closer to the level of full development (i.e., being marketable), this potential will decrease, following a learning curve. Technologies with a higher TRL value are developed very well, and further development may not be easy. In such a case, if the technologies are efficient, they may finally penetrate the market but probably not in the near future, and if they are not efficient, they will have a long and challenging way to go.

4.5.3.1 Future market of efficient and inefficient fast-response technologies

To explore the chance of each efficient or inefficient technology to access the market, we plot their median efficiency versus their TRL, as shown in Figure 10. The median efficiency score of fast-response technologies used in Figure 10 corresponds to the one obtained with DEA and previously reported in Figure 4. The technology's current TRL is retrieved from different literature sources, as reported in Table (B.12, chapter 8) of supplementary information. Each technology should meet specific criteria to qualify for a certain level [79], according to nine levels ranging from 1 (non-mature) to 9 (mature). Usually, a TRL lower than four is related to technology at the research or concept test stage. If TRL is between 4 and 6, the technology is in the demonstration or technical development stage. When TRL is above 7, the technology is at a specific test certification stage or is marketable (i.e., TRL close to 9) [107].

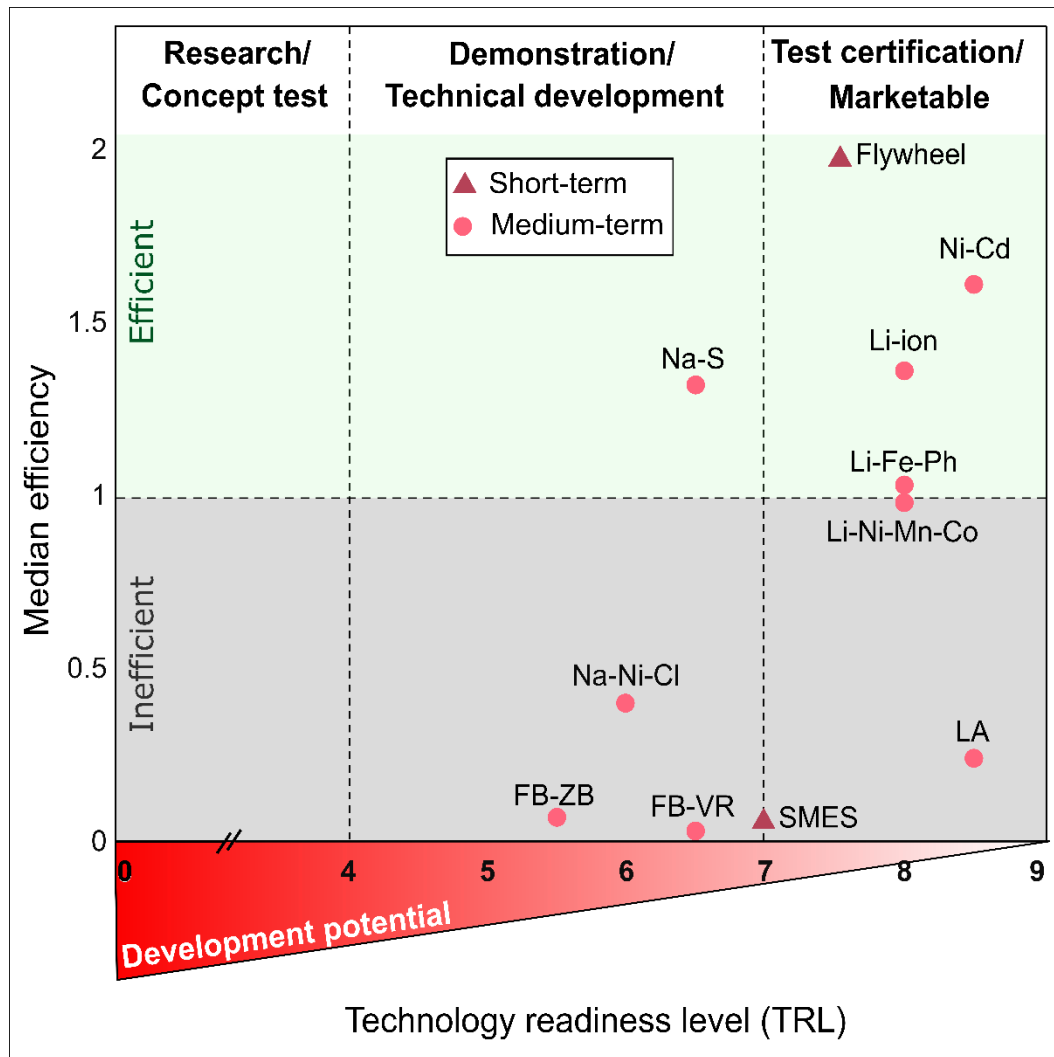


Figure 10. Market penetration chance of efficient and inefficient fast-response energy storage technologies. Short-term: Flywheel, SMES. Medium-term: Rest of the technologies. Grey region: Inefficient. Light green region: Efficient. Development potential decreases moving from TRL=0 to TRL=9.

Figure 10 is divided into different zones using dashed lines placed at an efficiency score of one (i.e., splitting the region between efficient and inefficient technologies), and TRLs of 4 and 7 (i.e., splitting the region according to how close the technology is to be marketable in the future). The combination of the different criteria met gives rise to the classification of the technologies assessed into different groups as follows:

- Efficient ($\delta^* \geq 1$) and marketable ($7 < TRL \leq 9$): flywheel, Ni-Cd, Li-ion, Li-Fe-Ph and, with a bit of optimism, Li-Ni-Mn-Co belong to this group. According to our results, all these technologies are winning choices since they show a competitive performance and a reliable level of development. The best technology selection from this group for a particular application can be underpinned by Figure 5, which provides the indicators that each of these technologies performs best. For instance, flywheel, Ni-Cd, and Na-S are promising options when creating new job opportunities is essential for developing a region. Meanwhile, Li-ion, Li-Fe-Ph, and Li-Ni-Mn-Co are also important

employment creators, on top of showing a good performance in energy density, which makes them suitable for electric vehicles [76]. It is forecasted that, by 2030, Li-ion batteries will remain the dominant technology in mobility applications, while for stationary applications, a broader choice of technologies will be used [89]. Continued research on Li-ion batteries makes solid-state Li-ion batteries marketable by 2025. From 2025 to 2030, solid-state lithium metal, advanced solid-state Li-ion, and metal-air batteries probably will access the market [89]. Despite this, their TRL is still lower than 9, which indicates that some aspects still need to be improved before they can effectively penetrate the market of electricity storage technologies. For instance, the gravimetric energy density and number of cycles during the lifetime of Li-ion batteries are about 250 Wh/kg and 3000 cycles, respectively [20]. These parameters are expected to reach 350 Wh/kg [106] and 15000 cycles [89] according to the 2030 set plan target offered by the European association for energy storage, which presents the roadmap of energy storage technologies development.

- Efficient ($\delta^* \geq 1$) but not marketable ($4 < TRL \leq 7$): only Na-S, the promising alternative of lithium-ion batteries [111], belongs to this group. The relatively low cost of this battery, the natural abundance of sodium resources [111], its high theoretical capacity, and the high energy density of sulphur [112], make the Na-S technology a promising candidate to attract investment, with real possibilities to infiltrate the market. Our DEA results confirm this, showing that Na-S is always efficient with a median efficiency score of 1.32. Although not a completely mature technology, its TRL is also relatively high, suggesting that Na-S is already highly developed, and that further development may not be easy or rapid. At this point, the main technical challenge of this battery is lowering its operational temperature [107]. The bottleneck to solving this problem is developing and designing suitable anode materials [111]. Hollow nanostructured materials capable of storing sodium ions in their structures through the combined conversion and alloying reactions are a class of promising materials for this purpose [113, 114]. For example, indium tin oxide nanoparticles decorated onto activated carbon cloth enable operations in sub-zero by immobilizing the higher-order Na-polysulfides and promoting their conversion into insoluble end-discharge products [74].
- Inefficient ($\delta^* < 1$) but marketable ($7 < TRL \leq 9$): LA and SMES are in this zone. Our analysis (Figure 6) revealed that significant improvement targets are necessary to increase the efficiency of these technologies. SMES requires more than 80% fall in all the indicators except for employment. On the other hand, LA asks for about 50% decrease in LCOE, energy consumption, and 1/energy density, while its required decline for water use and GWP is even higher and above 90%. The fact that these technologies are marketable suggests that considerable time has already been spent in their development. At this point, they no longer have remarkable development potential. In the absence of a technological breakthrough, it is hard to imagine how these technologies could reach the required performance. For all these reasons, they are not particularly promising alternatives at this point.
- Inefficient ($\delta^* < 1$) and not marketable ($4 < TRL \leq 7$): technologies in this zone are Na-Ni-Cl, FB-ZB, and FB-VR. These technologies need further improvement before they can become efficient. Still, since they are not yet at a marketable stage, it is not far from the expectation that they can move to the “efficient and marketable” zone. However, their improvement targets (Figure 6) do not reveal a smooth path ahead. For instance, Na-Ni-Cl needs to decrease its water use and GWP in the range of 70-80%, along with reductions in its LCOE, energy consumption, and 1/energy density (16-40%). Meanwhile, flow batteries (FB-ZB and FB-VR) need about 90% decrease in all the indicators except employment. For this latter group of batteries, extending the number of

operational cycles and increasing the power density are requested (e.g., from 12000 cycles [14, 20] to 50000 cycles [88] for FB-VR) [94].

- Research stage ($TRL \leq 4$): none of the technologies assessed qualified in this zone, whether efficient or inefficient. In this contribution, only the technologies whose data were available were considered. Usually, the data of technologies at the research step are not open to the public. It is expected that more players will be on the scene in the future, including organic batteries, metal batteries, onion shuttle-based batteries, high power primary regenerative batteries based on reactive metals [89], and hybrid energy storage technologies that include the advantages of different technologies [115]. Rapid growth is expected for technologies that manage to pass this step successfully.

Overall, the efficiency and TRL of all the energy storage technologies are influenced by some common factors. For instance, in addition to the environmental impacts and technical factors like energy capacity (kWh), energy density (Wh/kg), efficiency, response and discharge time, and the number of cycles during the lifetime of technology, the capital cost (\$/kW), and LCOE (\$/kWh) influence the technologies TRL value [116]. Almost all these factors are used in our DEA analysis explicitly (i.e., as an indicator) or implicitly (i.e., in calculations related to estimating the final value of the indicators). Therefore, the efficiency and TRL of these technologies will change simultaneously. So, in the next paragraph, we present some general improvement guides, the challenges ahead, and the solutions to deal with them.

The main challenge is developing advanced materials that enable high power and energy density to improve technical and environmental factors. To this end, the focus should be on adapting cathode and anode materials and stabilizing the formulation of electrolytes [89]. However, the unbalanced distribution of raw materials in different countries and the marginal extraction rate are obstacles to accelerating the development [89]. Reaching the production target of 300 GWh/a battery in the European Union alone will require 270000 tons battery-grade graphite, 30000 tons of silicon for the anode, 225000 tons of class 1 high purity nickel, 29000 tons of cobalt, 84000 tons of manganese, and 59000 tons of lithium for the cathode [89]. Mapping the availability of raw materials in different countries helps raise awareness regarding the available resources [106]. Beyond the application of sensing technologies, big data from sensors embedded in battery cells, the discovery of self-healing materials [117], artificial intelligence-based tools, physics-aware models, and autonomous synthesis robotics will enable scientists to learn the interplay between battery materials and interface. Therefore, several battery chemists will propose using novel developed materials and taking advantage of the knowledge obtained about the interplay between different materials [89].

Furthermore, according to the European 2030 technology development roadmap, liquid discharge from battery-grade material processing should be zero, and CO₂ emissions in material extraction and processing should be reduced by 50% [89]. To this end, currently used batch processes should be replaced by continuous processes, new smelting, and slag engineering technologies, and new recoverable reagents for battery metal leaching and extraction should be addressed [89]. Also, beyond 2025, some investments in the facilities that recycle materials from energy storage technologies will become necessary to reduce the pressure exerted on the environment [117], while recovery of metals from industrial or urban wastes can also contribute to this end [89]. Further, to decline the technology cost, its volume (i.e., large-scale manufacturing) and standardization (i.e., proper connection of system components, installation, maintenance, and performance) are factors that should be noted [106].

4.5.3.2 Future market of efficient and inefficient long-term energy storage alternatives

Figure 11 presents the median efficiency versus TRL for long-term energy storage alternatives. Their median efficiency is obtained from DEA analysis, as previously reported in Figure 7. Unfortunately, the TRL for many long-term storage options like hydrogen produced with solar, wind, or fossil fuels is not reported reliably and explicitly in the literature. However, generally, the TRL for grey processes is about 8-9 and is higher than for blue processes, which varies from 6 to 8. Finally, with a TRL of 1-3, green processes still have a long way ahead [118]. We select the median of the ranges reported as the TRL of each production method [106, 107]. In the case of NH_3 production, the TRL is not reported for any of the routes. Therefore, the TRL of each power-to- NH_3 production method is considered the same as its power-to- H_2 equivalent (see Table B.13 of chapter 8).

Figure 11 is equivalent to Figure 10, with the plotted area divided into six regions as given by the combination of the different categories achieved by the alternatives regarding their efficiency scores (efficient vs. inefficient) and their TRL level (research stage, not marketable, marketable). In this case, no alternative is both efficient and marketable. Only grey options, like power-to-gas based on water electrolysis using the grid mix, are close to a marketable situation. Despite this, grey alternatives are still far from efficient, with improvement targets on water use, GWP, and energy consumption asking for reductions beyond 80%. Considering that these alternatives are already well developed and almost marketable, these improvements seem out of reach.

The following alternatives in terms of TRL are blue options, such as power-to-gas using steam methane reforming or coal gasification, and both coupled with carbon capture and storage. Compared to grey ones, blue alternatives present a better situation regarding their GWP, which, combined with their lower TRL, may result in a better performance once they are completely developed. However, even if they manage to infiltrate the market, such domination will only be a transition period before growing environmental concerns put green alternatives in action.

Only the green power-to-gas-to-power routes, such as H_2 and NH_3 based on the water electrolysis powered with wind or solar, and NH_3 based on water electrolysis using hydropower, are found efficient. These alternatives are still at the research step and have good development potential, which could help them perform even better and achieve higher efficiency scores.

Overall, the bottleneck for developing the power-to-gas processes is water electrolysis. Due to different reasons, different electrolytic cells and processes have managed to achieve distinct TRL levels. For instance, alkaline electrolysis is well developed, with a TRL of almost 9, yet the technology is considered not marketable because of its high costs. Other options like polymer electrolyte membranes with a TRL of 8, solid oxide electrolytic cells, and the co-electrolysis of water and CO_2 , both with a TRL of 5.5, still need to increase their energy efficiency and lifespan while reducing maintenance costs and environmental impacts [107]. In this context, large-scale production might help decline costs [88]. At the same time, the use of nanomaterials to store the gas shows an improved environmental performance compared to other choices like caverns [119].

Finally, it is also essential to consider the market readiness level when predicting the future of energy storage alternatives. Market readiness level records a value of 7-8 (out of 12) for power-to-hydrogen, which means the market has identified the need for this storage alternative and its application [88]. In addition, it is forecasted that raising concerns about CO_2 emissions will increase motivations for further investments in power-to-gas energy storage alternatives. Hence, while mobility is the most significant anticipated market for hydrogen in the short term, balancing the energy system and grid reinforcement is expected to be the most demanding source for hydrogen in the longer term [88]. Further development of fuel cells, facilitation of gas storage, and cost reduction are the key factors

that will pave the development trajectory of power-to-gas energy storage alternatives [79]. Preparing the necessary infrastructures and certificates for gas production processes and their application operations will require political and financial support [88].

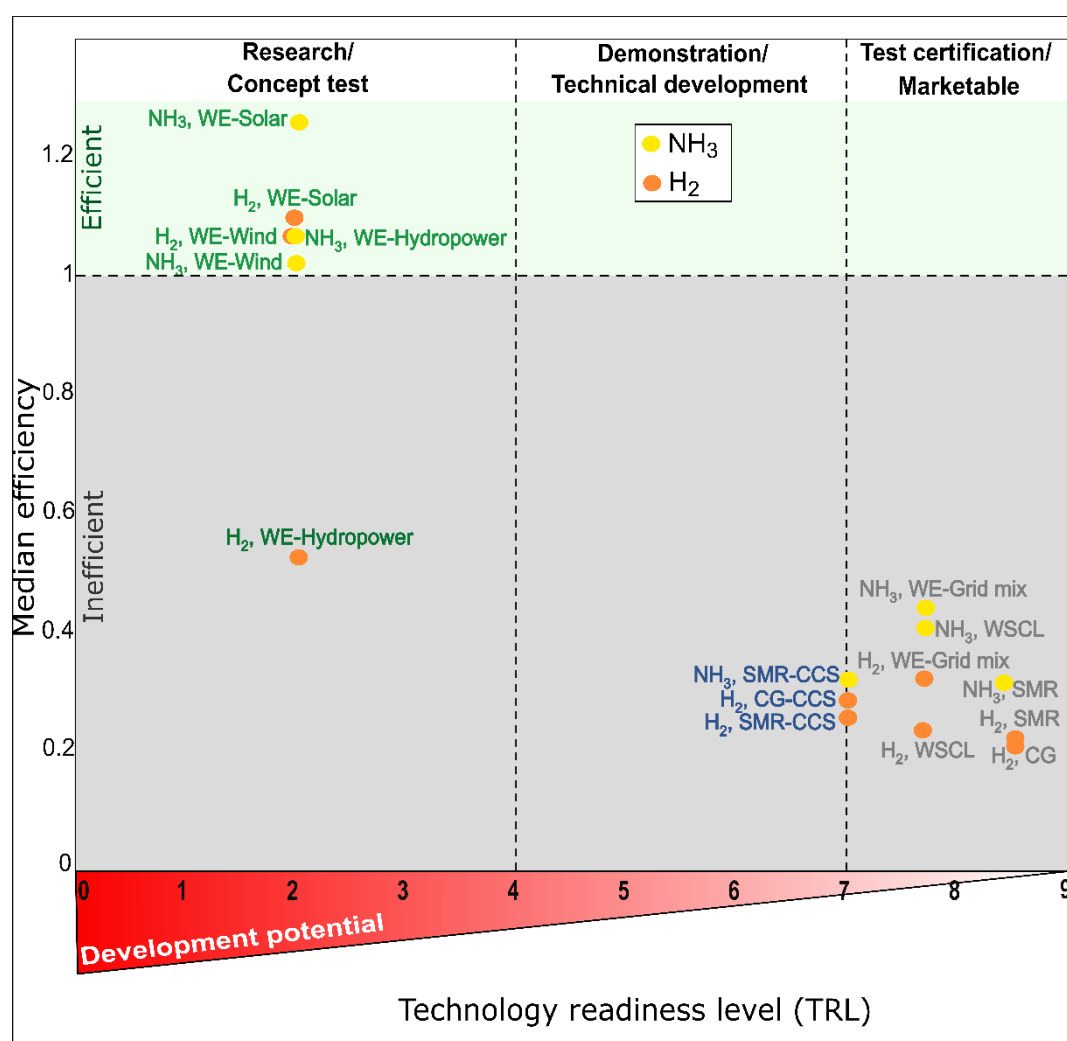


Figure 11. Market penetration chance of efficient and inefficient long-term energy storage alternatives. Grey region: Inefficient. Light-green region: Efficient. Development potential decreases moving from TRL=0 to TRL=9. Grey H₂/NH₃: H₂ or NH₃ produced using fossil fuels, Blue H₂/NH₃: H₂ or NH₃ produced using fossil fuels and the emitted carbon captured by CCS, Green H₂/NH₃: H₂ or NH₃ produced using renewable energy sources.

4.5.4 Incorporating concerns from stakeholders in the technology selection

In this contribution, we resorted to DEA to compare the energy storage options, where the absence of predefined weights is equivalent to implicitly assuming that all indicators are equally important. However, in real applications, the stakeholders' preferences or local contexts could challenge this assumption and even make some technologies rejected initially. Also, engineers, customers, or policymakers might show some preferences over selected indicators, which may vary with time, location, and the application of the technology. Therefore, we address the technologies comparison by presenting two additional investigations. In the first analysis, we include predefined weights as parameters in the model formulation. Indeed, we solved an additional problem where we assigned

80% of the total weight to environmental indicators and 20% to the rest. However, different weights could be used if stakeholders were more inclined towards other aspects of the problem (i.e., economic, or social). This exercise, discussed in detail in Appendix A.1, reflects the view of a stakeholder inclined towards using cleaner technologies.

This evaluation reveals that, between fast-response technologies, flywheel, Ni-Cd, Li-ion, Na-S, and Li-Fe-Ph face a significant decrease in their efficiency scores; nevertheless, they all remain efficient. This means that, although the main strengths of these technologies rest on their economic and social performance, they are also good choices for environmentally friendly applications. The efficiencies of Li-Ni-Mn-Co, Na-Ni-Cl, LA, FB-ZB, SMES, and FB-VR rise remarkably. However, only Li-Ni-Mn-Co moves from inefficient to efficient, raising its median efficiency marginally from 0.98 to 1. In general, the prioritization of environmental indicators causes the efficiency scores of efficient technologies to decrease and that of inefficient technologies to rise. However, these changes are not enough to cause modifications in the relative ranking of the different technologies, which remains unaltered.

Regarding alternatives in the long-term cluster, hydrogen production based on water electrolysis powered with solar (H_2 , WE-Solar) and wind energy (H_2 , WE-Wind), and ammonia production based on water electrolysis powered with solar (NH_3 , WE-Solar), wind (NH_3 , WE-Wind) and hydropower (NH_3 , WE-Hydropower) present a decline in their efficiencies. This happens because increasing the weight of environmental indicators reduces the weight assigned to employment, which is the most favourable indicator for most of these alternatives. Nonetheless, all these technologies remain efficient. In contrast, the rest of the alternatives face an increase in their efficiency scores, although insufficient to make them efficient.

Overall, the list of technologies recommended based on the results from our original DEA is still valid when environmental aspects are placed at the core of the assessment since the relative ranking of the technologies remains unaltered. Further discussion about this alternative study where environmental indicators are prioritized is presented in Appendix A.1.

Alternatively, other stakeholders may argue that the cost of reverting the damage caused by increased environmental impacts is higher than the cost of prevention [120]. To illustrate such an approach, in our second investigation, we monetized the different indicators, translating indicators into a consistent monetary term based on the corresponding externalities. Using monetized indicators in a unit-invariant DEA model, like the one used in this contribution, would result in the same efficiency scores as obtained with the original indicators since using monetization coefficients to transform the indicators is equivalent to changing their units. To overcome this, we avoid DEA and, instead, use the monetized indicators to estimate the efficiency of the DMUs using the basic definition of efficiency, that is, the summation of (monetized) desired outputs minus the summation of (monetized) undesired outputs, divided by the summation of (monetized) inputs. This provides a measure of the absolute efficiency of the technology, which is conceptually different from the relative efficiency score provided by DEA. Combining monetized indicators into a single score is helpful to rank alternatives, nevertheless, opposite to DEA, it does not provide information on how to improve the worst-performing technologies. In addition, it is improbable that two technologies will tie with precisely the same score and, hence, it might be more challenging to decide a threshold below which the remaining technologies should be discarded for further analysis. This issue is solved with DEA, which mathematically classifies all the alternatives between efficient and inefficient). Therefore, we avoid any comparison of the efficiency scores obtained with the two approaches and we only compare the relative ranking achieved by the energy storage options with each of the two methods.

According to the results obtained for fast-response technologies, only flywheel, Na-S, and SMES report a decline in their ranking. Although this ranking degradation is significant for the flywheel, it keeps its position as the best short-term option. The rest of the technologies improve their ranking. For instance, Ni-Cd, which is the second-best option in the original DEA, ranks first in this new analysis. Regarding the alternatives of the long-term cluster, some changes are observed in their relative ranking, but green alternatives still occupy the first positions, and usually green hydrogen alternatives rank better than the green ammonia alternatives. More details are reported in Appendix A.2.

4.6 Conclusions

Storage technologies improve grid flexibility, which is particularly appealing when there is a high share of renewables. However, insufficient attention to energy storage technologies has slowed down their development, hindering, in turn, the penetration of renewables. To unlock this situation, energy storage technologies need to be assessed considering all the sustainability dimensions concurrently to ensure that unsustainable practices in energy storage do not offset the benefits from the increased use of renewables in the grid.

In this contribution, we benchmark energy storage options using DEA, considering uncertainty in the data through the generation of 100 scenarios. Storage options are classified into two clusters according to their response time, the first for fast-response technologies and the second for long-term storage options. Independent DEAs are carried out for each cluster, finding the technologies with the best performance in each situation and providing evidence for policymakers to develop better-informed regulations.

Flywheel, with a median efficiency score of 2 and efficient in 99% of the scenarios, is the most efficient option among fast-response technologies. Since it is a short-term storage technology, it is the recommended choice for power applications such as power quality control. Ni-Cd, Li-ion, and Na-S batteries are standing at the next positions in terms of efficiency. Indeed, these medium-term technologies were found efficient in all or most scenarios and, therefore, should be promoted for applications like electric vehicles, where modular storage technologies are needed. In this case, it is suggested to employ a separator in the battery structure to improve its safety. Fortunately, most of them are well developed and easy to access. Only, Na-S needs further developments to be marketable. Conversely, FB-VR, SMES, and FB-ZB, with efficiencies lower than 0.1, are graded as the most inefficient technologies. For these technologies, quantitative improvement targets are reported to help technology developers improve and make them competitive. For instance, in the case of SMES, controlling energy loss would be key to increasing its performance. Also, in the case of flow batteries, increasing the number of operational cycles is several times recommended. The application of nanomaterials and recently developed membranes are beneficial for this purpose. According to their TRL, these technologies are not entirely developed and still can improve their performance and infiltrate the market. However, even technology like LA that is already developed is deemed inefficient in our evaluation. In such a case, the technology does not have an easy way ahead to improve its performance. Since the indicators influence each other, the developers should avoid worsening other indicators when improving one of them. For this case, the reported safe margin of changes gives insight into the worsening indicators can afford without turning a technology inefficient. We note that, in this contribution, we could not explore the effect of batteries on toxicity and human health owing to the lack of data for some of the options considered. This critical topic could be an object of future research since it might play an important role in shaping technological and political decisions.

Among the 16 long-term storage options evaluated, only ammonia produced from hydrogen obtained by water electrolysis powered by solar energy is efficient in all the scenarios. The most efficient options are green ammonia (median efficiency scores of 1.265 when based on solar and 1.07 if based on hydropower) and green hydrogen (1.09 using solar and 1.07 using wind). Grey hydrogen from coal gasification and from SMR processes are not efficient alternatives in any of the 100 scenarios considered. Apart from these two options, the other options in the long-term cluster emerge as efficient, at least in some scenarios. Again, we report improvement targets to guide developers in enhancing the different technologies. For instance, most options need reductions between 0.55-11.76% in their LCOE, which can be achieved by employing cheaper options like gas turbines instead of expensive fuel cells for gas reconversion, reducing the cost of renewable energies in the case of green alternatives and enhancing the availability and suitability of salt caverns for underground gas storage in the case of blue options. More significant actions are needed for other indicators like energy consumption of non-green hydrogen and ammonia, where technologies should target improvements between 38.45% and 89.29% to become efficient. These can be pursued by avoiding heat loss in reactors. Note, however, that it is expected that improving one of the indicators might affect others: for instance, insulation of reactors will result in a higher LCOE. In addition, the safe margin of change obtained for efficient alternatives reveals that most of them rest on employment generation for being deemed efficient. Despite this, their establishment may be challenging in regions with a high wage rate or lacking skilled laborers. Even in this case, automation may be helpful, and considering that these green alternatives are still at the research step, they have a promising development potential. Blue and green alternatives are close to being marketable according to their TRLs. However, they are not efficient, and they may dominate the market only during a transition period before a clean energy sector is completely developed. Meanwhile, we find that ammonia reveals better or at least the same performance compared with hydrogen. Therefore, when storing energy for the long-term is the target, using hydrogen to produce ammonia is better than its application as an energy storage alternative. Although the results presented are helpful to facilitate technology selection and improvement, each storage technology is especially suited for some specific applications due to its design and characteristics. Therefore, the technologies reported as efficient are not necessarily the best choices for all the applications, and inefficient ones are not completely useless. For a practical application, several additional aspects will affect the project's social, economic, environmental, and technical implications and should be considered before making the final decision. We dealt with some of these concerns by doing further analysis like weighted DEA and monetization. Our results revealed that although the efficiency score and relative ranking of technologies report some changes, still the results obtained by the original DEA are reliable. Other aspects including the location of the storage unit, the availability of raw materials, cost and availability of skilled labors, market energy prices, geographical limitations, deployment and construction time, the technology response time, the complicity of manufacturing, minimum and maximum charging rate, maximum operating temperature, packing issues, ease of installation-operation-and control, needed accessories, ability to join with other technologies, application purpose, commercial availability of technology, its strength and durability, maturity, safety, grid connection impacts, recyclability and after use impacts also should be considered. Therefore, while this study provides a powerful framework for comparing storage technologies considering multiple sustainability dimensions through DEA, more comprehensive evaluations are still necessary. Acknowledging that improving some technologies to make them efficient might take some time or even be impossible in some cases, it is suggested to design energy systems in a way that they do not

depend strongly on storage technologies found inefficient in this contribution. In this context, policies promoting the use of the most efficient technologies through incentives might be as effective as regulations based on the taxation of the poorest performing options while alleviating the direct economic burden placed on companies and citizens. Further, the evaluation of hybrid energy storage technologies is an unexplored necessity that should be considered in future studies.

Nomenclature

Table 3. Nomenclature

Nomenclature	
δ^*	Supper efficiency of DMU _o
ε	Non-Archimedean infinitely small
λ	Intensity vector that reports the weight of each DMU
Λ	Intensity vector that reports the weight of each DMU
τ^*	Efficiency of the DMU _o
CG	Coal gasification
CCS	Carbon Capture and Storage
DEA	Data envelopment analysis
DEDLF	Delivered energy during lifetime
DOD	Depth of discharge
ED	Energy Density
FEDLF	Feed Energy During Lifetime
FTEJ	Full Time Equivalent Jobs
GWP	Global Warming Potential
LCOE	Levelized cost of energy
LHV	Lower heating value
m	Number of inputs
NC	Number of cycles during lifetime of technology
RE	Renewable energy
REC	Rated energy capacity
RTE	Round-trip efficiency
WE	Water Electrolysis
WS	Water Splitting
s_1	Number of desired outputs
s_2	Number of undesired outputs
S_i^-	Slack of inputs in SBM model
S_r^g	Slack of desired outputs in SBM model
S_r^b	Slack of undesired outputs in SBM model
t	Charnes-Cooper linear transformation coefficient
x_{io}	Input i related to the DMU _o
X	Matrix of inputs
y_{ro}^g	Desired output r related to the DMU _o
y_{ro}^b	Undesired output r related to the DMU _o
Y^g	Matrix of desired outputs
Y^b	Matrix of undesired outputs

Abbreviation and full name of technologies and storage options

Table 4. Abbreviation and full name of fast-response technologies

Short-term	
Flywheels	Flywheels
SMES	Superconducting Magnetic Energy Storage
Medium-term	
FB-VR	Flow battery - Vanadium Redox
FB-ZB	Flow battery - Zinc Bromine
LA	Lead-Acid
Li-ion	Lithium-ion
Li-Fe-Ph	Lithium-Ferro-Phosphate
Li-Ni-Mn-Co	Lithium-Nickel-Manganese-Cobalt
Na-Ni-Cl	Sodium-Nickel-Chloride
Na-S	Sodium-Sulphur
Ni-Cd	Nickel-Cadmium

Table 5. Abbreviation and full name of long-term energy storage

H ₂ , CG	Power to H ₂ , Coal Gasification
H ₂ , CG-CCS	Power to H ₂ , Coal Gasification with carbon capture and storage (CCS)
H ₂ , SMR	Power to H ₂ , Steam Methane Reformation
H ₂ , SMR-CCS	Power to H ₂ , Steam Methane Reformation with CCS
H ₂ , WE-Grid mix	Power to H ₂ , Water Electrolysis by Grid mix
H ₂ , WE-Hydropower	Power to H ₂ , Water Electrolysis by Hydropower energy
H ₂ , WE-Solar	Power to H ₂ , Water Electrolysis by Solar energy
H ₂ , WE-Wind	Power to H ₂ , Water Electrolysis by Wind energy
H ₂ , WSCL	Power to H ₂ , Water Splitting by Chemical Looping
NH ₃ , SMR	Power to NH ₃ , Steam Methane Reformation
NH ₃ , SMR-CCS	Power to NH ₃ , Steam Methane Reformation with CCS
NH ₃ , WE-Grid mix	Power to NH ₃ , Water Electrolysis by Grid mix
NH ₃ , WE-Hydropower	Power to NH ₃ , Water Electrolysis by Hydropower energy
NH ₃ , WE-Solar	Power to NH ₃ , Water Electrolysis by Solar energy
NH ₃ , WE-Wind	Power to NH ₃ , Water Electrolysis by Wind energy
NH ₃ , WSCL	Power to NH ₃ , Water Splitting by Chemical Looping

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Declaration of competing interest

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

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4.8 Appendix A: Further analysis

In the evaluation presented in the main manuscript (models M1 and M2), the absence of predefined weights between indicators implicitly considers them equally important. However, in practice, stakeholders might be more concerned about certain facets of the sustainability problem. Bearing this in mind, we next present two additional analyses addressing the same problem of comparing energy storage technologies, but this time using different perspectives reflecting potential concerns from diverse stakeholders. In the first analysis, reported in Appendix A.1, we still use DEA but enforce environmental indicators to be more important than economic and social ones, thus prioritizing cleaner technologies for a sustainability transition. In the second one, provided in Appendix A.2., we explicitly account for the positive and negative externalities that would result from the deployment of each energy storage technology considered in this contribution.

4.8.1 Appendix A.1: Weighted-SBM

Without loss of generality, we explore a hypothetical situation where an environmentally conscious stakeholder assigns 80% of the total weight to environmental aspects and 20% to the rest (economic and environmental). We assume that these weights are divided equally between indicators within each sustainability dimension. For fast-response technologies, this translates to 20% weight for each of the four environmental indicators (i.e., $80/4=20$). For long-term alternatives, each of the three environmental indicators is assigned 26.67% weight (i.e., $80/3=26.67$). The dedicated weight to LCOE and employment in both clusters is 10%, as these are the only indicators in the economic and social categories, respectively. The weights considered are summarised in Table (A.1).

Table (A.1). Predefined weights for indicators of each cluster. LCOE: levelized cost of energy. GWP: global warming potential.

Indicators	Weight of indicators for the fast-response cluster (%)	Weight of indicators for the long-term cluster (%)
LCOE	10.00	10.00
Energy consumption	20.00	26.67
1/Energy density ¹	20.00	-
Water used	20.00	26.67
GWP	20.00	26.67
Employment	10.00	10.00
Total	100.00	100.00

¹This indicator is not considered in the evaluation of long-term energy storage alternatives.

Then, the undesired output slack-base model (i.e., model M1) is modified to consider these weights as parameters. The revised model (model M3 hereafter) is a weighted-SBM model presented in [43] and formulated next.

$$\begin{aligned}
 \tau^* = \min t - \frac{1}{m} \sum_{i=1}^m \frac{w_i^- S_i^-}{x_{i0}} & \quad (M3) \\
 s, t, \quad 1 = t + \frac{1}{s_1 + s_2} \left(\sum_{r=1}^{s_1} \frac{w_r^g S_r^g}{y_{r0}^g} + \sum_{r=1}^{s_2} \frac{w_r^b S_r^b}{y_{r0}^b} \right) \\
 x_0 t = X \Lambda + S^- \\
 y_0^g t = Y^g \Lambda - S^g \\
 y_0^b t = Y^b \Lambda + S^b \\
 w_{i=\text{energy consumption, water used, (1/energy density)}}^- = 0.2 \\
 w_{r=\text{GWP}}^b = 0.2 \\
 w_{i=\text{LCOE}}^- = 0.1 \\
 w_{r=\text{GWP}}^g = 0.1 \\
 S^- \geq 0. \quad S^g \geq 0. \quad S^b \geq 0. \quad \Lambda \geq 0. \quad t > 0,
 \end{aligned}$$

In this model, w_i , w_r^g , and w_r^b are the weights for input i , desired (good) output r , and undesired (bad) output r , respectively, as provided in Table A.1. The rest of the parameters and variables are the same as model M1. Analogous changes can be introduced in the super-efficiency model M2. The weighted undesired output SBM and the weighted super-efficiency model are solved for each DMU in the fast-response and long-term cluster for 100 scenarios. The scenarios were obtained by applying Monte Carlo sampling to the uncertain distributions associated with the sustainability indicators. The resulting median efficiency for each technology is compared with its median efficiency from the original DEA (i.e., equally important indicators) in Figure (A.1) and (A.2), with the former comparing fast-response technologies and the latter benchmarking long-term energy storage alternatives.

Figure (A.1) shows the median efficiency obtained for each technology in the fast-response cluster from both analysis. The Y-axis presents the median efficiency when 80% weight is dedicated to the environmental indicators, while the X-axis presents the median efficiency when the indicators are weighted equally (i.e., the median efficiency from the original DEA). This figure is divided into four quadrants; (i) light green region: the technologies are efficient regardless of the weight considered for the indicators; (ii) dark green region: the fate of the technology is affected by the weight of the indicators, and it is efficient only when the indicators are weighted unequally; (iii) grey region: technologies are always inefficient regardless of the relative importance assigned to the different indicators; and (iv) dark green region: the fate of the technology is affected by the weight of the indicators and is efficient only when all the indicators are considered equally important. Also, using a diagonal line, technologies are classified into two groups: those that report a higher efficiency when no predefined weights are assigned to indicators (i.e., located on the right side of the diagonal), and those that benefit from larger weights to the environmental indicators (i.e., located on the left side of the diagonal).

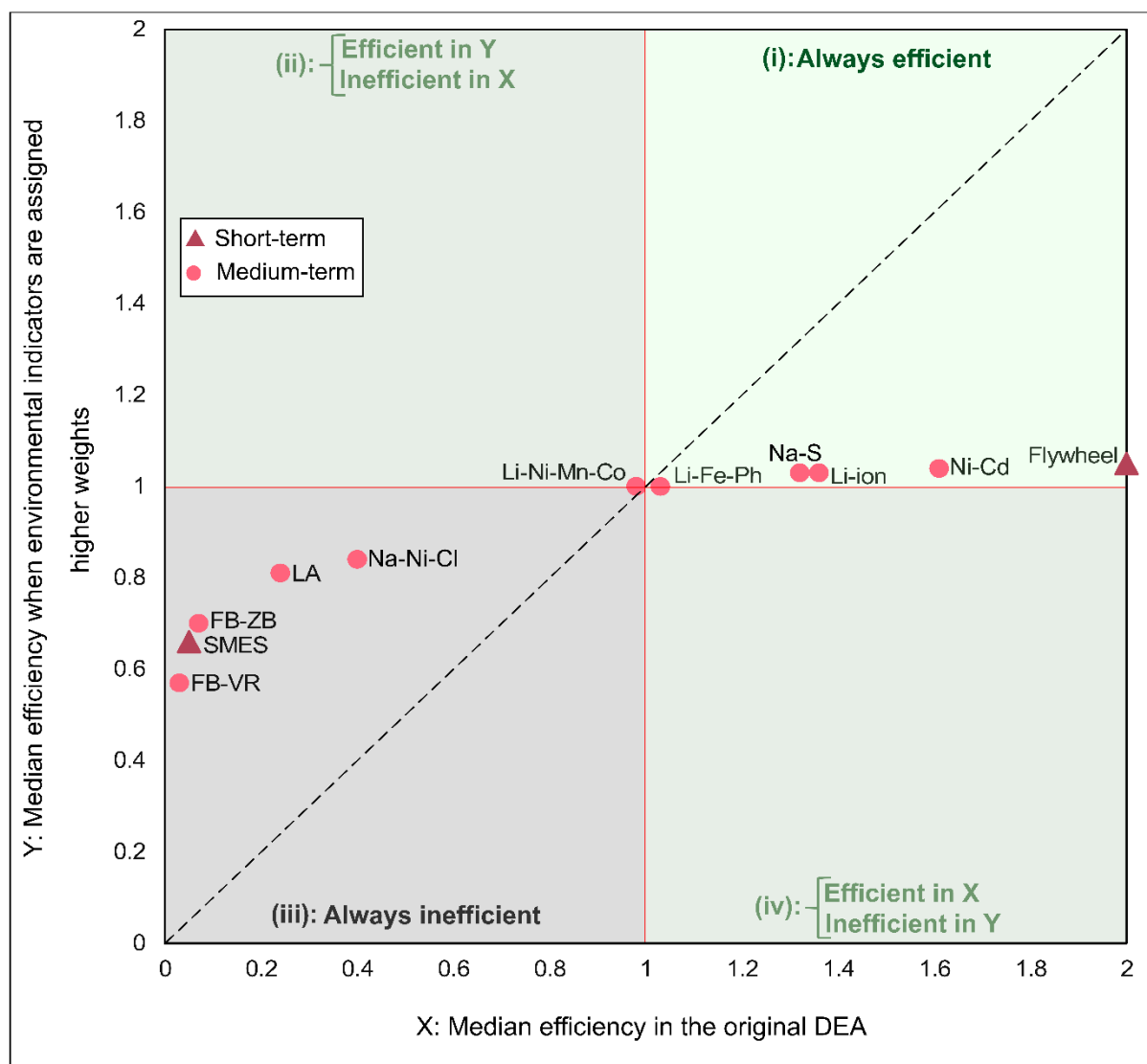


Figure (A.1). Comparing the median efficiency of fast-response energy storage technologies when the indicators are weighted equally and unequally. Grey region: always inefficient, Light green region: always efficient. Dark green region: inefficient when the indicators are equally weighted (i.e., X-axis) and efficient when the environmental indicators are weighted more (i.e., Y-axis), or vice versa.

As Figure (A.1) shows, using higher weights for environmental indicators results in important changes in the efficiency scores obtained. Technologies on the right side of the diagonal, namely flywheel, Ni-Cd, Li-ion, Na-S, and Li-Fe-Ph, see their efficiencies decrease from 2, 1.61, 1.36, 1.32, and 1.03, respectively, to 1.05, 1.04, 1.03, 1.03, and 1. This happens because increasing the weight of environmental indicators is equivalent to decreasing the weight of their most favourable indicator, which, in the case of the flywheel, Ni-Cd, Li-ion, and Na-S, is employment (see Figure 5 for more information). Li-ion and Li-Fe-Ph also rely on their energy density to be efficient. It is an environmental indicator and increasing its weight benefits the efficiency score. However, this benefit is counterbalanced by the other environmental indicators and results in a lower median efficiency score. In any case, all these technologies remain efficient in this analysis, too, which demonstrates they are still robust options with a solid environmental performance.

On the other hand, the technologies on the left side of the diagonal, namely Li-Ni-Mn-Co, Na-Ni-Cl, LA, FB-ZB, SMES, and FB-VR, benefit from increasing the weight of environmental indicators. They improve their median efficiency scores from 0.98, 0.4, 0.24, 0.07, 0.05, and 0.03, respectively, to 1, 0.84, 0.81, 0.7, 0.66, and 0.57. These improvements are enough for Li-Ni-Mn-Co to become efficient. Despite improving their median efficiency scores, the other technologies stay inefficient, although they now have a better chance for competition against efficient technologies. Indeed, using predefined weights in the analysis produced a narrower distribution of efficiency scores than in the original case: from 1.05 (flywheel) to 0.57 (FB-VR), compared to 2 (flywheel) and 0.03 (FB-VR). However, none of the technologies deemed efficient in the original DEA stops being so in this new analysis. From a mathematical point of view, model M1 is a relaxation of model M3 because (implicit) weights can take any value to favour the technology under assessment. Considering that the efficiency scores provided by DEA are relative (and not absolute) efficiency measures, in practice, this means that model M1 can produce more distinct results across the technologies. This is done, for instance, by assigning a high weight to employment for some technologies since this allows them to achieve high-efficiency values. Remarkably, the relative ranking of the technologies is not affected by increasing the weights of environmental indicators, i.e., sorting the technologies from highest to lowest median efficiency scores yields the same result as in the analysis presented in the main manuscript.

We next turn our attention to the long-term energy storage alternatives (Figure (A.2)). Again, the X-axis presents the median efficiency of the original DEA, while the Y-axis reports the median efficiency when 80% weight is dedicated to the environmental indicators. This figure is equivalent to Figure (A.1), with the plotted area divided into four quadrants achieved by the alternatives regarding their efficiency scores (efficient vs inefficient). Similarly, the diagonal divides the alternatives into two groups, with alternatives on the left side of the diagonal benefitting from unequal weights and alternatives on the right side of the diagonal being harmed.

As shown in Figure (A.2), the alternatives on the right side of the diagonal, including green alternatives like hydrogen based on water electrolysis powered with solar (H_2 , WE-Solar) and wind energy (H_2 , WE-Wind), and ammonia based on water electrolysis powered with solar (NH_3 , WE-Solar), wind (NH_3 , WE-Wind) and hydropower (NH_3 , WE-Hydropower) see their efficiencies decline when higher weights are dedicated to the environmental indicators. This change is particularly remarkable for (NH_3 , WE-Solar), with its efficiency score changing from 1.26 to 1.02. Despite this, all of them remain efficient, and this is a piece of evidence that they are reliable choices for environmentally friendly applications.

in their median efficiency compared to the results from the original DEA. This includes all the blue and grey options and power to hydrogen based on water electrolysis using hydropower energy (H₂, WE-Hydropower). Despite this, their improvements are not impressive, and none succeed in becoming efficient. Like fast-response technologies, the difference between the highest and the lowest median efficiency when unequal weights are used is lower (i.e., (1.02-0.73) vs. (1.26-0.23)). Also, in both types of analysis, (NH₃, WE-Solar) has the highest median efficiency, while (H₂, CG) presents the lowest median efficiency. The alternatives selected by the original DEA are attractive when social, economic, and environmental aspects are all essential. At the same time, the efficiency scores of this second “weighted” DEA look more reliable when environmental aspects are the most important.

4.8.2 Appendix A.2: Monetization of the indicators and monetized efficiency

Monetization uses predefined coefficients to translate environmental indicators into monetary terms. These coefficients are lower than one for some indicators and, therefore, decreases their value (e.g., water use, GWP), while the coefficients are greater than one for others, thus increasing the indicator values (e.g., energy consumption, Employment, and 1/energy density). In this way, monetization of the indicators helps to consider their relative importance from an economic point of view [121]. In this contribution, we monetize not only the environmental indicators but also employment. Employment provides the number of full-time equivalent jobs, as expressed in [number of jobs]. For its monetization, an average wage of 123816 \$/year is considered [122], together with a currency exchange rate of US\$=0.85€ [123]. Then, the received wage for 30 years is estimated (i.e., 123816 \$/year·0.85·30 years=3157308). The coefficients used to transform the value of the indicators (i.e., the values reported in Tables 1-2) to their monetary values are presented in Table B.14 of chapter 8. As stated in the main body of the manuscript, using monetized indicators in a unit-invariant DEA model as the one employed in this chapter would not affect DEA results since monetizing the indicators is equivalent to changing their units. Hence, in this case, we avoid the use of DEA and calculate efficiency as the summation of the monetized desired output (i.e., employment) minus the summation of the monetized undesired output (i.e., GWP), divided by the summation of the monetized inputs (i.e., LCOE, energy consumption, energy density, and water used). This provides a measure of the absolute efficiency of the technologies, which is conceptually different from the relative efficiency provided by DEA to the point that it is no longer possible to classify units as efficient or inefficient based on a score of 1 or any other cutoff value. Finally, Figures (A.3) and (A.4) show the results for fast-response and long-term clusters obtained using monetized indicators.

Figure (A.3) depicts the efficiency obtained using monetized indicators (i.e., Y) versus the median efficiency obtained from DEA (i.e., X) for each technology in the fast-response cluster. This figure is divided into two regions using the dashed line. On the left side, technologies are sorted according to their ranking in the original DEA, while on the right side, they are sorted based on their ranking in the monetized analysis. The signs and numbers inside the parenthesis beside the name of technologies introduce the changes in the ranking of technology in Y compared with X. The green line and a (+) sign reports an improvement in the ranking, while a red line and a (-) sign presents falling in the ranking. When the technology reports the same ranking, a blue line and an (=) sign are used.

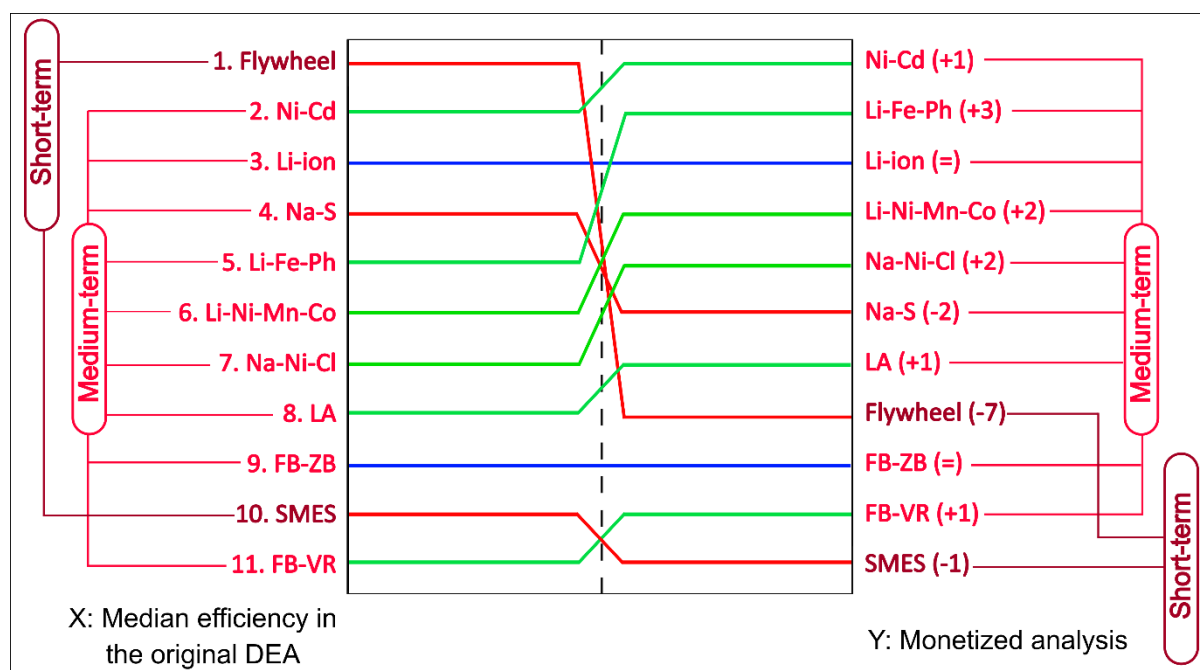


Figure (A.3). Comparing the median efficiency obtained from original DEA using per GJ values of indicators (i.e., X) with the efficiency obtained using monetized indicators (i.e., Y) for fast-response energy storage technologies. Left side: technologies' ranking in X. Right side: technologies' ranking in Y. Short-term: flywheel, SMES. Medium-term: rest of the technologies. The number of positions that each technology climbs (+) or drops (-) in the monetized analysis compared with the original DEA is reported by the numbers in the parenthesis. The (=) presents the case that there is no change in the ranking of the technology. Green, blue, and red lines, respectively, present the climbed, maintained, and dropped ranking.

Although in some cases, the technologies' ranking changes quite a lot in the monetized analysis compared with the original DEA, choices from the original DEA (i.e., flywheel for short-term and Ni-Cd for medium-term) still stand as the preferred options. Despite this, this new analysis unveils the potential of other technologies such as Li-Fe-Ph, which might also have certain opportunities to infiltrate the market.

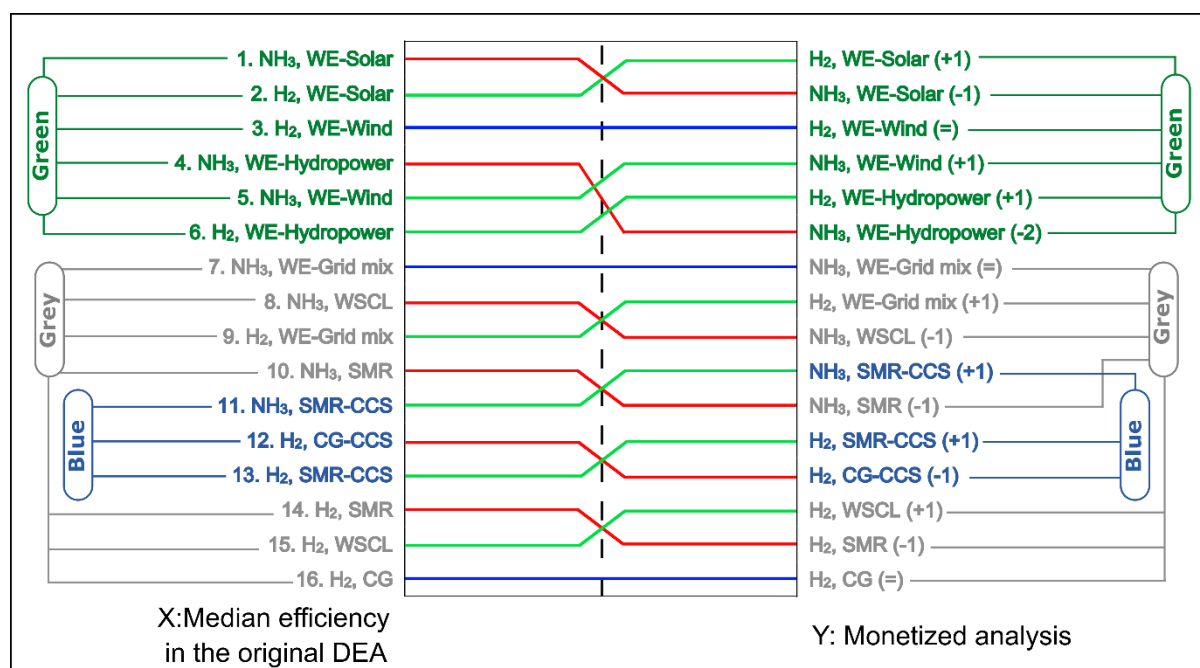


Figure (A.4). Comparing the median efficiency obtained from original DEA using per GJ values of indicators (i.e., X) with the efficiency obtained using monetized indicators (i.e., Y) for long-term energy storage alternatives. Left side: alternatives' ranking in X. Right side: alternatives' ranking in Y. The number of positions that each alternative climbs (+) or drops (-) in the monetized analysis compared with the original DEA is reported by the numbers in the parenthesis. The (=) presents the case that there is no change in the ranking of the alternative. Green, blue, and red lines, respectively, present the climbed, maintained, and dropped ranking. Grey H₂/NH₃: H₂ or NH₃ produced using fossil fuels, Blue H₂/NH₃: H₂ or NH₃ produced using fossil fuels and the emitted carbon captured by CCS, Green H₂/NH₃: H₂ or NH₃ produced using renewable energy sources. WE: Water Electrolysis.

Figure (A.4) is equivalent to Figure (A.3). On the left side of the dashed line, the alternatives are sorted based on their ranking in the original DEA (i.e., X), while on the right side, they are sorted regarding their ranking in the monetized analysis, which is marked by symbol Y. Similarly, an improvement in the ranking is presented by a green line and a (+) sign, the degradation with a red line and a (-) sign, and a maintained position with a blue line and an (=) sign. The number beside the sign accounts for the ranking changed.

As Figure (A.4) shows, several "pairs" swap their ranking. Overall, green alternatives are still the best, but, with externalities, they are sorted according to the power source, with green H₂ always preferred over green NH₃ because of its higher employment generation. For instance, the rankings of (NH₃, WE-Solar) and (NH₃, WE-Hydropower) fall from 1st and 4th, respectively, to 2nd and 6th, while the rankings of (H₂, WE-Solar) and (H₂, WE-Hydropower) climb from 2nd and 6th, respectively, to 1st and 5th. The opposite happens with blue and grey sources, where ammonia processes always rank above their H₂-based counterpart. Also, all processes based on water electrolysis are placed on the top of the list. Overall, these results show significant agreement with those from the original DEA and, therefore, demonstrate the robustness of the conclusions drawn.

Chapter 5

Summary and publications

Chapter 5

Summary

This chapter synthesizes the key findings of our research, emphasizing the challenges, limitations, and future directions identified in the study. Our goal was to provide a comprehensive and accurate analysis of the transition to clean energy technologies (CETs), highlighting the complexities and obstacles encountered along the way. We recognize that addressing these challenges is crucial for researchers and policymakers aiming to navigate the evolving landscape of energy transition.

In the following sections, we outline the main concerns and insights from our study, discuss the limitations faced during the research, and propose areas for future investigation to advance the global effort towards a sustainable and equitable energy future. Through this summary, we aim to encapsulate the essence of our findings, offering a clear pathway for continued exploration and policy development in the realm of clean energy technologies.

5.1 Challenges and Limitations

Although we aimed to do comprehensive and accurate analysis, we could identify the primary challenges and obstacles inherent in our research topics, pertain to data availability, methodological constraints, or conceptual complexities. Awareness of the complexities involved in our research, presented in the following, is a critical step for researchers following similar studies.

- **Dynamic Nature of Parameters:** The projections of technology capacities, market contributions, and material intensities, countries share in materials and technologies development are subject to change over time, introducing uncertainty into the conclusions. Mitigating this uncertainty requires revisiting estimates as newer data become available.
- **Assumption of Friction-Free Market:** Estimates for technology capacity based on material availability rely on the assumption of a friction-free market. Enhancing this assessment involves considering regional availability, transportation requirements, socio-economic factors, and environmental constraints for a more accurate representation of real-world practicalities.
- **Impact of Technological Advancements:** The discovery of new technological designs using alternative materials, material substitution, and recycling practices can significantly impact material demands. Incorporating these considerations into projections can enhance accuracy.
- **Broader Technological Spectrum:** The demand for technologies beyond those evaluated in the study, such as electric motors and fuel cells, also influences material markets. Recognizing and accounting for these broader technological spectrums is essential for a comprehensive understanding of material market dynamics.
- **Replacement of Obsolete CET Facilities:** The replacement of obsolete CET facilities is a minor contributor to material demands in the analysis due to the temporal scope considered. However, their importance may increase post-2050, depending on the lifespan achieved by different

technologies. Addressing this challenge requires forecasting the impact of technology turnover on material demands.

- **Dependence on Selected Indicators:** The results of this DEA study are highly dependent on the selected indicators and their accuracy. Any inaccuracies in these data points can lead to misleading conclusions, emphasizing the importance of reliable and precise data collection. In our study, it we had to omit toxicity due to data limitations. However, most studies are highlighting its importance, specifically in batteries manufacturing and disposal steps.
- **Challenges in Improving Technologies:** Despite the identification of improvement targets for energy storage options, enhancing the efficiency of certain technologies may be challenging due to various factors such as technological limitations, market dynamics, and environmental considerations.
- **Policy Implications:** Decision-makers can consider the findings of this study when formulating policies related to renewable energy deployment, material sourcing, and technological innovation. Their approach should remain unbiased, considering the importance of all energy supply routes including CETs, biorefineries, and fossil fuels. In any case, navigating political landscapes and garnering support for such policies may present significant challenges, requiring further discussions and negotiations with various stakeholders.

5.2 Future Work

Based on our findings, the following areas represent potential for further investigation:

- Streamlining the supply chain of materials necessary for the development of CETs on a global scale.
- Establishing standards and regulations to safeguard the rights of stakeholders impacted by this transition, whether through material contributions or its externalities, and regularly monitoring and updating these measures to ensure equitable distribution of benefits and burdens among nations/actors involved.
- Expanding the parameters included in DEA studies of energy storage options, particularly those pertaining to toxicity and human health, to reevaluate the rankings of options after considering these significant indicators. Also, considering other alternatives such as thermal storage options in the evaluations.

5.3 Conclusions

The transition to CETs stands as a pivotal step towards mitigating the wide-ranging impacts of fossil fuel usage on the environment, health, and social equity. However, this shift necessitates a comprehensive evaluation to ensure its sustainability across various dimensions. Our examination underscored the intricate challenges and opportunities entwined within the transition.

Firstly, we confronted the disconnect between IAM projections and real-world constraints, particularly regarding critical materials essential for CETs. By quantifying tangible challenges like material shortages and technological limitations, we strove to bridge this gap, offering insights crucial for informed decision-making and policy formulation.

Secondly, we delved into the geopolitics surrounding mineral extraction and supply chains, recognizing the imperative of CET development while addressing concerns over human rights and sustainable development goals. Through evidence-based analysis, we unravelled the multifaceted challenges inherent in achieving sustainable energy solutions, highlighting disparities and risks across various dimensions.

Lastly, we explored the role of energy storage technologies in facilitating grid stability and decarbonization, conducting a comprehensive evaluation across economic, environmental, and social dimensions. By providing quantitative insights, we aimed to guide stakeholders towards adopting sustainable energy storage solutions, crucial for realizing a low-carbon, resilient future.

In essence, we believe that our research contributes to a nuanced understanding of the complexities surrounding the transition to clean energy. By shedding light on the challenges, proposing strategies for enhancement, and offering actionable insights, we strived to advance global efforts towards a just, equitable, and sustainable energy transition for all.

In the following, we briefly overview the main concerns addressed in this study:

- **Plausibility of IAM Scenarios:** We found that IAM projections are overly optimistic when considering materials availability. Consequently, we recommend incorporating materials availability constraints into IAM formulations to improve their reliability.
- **Material Supply and Availability:** We provided realistic assessments of material availability, considering production rates and reserve capacities. We identified 16 materials with challenging supply issues. Additionally, the cumulative demand for cobalt, indium, lithium, selenium, silver, and tellurium by 2050 for CETs development may result in using almost their entire current reserve capacity. To address these concerns, increased production rates, mine explorations, and expansion activities should be prioritized.
- **Importance of Materials Recycling:** We determined the minimum recycling rates necessary to align with IAMs' projected capacities. For instance, lithium requires a recycling rate of about 325%, necessitating significant investments in establishing the necessary facilities.
- **Feasibility of Achieving IAM Projections:** Using a bottom-up approach that considers material availability constraints and higher technological resolution, we identified significant shortages in projected clean energy capacities. Depending on the IAM scenario, shortages could exceed 93% for batteries, PV, and wind turbines.
- **Potential Temperature Deviations from Paris Agreement Targets:** Due to shortages in CET capacity development, temperature deviations from the Paris Agreement target could range from 0.11-0.95°C.
- **Externalities of Transition to CETs:** We estimated the energy requirements, GHG emissions, waste rock generation, and human health impacts, associated with materials production. By 2050, the cumulative energy demand is projected to be 55.8 exajoules, equivalent to 61% of global net electricity consumption in 2022. Additionally, cumulative GHG emissions could reach 4.2 Gt, representing almost 11% of 2022 energy-related emissions. Waste rock generation could reach the equivalent of 28 Mount Everests in the worst case, with a median estimate of 58.4 Gt among different scenarios, which is 29.1 times higher than the global municipal solid waste generated in 2022. The cumulative human health impact is projected to be approximately 140 million years, equating to around 2 million human lifetimes, comparable to the total deaths from COVID-19 by May 2024.

- **Highlighting Disparities within Supply Chains:** We used the Gini index to highlight disparities in the supply of required materials and its associated externalities among 169 countries, illustrating the geopolitical significance of this transition. The Gini index for materials supply and its associated externalities is nearly 0.6 or higher, indicating high inequality among countries. Armenia, Australia, Congo, Chile, China, Germany, Japan, and Korea show significant per capita contributions to materials supply or associated externalities.
- **Guiding Policymakers in Fair Allocation:** The insights from our quantitative analysis aim to guide policymakers in identifying responsibilities and equitably distributing the benefits and burdens of the transition. Tracking materials supply routes can help in identifying the benefits and burdens at each step, ensuring fair distribution. For example, if country A uses material m – which significantly impacts GHG emissions – produced in country B, assigning a carbon tax on material m imports to country B could help fund carbon capture initiatives in country A.
- **Need for Comprehensive Assessment of Energy Storage Options:** To unlock the potential of energy storage technologies, we conducted a comprehensive assessment considering all sustainability dimensions. This ensures that unsustainable practices in energy storage do not offset the benefits of increased renewable energy use. Based on our indicators, nickel-cadmium appears attractive among medium-term alternatives, while green ammonia produced by water electrolysis using solar energy is promising among long-term alternatives, though not yet widely marketable. Provided improvement targets that can be very useful for technology developers highlight the significant need to reduce GHG emissions from grey power-to-hydrogen and power-to-ammonia production routes.

5.4 List of publications

5.4.1 Research articles

- F. Rostami, Z.Kis, R. Koppelaar, L. Jimenez, C.Pozo, “Comparative sustainability study of energy storage technologies using data envelopment analysis”, Energy storage materials, DOI: 10.1016/j.ensm.2022.03.026
- F. Rostami, P. Patrizio, L. Jimenez, C. Pozo, N. Mac Dowell, “Assessing the Realism of Clean Energy Projections”, Energy and Environmental Science, revision submitted on 22 May.

5.4.2 Oral presentations

- Fateme Rostami, Richard Cabrera- Jiménez, Laureano Jiménez, Carlos Pozo, “Pioneer Options for Sustainable Energy Storage: A Comparative Study of 25 Alternatives Using Data Envelopment Analysis “, ESCAPE, 2-6 June 2024, Florence, Italy.
- Fateme Rostami, Youssef Elomari, Laureano Jiménez, Carlos Pozo, “A DEEP DIVE INTO ENERGY STORAGE ALTERNATIVES”, ECOS, June 30 – July 5, 2024, Rhodes, Greece.

5.4.3 Poster presentations

- Fateme Rostami, Richard Cabrera-Jimenez, Laureano Jiménez, Carlos Pozo, “Evaluating Sustainability of Energy Storage Options”, SETAC, 5-9 May 2024, Sevilla, Spain.

5.4.4 Workshop presentations

- Fateme Rostami, “A Data-Driven Approach to Facilitate Smart Decision-Making in Comparative Analysis”, TECNATOX, January 30, 2024, Reus, Spain.

5.4.5 Project reports

- Fateme Rostami, Niall Mac Dowell, “Decarbonising materials for the energy system transition”, Clean Air Task Force.

Chapter 6

Supplementary information: Assessing the Realism of Clean Energy Projections

Chapter 6

Supplementary information for chapter 2:

Assessing the Realism of Clean Energy Projections

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6.1 Technologies projected capacity

This section focuses on estimating the projected capacity of clean energy technologies (CETs) from 2020 to 2050 based on the Integrated Assessment Models (IAMs) for 1.5°C and 1.5°C with low overshoot temperature targets. The steps are as follows:

- **6.1.1: Technology selection:** We choose specific CETs along with their diverse types.
- **6.1.2: Exploring IAMs:** We use IAMs, particularly 8 different models including 25 scenarios in total, to estimate the capacity for each selected technology in terms of gigawatts (GW) for 1.5°C and 1.5°C with low overshoot targets.
- **6.1.3: Assigning capacity to each technology type:** IAMs typically provide capacity for an overall technology (e.g., photovoltaics) without specifying individual types (e.g., CdTe, CIGS, and CSi). To address this, we use market contribution data for diverse types of a technology to estimate their allocated capacity.
- **6.1.4: Presenting the capacity values:** We depict the annual and cumulative capacity for each selected technology and compare cumulative values with estimates from other sources such as International Energy Agency (IEA) and the International Renewable Energy Agency (IRENA). This comparative analysis helps realize the additional or reduced capacity needed to meet the temperature targets.

Each step will be elaborated on in the subsequent sections.

6.1.1: Technology selection

The list of technologies under consideration is presented in Table S1. While it appears in the manuscript, we have included it here for the sake of completeness.

Table S1: Considered CETs and technology types.

Technology category	Technology type	Technology full name and description
Battery	LFP	Lithium Ferro Phosphate
	NCA	Lithium Nickel Cobalt Aluminium
	NMC111	Lithium Nickel Manganese Cobalt (composition Ni/Mn/Co = 1/1/1)
	NMC622	Lithium Nickel Manganese Cobalt (composition Ni/Mn/Co = 6/2/2)
	NMC811	Lithium Nickel Manganese Cobalt (composition Ni/Mn/Co = 8/1/1)
	LiS	Lithium sulfide
	LiO	Lithium oxide
Concentrated solar power	FC	Fresnel Collector
	PT	Parabolic Trough
	ST	Solar Tower
Electrolyzers	Alkaline	Alkaline electrolyzer
	PEM	Proton Exchange Membrane electrolyzer
Photovoltaics	C-Si	Crystalline Silicon
	CIGS	Copper Indium Gallium Diselenide
	CdTe	Cadmium-Telluride
Wind turbines	AG	Asynchronous generator
	HTS-DD	High temperature superconductor - direct drive
	SG-E-DD	Synchronous generator - electrically excited - direct drive
	SG-PM-HS	Synchronous generator - permanent magnet - high speed gear
	SG-PM-MS	Synchronous generator - permanent magnet - middle speed gear
	SG-PM-DD	Synchronous generator - permanent magnet - direct drive

6.1.2: Exploring IAMs

Acknowledging that each IAM possesses unique scenario designs and technological resolutions, our analysis encompasses multiple IAMs to capture a broader spectrum of perspectives and account for variations in model assumptions. Specifically, we include eight distinct IAMs, encompassing a total of 25 scenarios which are presented in Table S2.¹

The anticipated capacity for concentrated solar power systems (CSP), photovoltaics (PV), and wind turbines, as projected by IAMs, is generally based on their GW capacity. However, IAMs do not provide a direct projection for the capacity of batteries and electrolyzers in GW. Furthermore, IAMs provide cumulative capacity for CSP, PV, and wind, while our analysis requires annual capacity values. To address these discrepancies, additional calculations were performed, as explained next.

Table S2. Employed IAMs and scenarios under the "Below 1.5" and "1.5 low overshoot" targets.¹

Model	Scenario	Technologies					
		Battery (Stationary)	Battery (EV)	CSP	Electrolyzer	PV	Wind
GCAM 4.2	SSP1-19				√	√	√
IMAGE 3.0.1	IMA15-AGInt			√	√	√	√
	IMA15-Def			√	√	√	√
	IMA15-Eff			√	√	√	√
	IMA15-LiStCh			√	√	√	√
	IMA15-Pop			√	√	√	√
	IMA15-TOT			√	√	√	√
	SSP1-19				√	√	√
MERGE-ETL 6.0	DAC15_50				√	√	√
MESSAGE-GLOBIOM 1.0	ADVANCE_2020_1.5C-2100			√		√	√
	EMF33_1.5C_cost100					√	√
	EMF33_1.5C_full					√	√
	SSP1-19				√	√	√
	SSP2-19				√	√	√
MESSAGEix-GLOBIOM 1.0	Low Energy Demand	√	√	√	√	√	√
POLES ADVANCE	ADVANCE_2020_1.5C-2100			√		√	√
REMIND-MAGPIE 1.7-3.0	PEP_1p5C_red_eff	√	√	√	√	√	√
	SMP_1p5C_Def	√	√	√	√	√	√
	SMP_1p5C_lifesty	√	√	√	√	√	√
	SMP_1p5C_regul	√	√	√	√	√	√
	SMP_2C_Sust	√	√	√	√	√	√
	SMP_1p5C_Sust*	√	√	√	√	√	√
	SMP_1p5C_early*	√	√	√	√	√	√
WITCH-GLOBIOM 4.4	CD-LINKS_NPi2020_1000			√		√	√
	CD-LINKS_NPi2020_400			√		√	√

* Scenarios belonging to the "Below 1.5" target.

Each model and scenario contribute to a broader understanding of potential futures and informs policy discussions. Awareness of the assumptions behind these scenarios, can provide insights into their effectiveness and feasibility.¹

- GCAM 4.2, scenario SSP1-19 (Sustainability – Taking the Green Road):

This scenario envisions a gradual shift toward a sustainable path emphasizing inclusive development, improved global commons management, demographic transition, and reduced inequality. It focuses on human well-being, low material growth, and lower resource and energy intensity.

- IMAGE Model:

IMA15AGInt: Assumes high agricultural yields and intensified animal husbandry globally.

IMA15-Def: Implements climate policy through a uniform carbon tax in all regions and sectors from 2020 onward.

IMA15-Eff: Rapid application of best-available technologies for energy and material efficiency.

IMA15-LiStCh: Promotes a lifestyle change towards lower greenhouse gas (GHG) emissions, including dietary shifts and reduced use of CO₂-intensive transport.

IMA15-Pop: Based on SSP1 with low population growth projections.

IMA15-TOT: Combination of all the above options.

- MESSAGE-GLOBIOM 1.0 Model:

ADVANCE_2020_1.5C-2100: Strengthened ambition post-2020 to align with a long-term target of limiting warming to 1.5°C by 2100.

EMF33_1.5C_cost100 and EMF33_1.5C_full: Consider bioenergy technologies, such as Bio Energy with Carbon Capture and Storage (BECCS), Cellulosic fuels and Hydrogen.

SSP1-19: Choosing the Green Pathway (Minimal challenges to mitigation and adaptation) the global trajectory gradually veers towards sustainability, with a pervasive shift emphasizing inclusive development within perceived environmental limits. Progress in managing shared resources steadily enhances, while investments in education and healthcare accelerate demographic shifts. Economic priorities broaden to prioritize human well-being over mere growth. A growing commitment to development goals leads to decreased inequality both among and within nations. Consumption patterns favour minimal material growth and reduced resource and energy usage.

SSP2-19: In a Middle-of-the-road scenario (with moderate challenges to mitigation and adaptation), global trends in social, economic, and technological spheres remain relatively stable, aligning closely with historical patterns. Development and income growth vary across nations, with some countries achieving notable progress while others struggle to meet expectations. Efforts by global and national institutions to address sustainable development goals are ongoing but slow-moving. While environmental degradation persists, there are some signs of improvement, and overall, there's a gradual decline in resource and energy consumption. Global population growth maintains a moderate pace, reaching a plateau in the latter half of the century. Income inequality persists or improves at a sluggish rate, and challenges in reducing vulnerability to societal and environmental shifts persist.

- MESSAGEix-GLOBIOM 1.0, scenario LowEnergyDemand:

Limits global mean temperature increase to 1.5°C and achieves remarkable co-benefits for other sustainable development goals.

- REMIND-MAGPIE 1.7-3.0:

PEP_1p5C_red_eff: Scenario with a carbon budget of 400 Gt CO₂ from 2011-2100, reduced availability of carbon dioxide removal (CDR), and comprehensive carbon pricing.

SMP_1p5C_Def, SMP_1p5C_Sust, SMP_1p5C_early, SMP_1p5C_lifesty, SMP_1p5C_regul: Various scenarios with a 400 Gt CO₂ budget from 2011-2100, each emphasizing different policy approaches (default carbon pricing, sustainability policies, early action, lifestyle changes, regulation policies).

SMP_2C_Sust, SMP_2C_early: Scenarios with a 1000 Gt CO₂ budget from 2011-2100, focusing on sustainability and early action policies to limit warming to 2°C.

- WITCH-GLOBIOM 4.4:

CD-LINKS_NPi2020_1000, CD-LINKS_NPi2020_400: Transition scenarios from a New Product Introduction (NPi) scenario until 2020 to globally cost-effective carbon budget implementation for the period 2011-2100 (1000 Gt CO₂ for 2°C limit, 400 Gt CO₂ for 1.5°C limit).

6.1.2.1: Photovoltaics, concentrated solar power systems, and wind turbines

We extracted cumulative PV capacity data from 8 IAMs, including 25 scenarios, covering years 2005 to 2050 in five-year intervals (e.g., 2020, 2025, 2030, ...). The process to estimate the capacity added annually involved several steps:

- We created a plot of cumulative capacity against years and extracted the cumulative capacity for the remaining years (e.g., 2021, 2022, ...), since neither linear nor nonlinear regression proved to be a suitable fit.
- By calculating the capacity difference between consecutive years, we determined the capacity added annually.
- We estimated the Replaced Capacities (RC) resulting from the retirement of Previously Installed Capacities (PIC) for each year (n), assuming a 30-year lifespan for a typical PV panel, and using Eq. S1. Note that, in this analysis, we are investigating the period from 2020 to 2050. However, to estimate the required replacements, we extracted data from as early as 2005, which is the first year that IAMs have some capacity projections.

$$RC_{(n + \text{lifespan})} = PIC_n \quad \forall n \quad (S1)$$

- The total annual added capacity was then derived by summing the estimated annual capacity values from step two and the replaced capacities from step three.

We followed the same approach for concentrated solar power systems and wind turbines, considering a lifespan of 30 years.

While most IAM scenarios provide capacity projections for these technologies in GW, four of them - DAC15_50 from MERGE-ETL 6.0 model, EMF33_1.5C_cost100 and EMF33_1.5C_full from MESSAGE-GLOBIOM 1.0 model, and LowEnergyDemand from MESSAGEix-GLOBIOM 1.0 model - offer projections in EJ/yr. Therefore, for these scenarios, we initially divide the provided projections by the energy delivered annually from each of these technologies. Details on estimating the delivered energy for these technologies are provided in section 6.4.1 (Eq. S27).

6.1.2.2: Batteries used for stationery and mobility applications

We distinguish between batteries used for stationery and mobility applications. For the former, we extracted Annual Investment (AINV) data for electricity storage between 2015 and 2050 from MESSAGEix-GLOBIOM 1.0 and REMIND-MAGPIE 1.7-3.0 models including 8 scenarios (see Table S2). These data are expressed in billions of US\$2010 per year and provided for five-year intervals (e.g., 2020, 2025, 2030, ...). Values for the remaining years were estimated using linear regression. Since batteries are just one alternative among other energy storage options, these values are multiplied by $Share^{BAT}$, providing the share of batteries in electricity storage [%]^{2,3}. Then, we converted the resulting values to current € (2023), considering appropriate currency conversion (Con, [€/USD]⁴), and, subsequently, translated them to energy storage capacity using the price of a typical battery ($PRICE^{BAT}$, [€/Wh]). Finally, we transform these values into power capacity using the ratio between the power density (PODENS, [W/kg]) and the energy density (ENDENS, [Wh/kg]). The overall calculation used to obtain the capacity installed annually based on each IAMs scenario for batteries in year n ($CC_{n,s}^{BATSTO}$, [W]) is given by Eq. S2.

$$CC_{n,s}^{BATSTO} = AINV_{n,s}^{STO} \cdot Share^{BAT} \cdot Con \cdot \frac{1}{PRICE^{BAT}} \cdot \frac{PODENS}{ENDENS} \quad \forall n=2020, \dots, 2050, s \quad (S2)$$

Values for battery price (e.g., 200 euros/kWh), power density (e.g., 750 W/kg), and energy density (e.g., 250 Wh/kg) are sourced from the literature^{2,3}. It is important to highlight that power and energy density exhibit considerable variability. For instance, power density varies within the range of 50-2000 W/kg, while energy density changes from 150 to 350 Wh/kg³. For our calculations, we opted for 750 W/kg for power density and 250 Wh/kg for energy density, aligning with the characteristics of batteries used in power applications and electric vehicles. Importantly, as will be discussed in section 6.2.1, selected values do not impact the estimated demand for materials. Still, accounting for these ranges allows to assess uncertainties in installed capacities. These are reported as error bars in Figures S1 and S2, where we compare the power capacity across different technologies.

Replaced capacities for batteries were calculated assuming a 15-year lifespan⁵ (Eq.S1). Hence, the total capacity added is determined by adding the replaced capacities to the newly installed annual capacities⁶. Note that in this case data are available since 2015.

In addition to its primary role in electricity storage, batteries are anticipated to play a crucial role in electric mobility. As outlined by the European Technology and Innovation Platform on Batteries (2020)⁷, there is a notable shift in the ratio of battery utilization for electric mobility compared to its application in energy storage ($\frac{BAT^{EV}}{BAT^{STO}}$ in Eq. S3). This ratio is projected to transition from approximately 23 in 2020 to 7.6 in 2025. Utilizing these varying ratios over time, and the capacity of batteries for energy storage determined previously, we calculated the capacity of batteries required for electric mobility ($CC_{n,s}^{BATEV}$) up to 2025 (Eq. S3).

$$CC_{n,s}^{BATEV} = CC_{n,s}^{BATSTO} \cdot \frac{BAT^{EV}}{BAT^{STO}} \quad \forall n \leq 2025, s \quad (S3)$$

Based on the global electric vehicle outlook⁸, the number of electric vehicles (EV) on the road was approximately 10 million in 2020. According to the Energy Technology Perspectives report, the

projected manufacturing output for EV is 60 million units by 2030 and increases to 90 million by 2050⁹. These estimations align with the 1.5°C target.

Having the $CC_{n,s}^{BATEV}$ for 2020 from Eq.S3, as well as the Number of Electric Vehicle (NEV) in that year, we assumed a proportional ratio to estimate the capacity of batteries used in EV for 2030 and 2050 (Eq. S4-S5). Then, we employed a linear regression to estimate the capacity for intermediate years. Subsequently, we calculated the required replacements using Eq. S1, and added them to the annual capacities of new batteries to determine the final capacity added each year.

$$CC_{2030,s}^{BATEV} = CC_{2020,s}^{BATEV} \cdot \frac{NEV_{2030}}{NEV_{2020}} \quad s \quad (S4)$$

$$CC_{2050,s}^{BATEV} = CC_{2030,s}^{BATEV} \cdot \frac{NEV_{2050}}{NEV_{2030}} \quad s \quad (S5)$$

Acknowledging that these ratios may not necessarily yield a capacity value in alignment with the 1.5°C target, we employ them due to the absence of better data.

6.1.2.3: Electrolyzers

Under the secondary energy category, IAMs provide data on Annual Production (APROD) of hydrogen through electrolyzers between 2020 and 2050, with measurements given in [EJ/year] in five-year intervals, for each of the scenarios. Then, the capacity of the electrolyzers in year n and based on IAMs scenario s ($CC_{n,s}$, [W]) is determined using Eq. S6.

$$CC_{n,s}^{ELCTZ} = APROD_{n,s}^{H_2} \cdot \frac{1}{LHV^{H_2}} \cdot \frac{1}{ENGEN^{ELCTZ}} \cdot \frac{1yr}{365d} \quad \forall n, s \quad (S6)$$

Here, $CC_{n,s}^{ELCTZ}$ is the capacity installed for electrolyzers in year n according to IAMs scenario s [GW] and LHV^{H_2} is the lower heating value of hydrogen [EJ/kg H₂]. Then, $ENGEN^{ELCTZ}$ is the hydrogen generation capacity of a typical electrolyzer [kg H₂/day·GW]. We acknowledge this value changes in a range for different types of the electrolyzers, so we considered it equal to 400 kg H₂/day·MW, which is a valid values for both, alkaline and PEM electrolyzers¹⁰.

In all IAM scenarios, electrolyzer development starts mainly after 2030 with very minor values, and given its lifespan of more than 10 years, the replaced capacity before 2050 is negligible. Therefore, Eq.S6 directly provides the total capacity added annually.

6.1.3: Assigning capacity to each technology type

IAMs provide capacity projection for each technology but they do not distribute it among different technology types owing to a low technological resolution. Therefore, we employed the potential market share evolution of different technology types, as reported by the German Aerospace Centre¹¹, to allocate the total capacity projected for each technology to their respective types. Two different market contribution scenarios are available in the report, one based on a “continued market trend” and another based on a “technological change market trend” for technologies deployment and diffusion. The former trend considers a smooth evolution of technologies, while the later one assumes that sudden technological changes might occur. Eq. S7 provides the details of the calculations, while

Tables S3-S4 present the market contribution values for each technology (T) and its respected types (t)¹¹.

$$CCI_{t,n,s,k}^T = CC_{n,s}^T \cdot MC_{t,n,k} \quad \forall n, k, t \in TT_T, s, T = \{BAT, CSP, ELECTZ, PV, WIND\} \quad (S7)$$

Here, $CCI_{t,n,s,k}^T$ is the capacity installed for individual type t of technology category T in year n according to IAMs scenario s and market trend k [GW], $CC_{n,s}^T$ is the capacity installed for technology category T in year n and according to IAMs scenario s [GW], and $MC_{t,n,k}$ is the market contribution of technology type t in year n according to market trend k [%]. The relationship between technology types t (e.g., SG-E-DD wind turbine) and technology categories T (e.g., wind turbines) is given by set TT_T , providing the technologies of type t that belong to category T .

Table S3: Market contribution of different technology types based on continued market¹¹.

Technology	Type	2020	2030	2040	2050
Battery (EV)	LFP	11	5	3	0
	NCA	13	8	13	13
	NMC111	20	0	0	0
	NMC622	50	32	20	15
	NMC811	6	55	64	72
Battery (Stationary)	LFP	39.8	39.8	39.7	39.7
	NCA	0	0	0	0
	NMC111	23.9	0	0	0
	NMC622	13.3	16.7	12.5	6.63
	NMC811	3.3	33.6	37.9	43.8
	Non lithium types	19.7	9.9	9.9	9.9
Concentrated solar power	FC	5	5	5	5
	PT	90	90	90	90
	ST	5	5	5	5
Electrolyzer	Alkaline	50	42	40	35
	PEM	50	58	60	65
Photovoltaic	C-Si	94	94	94	94
	CIGS	1	1	1	1
	CdTe	5	5	5	5
Wind turbine	AG	15	18	16	14
	SG-E-DD	57	50	50	50
	SG-PM-HS	28	30	31	31
	SG-PM-MS	0	2	3	5

Table S4: Market contribution of different technology types based on technological change trends¹¹.

Technology	Types	2020	2030	2040	2050
Battery (EV)	LFP	9.8	4.8	0	0
	NCA	14.7	10.1	5.6	0
	NMC111	25.5	0	0	0
	NMC622	44.5	27.8	10.9	0
	NMC811	5.5	47.9	32.7	0
	LiS	0	9.4	49.4	91.4
	LiO	0	0	1.4	8.6
Battery (Stationary)	LFP	39.1	22.3	20.3	19.9
	NCA	0	0	0	0
	NMC111	23.9	0	0	0
	NMC622	13.2	8.14	4.9	2.09
	NMC811	3.2	16.6	14.7	15.41
	Non lithium types	20.6	53	60.1	62.6
Concentrated solar power	FC	5	7	12	15
	PT	90	75	60	45
	ST	5	18	28	40
Electrolyzer	Alkaline	50	25	15	0
	HT SOEL (Yttrium)	0	3	12	25
	PEM	50	72	73	75
Photovoltaic	C-Si	96	83	73	63
	CIGS	1	5	9	12
	CdTe	3	12	18	25
Wind turbine	AG	12	7	3	1
	SG-E-DD	28	15	7	2
	SG-PM-HS	50	50	45	50
	SG-PM-MS	0	8	8	10
	HTS-DD	0	0	0	12
	SG-PM-DD	10	20	37	25

6.1.4: Presenting the capacity values

Figures S1 and S2, respectively, depict the anticipated annual and cumulative capacity of CETs until 2050. Note that since we use the annual capacities of CETs in our calculations, we provide their median values obtained from 25 scenarios. In addition, we compare our estimates with data from reports from the International Energy Agency (IEA)^{7,12–17}, the International Renewable Energy Agency (IRENA)¹⁷, or any other source where projections are available. As depicted in Figure S2, the demand for batteries is predominantly influenced by their usage in electric vehicles. Furthermore, our estimated ranges based on IAMs projections align with the data reported from other sources.

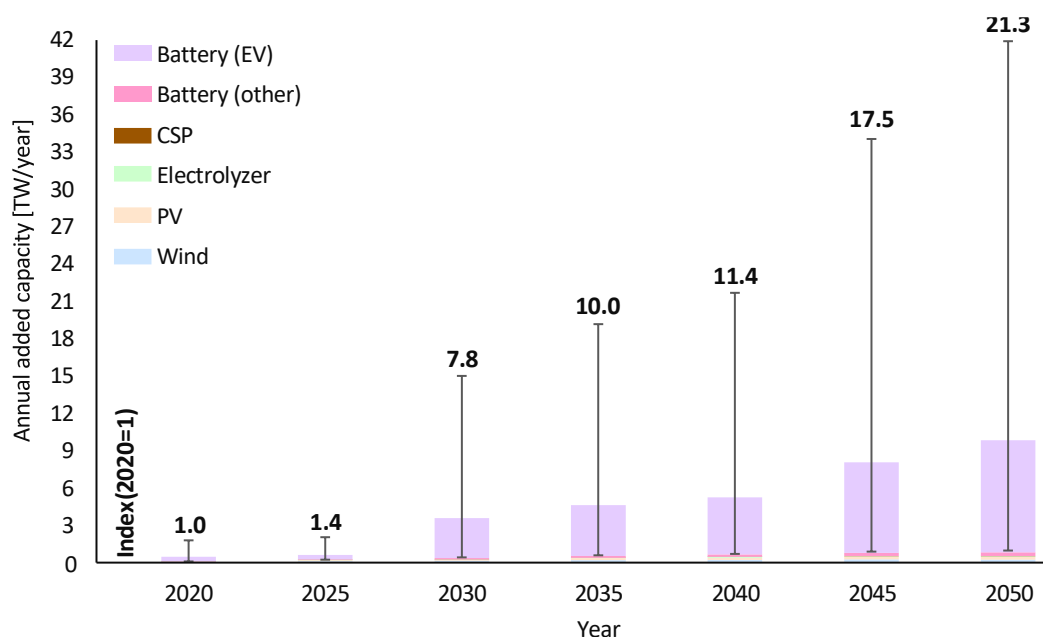


Fig.S1 Projections for the aggregated capacity of clean energy technologies added annually based on IAMs scenarios (Table S2). The numbers on top of the bars present the ratio of capacity added in each year over the capacity added in 2020. The error bars present the variations in the capacity added for batteries, depending on the battery characteristics, as discussed in section 6.1.2.2.

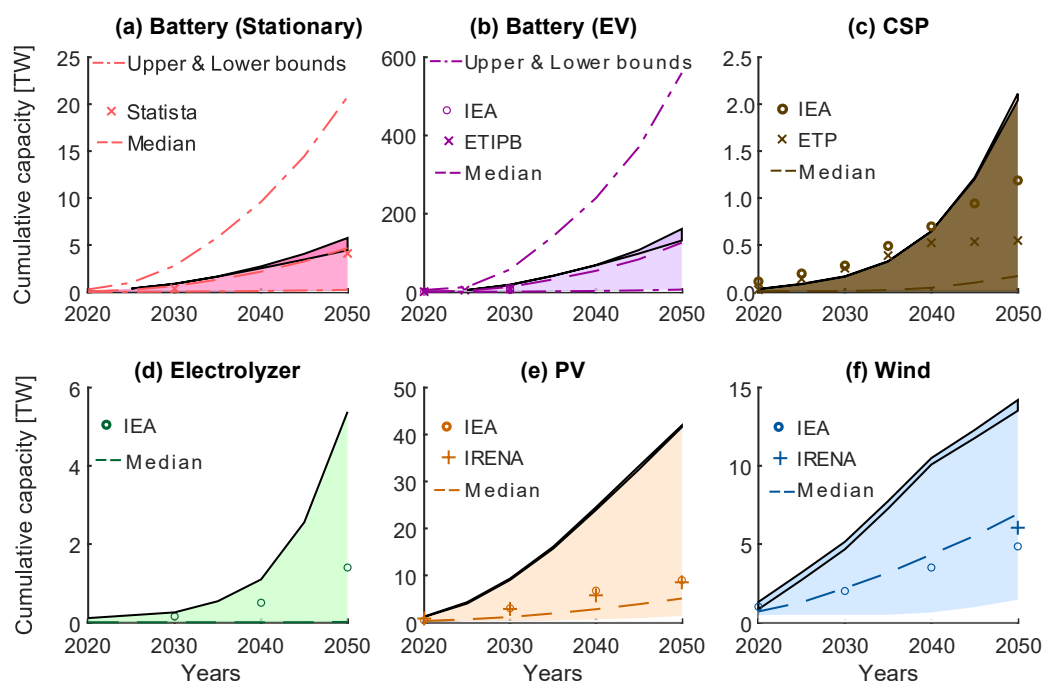


Fig.S2 Cumulative projected capacity of clean energy technologies based on IAMs (Table S2). For each technology, the projected capacity in 2020 is used as a base to estimate the ratio of projected capacity in 2050 over it, except for the electrolyzers, since their development starts mainly after 2030. In addition, the replaced capacity of each technology is presented in its panel by a dashed area. Markers in each panel represent data from additional sources used for comparison: circles show IEA projections,^{14,18,19} plus signs denote IRENA data,¹⁷ and cross signs correspond either to data from the European Technology and Innovation Platform for Battery (ETIPB),⁷ from Statista (for stationary batteries projections),¹³ or from the Energy Technology Perspectives (ETP) (for CSP).¹² Dashed lines present the median of projections. Notably, long dash dot lines present the upper bound and lower bound capacity for batteries (more on this can be seen in section 6.1.2.2).

6.2 Materials demand estimation

This section is dedicated to estimating materials demand associated with the projected capacity of CETs from 2020 to 2050, as per IAMs and for selected temperature targets. The outlined steps are as follows:

- **6.2.1: Material intensities:** We conducted an extensive literature review to compile current intensity values (i.e., ton/GW capacity) for 36 different materials across various technology types. We also included the effect of learning curves to estimate a decrease in material intensity values over time.
- **6.2.2: Resulting classifications:** We derived material demand estimates for four distinct classes. Two market contribution scenarios to estimate allocated capacity for technology types (Continued and Technological change, section 6.1.3), and two material intensity scenarios (Base and Learning). These are combined by 25 IAM scenarios (Table S2).
- **6.2.3: Calculation of material demands:** We multiplied the capacity allocated to each technology type by its respective material intensity values to derive the material demands. Specifically, we estimated material demand values for 25 IAM scenarios, providing detailed discussions.
- **6.2.4: Current production rate of materials, their reserve capacities, and recycling rate:** We provided a scale to the demand values estimated by comparing them with their current production rates, illustrating how demand will evolve over time.
- **6.2.5: Exploring the possibilities of by-products:** For materials generated as byproducts of others, we estimated their production by considering their relative concentration in the ores.
- **6.2.6: Estimated material demands:** We compared the estimated demand for materials over time with (i) their current production rate, and (ii) their current (i.e., 2020 due to data limitations) demand. Results for materials whose ratios are greater than one in both cases are discussed in the manuscript, while, in this section, we focus on the remaining materials. In addition, median values for material demands across scenarios in selected years are also presented. Results are compared with those from similar studies for validation.
- **6.2.7: Links between problematic materials and technology types:** We explored the relationship between problematic materials and the technology types expected to dominate the 2050 market.
- **6.2.8: Demand-to-reserves comparison:** Additionally, we provide an analysis of demand-to-reserves capacity ratios for problematic materials where this ratio approaches or exceeds one.

6.2.1: Material intensities

In this step, material intensity values for each technology type are collected. Technology learning curves are then used to estimate the impact of technology evolution. Table S5 provides a list of the materials considered, while a summary of material intensity values is presented in Tables S6-S8. Note that, for the case of PV and wind turbines, material intensity estimations consider the cabling requirements to connect the PV panels or the wind turbines to the grid²⁰. Where more than a single value was available, we used the average of reported values. Additionally, material intensity values for some materials change over time due to the effects of technology learning curves, specifically for PV panels and wind turbines. However, for the types of batteries and electrolyzers included in our assessment, no significant changes are reported in their material intensities^{11,20}.

The values for aluminium, cadmium, concrete, copper, gallium, glass, indium, nickel, plastic, selenium, silicon, silver, steel, and tellurium used in PV panels, and Dy, Mn, Nd, Ni, and V used in wind turbines, are updated for the next decades using the learning curves of the technologies as reported in Tables S7 and S8 ^{11,20}. Apart from these, the intensity of the iridium used in PEM electrolyzers changes from 0.88 ton/GW in 2020 to 0.20 ton/GW in 2030, 0.05 ton/GW in 2040 and stays constant until 2050. For platinum used in the same technology, the material intensity changes from 0.25 in 2020 to 0.07 in 2030, 0.04 in 2040 and stays constant until 2050 ¹¹. Similarly, the lithium used in LFP batteries drops from 43 ton/GW in 2020 to 40 ton/GW in 2050, while nickel intensity in NMC622 batteries changes from 197 ton/GW in 2020 to 141.5 ton/GW in 2050.

It is essential to note that material intensities for batteries is commonly expressed in ton/GWh in the literature. To convert these values to ton/GW, we multiply them by the energy density of batteries (e.g., 250 Wh/kg) and then divide it by their corresponding power density (i.e., 750 W/kg) ³. It is worth emphasizing that, for estimating the capacity of batteries in GW, we multiplied the available data by power density and then divided the result by the corresponding energy density, as detailed in section 6.1.2.2. Therefore, the final multiplication of capacity time intensity cancels out the power and energy density values. Ultimately, the material demand value, presented in tons, remains independent of these values.

In addition to the values provided in Table S6, we use the following values for CSP technologies: FC require 2045 [ton Mn/GW], 471 [ton Ni/GW], 31 [ton Ag/GW] and 2 [ton V/GW]; PT need 2047 [ton Mn/GW], 471 [ton Ni/GW], 25 [ton Ag/GW] and 1.9 [ton V/GW]; and ST demand 5600 [ton Mn/GW], 1785 [ton Ni/GW], 36 [ton Ag/GW] and 1.7 [ton V/GW].^{11,20}

Table S5: List of the materials considered and their symbols.

Materials	Symbols	Materials	Symbols	Materials	Symbols	Materials	Symbols
Activated carbon	C	Gallium*	Ga	Manganese	Mn	Silica ^a	Sil.
Aluminium	Al	Glass ^a	Gla.	Molybdenum	Mo	Silicon	Si
Cadmium	Cd	Glass/Carbon composites/fiberglass ^a	GCC	Neodymium*[R]	Nd	Silver	Ag
Cement ^a	Cem.	Gold	Au	Nickel	Ni	Steel ^a	Ste.
Chromium	Cr	Graphite ^{a, *}	Gra.	Plastic ^a	Pla.	Tellurium	Te
Cobalt*	Co	Indium*	In	Platinum*[P]	Pt	Terbium*[R]	Tb
Concrete ^a	Con.	Iridium*[P]	Ir	Praseodymium*[R]	Pr	Titanium*	Ti
Copper	Cu	Iron	Fe	Resin PPS ^b - Glass fiber ^a	Res.	Vanadium*	V
Dysprosium*[R]	Dy	Lithium*	Li	Selenium	Se	Zinc	Zn

*: Critical material, *[R]: Critical and rare earth element (REE), *[P]: Critical and platinum group metal (PGM) ²¹.

^aThe presented symbol is not a standard symbol assigned to this material. It is defined by the author for the sake of simplicity in later referring.

^bPPS: Polyphenylene Sulfide.

Table S6: Material intensities for CETs, except for CSP^{a,b,c}.

Technologies	Battery							Electrolyzer		PV			Wind				
Materials	LFP	NCA	NMC 111	NMC 622	NMC 811	LiS	LiO	Alkaline	PEM	CSi	CIGS	CdTe	AG	HTS-DD ^d SG-E-DD ^d	SG-PM-HS	SG-PM-MS	SG-PM-DD
Ag										18							
Al	353	539	451	409	366	353	353	75	65	7,500	7,500	7,500	4,990	700	1,600	1,600	500
Au									0.29								
C									13								
Cd											1	47					
Cem. ^a										7.7	7.7	7.7	55.3	48.5	54.3	54.3	32.0
Co	0	190	178	67	47	0	120										
Con. ^a										60.7	60.7	60.7	420	369	413	413	243
Cr														525	580	580	525
Cu	46	55	62	59	56	46	46	333	11	4,600	4,600	4,600	1,764	5,000	950	950	3,000
Dy														6	4.3	5	17
Fe ^a														20.1	20.8	20.8	20.1
Ga											4						
GCC ^a													7.7	8.1	8.1	8.1	8.1
Gla. ^a										46.4	46.4	46.4					
Gra.	274	352	325	340	354	274	274	72									
In											18	8					
Ir									0.88								
Li	43	60	50	57	57	120	53										
Mn		129	175	63	54	0	105						780	790	550	500	600
Mo														109	119	119	109
Nd														28	35	42	155
Ni	23	190	181	197	375	0	193	3167		2			410	340	420	442	410
Pla.	24	30	30	29	28	24	24	130		8,600	8,600	8,600	7,817	7,817	7,817	7,817	7,817
Pr														9	4	4	35
Pt									0.25								
Res.									136								
Se											39						
Si										4,000							
Sil.	4	7	7	7	7	6	6										
Ste.	11	13	14	14	14	11	11		1,928	67,900	67,900	67,900	124,654	66,000	107,000	107,000	119500
Tb														1	1	1	7
Te												51					
Ti									34								
V															90	90	90
Zn ^a													5,500	5,500	5,500	5,500	5500
Ref.	11,22,23							11,23,24		6,11,20,22			6,11,20,22,25,26				

^aValues are in [ton/GW capacity], except for cem., con., gla., GCC, Fe, and Zn which are in [ton/MW capacity].

^bMaterials complete name is presented in Table S5.

^cValues for CSP technology are provided in text before Table S5.

^dValues for SG-E-DD wind turbines are also used for HTS-DD as this is the most similar technology²⁰.

Table S7: Change in material intensities driven by learning curves for PV panels [ton/GW capacity] ^{11,20}.

Year	2020			2030			2040			2050		
Materials	C-Si	CIGS	CdTe	C-Si	CIGS	CdTe	CIGS	C-Si	CdTe	C-Si	CIGS	CdTe
Aluminium	7,500	7,500	7,500	7,200	7,200	7,200	7,000	7,000	7,000	6,800	6,800	6,800
Cadmium	0	1	46.5	0	1	42	0	1	23	0	1	21
Concrete	60,700	60,700	60,700	58,400	58,400	58,400	56,500	56,500	56,500	54,600	54,600	54,600
Copper	4,600	4,600	4,600	4,500	4,500	4,500	4,350	4,350	4,350	4,200	4,200	4,200
Gallium*	0	4.3	0	0	2.5	0	0	2	0	0	1.5	0
Glass	46,400	46,400	46,400	44,700	44,700	44,700	43,050	43,050	43,050	41,800	41,800	41,800
Indium*	0	17.7	8	0	15	4	0	11	1	0	9	0
Nickel	2	0	0	2	0	0	2	0	0	2	0	0
Plastic	8,600	8,600	8,600	8,300	8,300	8,300	8,000	8,000	8,000	7,700	7,700	7,700
Selenium	0	38.5	0	0	29	0	0	16	0	0	12	0
Silicon	4,000	0	0	2,750	0	0	2,325	0	0	2,000	0	0
Silver	18	0	0	10	0	0	4	0	0	3	0	0
Steel	67,900	67,900	67,900	67,900	67,900	67,900	63,150	63,150	63,150	61,100	61,100	61,100
Tellurium	0	0	50.7	0	0	34.6	0	0	25.3	0	0	22.9

Table S8: Change in material intensities driven by learning curves for wind turbines [ton/GW capacity] ^{11,20}.

Year	2020					2030					2040					2050				
Materials	AG	SG-E-DD ^{a,b}	SG-PM-HS	SG-PM-MS	SG-PM-MS	AG	SG-E-DD ^{a,b}	SG-PM-HS	SG-PM-MS	SG-PM-MS	AG	SG-E-DD ^{a,b}	SG-PM-HS	SG-PM-MS	SG-PM-MS	AG	SG-E-DD ^{a,b}	SG-PM-HS	SG-PM-MS	SG-PM-MS
Dysprosium*[R]	0	6	4.3	5	17	0	NA	1	2	11	0	NA	1.2	2	11.3	0	NA	1.3	2	11.5
Manganese	780	790	550	500	600	780	790	550	500	600	780	790	550	500	600	780	790	550	500	600
Neodymium*[R]	0	28	35	42	155	0	NA	18	37	145	0	NA	17	34	128	0	NA	16	31	125
Nickel	410	340	420	442	410	410	340	420	442	410	410	340	420	442	410	410	340	420	442	410
Vanadium*	0	0	90	90	90	0	0	90	90	90	0	0	90	90	90	0	0	90	90	90

^aFor this technology type, there is no available prediction on its dysprosium and neodymium intensity. Therefore, the values reported for 2020 are used in the estimations.

^bValues for SG-E-DD wind turbines are also used for HTS-DD as this is the most similar technology²⁰.

6.2.2: Resulting classifications

The scenarios considered for the estimation of material demands are presented in Table S9. While it appears in the manuscript, we have included it here to enhance the text coherence and simplify the review process.

Table S9: Classifications resulting by combining IAM capacity projections, market contributions, and material intensity scenarios.

Scenario	Market contribution	Intensity	Colour/symbol
C_B	Continued	Base	Red
C_L	Continued	Learning	Red (*)
T_B	Technological change	Base	Blue
T_L	Technological change	Learning	Blue (*)

6.2.3: Calculation of materials demands

To estimate the demand for materials, various factors such as projected technology capacities, the market contribution of technology types, materials intensity values, and technology learning curves are taken into account. The specific equation or method used to estimate material demand is not provided in the other relevant studies. However, we can calculate the material demand by multiplying the projected technology capacities (which already considers the effect of varying market shares) by material intensity values (with or without considering the impact of technology evolution on material intensity), as reported in Eq. S8.

$$MD_{m,t,n,s,k,i}^T = CCI_{t,n,s,k}^T \cdot MI_{m,t,n,i} \quad \forall m,n,s,k,i, t \in TT_T, T=\{BAT, CSP, ELECTZ, PV, WIND\} \quad (S8)$$

Here, $MD_{m,t,n,s,k,i}^T$ is the demand for material m driven by technology type t , belonging to technology category T , at year n according to IAMs scenario s , market trend k , and material intensity i [ton]. $CCI_{t,n,s,k}^T$ is the capacity installed for individual type t of technology T at the year n according to IAMs scenario s and market trend k [GW] (as estimated in section 6.1). $MI_{m,t,n,i}$ is the intensity i (e.g., base or with learning curves) of material m used in type t of technology T in year n [ton/GW]. The inclusion of set n in the material intensity accounts for the effect of varying material intensities over the years that might result from technology learning curves (as given by set i). Finally, the material demand considering all types t of technologies T can be aggregated to provide the lumped material demand of a given technology category (e.g., electrolyzers) for a specific scenario (combination of IAMs capacity projection, market trend, and material intensity), as given by $LMD_{m,n,s,k,i}^T$ in Eq. S9.

$$LMD_{m,n,s,k,i}^T = \sum_{t \in TT_T} MD_{m,t,n,s,k,i}^T \quad \forall m,n,s,k,i \quad T=\{BAT, CSP, ELECTZ, PV, WIND\} \quad (S9)$$

Referring back to section 6.2.2, it is important to note that depending on IAMs and market contribution scenarios, $CCI_{t,n,s,k}^T$ takes 50 different values for each technology type and year. Additionally, based on materials intensity scenarios, $MI_{m,t,n,i}$ assumes two different values for each technology type, material, and year. Consequently, we end up with 100 resulting values for both $MD_{m,t,n,s,k,i}^T$ and $LMD_{m,n,s,k,i}^T$.

6.2.4: Current production rate of materials, their reserve capacities, and production rate

To provide context for the material demands estimated, we compare them with the current production rates, as presented in Table S10. The information about data collection from the U.S. Geological Survey (USGS) and the specific webpage of USGS Commodity Statistics and Information. Generally, the production rates reported are based on values for 2020. However, in some cases the base year is later (i.e., 2021, or 2022), and, only in one case, it is 2018 (i.e., production rate of praseodymium). In any case, there is no remarkable change in material reserve capacity or global production rate between 2020 and 2022.

Table S10: Annual production rate of the different materials.

Materials	Annual production rate [kton/year]	Ref.	Materials	Annual production rate [kton/year]	Ref.
Activated carbon	5700	27	Manganese	21500	28
Aluminium	65200	28	Molybdenum	298	28
Cadmium	25	28	Neodymium	21	6
Cement	4190000	28	Nickel	2240	28
Chromium	44000	28	Plastic	390700	29
Cobalt	132	28	Platinum	0.180	28
Concrete	4400000	30	Praseodymium	9.723	28,31
Copper	20300	28	Resin PPS - Glass fiber	5851	32
Dysprosium	1.800	28,33	Selenium	2.800	28
Gallium	0.327	28	Silica	266500	34
Glass	209000	35	Silicon	7000	28
Glass/Carbon composites/ fiberglass	5851	32	Silver	23.700	28
Gold	3.030	28	Steel	1958450	36
Graphite	966	28	Tellurium	0.470	28
Indium	0.957	28	Terbium	0.340	28,37
Iridium	0.004	28,38	Titanium	7600	28
Iron	1300000	28	Vanadium	105	28
Lithium	77	28	Zinc	13000	28

We also present Table S11 and S12, reporting the capacity of the reserves for minerals and their current recycling rate that will be used later in section 6.2.7 and section 6.3 which dedicated to our optimization models.

Table S11: Capacity of the reserves for different materials.²⁸

Mineral	Reserve capacity [ton]	Mineral	Reserve capacity [ton]
Aluminium	$3 \cdot 10^{10}$	Manganese	810,000,000
Cadmium	600,000	Molybdenum	18,000,000
Chromium	570,000,000	Neodymium	8,000,000
Cobalt	7,000,000	Nickel	89,000,000
Copper	$8.7 \cdot 10^8$	Platinum	69,000
Dysprosium	1,410,000	Praseodymium	4,000,000
Gallium	279,300	Selenium	99,000
Gold	50,000	Silver	560,000
Graphite	$3 \cdot 10^8$	Tellurium	31,000
Indium	5,700	Terbium	$1.2 \cdot 10^8$
Iridium	69,000	Titanium	47,000,000
Iron	$8.1 \cdot 10^9$	Vanadium	22,000,000
Lithium	17,000,000	Zinc	250,000,000

Table S12: Current recycling rate for different materials.^{28,39}

Mineral	Recycling rate* [%]	Mineral	Recycling rate* [%]	Mineral	Recycling rate* [%]
Cadmium	17.5	Indium	37.5	Praseodymium	5.5
Cobalt	37.5	Iridium	17.5	Selenium	5.5
Copper	34	Lithium	1	Silicon	-
Dysprosium	5.5	Manganese	56	Silver	37.5
Gallium	17.5	Neodymium	5.5	Tellurium	-
Graphite	-	Nickel	50	Terbium	1

* It is defined as the fraction of secondary metal in total metal input in metal production process.³⁹

6.2.5: Exploring the possibilities of by-products

For a comprehensive understanding of the dynamics between host elements and their associated by-products, it is vital to consider the broader context and competing demands from different sectors and applications. Here, we estimate the by-product production that would be obtained when sourcing the host elements to develop CETs. Table S13 presents the companion elements and the parameters used to estimate the amount of by-product produced. Notably, the column “dependency” in this table presents the percentage of guest that is currently product as a by-product of its host at global scale. This value, which is not directly used in the calculations, is presented as an indicator of the strength of the relationship between each pair of elements.

Depending on data availability, one of the Eqs. S10-S12 is employed to calculate the resulting amount of by-product that will be obtained as a result of mining the host element. This is indicated in the last column of Table S13.

Table S13: Companion elements and their relevant data.

Guest	Host	Dependency ^{a,b} [%]	Concentration of guest in concentrated host ($CGCH_{g,m}$)	Concentration of guest in host's ore ($CGOre_g$)	Relative concentration of guest to host in their ore [%] $\left(\frac{CGOre_g}{CHOre_g}\right)$	Ore to metal ratio ($OreMR_m$) ⁴⁰	Recovery rate [%] ($RR_{g,m}$)	Equation used
Cadmium	Zinc	90 ⁴¹	0.4% ⁴²	-	-	-	94 ⁴²	S10
Gallium	Aluminium	95 ²⁸	-	50 ppm ²⁸	-	4.2	10 ²⁸	S11
Gallium	Zinc	-	-	<50 ppm ²⁸	-	52.8	10 ²⁸	S11
Indium	Zinc	75 ⁴¹	-	1-100 ppm ²⁸	-	52.8	(100) ^c	S11
Iridium	Platinum	98 ⁴¹	-	-	7 over 92.55 ⁴³	-	(100) ^c	S12
Silver	Zinc	40 ⁴¹	-	-	116.32·10 ⁻⁴ over 6.49 ⁴⁴	-	(100) ^c	S12
Silver	Copper	25 ⁴¹	100 - 700 ppm ⁴⁵	-	-	-	(100) ^c	S10

^aGlobal production percentage of host element derived as a by-product of its host element.

^bIt is reported to demonstrate the dependency between the production of the guest and the host elements, although it is not directly used in any calculations.

^cIn the absence of reported data, it is assumed to be 100%.

$$PG_{g,n,s,k,i} = \sum_{m \in \text{HOST}_g} \left(\sum_T \text{LMD}_{m,n,s,k,i}^T \cdot \text{CGCH}_{g,m} \cdot \text{RR}_{g,m} \right) \quad \forall g,n,s,k,i \quad (\text{S10})$$

$$PG_{g,n,s,k,i} = \sum_{m \in \text{HOST}_g} \left(\sum_T \text{LMD}_{m,n,s,k,i}^T \cdot \text{OreMR}_m \cdot \text{CGOre}_g \cdot \text{RR}_{g,m} \right) \quad \forall g,n,s,k,i \quad (\text{S11})$$

$$PG_{g,n,s,k,i} = \sum_{m \in \text{HOST}_g} \left(\sum_T \text{LMD}_{m,n,s,k,i}^T \cdot \frac{\text{CGOre}_g}{\text{CHOre}_g} \cdot \text{RR}_{g,m} \right) \quad \forall g,n,s,k,i \quad (\text{S12})$$

Here, $PG_{g,n,s,k,i}$ is the amount of guest element g that would be produced at year n , according to IAMs scenario s market trend k and materials intensity i [ton], $\text{LMD}_{m,n,s,k,i}^T$ is the demand for material m which is the host for element g (as given by set HOST_g) driven by all the technology types in category T at year n [GW], as estimated in section 6.2.4, and $\text{RR}_{g,m}$ is the recovery rate of guest element g from its host element m [%]. Apart from these parameters, that are common between the three equations, each equation has a specific parameter. The term $\text{CGCH}_{g,m}$ is the concentration of guest g in concentrated host m [%], while CGOre_g is the concentration of guest g in the ore [ppm], OreMR_m is the ore to metal ratio [$\text{ton}_{\text{ore}}/\text{ton}_{\text{metal}}$], and CHOre_m is the concentration of the host m in the ore [ppm].

6.2.6: Estimated material demands

We computed annual demands for 36 materials (Table S5) across 25 IAM scenarios (Table S2), and four categories (Table S9), with minimum and maximum values presented in Tables S14-S15. In Table S16, we compared our estimated range with a recent study⁶, and with IEA data explorer, where data are available. Also, Figure S3 visualizes 20 materials with demand-to-production ratios below one.

Table S14: Materials annual demand, based on minimum values across scenarios [ton].

Materials	2020	2025	2030	2035	2040	2045	2050
Activated carbon	0.0	0.0	0.0	0.0	0.0	0.0	0.1
Aluminium	63290.8	56571.7	3919.9	135354.0	405027.6	791845.1	732071.0
Cadmium	6.7	15.8	1.1	31.2	55.6	100.9	93.5
Cement	388735	196925	4194.9	146888	2946016	6157336	5537179
Chromium	3053.0	1299.2	0.0	0.0	25928.8	54023.4	45637.5
Cobalt	0.0	0.0	16059.1	12597.3	9393.4	10340.4	4502.3
Concrete	2969770	1503798	31795	1095223	22293525	46518098	41627387
Copper	48130.5	38555.5	2450.0	84357.9	322257.2	637239.2	588959.3
Dysprosium	30.6	11.5	0.0	0.0	193.6	402.4	339.2
Fiberglass	53197.1	22958.8	0.0	0.0	453504.3	933548.7	779292.8
Gallium	0.2	0.2	0.0	0.4	1.0	1.6	1.3
Glass	218985	322916	24336	836430	2063664	3854748	3687399
Gold	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Graphite	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Indium	2.0	3.3	0.2	4.9	7.7	11.4	7.9
Iridium	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Iron	114283.1	48535.5	0.0	0.0	965745.3	2011225.5	1698261.7
Lithium	0.0	0.0	15317	15037	15890.7	27647.5	31020.2
Manganese	4824.4	2350.6	191.2	3823.1	42702.6	90147.1	93413.5
Molybdenum	631.2	268.5	0.0	0.0	5356.1	11158.6	9425.7
Neodymium	170.4	65.9	0.0	0.0	1144.4	2369.3	1986.1
Nickel	2606.3	1286.3	50.3	956.9	23149.1	48127.0	43834.3
Plastic	112170.1	82230.5	4518.8	155371.1	824399.7	1645356.1	1517297.1
Platinum	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Praseodymium	41.3	17.2	0.0	0.0	330.5	684.7	575.2
Resin	0.0	0.0	0.0	0.0	0.0	0.0	1.0
Selenium	1.8	2.4	0.2	4.3	7.7	12.7	10.6
Silica	0.0	0.0	1819.6	1789.6	1818.0	3147.4	3430.7
Silicon	17745.3	21414.0	1242.7	37732.3	81360.1	133610.1	111151.3
Silver	79.9	98.3	7.0	150.7	229.5	388.6	308.6
Steel	1048043	732636	36967	1249165	8065432	16187947	14874057
Tellurium	7.2	15.1	0.9	28.5	60.6	109.5	101.0
Terbium	5.6	2.4	0.0	0.0	47.4	98.6	83.3
Titanium	0.0	0.0	0.0	0.0	0.0	0.0	0.3
Vanadium	167.1	77.8	0.2	3.2	1731.9	3669.1	3159.2
Zinc	36372.7	15708.7	0.0	0.0	310220.7	638300.1	532582.9

Table S15: Materials annual demand, based on maximum values across scenarios [ton].

Materials	2020	2025	2030	2035	2040	2045	2050
Activated carbon	58.8	106.7	199.1	739.1	1439.6	3867.9	7392.8
Aluminium	1812202	4791170	9690448	13260975	15370312	17341446	18865155
Cadmium	435.1	2029.7	5780.8	10113.6	14142.1	17655.3	21379.0
Cement	5546556	22499308	22584053	33490551	33485745	31520519	30995030
Chromium	39467.2	197658.5	203658.8	275285.4	280031.5	220114.3	298248.7
Cobalt	72145.6	44630.8	255440.7	337313.5	403271.7	646266.6	800623.1
Concrete	42552544	171674480	172318684	256402911	256366393	243276922	239436170
Copper	1160247	3197534	5692857	7797968	9009154	9576423	10004045
Dysprosium	445.9	2423.6	2682.0	4133.6	4704.5	3386.0	4176.3
Fiberglass	649475	3157588	3161239	4203255	4207135	3264965	4368525
Gallium	7.9	68.5	203.2	397.7	595.5	726.3	864.5
Glass	8554225	26492213	47140203	65908593	76747704	80235609	83570669
Gold	1.3	2.4	4.5	16.8	32.7	87.8	167.8
Graphite	228919	190830.9	1429555	1818315	2095153	3357108	4169166
Indium	106.9	650.9	1889.7	3494.3	5061.4	6242.5	7492.5
Iridium	4.0	7.2	13.5	50.0	97.5	261.8	500.4
Iron	1454362	7270284	7477996	10133718	10333703	8106797	10963575
Lithium	37487.0	31918.5	255259.4	387581.9	518810.1	951188.5	1325084
Manganese	118242	280282.9	425237.7	541609.1	638782.2	952438.9	1180557
Molybdenum	8136.9	40737.6	41961.2	56744.9	57748.7	45376.4	61462.7
Neodymium	3292.8	18970.0	21949.7	34972.7	40787.6	28804.6	34732.3
Nickel	158359	192178.1	1270745	1654463	1948754	3197836	4178685
Plastic	2235640	6222393	10822731	14796901	17070479	17881345	18430439
Platinum	1.1	2.1	3.8	14.2	27.7	74.4	142.2
Praseodymium	646.6	3658.9	4177.7	6857.8	8165.9	5670.5	6696.1
Resin	614.9	1116.7	2082.7	7731.8	15060.7	40464.5	77339.9
Selenium	71.9	668.0	1981.1	3877.8	5805.7	7081.1	8429.1
Silica	4606.4	3774.2	28284.0	35955.7	41417.2	66490.6	82668.6
Silicon	707936	2146783	3819982	5340869	6219211	6501851	6772106
Silver	3194.8	9661.8	17189.9	24033.9	27991.5	29436.5	30538.1
Steel	20500420	60788239	95375058	129796162	149790125	155726664	157464932
Tellurium	470.1	2183.9	6217.6	10866.4	15184.1	18960.9	22963.9
Terbium	119.3	706.7	834.0	1383.5	1659.2	1145.8	1343.5
Titanium	153.7	279.2	520.7	1932.9	3765.2	10116.1	19335.0
Vanadium	4354.6	24314.5	27486.0	39320.9	42129.6	31796.1	41353.2
Zinc	443452	2153462	2153462	2860649	2860649	2218995	2967649

Table S16: Comparison of estimated values with similar studies.

Material	comparison with similar studies ⁶	Comparison with “IEA data Explorer” ⁴⁶	Reason
Ag	OV_U	√	
Al	OV_L	-	
Cd	OV	√	
Cem.	OV_L	-	
Co	-	√	
Cr	-	√	
Cu	-	√	
Dy	X	√	Electric motors and in turn the demand driven by them is not included in our study.
Ga	X	√	It is used in certain types of PV panels, and variations in its demand are possible depending on the capacity assigned to each type
GCC	OV_L	-	
Gla.	OV_U	-	
Gra.	-	√	
In	X	√	It is used in certain types of PV panels, and variations in its demand are possible depending on the capacity assigned to each type
Ir	-	√	
Li	-	√	-
Mn	OV_U	√	
Mo	-	√	
Nd	X	√	Electric motors and in turn the demand driven by them is not included in our study.
Ni	X	√	Electric motors and in turn the demand driven by them is not included in our study.
Pt	-	√	
Pr	-	√	
Se	X	√	It is used in certain types of PV panels, and variations in its demand are possible depending on the capacity assigned to each type
Si	-	√	
Ste.	OV_L	-	
Te	X	√	It is used in certain types of PV panels, and variations in its demand are possible depending on the capacity assigned to each type
Tb	-	√	
V	-	√	
Z	-	√	

OV_U: There is considerable overlap in the range of estimations, and our estimate represents a conservative upper bound.

OV_L: There is considerable overlap in the range of estimations, and our estimate represents a conservative lower bound.

X: While there are some overlaps in the data, it does not seem enough to consider them at the same range.

√: While the ranges provided may not align precisely, they exhibit striking similarity. It is noteworthy that for certain elements, like those used in the electrolyzers, while the IEA's range follows an inverted U-shaped pattern, our estimations derived from IAMs consistently show a rising trend.

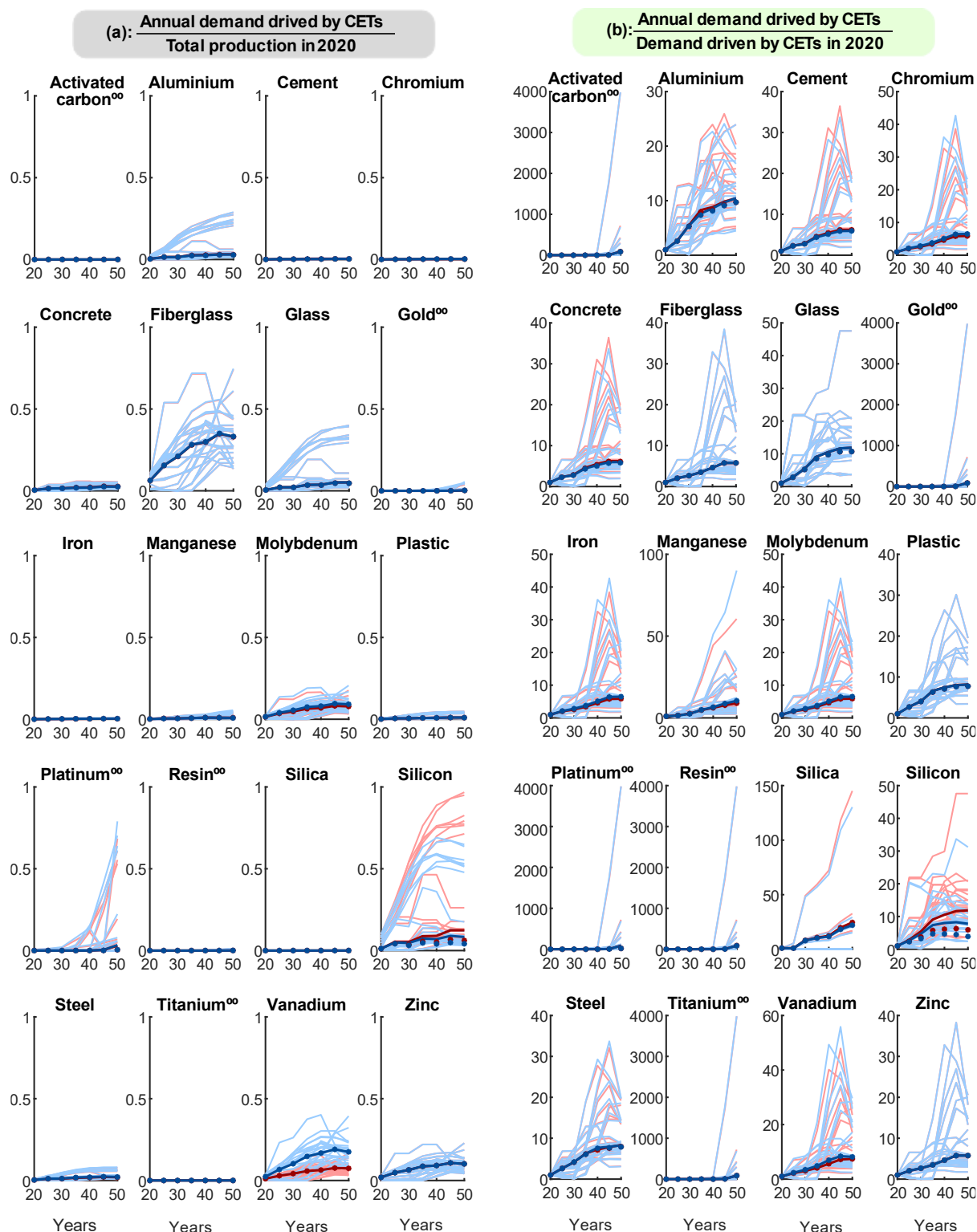


Fig.S3 Material demands from clean energy technologies. Panel (a) compares the demand for materials from CETs with their production rate dedicated to all sectors in 2020. Panel (b) represents materials demand from CETs compared with their estimated demand in 2020. ^{oo}: Materials primarily used in electrolyzers, does not exhibit demand until 2030 and therefore rely on this year or later years, depending on the scenario, as the basis for calculations. Timeframes are indicated as follows: 20: 2020, 30: 2030, 40: 2040, 50: 2050. The results of the continued trend and technological change are distinguished by red and blue colors, respectively. In both cases, the median is depicted with a thicker line. The effect of the reductions in material intensities due to learning curves is indicated with star signs, only for median projections. CETs: clean energy technologies.

6.2.7: Links between problematic materials and technology types

Figure S4 presents the intricate relationships among different types of clean energy technologies and materials, addressing potential challenges in terms of supply and pricing. On the right side, we list various technology types contributing to the 2050 market, with box widths indicating their reliance on featured materials compared to other technologies. On the left side, we show problematic materials highlighted (i.e., those whose demand-to-production ratio is more than 0.5). The ribbons in the figure represent connections between materials and their respective technology hosts, affected by technologies learning curve. Shortages or price increases in these materials may impact the development and market penetration of the associated CETs.

Fig.S4 corresponds to Fig.5 in the main manuscript, illustrating the connections between materials and clean energy technologies for the years 2050 and 2020, respectively. It is important to note that in both figures, the intensity values are normalized, meaning that the intensity value for each material is divided by the largest intensity value for that year.

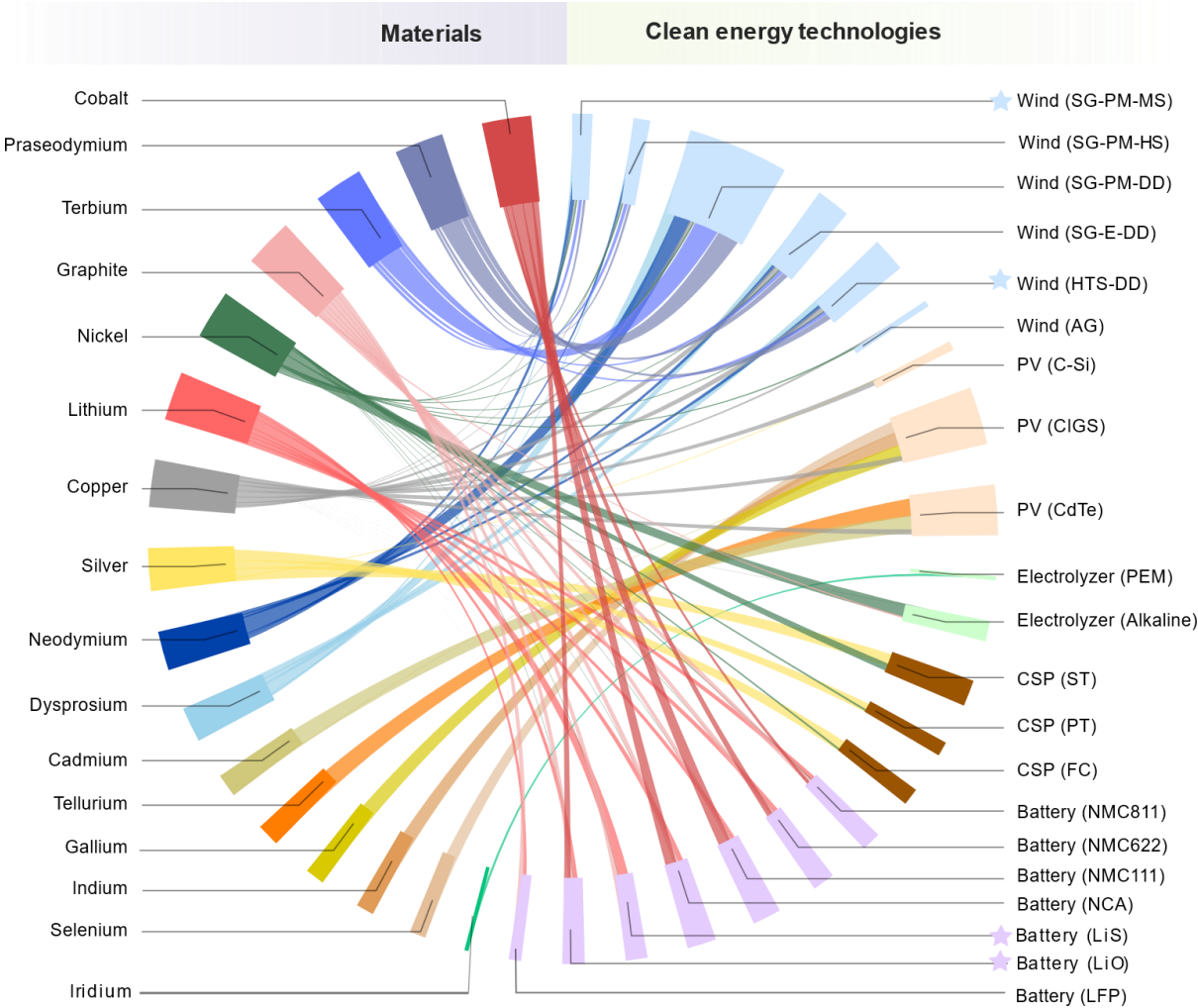


Fig.S4 Links between the materials (left-hand side) and clean energy technologies (right-hand side), based on material intensity values in 2050, considering the effect of learning curves. The width of the ribbons is proportional to material intensity values. Technologies that penetrate the market after 2020 are distinguished by a star. Note that to make all the materials visible and comparable with 2020 values, the materials relative to 2020 intensity values are normalized. For clarity, technology types are enclosed in brackets, with the corresponding acronyms found in Table S1.

6.2.8: Demand-to-reserves comparison

We also made a comparison between the demand values of materials and their reserve capacities (refer to Table S11). We found that cobalt, indium, selenium, silver, and tellurium exhibited a demand-to-reserve ratio potentially exceeding one in some scenarios. Additionally, cadmium, copper, lithium, nickel, and zinc although display demand-to-reserve ratios smaller than one, are noteworthy. Figure S5 illustrates these minerals.

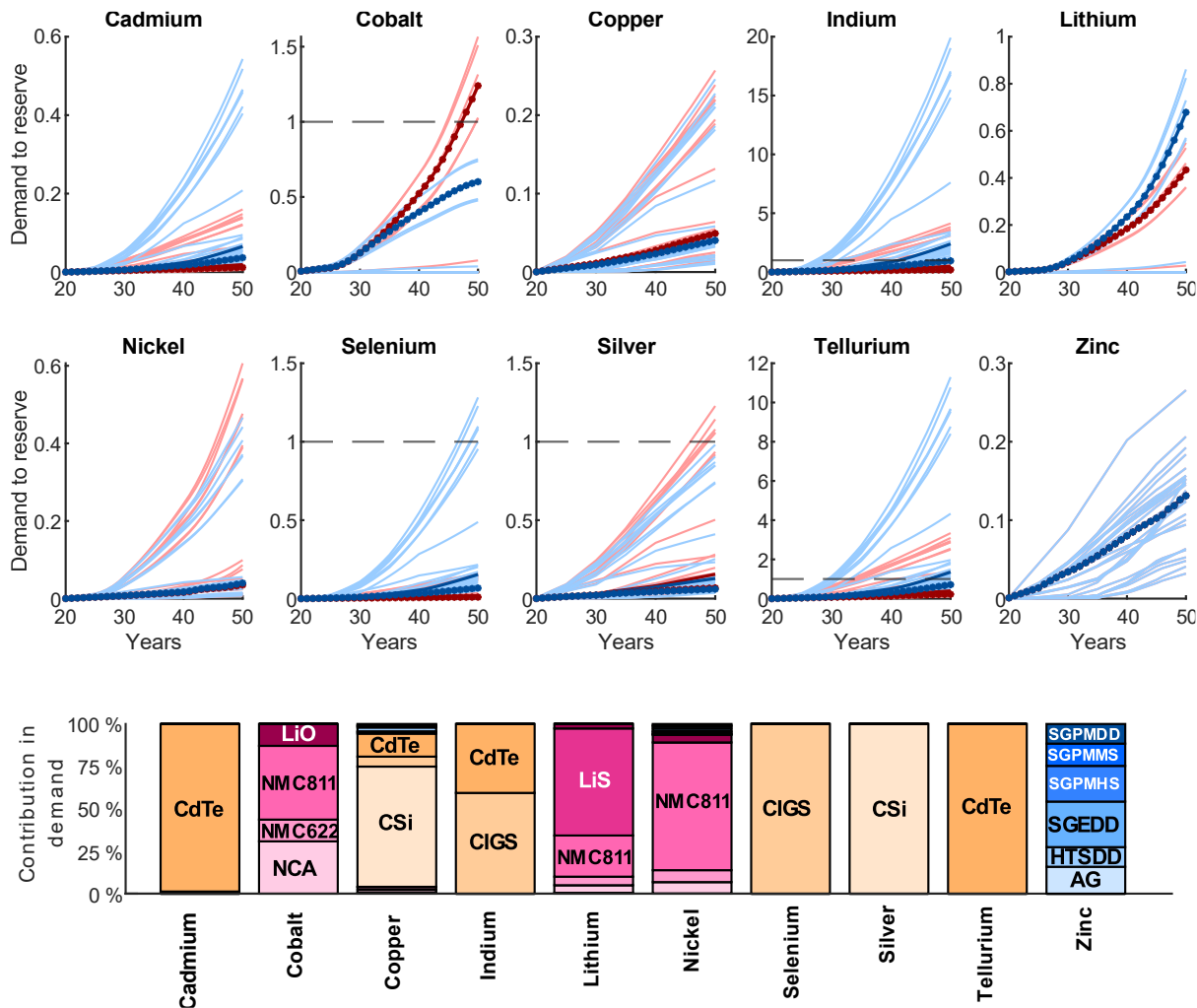


Fig.S5 Materials demand over their reserve capacities. To aid comparison, dashed horizontal lines are included. Timeframes are indicated as 20: 2020, 30: 2030; 40: 2040, 50: 2050. The results of the continued trend and technological change are distinguished by red and blue colors, respectively. In both cases, the median is depicted with a thicker line. Additionally, the resulting median, accounting for reductions in materials intensity based on learning curves, is indicated by star signs. The stacked bars chart presents the share of different technology types in specific material demands. Technology type acronyms as given in Table S1.

6.3 Optimization model to estimate realistic capacities

This section is dedicated to estimating the achievable capacity of clean energy technologies while accounting for constraints on materials availability. Additionally, we calculate the necessary recycling rates of materials to meet their projected capacity by IAMs. The steps involved are as follows:

- **6.3.1: Estimating shortages in technologies developed capacity:** Utilizing the projected capacity of technologies by IAMs as a starting point, we impose constraints based on materials reserve capacity and allocated demand to reassess their achievable capacity and compare them with IAMs projections.
- **6.3.2: Estimating required recycling:** Taking into account similar constraints, we estimated the required recycling range for each of the materials needed to meet the capacity of clean energy technologies as projected by IAMs.

6.3.1 Estimating shortages in technologies developed capacity

Previous analyses suggest that IAM projections on the of CETs are probably too optimistic when factoring in material supply rates, and a higher technological resolution. To assess how far these might be from reality, we evaluate the capacity of CETs that could be realistically deployed considering material availability. To this end, we formulate an optimization model (M1) to minimize the disparity in capacities between IAM projections and what could be realistically manufactured. In all the equations, variables are written in *italics* while parameters are in normal style.

Model M1: minimizing disparities

$$\text{Min} \sum_{T,n,s} \text{Diff}_{n,s}^T \quad (S13)$$

$$\text{s.t: } \text{Diff}_{n,s}^T = \sum_{t \in T_t} (CCI_{t,n,s}^{T,Opt}) - CC_{n,s}^{T,IAMs} \quad \forall n,s,T=\{BAT, CSP, ELECTZ,PV,WIND\} \quad (S14)$$

$$\text{Diff}_{n,s}^T \geq 0 \quad \forall n,s,T=\{BAT, CSP, ELECTZ,PV,WIND\} \quad (S15)$$

$$\sum_{T,t} CCI_{t,n,s}^{T,Opt} \cdot MI_{m,t,n} \leq PR_{m,n} \cdot \text{SHARE}_{m,2020}^{CETs} \quad \forall m,s,n=2021, ..., 2050 \quad (S16)$$

$$\sum_{t,n,T} CCI_{t,n,s}^{T,Opt} \cdot MI_{m,t,n} \leq \text{Res}_m \quad \forall m,s \quad (S17)$$

$$\text{Diff}_{n,s}^T, CCI_{t,n,s}^{T,Opt} \in \mathbb{R}^+ \quad \forall n,s,t,T=\{BAT, CSP, ELECTZ, PV, WIND\} \quad (S18)$$

The objective of M1 (Eq. S13) is to minimize the disparities in capacity across different technology categories T (e.g., PV), IAMs scenario s , and years n , as denoted by $\text{Diff}_{n,s}^T$. These disparities are quantified in Eq.S14 as the difference between the capacity assigned to each technology based on IAM projections ($CC_{n,s}^{T,IAMs}$) and the “realistic” estimates obtained with this model ($\sum_t CCI_{t,n,s}^{T,Opt}$). For each technology, this difference should be positive to ban situations where excess capacity for a technology category compared with IAMs projections offsets deficits for other categories (Eq. S15). $CC_{n,s}^{T,IAMs}$ is obtained with Eqs. S2-S6, for the corresponding IAM scenario and material intensity values.

We acknowledge that not all the materials produced can be allocated to the development of CETs since they are also used in other sectors. Hence, we restrict the amount of each material that can be used for manufacturing CETs according to the shares observed in 2020 ($\text{SHARE}_{m,2020}^{CETs}$). Hence, the left-hand side of Eq. S16 estimates the demand for material m driven by all types of technology T developed at year n , by multiplying the capacity of each technology type by its material intensity

($MI_{m,t,n}$), while the right-hand side accounts for the (share of) the realistic production rate that is expected for material m in year n ($PR_{m,n}$). As aforementioned, the available share of each material m is obtained based on 2020 values (Eq. S19).

$$SHARE_{m,2020}^{CETs} = \frac{\sum_{t,T} CCIT_{t,2020}^{IAMs} \cdot MI_{m,t,2020}}{PR_{m,2020}} \quad \forall m, n = 2021, \dots, 2050 \quad (S19)$$

Capacity projections and material intensities are set at appropriate values depending on the corresponding scenario studies, while production rates for 2020 ($PR_{m,2020}$) are detailed in Table S10. Exceptionally, for iridium, used in electrolyzers, we conducted the estimation based on the initial year of the technology (i.e., after 2030, depending on the IAM scenario), instead of in 2020.

The production rates for future years appearing in Eqs. S16 and S19 ($PR_{m,n}$) are obtained by allowing a certain annual growth α , starting from the production rate of 2020 (see Eq. S20). Specifically, we used $\alpha = 2.7\%$, which is the average annual growth of metals mining⁴⁷, and changed this value to 0.7 and 4.7 for the sensitivity analysis. (i.e., average $\pm 2\%$).

$$PR_{m,n} = (1 + \alpha) \cdot PR_{m,n'} \quad n' = (n-1), \forall n = 2021, \dots, 2050 \quad (S20)$$

Finally, Eq.S17 is employed to restrict the cumulative demand for material m by year n driven by all the technologies according to the capacity of its reserves (Res_m), as given in Table S11.

Notably, by combining three production rates with two materials intensity projections, six sets of results are created for each of the 25 IAMs scenario. Figure S6 presents the median shortage values for each set and each IAM scenarios.

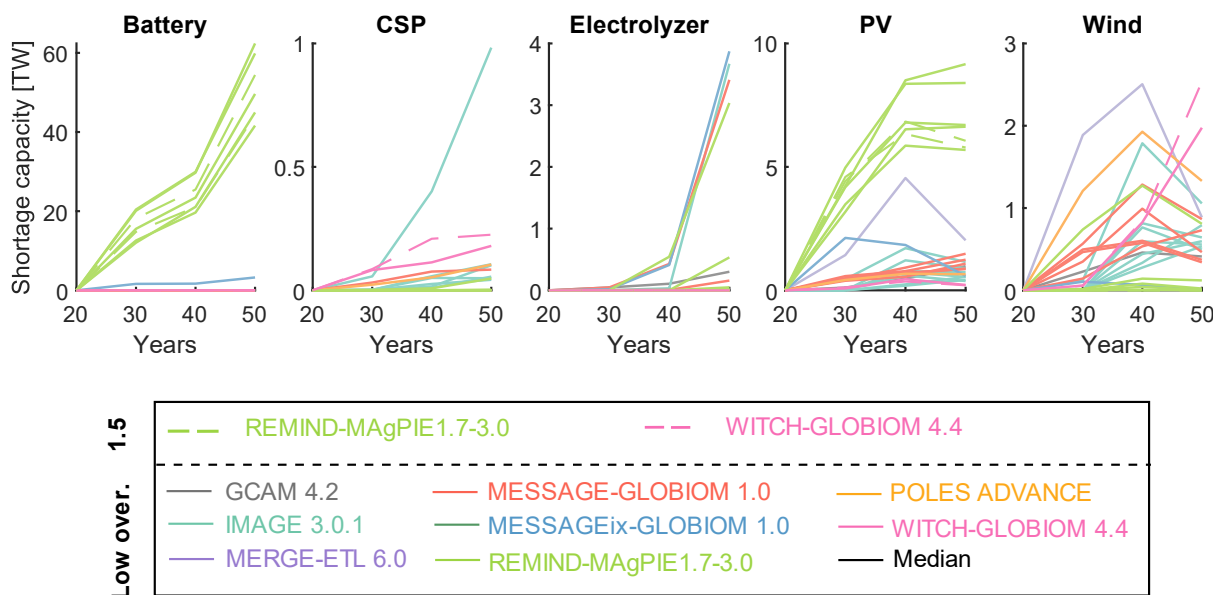


Fig.S6 Shortages in technologies annual developed capacity based on different IAMs scenarios.

6.3.2 Estimating required recycling:

To assess the minimum recycling rate for materials to meet the demand from CETs, we construct another model with similar constraints. This aids in understanding the significance of materials recycling and gauging the disparity between our expectations and their current recycling rates (see Table S12). For this purpose, we formulate an optimization model (M2) aimed at minimizing the recycling rate required for materials to fulfil IAM's projected capacities. In all equations, variables are denoted in *italics* while parameters are in normal style.

Model M2: minimizing recycling rates

$$\text{Min} \sum_{i,n,s} \text{Rec}_{i,n,s} \quad (\text{S21})$$

$$\sum_{T,t} \text{CCI}_{t,n,s}^{T,Opt} \cdot \text{MI}_{m,t,n} \leq \text{PR}_{m,n} \cdot \text{SHARE}_{m,2020}^{\text{CETs}} + \text{Rec}_{i,n,s} \quad \forall m,s,n=2021, \dots, 2050 \quad (\text{S22})$$

$$\sum_{t,n,T} \text{CCI}_{t,n,s}^{T,Opt} \cdot \text{MI}_{m,t,n} \leq \text{Res}_m + \text{Rec}_{i,n,s} \quad \forall m,s \quad (\text{S23})$$

$$\text{CCI}_{t,n,s}^{T,Opt} = \text{CCI}_{t,n,s}^{T,IAMs} \quad \forall n,s,t,T=\{BAT, CSP, ELECTZ, PV, WIND\} \quad (\text{S24})$$

$$\text{Rec}_{i,n,s}, \text{CCI}_{t,n,s}^{T,Opt} \in \mathbb{R}^+ \quad \forall n,s,t,T=\{BAT, CSP, ELECTZ, PV, WIND\} \quad (\text{S25})$$

Model M2, outlined in equations (S21) to (S25), seeks to minimize the material recycling across materials intensity projections i , IAM scenarios s , and years n . The objective (Eq. S21) aims to minimize the recycled materials indicated by $\text{Rec}_{i,n,s}$, while considering IAM projections. This term is incorporated into the right-hand side of Eqs. S22 and S23 to increase material availability. Eqs. S22 and S23 are equivalent to Eqs. S16 and S17 in model M1. However, in model M2, we enforce the exact capacity values based on IAM projections through Eq. S24. Note that the $\text{CCI}_{t,n,s}^{T,IAMs}$ contains the market contribution trends (see Eq. S7).

It is important to note that, for each material m and IAM scenario s , 12 sets of results are obtained, each considering one of three production rates, one of two material intensity projections, and one of two market contribution trends. This comprehensive approach allows for a thorough assessment of the recycling rates required across various scenarios and parameters.

6.4 Extra warming due to shortages in technology developed capacities

Our optimization model highlights a potential challenge: achieving the capacities projected by IAMs for 1.5°C and 1.5°C with low overshoot temperature targets may be constrained by material supply. This section delves into estimating the additional warming that could result from these shortages. Here, "shortage" denotes the disparity between the capacity projected by IAMs and the more realistic capacity that could be deployed according to our model. It is important to note that electrolyzers are excluded from this analysis as we conservatively assume that the hydrogen generated would be utilized in chemical industries (i.e., not for energy applications). The steps involved in this estimation are outlined below:

- **6.4.1 Expected energy delivered:** First, we estimate the energy that could be delivered by CETs if we could achieve the capacity projected by IAMs.
- **6.4.2 Real energy delivered:** Then, we calculate the energy that can be delivered by the capacity of technologies obtained from our optimization model, which includes constraints on material supplies.
- **6.4.3 Replacement energy:** The difference between the energy expected to be delivered and that actually delivered should be substituted by alternative sources.
- **6.4.4 Additional greenhouse gas emissions:** Shortages in the capacity developed for CETs requires contributions from business-as-usual sources for compensation. Specifically, we assume the electricity mix would supply shortages in CSP, PV and wind capacity, while diesel-engine trucks would replace missing EVs due to shortages in the capacity of batteries. This substitution would result in the release of additional CO₂-eq emissions compared to the original IAM estimates. To quantify them, we resort to prospective life cycle assessment.
- **6.4.5 Additional warming:** We translate non-avoided CO₂-eq emissions into additional warming.

Each step is discussed in detail in the following sections.

6.4.1 Expected energy delivered

To estimate the amount of energy delivered (ED) by all the capacity installed in each year for all technologies during their lifetime, Eqs. S26-S27 have been employed.

$$ED_{n,s}^{BATEV,IAMS} = CC_{n,s}^{BATEV,IAMS} \cdot \frac{REC^{BAT}}{RPC^{BAT}} \cdot OCLT^{BAT} \cdot DOD^{BAT} \cdot RTEff^{BAT} \quad \forall n,s \quad (S26)$$

$$ED_{n,s}^{T,IAMS} = CC_{n,s}^{T,IAMS} \cdot GCF^T \cdot \left(\frac{365 \text{ days}}{\text{year}} \cdot \frac{24 \text{ h}}{\text{day}} \cdot LF \right) \quad \forall n,s, T=\{CSP, PV, WIND\} \quad (S27)$$

The term $ED_{n,s}^{BATEV,IAMS}$ used in Eq. S26 indicates the energy delivered by installed capacity of batteries according to IAMs scenario s in year n [GWh]. In this equation, REC^{BAT} is the rated energy capacity of batteries [GWh], while RPC^{BAT} is its rated power capacity [GW]. These parameters represent the nominal energy or power output of a battery in each cycle, respectively. Here, the ratio of 20/6 is used as rated energy-to-rated power capacity of batteries⁴⁸. $OCLT^{BAT}$ is the number of operational cycles expected during the lifetime of the battery (e.g., 3000 cycles during 15 years). Then, DOD^{BAT} is the depth of discharge, providing the amount of energy discharged compared with the total storage capacity (e.g., 80%). $RTEff^{BAT}$ denotes the battery round-trip efficiency, which reflects the efficiency

(%) achieved through converting electricity from alternating current to stored energy and back to alternating current (e.g., 86%)⁵. Finally, $CC_{n,s}^{BATEV, IAMs}$ is the annual capacity of batteries used in EVs [GW], estimated from IAM projections using Eqs. S3-S5.

$ED_{n,s}^{T, IAMs}$ in Eq. S27 represents the energy delivered from the capacity of CSP, PV or wind installed in year n according to IAM scenario s [GWh]. In this equation, GCF^T is the global capacity factor for the desired technology [%], equal to 32.8% for wind and 22.4% for PV⁴⁹. For CSP, the value of 45% related to CSP systems with thermal storage is used⁵⁰. Also, LF is the lifespan, which is assumed to be 30 years for these technologies. $CC_{n,s}^{T, IAMs}$ is the capacity of each technology installed in year n [GW], which is directly reported by IAMs for CSP, PV, and wind.

We aim to emphasize that our goal in conducting these estimations is to calculate the additional warming resulting from capacity shortages and add it into the initial target of limiting global warming to 1.5°C by 2100. Hence, even if part of the energy generated by some technologies installed in the 2020-2050 will occur after 2050, it will still occur before 2100 (note the lifespan of 30 years). Thus, this approach is relevant and meaningful in this context.

6.4.2 Real energy delivered

Analogous to the estimation of the expected energy delivered, we calculate the amount of energy that would be delivered in practice during the lifetime of the technologies installed with the available capacity according to the optimization model (Eqs. S28-S29). The only difference compared with Eqs. S26 and S27 is the replacement of the capacities obtained by the IAMs by those obtained from model M1 (see section 6.3).

$$ED_{n,s}^{BATEV, Opt} = CC_{n,s}^{BATEV, Opt} \cdot \frac{REC^{BAT}}{RPC^{BAT}} \cdot OCLT^{BAT} \cdot DOD^{BAT} \cdot RTEff^{BAT} \quad \forall n, s \quad (S28)$$

$$ED_{n,s}^{T, Opt} = CC_{n,s}^{T, Opt} \cdot GCF^T \cdot \left(\frac{365 \text{ days}}{\text{year}} \cdot \frac{24 \text{ h}}{\text{day}} \cdot LF \right) \quad \forall n, s \text{ } T=\{\text{CSP, PV, WIND}\} \quad (S29)$$

The term $ED_{n,s}^{BATEV, Opt}$ used in Eq. S28 indicates the energy delivered by the capacity of batteries according to scenario s installed in year n according to the optimization model [GWh], while $ED_{n,s}^{T, Opt}$ in Eq. S29 represents the same for CSP, PV, or wind [GWh].

As discussed in the previous section, our aim is to calculate the additional warming and add it into the target of limiting global warming to 1.5°C by 2100, even for technologies installed close to 2050, as the energy they will generate will be expended by 2100.

6.4.3 Replacement energy

To estimate the amount of energy that could not be delivered because of shortages in the capacity of each technology and needs to be provided by business-as-usual options, we employ Eqs. S30-S32.

$$SED_{n,s}^{BATEV} = ED_{n,s,k,i}^{BATEV, IAMs} - ED_{n,s}^{BATEV, Opt} \quad \forall n, s \quad (S30)$$

$$MSED_{n,s}^T = ED_{n,s}^{T, IAMs} - x_n^T \cdot SED_{n,s}^{BATEV} \quad \forall n, s \text{ } T=\{\text{CSP, PV, WIND}\} \quad (S31)$$

$$SED_{n,s}^T = MSED_{n,s}^T - ED_{n,s}^{T, Opt} \quad \forall n, s, T = \{CAP, PV, WIND\} \quad (S32)$$

Eq. S30 is used for batteries, with the term $SED_{n,s}^{BATEV}$ [GWh] representing the substitute energy that should be delivered in year n to compensate for the capacity that could not be developed owing to shortages in material supplies. Parameters $ED_{n,s}^{BATEV, IAMS}$ and $ED_{n,s}^{BATEV, Opt}$ are estimated using Eq. S26 and Eq. S28, respectively.

We could use the same approach for the case of CSP, PV, and wind. However, we adopt a conservative approach and assume that part of the capacity that was projected for CSP, PV, and wind by IMAs was going to be dedicated to batteries used in EVs. Hence, if the expected capacity of batteries (and consequently EVs) could not be developed, there is also no need to develop the corresponding capacity of CSP, PV panels, and wind turbines required to feed them. To account for this, we introduce Eq. S31, where we deduct the energy that does not need to be delivered anymore owing to the shortage in batteries. To allocate this capacity between CSP, PV, and wind the term x_n^T is used to reflect the contribution of each of these technologies in feeding the batteries. This value is given by the share of CSP, PV, and wind capacities in year n according to IAM estimates. At the end, the equation estimates the “modified” replacement energy that needs to be delivered according to IAMs scenario s in year n ($MSED_{n,s}^T$). $SED_{n,s}^T$ in Eq. S32 represents the energy that could not be supplied by CSP, PV panels, or wind turbines because of material shortages, and, therefore, should be replaced by the grid in each year n [GWh]. Finally, $ED_{n,s}^{T, Opt}$ and $MSED_{n,s}^T$ are estimated using Eqs. S29 and S31, respectively. Fig. S7 depicts this approach.

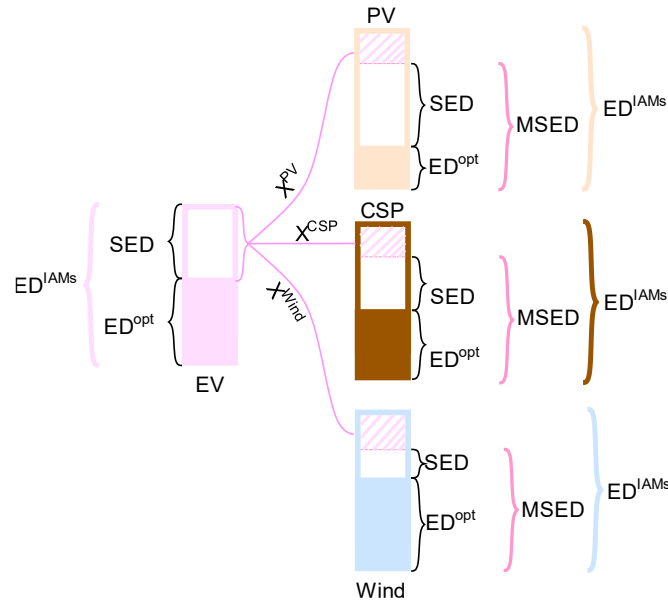


Fig.S7: Approach used to estimate the replacement energy requirements for each clean energy technology.

6.4.4 Additional greenhouse gas emissions

In order to calculate the extra greenhouse gas emissions, it is important to note that IAMs anticipate a specific level of emissions for the projected capacity of clean energy technologies for a particular temperature target. Indeed, their projections are based on expected emission levels. Therefore, to estimate the additional emissions, we need to determine the difference between their expected

emissions and the emissions that would occur based on the realistic capacities derived from our optimization model (Section 6.3). We also consider the services, such as transportation or electricity, that these technologies would provide but they cannot due to capacity shortages (i.e., difference between IAMs and optimized capacities). We replace these unmet services with equivalent options and estimate the corresponding resulting emissions, which are included in our additional greenhouse gas emissions calculation.

We provide a detailed methodology for estimating emissions related to batteries, followed by similar methodologies for CSP, PV panels, and wind turbines. Electrolyzers' hydrogen generation is excluded from this analysis as it is assumed to be used as feedstock in the chemical sector. It is important to note that we use prospective life cycle assessment results, as carbon intensity values vary over time. Having this roadmap in mind, we turn your attention to the D.4.1 subsection which is related to batteries.

6.4.4.1 Battery electric vehicles

As aforementioned, we assume that batteries are primarily designed for EVs (Figure S1). Hence, we estimate the difference in greenhouse gas emission stemming from shortages in battery capacities ($ACE_{n,s}^{BATEV}$, in [ton CO₂-eq]) by assuming that the missing transportation service by electric vehicles would be replaced by an alternative mean ($ACE_{n,s}^{BATEV, Service}$) (Eq. S33).

$$ACE_{n,s}^{BATEV} = -ACE_{n,s}^{BATEV, IAMs} + (ACE_{n,s}^{BATEV, Opt} + ACE_{n,s}^{BATEV, Service}) \quad \forall n, s \quad (S33)$$

Here, $ACE_{n,s}^{BATEV, IAMs}$ and $ACE_{n,s}^{BATEV, Opt}$ represent the greenhouse gas emissions incurred by EVs according to the capacity estimated by IAMs and our optimization model, respectively [ton CO₂-eq]. Note that we calculate life cycle (instead of direct) emissions, thus considering also the emissions incurred while producing the energy required to feed the batteries.

In turn, the life cycle greenhouse gas emissions that would occur if we could develop the capacity of batteries projected by IAMs ($ACE_{n,s}^{BATEV, IAMs}$) are calculated from the energy delivered by batteries ($ED_{n,s}^{BATEV, IAMs}$, estimated with Eq. S26 [MJ]), the energy required by a battery EV to transport a tonne over a km in year n (ER_n^{BATEV} , in [kJ/t·km]), and the carbon intensity of a battery EV in year n (CI_n^{BATEV} , in [ton CO₂-eq/t·km_{BEV}]) (see Eq. S34).

$$ACE_{n,s}^{BATEV, IAMs} = ED_{n,s}^{BATEV, IAMs} \cdot \frac{1}{ER_n^{BATEV}} \cdot CI_n^{BATEV} \cdot 1000 \quad \forall n, s \quad (S34)$$

Acknowledging that EVs performance improves over time and also their carbon intensity will vary over time, we resort to prospective LCA to estimate the value of CI_n^{BATEV} for different years n (Table S17). Prospective LCA methodology is discussed in section 6.4.4.3

Next, we use Eq. S35 to estimate the life cycle greenhouse gas emissions for the actual capacity of batteries that could be manufactured according to the optimization model ($ACE_{n,s}^{BATEV, Opt}$, in [GWh]).

$$ACE_{n,s}^{BATEV,Opt} = ED_{n,s}^{BATEV,Opt} \cdot \frac{1}{ER_n^{BATEV}} \cdot CI_n^{BATEV} \cdot 1000 \quad \forall n,s \quad (S35)$$

This equation is analogous to Eq. S34, but uses $ED_{n,s}^{BATEV,Opt}$ instead of $ED_{n,s}^{BATEV,IAMs}$. The values for CI_n^{BATEV} are also provided in Table S17.

Finally, Eq. S36 is used to estimate the life cycle greenhouse gas emissions incurred by replacing the service that would have been delivered by means of the "missing" battery EVs, with the corresponding replacement service (i.e., a diesel truck).

$$ACE_{n,s}^{BATEV,Service} = SED_{n,s}^{BATEV} \cdot \frac{1}{ER_n^{BATEV}} \cdot ER_n^{DICT} \cdot CI_n^{DICT} \cdot 1000 \quad \forall n,s \quad (S36)$$

Here, $SED_{n,s}^{BATEV}$ is the energy that will need to be substituted (in [GWh], as estimated by Eq. S30), ER_n^{BATEV} and ER_n^{DICT} denote the energy required by a battery electric vehicle and a diesel ignition combustion truck, respectively, to transport a tone over a km in year n [kJ/t-km], and CI_n^{DICT} is the carbon intensity of the diesel ignition combustion truck in year n [ton CO₂-eq/kJ_{diesel}] (Table S17).

Table S17: Results for the prospective life cycle assessment of the energy consumption and carbon intensity of diesel-engine trucks and battery EVs.

Term	Unit	2020	2025	2030	2035	2040	2045	2050
CI_n^{BATEV}	Kg CO ₂ -eq/t-km	0.132	0.101	0.081	0.068	0.059	0.052	0.046
CI_n^{DICT}	kg CO ₂ -eq/kJ	$7.56 \cdot 10^{-5}$	$6.98 \cdot 10^{-5}$	$6.60 \cdot 10^{-5}$	$6.78 \cdot 10^{-5}$	$6.94 \cdot 10^{-5}$	$6.98 \cdot 10^{-5}$	$6.98 \cdot 10^{-5}$
ER_n^{BATEV}	kJ/t-km	480	386	316	297	281	265	249
ER_n^{DICT}	kJ/t-km	1296	1239	1187	1142	1102	1069	1042

6.4.4.2 Concentrated solar power, photovoltaic panels, and wind turbines

An analogous procedure is followed to estimate the additional greenhouse gas emissions incurred by providing an alternative service to CSP, PV, and wind ($ACE_{n,s,Sc}^T$ in [ton CO₂-eq]).

$$ACE_{n,s,Sc}^T = -ACE_{n,s}^{T,IAMs} + (ACE_{n,s}^{T,Opt} + ACE_{n,s,Sc}^{T,Service}) \quad \forall n,s, T=\{CSP, PV, WIND\}, Sc=\{CP, NZ\} \quad (S37)$$

In this equation, $ACE_{n,s}^{T,IAMs}$ and $ACE_{n,s}^{T,Opt}$ are the life cycle greenhouse gas emissions that would be released from these technologies according to the capacity estimated by IAMs (Eq. S38) and our optimization model (Eq. S39), respectively. Finally, $ACE_{n,s,Sc}^{T,Service}$ denotes the greenhouse gas emissions from the replacement energy (i.e., Eq. S40). The first two terms ($ACE_{n,s}^{T,IAMs}$ and $ACE_{n,s}^{T,Opt}$) are obtained with Eqs. S38-S39:

$$ACE_{n,s}^{T,IAMs} = ED_{n,s}^{T,IAMs} \cdot CI_n^T \quad \forall n,s, T=\{CSP, PV, WIND\} \quad (S38)$$

$$ACE_{n,s}^{T,Opt} = ED_{n,s}^{T,Opt} \cdot CI_n^T \quad \forall n,s, T=\{CSP, PV, WIND\} \quad (S39)$$

Here, $ED_{n,s}^{T, IAMs}$ and $ED_{n,s}^{T, Opt}$ correspond to the energy delivered by CSP, PV panels, or wind turbines according to the capacities derived from IAMs or our optimization model, respectively (see Eqs. S27 and Eq. S29). These are multiplied by the carbon intensity of the desired technology T for year n (CI_n^T , in [ton CO₂-eq/GWh]), as obtained from prospective LCA data reported in relevant studies^{51–53} (see Table S18).

Table S18: Collected data for the prospective life cycle carbon intensity of CSP systems, PV panels and wind turbines.

Term	Unit	2020	2025	2030	2035	2040	2045	2050
CSP*	ton CO ₂ -eq/GWh	34	32	29	27	25	22	20
PV	ton CO ₂ -eq/GWh	80	72	64	56	55.2	54.4	53.6
Wind	ton CO ₂ -eq/GWh	20.1	19.95	19.8	17.8	15.9	15.9	15.9

* Data are related to a SCP system with storage option. Only two value (i.e., 20-34) were available and a linear regression is used.⁵⁴

In this case, we assume electricity from the grid will replace the energy that CSP, PV, or wind should deliver ($SED_{n,s}^T$, as estimated by Eq.32). The emissions stemming from this substitution depend on the carbon intensity of the mix ($CI_{n,Sc}^{EM}$, in [ton CO₂-eq/GWh]), which, in turn, could vary differently over time depending on the evolution of the different technologies in the mix. Hence, two prospective scenarios Sc , Current Policy (CP) or Net Zero (NZ), are used to derive two different sets of carbon intensities over time, as discussed in section 6.4.4.3 (Table S19).

$$ACE_{n,s,Sc}^{T, Service} = SED_{n,s}^T \cdot CI_{n,Sc}^{EM} \quad \forall n, s \quad T=\{CSP, PV, WIND\}, Sc=\{CP, NZ\} \quad (S40)$$

Ultimately, $ACE_{n,s,Sc}^{T, Service}$ denotes the greenhouse gas emissions released from the replacement service offered by the grid according to IAM scenario s and policy scenario Sc in year n [ton CO₂-eq].

6.4.4.3 Prospective life cycle assessment

To estimate the carbon intensity and energy requirements of battery electric vehicles and diesel ignition combustion truck, as well as the carbon intensity of grid mix, we use the data provided by prospective life cycle analysis. In contrast to traditional LCA, prospective LCA takes into account the impacts of future changes in the background system of LCA datasets. This approach considers potential shifts that could influence environmental impacts over time, ensuring that decisions are not solely reliant on present circumstances. To conduct a prospective analysis, we need to generate future life cycle inventories under different socioeconomic and environmental policy scenarios.

Our estimation begins with the data provided by IAMs, which project the potential development of the energy system, GHG sources, and mitigation technologies across various socioeconomic scenarios and climate policies. Next, we create a series of LCA databases, each corresponding to a specific year and scenario considered in the analysis. Here, we leverage the IAM data for the chosen scenarios and use the Premise v1.5.0 toolbox⁵⁵, to adapt the Ecoinvent v3.8 LCA database accordingly. Premise toolbox is an open-source Python library, operating on BrightWay2 V.0.8.7⁵⁶, which is specifically crafted to enhance the Ecoinvent v3.8 database by integrating scenario data from IAMs related to five pivotal energy-intensive sectors: electricity generation, cement and steel production, road freight and

passenger transport, and both conventional and alternative fuel supplies. This approach helps us to ensure that our LCA databases accurately reflect the evolving environmental impacts associated with different policy pathways and socioeconomic conditions over time.

Notably, our starting point involves using results from the REMIND model under Current Policy (CP) and Net Zero (NZ) narratives spanning the 2020-2050 timeframe. These narratives account for alterations in both technological aspects (e.g., vehicle weight) and policy implementations (e.g., decarbonization of the electricity matrix). Table S19 presents the results obtained for grid mix, while the results for battery electric vehicles are already presented in Table S17.

Table S19: Perspective life cycle results for carbon intensity of the grid mix electricity [kg CO₂-eq/kWh].

Scenarios	2020	2025	2030	2035	2040	2045	2050
Current Policy	0.508	0.425	0.361	0.310	0.274	0.236	0.207
Net zero	0.508	0.316	0.194	0.110	0.081	0.076	0.074

Although prospective LCA can help us to provide more accurate estimations, our calculations are still imperfect. First, it is worthnoting that these carbon intensity values are related to a typical battery, PV panel, or wind turbine, and are not available for specific types. Notably, life cycle greenhouse gas emissions from a battery EV only become lower than those from diesel-based cars after 2031. Therefore, in this case, only the extra emissions from 2032 untill 2050 are considered in our calculations (i.e., the negative difference that would be generated between 2020-2031 is neglected).

In addition, we acknowledge that a share of the energy provided by CSP, PV panels, and wind turbines during the period analysed (2020-2050) would be delivered beyond 2050 in practice (note the technology lifespan). Therefore, the carbon intensity of these technologies and that of the grid electricity used to compensate for shortages should include years beyond 2050. Unfortunately, these data are not available. Hence, in the absence of better data, we estimate the emissions for the whole life cycle of the technologies based on the carbon intensity of the year they would be installed.

6.4.5 Additional warming

In this step, we convert the additional greenhouse gas emissions into a temperature increase, using Eq. S41, as suggested by Hare and Meinshausen⁵⁷.

$$\Delta T_{n',Sc}^T = \frac{0.16^\circ\text{C}}{100 \text{ GtCO}_2} \cdot \sum_{n=2020}^{n'} ACE_{n,s,Sc}^T \quad \forall n,s, T=\{\text{Battery, CSP, PV, WIND}\}, Sc=\{\text{CP, NZ}\} \quad (\text{S41})$$

This equation establishes a temperature change of approximately 0.16°C for every 100 GtCO₂ cumulative fossil CO₂ emissions released until year n' . The additional fossil CO₂ emissions resulting from shortages in the capacity developed for each technology, denoted by $ACE_{n,s,Sc}^T$, are derived from Eqs. S33-S40. Hence, the term $\Delta T_{n',Sc}^T$ provides the temperature increase associated with the “lack” of each technology, according to CP and NZ scenarios, up to the specific year n' [°C].

6.5 Materials and their potential substitutes

Table S20 presents the list of materials that can be used for replacement.

Table S20: Materials and their potential substitutes²⁸.

Material	Replace by	Material	Replace by	Material	Replace by
Aluminium	Glass	Gold	Silver	Selenium	Silicon
	Paper		Palladium		Cerium oxide
	Plastic		Platinum		Tellurium
	Steel	Graphite	Molybdenum disulfide		Bismuth
	Manganese	Indium	Antimony		lead
	Titanium		Carbon		Sulphur dioxide
	Wood		PEDOT ^e	Silicon	Aluminium
	Vinyl		Copper		Gallium
	Copper		Silver		Germanium
Cadmium	Zinc	Iron/steel	Graphene	Silver	Steel
	Nickel		Zinc		Tantalum
	Aluminium		Hafnium		Titanium
	Tin		Aluminium		Aluminium
Cement	Fly ash	Iron/steel	Plastic		Rhodium
	GGBFS ^a		Concrete	Tellurium	Bismuth
Cobalt	Barium		Wood		Calcium
	SF ^b		Glass		Lead
	Cerium		Paper		Phosphorus
	Iron	Lithium	Calcium		Selenium
	Lead		Magnesium		Sulphur
	Manganese		Mercury		Niobium
	Vanadium		Zinc		Tantalum
	Copper		Aluminium	Titanium	Ilmenite
	Ceramics		Sodic fluxes		Leucosene
	Nickel		Potassic fluxes		Rutile
	Rhodium	Molybdenum	Boron		Slag
	Titanium		Chromium		Synthetic rutile
Copper	Aluminium		Niobium	Vanadium	Manganese
	Titanium		Vanadium		Molybdenum
	Steel		Tungsten		Niobium
	Plastic		Graphite		Titanium
Gallium	LC ^c		Tantalum		Tungsten
	SiMeOx ^d		Cadmium	Zinc	Aluminium
	In-Phosphide	Nickel	Titanium		Cadmium
	Helium-Neon	Platinum	Palladium		Plastic
	Silicon-Germanium	REE ^f	-		Molybdenum

^a Ground granulated blast furnace slag.

^b Strontium Ferrites.

^c Liquid crystals from organic compounds.

^d Silicon based complementary metal oxides.

^e Poly (3,4-ethylene dioxythiophene).

^f Substitutes are available for many applications but generally are less effective.

6.6 References

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Chapter 7

Supplementary information: Navigating the Geopolitics and Justice of transition to Renewable Energy

Chapter 8

Supplementary information: Comparative sustainability study of energy storage technologies using data envelopment analysis

Chapter 8

Supplementary information for chapter 4:

Comparative sustainability study of energy storage technologies using data envelopment analysis

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8.1 Calculation of delivered energy

The details on the calculation of the energy delivered during the lifetime of fast-response technologies is reported in section 8.1, together with the values and sources of the technical parameters used in the calculations. Analogously, section 8.2 presents the method employed to estimate the electricity delivered from 1 kg of H₂ and 1 kg of NH₃, while also providing details on the production processes of the two energy carriers. The following assumptions apply to all the tables in the supplementary information:

1. Values underlined represent data gaps estimated based on similar technologies.
2. The selected value for each indicator of each DMU reported in tables corresponds to the median of the range reported for it in the literature.
3. Indicators should be expressed per 1 GJ of energy delivered for consistency with the choice of a CRS model. In cases that the selected value is expressed in [MWh], it is multiplied by 3.6 to estimate the used value in [GJ]. Similarly, the $3.6 \cdot 10^{-3}$ and $3.6 \cdot 10^{-6}$ conversion coefficients are used, respectively, to convert kWh and Wh to per GJ.
4. Currency exchange rates of AUS\$=0.63€ and US\$=0.85€ are used to express all costs in € [1].
5. The abbreviations and full names of fast-response technologies and long-term energy storage options are reported in Tables 4-5 of the manuscript.

8.1.1 Delivered energy for fast-response technologies

The amount of energy delivered during the lifetime of a fast-response energy storage technology is calculated using Eq. (A.1) [2].

$$\text{DEDLF} = \text{REC} \cdot \text{NC} \cdot \text{DOD} \cdot \text{RTE} \quad (\text{A.1})$$

In this equation, DEDLF is the energy delivered during the lifetime of storage technology in [GJ], REC refers to the rated energy capacity (i.e., the nominal energy output of each cycle, expressed in [GJ]), NC is the number of cycles during the lifetime of technology, and DOD (%) refers to the depth of discharge, providing the amount of energy discharged compared with the total storage capacity. Finally, RTE is the round-trip efficiency, which reflects the efficiency (%) achieved through converting electricity from alternating current to stored energy and back to alternating current [3]. Values used for REC, NC, DOD, and RTE are based on the median of the range reported in the literature for the corresponding technologies, as provided in Tables (A.1), (A.2), (A.3), and (A.4), respectively. Finally, the estimated energy delivered for each fast-response technology is reported in Table (A.5).

Table (A.1). Rated energy capacity (REC) of each fast-response technology. Values underlined represent data gaps, which are estimated based on similar technologies.

Technology	Reported range (MWh)	Selected value (MWh)	Used value ² (GJ)	References
Flywheels	$5.0 \cdot 10^{-3}$ -5.0	2.5	9.0	[4]
SMES	$0.8 \cdot 10^{-3}$ - $15.0 \cdot 10^{-3}$	$8.0 \cdot 10^{-3}$	$28.4 \cdot 10^{-3}$	[4]
FB-VR	2.0-60.0	31.0	111.6	[4]
FB-ZB	$50.0 \cdot 10^{-3}$ -4.0	2.2	8.1	[4]
LA	$0.5 \cdot 10^{-3}$ -40.0	20.0	72.0	[4]
Li-ion	$4.0 \cdot 10^{-3}$ -10.0	5.0	18.0	[4]
Li-Fe-Ph ¹	<u>$4.0 \cdot 10^{-3}$-10.0</u>	<u>5.0</u>	<u>18.0</u>	-
Li-Ni-Mn-Co ¹	<u>$4.0 \cdot 10^{-3}$-10.0</u>	<u>5.0</u>	<u>18.0</u>	-
Na-Ni-Cl	$120.0 \cdot 10^{-3}$ -5.0	2.6	9.2	[5]
Na-S	0.4-244.8	122.6	441.4	[4, 5]
Ni-Cd	6.8-6.8	6.8	24.3	[4, 5]

¹Considered the same as for Li-ion.

²The 3.6 conversion coefficient is used to convert the selected value (MWh) to the used value (GJ).

Table (A.2). Number of cycles (NC) during the lifetime of each fast-response technology. Values underlined represent data gaps, which are estimated based on similar technologies¹.

Technologies	Reported range	Used value	References
Flywheels	20000-100000	60000	[3]
SMES	20000-100000	60000	[4]
FB-VR	10000-13342	11671	[3, 4]
FB-ZB	1500-10000	5750	[3, 4]
LA	500-4500	2500	[3, 4]
Li-ion	1500-4500	3000	[3]
Li-Fe-Ph ²	<u>1500</u> -3500	<u>2500</u>	[6]
Li-Ni-Mn-Co ²	<u>1500</u> -3500	<u>2500</u>	[6]
Na-Ni-Cl	1000-3500	2250	[5, 6]
Na-S	2500-5000	3750	[4, 6]
Ni-Cd	800-3500	2150	[4, 5]

¹The lifespan range of each technology, for which the number of cycles is reported, is as follows: Flywheel: 15-20 [3], SMES: 15-20 [3], FB-VR: 5-10 [3], FB-ZB: 5-10 [3], LA: 5-15 [3], Li-ion: 5-16 [3, 4], Li-Fe-Ph: 5-15 [3], Li-Ni-Mn-Co: 5-15 [3], Na-Ni-Cl: 15-15 [3], Na-S: 10-20 [3, 4], and Ni-Cd: 10-20 [3]. All the numbers are in years. Note that, in general, standardized lifespan information in years is difficult to obtain as it is highly context-specific and may be different from the reported value.

²Lower bound is considered the same as for Li-ion.

Table (A.3). Depth of discharge (DOD) of each fast-response technology.

Technologies	Estimated range (%)	Used value (%)	References
Flywheels	80-80	80	[7]
SMES	80-80	80	[7]
FB-VR	80-100	90	[3, 6]
FB-ZB	80-100	90	[6, 7]
LA	50-80	65	[6, 7]
Li-ion	80-80	80	[5, 7]
Li-Fe-Ph	90-90	90	[6]
Li-Ni-Mn-Co	90-90	90	[6]
Na-Ni-Cl	80-100	90	[3, 6]
Na-S	80-100	90	[6, 7]
Ni-Cd	80-80	80	[7]

Table (A.4). Round-trip-efficiency of each fast-response technology

Technologies	Reported range (%)	Used value (%)	References
Flywheels	90-95	92.5	[4]
SMES	90-98	94.0	[4, 5]
FB-VR	60-90	75.0	[4, 5]
FB-ZB	60-80	70.0	[3, 4]
LA	63-90	76.5	[4]
Li-ion	75-97	86.0	[4]
Li-Fe-Ph	86-86	86.0	[6]
Li-Ni-Mn-Co	92-92	92.0	[6]
Na-Ni-Cl	85-90	87.5	[5, 6]
Na-S	75-90	82.5	[4]
Ni-Cd	60-85	72.5	[4, 6]

Table (A.5). Estimated values for delivered energy during the lifetime of each fast-response technology.

Technologies	DEDLF (MWh)	DEDLF (GJ)
Flywheels	111111	400000
SMES	356.4	1283
FB-VR	244216	879176
FB-ZB	8150.6	29342
LA	24863	89506
Li-ion	10324	37167
Li-Fe-Ph	9679	34844
Li-Ni-Mn-Co	10354	37275
Na-Ni-Cl	4536	16330
Na-S	341364	1228912
Ni-Cd	8417	30302

8.1.2 Delivered energy for long-term storage alternatives

For long-term storage options, the electricity obtained from 1 kg H₂ or NH₃ is used to normalize the data. The starting point is 1 kg of the corresponding gas, taken here as the calculation basis. Then, the gravimetric energy density of the gas (as reported in Table (A.6)) is multiplied by the efficiency of the compression, storage, and reconversion processes, as shown in Figure 2. The final values for the delivered energy of long-term storage options are reported in Table (A.7).

Table (A.6). Gravimetric energy values of long-term storage options

Energy career	Gravimetric energy density (kWh/kg)	Gravimetric energy density (GJ/kg)	References
H ₂	5.4	$19.4 \cdot 10^{-3}$	[8]
NH ₃	3.0	$10.8 \cdot 10^{-3}$	[3]

Table (A.7). Estimated delivered energy from 1 kg H₂ and 1 kg NH₃

Energy career	Delivered energy (kWh)	Delivered energy (GJ)
H ₂	1.9	$6.86.4 \cdot 10^{-3}$
NH ₃	1.5	$5.47 \cdot 10^{-3}$

8.2 Data, calculations, and references

In this contribution, the CRS version of the undesired SBM model is used, and, for consistency, all the indicators are estimated per GJ of delivered energy so that scale economies are left out from the comparison. Therefore, the data collected are sometimes divided by the delivered energy estimated with Eq. (A.1) to obtain normalized unitary indicators (i.e., per GJ of energy delivered).

In the case of fast-response technologies, data found in the literature are often expressed per kg of the storage technology or its energy capacity (kWh), especially in the case of environmental data. In the case of data reported per kg of the storage technology, the data is first divided by its gravimetric energy density to obtain the value of the indicator per unitary capacity of the storage technology and then divided by the delivered energy calculated based on one GJ of storage capacity (Eq. (A.1), 1 GJ capacity).

For long-term energy storage options, reported values are usually expressed per kg of gas. Thus, these data are divided by the gravimetric energy density of the corresponding gas. Also, in some cases, the data are based on the gas's available heat (instead of deliverable electricity). So, at first, they are multiplied by the heating value of the gas so that the indicator is expressed per kg, then divided by the gravimetric energy density to become per GJ of electricity output. The details of calculations are discussed in the next subsections for each indicator.

8.2.1 Levelized cost of energy (LCOE)

For most fast-response technologies, the LCOE is reported directly in the literature. Exceptions are Li-Fe-Ph and Li-Ni-Mn-Co batteries, whose LCOE is assumed to be the same as Li-ion. The data collected are reported in Table (B.1).

In the case of long-term storage options based on gas, the LCOE is seldom reported as this concept is associated with technologies that, unlike gases, are only intrinsic to the power sector. To overcome this limitation, we compute the cost of delivering one unit of energy with power-to-gas-to-power technologies, analogously as it would be provided by the LCOE. We use the cost of producing one kg of gas as a starting point, which is often reported in the literature (e.g., see hydrogen obtained from electrolysis powered by the grid in Table (B.2)). In other cases, the cost of producing the gas is estimated using reported data on the equivalent annual cost (expressed in US M\$/year) and the plant capacity (kg H₂/day) [9], assuming 365 operating days per year (i.e., equivalent annual cost/(plant capacity · 365)). In both cases, the cost of producing the gas needs to be divided by the energy that can be obtained from it (Table (A.7)) to obtain the cost of producing one GJ with this technology, i.e., a cost metric we use as a proxy of the LCOE (and which we will refer to as LCOE hereafter for simplicity). Indeed, dividing the original costs reported, which are usually based on a particular weight of H₂ or ammonia, by their delivered energy, which covers the effects of after-production steps, we estimated the costs per unit of delivered energy.

Manufacturing costs are not reported explicitly for ammonia production using the chemical looping process. However, it is expected to be 1.5% lower than ammonia based on SMR [10]. Therefore, the reported values for ammonia based on SMR are multiplied by 98.5% to estimate the cost of ammonia production using the chemical looping process. In addition, the cost of ammonia production using grid mix energy as the energy source (NH₃, Grid mix) and its production cost using renewable energy sources like hydropower, solar, and wind are not reported explicitly. To have an estimation for these cases, the cost of hydrogen and ammonia production based on SMR are used to estimate the missing data. Indeed, their difference is estimated and used to find the missing data (cost of ammonia=cost of hydrogen + estimated difference). The cost of hydrogen production based on SMR is 0.96 €/kg H₂, while for ammonia, it is 1.53 €/kg NH₃. To subtract them, we divide each one by its gravimetric energy density, which results in 49.38 and 141.66 €/GJ, respectively. This results in a cost difference of 92.28 €/GJ between them. Then, this value is added to the cost of desired hydrogen production to estimate the relevant cost of ammonia production (e.g. cost of NH₃ using Grid mix= [(cost of H₂ using Grid mix/gravimetric energy density of H₂) + 92.28]/efficiency of after production steps). Similarly, the cost of hydrogen production based on the water-splitting by chemical looping method (H₂, WSCL) is obtained by subtracting 92.28 (€/kg) from the cost of ammonia production using the same method. Data for the LCOE of long-term storage alternatives are reported in Table (B.2).

Table (B.1). LCOE for fast-response technologies

Technologies	Reported range (€/MWh)	Selected value (€/MWh)	Used value (€/GJ delivered)	References
Flywheel ¹	590-590	590.0	163.89	[7]
SMES ¹	369-369	369.0	102.50	[7]
FB-VR	330-380	355.0	98.61	[3]
FB-ZB	198-230	214.0	59.44	[3]
LA	300-350	325.0	90.28	[3]
Li-ion	600-645	622.5	172.92	[3]
Li-Fe-Ph ²	<u>600-645</u>	<u>622.5</u>	<u>172.92</u>	-
Li-Ni-Mn-Co ²	<u>600-645</u>	<u>622.5</u>	<u>172.92</u>	-
Na-Ni-Cl	320-380	350.0	97.22	[3]
Na-S	225-265	245.0	68.06	[3]
Ni-Cd	370-475	422.5	117.36	[3]

¹The original data reported are 59.02 (c€/kWh) for flywheel and 36.92 (c€/kWh) for SMES.

²The LCOE is estimated using the data of Li-ion.

Table (B.2). LCOE for long-term storage options

Storage options	Reported values (original units)	Selected value (original units)	Selected value ³ (€/kg)	Used value (€/GJ delivered)	Ref.
H ₂ , CG	104.4-104.4 (US M\$/year)	104.4	0.86	124.82	[9]
H ₂ , CG-CCS	2.6-3.1 (A\$/kg)	2.8	1.79	261.81	[11]
H ₂ , SMR	156.0-156.0 (US M\$/year)	156.0	0.96	139.79	[9]
H ₂ , SMR-CCS	2.3-2.8 (A\$/kg)	2.6	1.61	234.25	[11]
H ₂ , WE-Grid mix	2.5-8.0 (\$/kg)	5.3	4.46	650.67	[12]
H ₂ , WE-Hydropower	140.7-140.7 (US M\$/year)	140.7	6.30	918.86	[9]
H ₂ , WE-Solar	298.5-298.5 (US M\$/year)	298.5	13.37	1949.45	[9]
H ₂ , WE-Wind	165.5-165.5 (US M\$/year)	165.5	7.41	1080.48	[9]
H ₂ , WSCL ¹	NA	NA	<u>0.92</u>	<u>134.72</u>	-
NH ₃ , SMR	1300-2300 (\$/1000 kg)	1800	1.53	279.64	[13]
NH ₃ , SMR-CCS	1425-2450 (\$/1000 kg)	1937	1.65	301.57	[13]
NH ₃ , WE-Grid mix ¹	NA	NA	<u>3.47</u>	<u>635.02</u>	-
NH ₃ , WE-Hydropower ¹	NA	NA	<u>4.50</u>	<u>821.84</u>	-
NH ₃ , WE-Solar ¹	NA	NA	<u>8.42</u>	<u>1539.72</u>	-
NH ₃ , WE-Wind ¹	NA	NA	<u>5.11</u>	<u>934.56</u>	-
NH ₃ , WSCL ²	<u>1280.5-2265.5 (\$/1000 kg)</u>	<u>1773</u>	<u>1.51</u>	<u>275.98</u>	-

¹The estimation method is discussed before the table.

²Estimated using the cost of ammonia production based on SMR (NH₃, SMR).

³Currency exchange rates of A\$=0.63€ and US\$=0.85€ are used to express all costs in € [1].

8.2.2 Energy consumption

For fast-response technologies, energy consumption is the sum of two contributions. The first one is the energy consumed for manufacturing the technology. The second one is the energy needed to charge the technology, which varies for a common energy output owing to different depths of discharge and round-trip efficiencies. Assuming the efficiency of feeding energy is 100%, the amount of energy fed during the complete lifespan can be estimated with Eq. (B.1).

$$\text{FEDLF} = \text{REC} + (\text{NC} - 1) \cdot \text{REC} \cdot \text{DOD} \quad (\text{B1})$$

Here, FEDLF is the energy fed during the whole lifetime of the technology, while REC is the rated energy capacity, NC is the number of cycles, and DOD is the depth of discharge. Note that the whole capacity of the technology is only filled the first time; after this, part of the energy will always remain in the storage system due to a DOD lower than 100%, reducing its capacity for the following cycles (i.e., $(\text{NC} - 1) \cdot \text{REC} \cdot \text{DOD}$).

Hence, the sum of the energy consumption for manufacturing and the energy consumed to feed the technology gives the total energy consumption, as reported in Table (B.3). Note that different factors like aging may affect the characteristics of technology and, consequently, its delivered energy. The employed uncertainty analysis helps us to cover such potential variabilities. Values are finally divided by the delivered energy during the lifetime of the technology for consistency with the CRS assumption. For long-term energy storage alternatives, the energy consumption to produce 1 kg of gas, as reported in the literature, is divided by delivered energy from that kg of gas (Table (A.7)). This energy consumption can range between 6.03-15 kWh/kg H₂ for hydrogen [21] and between 6.4-10.08 kWh/kg NH₃ for ammonia [22].

For processes based on the fossil fuel energy sources (i.e. H₂ production using coal gasification, H₂ production based on the SMR, and NH₃ based on SMR), a CCS unit becomes necessary to reduce emissions. In such cases, the energy consumption of the CCS unit is added to the energy consumption of gas production. Note that this can range from 1.22 GJ/ton CO₂ [23, 24] to 2.45 GJ/ton CO₂ [24], depending on the type of carbon capturing process. For simplicity, we use the average of this range (1.83 GJ/ton CO₂) and multiply it by the amount of CO₂ captured to estimate the energy consumption of the CCS system. In the absence of specific CO₂ emissions, we adopt a conservative approach and use CO₂-eq emissions instead. Values for CO₂-eq emission are reported in Table (B.9). The amount of captured CO₂ is obtained as the difference between the CO₂-eq emissions of a production unit with and without CCS, with both data based on references. According to Table (B.9), 15.702 kg CO₂-eq emissions/kg H₂ in CG process, 10.294 kg CO₂-eq emissions/kg H₂ in SMR process, and 1.136 kg CO₂-eq emissions/kg NH₃ in SMR process is captured by the corresponding CCS units. These result in 4.196, 2.751, and 0.380 GJ energy consumption per 1GJ delivered energy associated with the CCS units.

The estimated values for energy consumption of long-term storage options are reported in Table (B.4).

Table (B.3). The energy consumption of fast-response technologies

Technologies	Reported value/range for manufacturing (original units)	Selected value for manufacturing (original units)	Selected value for manufacturing (GJ consumed/GJ delivered)	FEDLF (GJ feed/GJ delivered)	Used value (GJ total energy consumption/GJ delivered)	Ref.
Flywheel ¹	1225-1225 (GJ/1095 MWh net delivered)	1225	0.31	1.80	1.39	[14]
SMES ¹	2669-2669 (GJ/1095 MWh net delivered)	2669	0.68	1.06	1.74	[14]
FB-VR ²	827.1-3080 (MJ/1 kWh storage)	1953	0.07	1.33	1.40	[14, 15]
FB-ZB ³	<u>827.1-3080 (MJ/1 kWh storage)</u>	<u>1953</u>	<u>0.15</u>	<u>1.43</u>	<u>1.58</u>	-
LA ¹	1062-1593 (GJ/1095 MWh net delivered)	1327	0.34	1.31	1.64	[14]
Li-ion ²	1766.5-1766.5 (MJ/1 kWh storage)	1766	0.24	1.16	1.40	[15]
Li-Fe-Ph ⁴	1.8-3.5 (delivered/invested)	2.65	0.38	1.16	1.54	[16]
Li-Ni-Mn-Co ⁴	1.8-4.5 (delivered/invested)	3.15	0.32	1.09	1.40	[16]
Na-Ni-Cl ⁵	234.3-234.3 (MJ/kg)	234.30	0.31	1.14	1.45	[17]
Na-S ⁶	12.0·10 ⁻³ -22.0·10 ⁻³ (kg oil /kWh delivered)	0.02	0.20	1.21	1.41	[18]
Ni-Cd ⁷	3-5 (fossil depletion/MJ capacity)	4.00	0.14	1.38	1.51	[19]

¹The reported data are per net delivered energy (GJ consumed/MWh delivered). Hence only the units are converted from GJ consumed/MWh delivered to GJ consumed/GJ delivered.

²Since the reported data are per 1 kWh storage, considering 1kWh as capacity and using Eq. (A.1), the DEDLF is estimated, and the selected value is divided by it.

³Is considered the same as vanadium redox flow battery

⁴The inverse (i.e., 1/ reported value) is used.

⁵The reported values are expressed in (MJ/kg). Therefore, they are divided by gravimetric energy density (Table (B.5)). Then, divided by DEDLF of technology (Eq. (A.1), assuming 1GJ capacity).

⁶The reported data are (kg oil/kWh). Hence, they are multiplied by the energy content of oil (0.042 GJ/kg oil [20]). Then, the unit is converted to GJ consumed/GJ delivered.

⁷The reported data is (fossil fuel depletion-kg oil/MJ capacity). So, it is multiplied by the energy content of oil (0.042 GJ/kg oil [20]). Then, divided by DEDLF (Eq. (A.1), 1 GJ capacity).

Table (B.4). The energy consumption of long-term storage options

Storage options	Reported/estimated range for H ₂ and NH ₃ production without CCS (kWh/kg)	Selected value for H ₂ and NH ₃ production without CCS (kWh/kg)	Selected value for H ₂ and NH ₃ production considering all processes (GJ/GJ delivered)	Used value for H ₂ and NH ₃ production considering all processes (GJ/GJ delivered)	Ref.
H ₂ , CG	6.03-15.00	10.52	5.52	5.52	[21]
H ₂ , CG-CCS ¹	6.03-15.00	10.52	5.52+4.20	9.72	[21]
H ₂ , SMR	6.03-15.00	10.52	5.52	5.52	[21]
H ₂ , SMR-CCS ¹	6.03-15.00	10.52	5.52+2.75	8.27	[21]
H ₂ , WE-Grid mix	6.03-15.00	10.52	5.52	5.52	[21]
H ₂ , WE-Hydropower	6.03-15.00	10.52	5.52	5.52	[21]
H ₂ , WE-Solar	6.03-15.00	10.52	5.52	5.52	[21]
H ₂ , WE-Wind	6.03-15.00	10.52	5.52	5.52	[21]
H ₂ , WSCL	6.03-15.00	10.52	5.52	5.52	[21]
NH ₃ , SMR	6.40-10.08	8.24	5.42	5.42	[22]
NH ₃ , SMR-CCS ¹	6.40-10.08	8.24	5.42+0.38	5.80	[22]
NH ₃ , WE-Grid mix	6.40-10.08	8.24	5.42	5.42	[22]
NH ₃ , WE-Hydropower	6.40-10.08	8.24	5.42	5.42	[22]
NH ₃ , WE-Solar	6.40-10.08	8.24	5.42	5.42	[22]
NH ₃ , WE-Wind	6.40-10.08	8.24	5.42	5.42	[22]
NH ₃ , WSCL	6.40-10.08	8.24	5.42	5.42	[22]

¹The energy consumption of the carbon capturing unit is estimated and added to the selected value

8.2.3 Energy density

In this contribution, energy density is used as an indicator for evaluating fast-response technologies. The collected data are reported in Table (B.5). Since the indicators are per GJ, 1/energy density is used as an input in DEA.

Table (B.5). The gravimetric energy density for fast-response technology

	Reported range (Wh/kg)	Selected value (Wh/kg)	Used value (1/(GJ/kg))	References
Flywheels	5-100	52.5	5291.0	[3]
SMES	0.5-5	2.8	101010.1	[3]
FB-VR	10-35	22.5	12345.7	[3]
FB-ZB	30-85	57.5	4830.9	[3]
LA	30-50	40.0	6944.4	[3]
Li-ion	150-350	250.0	1111.1	[3]
Li-Fe-Ph ¹	<u>150-350</u>	<u>250.0</u>	<u>1111.1</u>	-
Li-Ni-Mn-Co ¹	<u>150-350</u>	<u>250.0</u>	<u>1111.1</u>	-
Na-Ni-Cl	100-140	120.0	2314.8	[3]
Na-S	150-250	200.0	1388.9	[3]
Ni-Cd	15-300	157.5	1763.7	[3]

¹Considered the same as for Li-ion.

8.2.4 Water use

For fast-response technologies, water is used mainly in their manufacturing step and retrieved from the literature. For Na-Ni-Cl batteries, the reported value is per one cell only. Considering that 100 cells are used to build a battery with 105 kg weight [17], the reported value for one cell is multiplied by 100 and divided by 105 so that water use in m³ of water per kg of battery is obtained. Then, this value is divided by the gravimetric energy density of the battery (91 Wh/kg [17]), yielding water use per GJ of capacity. Finally, this value is divided by DEDLF (Eq. (A.1), assuming one GJ capacity) to obtain the water use per GJ of delivered energy during the lifetime of the technology.

In most studies, the water used for manufacturing a FB-ZB and a Na-S battery is ignored from the list of their components [25]. Here, the water use of FB-ZB is considered the same as FB-VR. For Na-S, the average value of water used for manufacturing the other batteries is used. All the collected and estimated values for water use of fast-response technologies are reported in Table (B.6).

Table (B.6). Water use of fast-response technologies

Technologies	Reported value/range (original units)	Selected value (original units)	Used value (m ³ /GJ delivered)	Reference
Flywheel ¹	7200-7200 (m ³ /1095 MWh net delivered)	7200	1.8	[14]
SMES ¹	4718-4718 (m ³ /1095 MWh net delivered)	4718	1.2	[14]
FB-VR ¹	11.3-11.3 (m ³ /1095 MWh net delivered)	11.3	2.9·10 ⁻³	[14]
FB-ZB ²	<u>11.3-11.3 (m³/1095 MWh net delivered)</u>	<u>11.3</u>	<u>2.9·10⁻³</u>	-
LA ¹	6.4-9.6 (m ³ /1095 MWh net delivered)	8	2.0·10 ⁻³	[14]
Li-ion ³	1.97-1.97 (kg/1000 kWh delivered)	1.97	0.5·10 ⁻³	[26]
Li-Fe-Ph ⁴	<u>1.97-1.97 (kg/1000 kWh delivered)</u>	<u>1.97</u>	<u>0.5·10⁻³</u>	-
Li-Ni-Mn-Co ⁴	<u>1.97-1.97 (kg/1000 kWh delivered)</u>	<u>1.97</u>	<u>0.5·10⁻³</u>	-
Na-Ni-Cl ⁵	2.94-2.94 (kg/1 cell of Na-Ni-Cl)	2.94	4.80·10 ⁻³	[17]
Na-S ⁶	-	-	<u>1.8·10⁻³</u>	-
Ni-Cd ⁷	16.47-16.47 (gr/100 gr battery)	16.47	0.2·10 ⁻³	[27]

¹The reported data are per net delivered energy (m³/1095MWh delivered). Only the units are converted from m³/MWh delivered to m³/GJ delivered.

²Is considered the same as vanadium redox flow battery (FB-VR).

³The reported data are divided by the density of water and 1000 to be (m³/kwh delivered). Then, unit conversion to be (m³/GJ delivered).

⁴Are considered as the same as lithium ferro phosphate (Li-Fe-Ph).

⁵The reported data is per one cell. The estimation method is discussed in the text before this table.

⁶Is considered the same as the average of batteries.

⁷The reported value is divided by the density of water and gravimetric energy density. Then, it is divided by the DEDLF (Eq. (A.1), assuming 1GJ capacity).

We neglect water used to manufacture long-term storage alternatives since this is expected to be orders of magnitude lower than the water consumed as raw material for hydrogen production (and therefore for ammonia manufacturing, too). According to the reports from experimental efforts to produce hydrogen, about 9 kg of water is used to produce 1 kg of hydrogen via renewable energy sources (electrolysis) [11]. In the case of ammonia production using renewable energies that the water consumption is not reported, the stoichiometry of the reactions and the coefficient of converting hydrogen to ammonia (97.06% [28]) dictate that 1.636 kg of water are needed per kg of ammonia. For the rest of the processes, the water consumption is reported as kg of water per kg of H₂ or NH₃. Then, it is divided by the energy delivered from 1 kg H₂ or NH₃. The estimated values for water use of long-term storage options are reported in Table B7.

Table (B.7). Water use of long-term storage options

Storage options	Water used (Kg water/kg H ₂ or NH ₃)	Water used (m ³ /GJ delivered)	References
H ₂ , CG ¹	<u>18.8</u>	<u>2.74</u>	-
H ₂ , CG-CCS ¹	<u>18.8</u>	<u>2.74</u>	-
H ₂ , SMR	18.8	2.74	[29]
H ₂ , SMR-CCS ¹	<u>18.8</u>	<u>2.74</u>	-
H ₂ , WE-Grid mix ¹	<u>18.8</u>	<u>2.74</u>	-
H ₂ , WE-Hydropower	9.00	1.31	[11]
H ₂ , WE-Solar	9.00	1.31	[11]
H ₂ , WE-Wind	9.00	1.31	[11]
H ₂ , WSCL	31.67	4.61	[29]
NH ₃ , SMR	2.50	0.46	[30]
NH ₃ , SMR-CCS	2.50	0.46	[30]
NH ₃ , WE-Grid mix	2.50	0.46	[30]
NH ₃ , WE-Hydropower	1.59	0.29	[31]
NH ₃ , WE-Solar ²	<u>1.64</u>	<u>0.30</u>	-
NH ₃ , WE-Wind ²	<u>1.64</u>	<u>0.30</u>	-
NH ₃ , WSCL	1.64	0.30	[30]

¹Considered the same as hydrogen production based on SMR (H₂, SMR).

²Estimated using the data of hydrogen as discussed before the table.

8.2.5 Global warming potential

For fast-response technologies, the data on CO₂-eq emissions are collected from LCA studies (see Table (B.8)). This is also true for most of the long-term storage options, yet there are some exceptions. Greenhouse gases emission of hydrogen production based on coal gasification with CCS (H₂, CG-CCS) and (H₂, SMR-CCS) are gathered from a report by Australia's Commonwealth [11], which provides only CO₂ (and not CO₂-eq) emissions. Therefore, in this case, CO₂ emissions are used as a proxy for the CO₂-eq emissions. Although underestimating greenhouse gases, this assumption is reasonable in power-to-gas-to-power processes, where CO₂ emissions tend to be, by far, the main contributor to CO₂-eq emissions since this stem mainly from energy production.

In the case of ammonia based on SMR with CCS, the CO₂-eq emissions are not reported explicitly; instead, it is stated that 1136.62 CO₂-eq emission/t NH₃ should be stored in a SMR with CCS process [32]. This value is deducted from the CO₂-eq emission of the conventional SMR process (i.e., without CCS) to have an estimation for SMR-CCS. Table (B.9) presents the collected and estimated data for CO₂-eq emissions of long-term options.

Table (B.8). Global warming potential of fast-response technologies

Technologies	Reported value/range (original units)	Selected value (original units)	Selected value (kg CO ₂ -eq/GJ delivered)	Used value (kgCO ₂ -eq/GJ delivered) ⁴	Ref.
Flywheel ¹	159-159 (gr CO ₂ -eq/kWh delivered)	159.0	44.2	44.2	[14]
SMES ¹	416-416 (gr CO ₂ -eq/kWh delivered)	416.0	115.5	115.5	[14]
FB-VR ^{1,2}	44-44 (gr CO ₂ -eq/kWh delivered)	44.0	12.2	8.9	[14]
	136.5-184 (kg CO ₂ -eq/kWh capacity)	160.2	5.6		[15, 33]
FB-ZB ²	158-158 (kg CO ₂ -eq/kWh capacity)	158.0	12.1	12.1	[33]
LA ^{1,2}	51.6-51.6 (kg CO ₂ -eq/kWh capacity)	51.6	11.5	20.0	[15]
	102.76-102.76 (kg CO ₂ - eq/1000 kWh delivered)	102.8	28.5		[26]
Li-ion ²	17-27 (kg CO ₂ -eq/kWh capacity)	22.0	3.0	3.0	[19]
Li-Fe-Ph ^{1,2}	168.5-168.5 (kg CO ₂ -eq/kWh capacity)	168.5	24.2	14.3	[15]
	16.1-16.1 (kg CO ₂ -eq/1000 kWh delivered)	16.1	4.5		[26]
Li-Ni-Mn-Co ³	22-22 (kg CO ₂ -eq / kg battery)	22.0	11.8	11.8	[17]
Na-Ni-Cl ²	116-116 (kg CO ₂ -eq/kWh capacity)	116.0	18.2	18.2	[15]
Na-S ²	2-2 (kg CO ₂ -eq/kWh capacity)	2.0	0.2	0.2	[19]
Ni-Cd ²	10-15 (kg CO ₂ -eq/kWh capacity)	12.5	2.8	2.8	[19]

¹Only the units are converted to (kg CO₂-eq/GJ delivered).

²Reported data are divided by DEDLF (Eq. (A.1), based on 1 GJ capacity) to be per GJ delivered.

³Reported data are divided by gravimetric energy density (Table (B.5)) and by DEDLF (Eq. (A.1), based on 1 GJ capacity).

⁴For cases that more than one value is selected, the used value is their average.

Table (B.9). Global warming potential of long-term storage options

Storage options	Reported value/range (original units)	GWP (kg-CO ₂ - eq/ GJ delivered)	Used value (kg- CO ₂ -eq/ GJ delivered) ⁴	Ref.
H ₂ , CG ^{1,2}	0.076-0.076 (kg CO ₂ -eq/MJ H ₂)	1329.8	2392.7	[9]
	23.7-23.7 (kg CO ₂ -eq/kg H ₂)	3455.6		[34]
H ₂ , CG-CCS ¹	5.9-5.9 (kg CO ₂ /GJ H ₂)	103.2	103.2	[11]
H ₂ , SMR ¹	0.08-0.08 (kg CO ₂ -eq /MJ H ₂)	1399.7	1611.2	[9]
	12.50-12.50 (kg CO ₂ -eq/kg H ₂)	1822.6		[34]
H ₂ , SMR-CCS ¹	6.30-6.30 (kg CO ₂ /GJ H ₂)	110.2	110.2	[11]
H ₂ , WE-Grid mix ²	28.6-28.6 (kg CO ₂ -eq/kg H ₂)	4170.0	4170.0	[34]
H ₂ , WE-Hydropower ¹	0.01-0.01 (kg CO ₂ -eq /MJ H ₂)	175	175	[9]
H ₂ , WE-Solar ¹	0.04-0.04 (kg CO ₂ -eq /MJ H ₂)	699.9	699.9	[9]
H ₂ , WE-Wind ¹	0.005-0.005 (kg CO ₂ -eq /MJ H ₂)	87.5	87.5	[9]
H ₂ , WSCL ¹	0.012-0.012 (kg CO ₂ -eq /MJ H ₂)	210	210	[9]
NH ₃ , SMR ²	3.032-3.032 (kg CO ₂ -eq/kg NH ₃)	554.2	554.2	[32]
NH ₃ , SMR-CCS ^{2,3}	<u>1.895-1.895 (kg CO₂-eq/kg NH₃)</u>	<u>346.3</u>	<u>346.3</u>	-
NH ₃ , WE-Grid mix ²	2804.69-2804.69 (kg CO ₂ - eq/t NH ₃)	512.6	512.6	[30]
NH ₃ , WE-Hydropower ²	0.38-0.38 (kg CO ₂ -eq/kg NH ₃)	69.5	69.5	[31]
NH ₃ , WE-Solar ²	1.277-1.277 (kg CO ₂ -eq/kg NH ₃)	233.4	233.4	[32]
NH ₃ , WE-Wind ²	0.496-0.496 (kg CO ₂ -eq/kg NH ₃)	90.7	90.7	[32]
NH ₃ , WSCL ²	373.54-373.54 (kg CO ₂ - eq/t NH ₃)	68.3	68.3	[30]

¹The reported values are per energy content of H₂ based on its heating value. They are multiplied by the heating value of hydrogen (120MJ/kg [11]) and divided by the electricity delivered from 1 kg H₂ (Table (A.7)).

²Divided by energy delivered from 1 kg gas (Table (A.7)).

³Estimated from the data of ammonia production based on SMR (NH₃, SMR) as discussed in the text.

⁴For cases that more than one value is selected, the used value is their average.

8.2.6 Employment

As discussed in section 4.2.2.3, we assume employment as an output indicator because of its positive social impacts. In the absence of explicitly reported data or a standard and accurate way for estimating employment, for both clusters, fast-response, and long-term, we use economic data to estimate the employment. We compute employment from the total capital cost (TCC) of the technology for fast-response technologies. For long-term energy storage options, we compute it using the cost of gas production. A factor of 7.605 full-time eq. jobs per M\$ (i.e., the average between the ranges reported in [35], i.e., 7.49-7.72 full-time eq. jobs per M\$) is used for this goal. This number presents the number of full-time equivalent jobs created per million USD investment in the energy sector, whether to buy equipment to establish a new power plant or improve the efficiency of the current unit.

Therefore, for fast-response technologies, the employment offered per GJ of energy delivered during the lifetime of the technology is obtained by multiplying 7.605 by the total capital cost (€/kWh capacity) and dividing it by the energy delivered during the lifetime of technology considering 1GJ as the rated capacity of the technology (Eq. (A.1), based on 1GJ capacity).

For long-term energy storage options, 7.605 is multiplied by the cost of producing 1 kg gas (Table (B.2)). This is equivalent to assuming that capital costs completely dominate the total cost of these technologies and ultimately overestimates the employment generated with these technologies. Note, however, that the same overestimation is done for all the technologies in the cluster, which ensures that no alternatives are significantly benefited or harmed. Finally, this value is divided by the energy delivered from 1 kg gas (Table (A.7)). The final data are reported in Tables (B.10) and (B.11).

Table (B.10). Estimated employment for each fast-response technology

Technologies	Reported range for total capital cost (TCC, €/kWh)	Selected value for total capital cost ² (TCC, €/kWh) ²	Estimated employment (FTEJ ³ /GJ delivered)	Reference of TCC
Flywheels	1850-25049	4791	$2.68 \cdot 10^{-4}$	[3]
SMES	5310-6870	6090	$3.35 \cdot 10^{-4}$	[3]
FB-VR	459-560	546	$1.72 \cdot 10^{-4}$	[3]
FB-ZB	257-433	307	$2.11 \cdot 10^{-4}$	[3]
LA	346-721	457	$9.14 \cdot 10^{-4}$	[3]
Li-ion	973-1211	1095	$13.19 \cdot 10^{-4}$	[3]
Li-Fe-Ph ¹	<u>973-1211</u>	<u>1095</u>	<u>$14.06 \cdot 10^{-4}$</u>	-
Li-Ni-Mn-Co ¹	<u>973-1211</u>	<u>1095</u>	<u>$13.15 \cdot 10^{-4}$</u>	-
Na-Ni-Cl	596-808	699	$9.80 \cdot 10^{-4}$	[3]
Na-S	328-398	343	$3.06 \cdot 10^{-4}$	[3]
Ni-Cd	1071-1153	1147	$22.86 \cdot 10^{-4}$	[3]

¹TCC is considered the same as for Li-ion batteries.

²The original value computed using statistical methods in the reference paper and reported here is used to estimate the employment. Note that the reported value is not the median of the reported range in this case.

³FTEJ: Full Time Equivalent Jobs

Table (B.11). Estimated employment for each long-term storage option

Storage options	Estimated value/range for LCOE (€/kg) ¹	Selected value for LCOE (€/kg) ¹	Estimated employment (FTEJ ² /GJ delivered)
H ₂ , CG	0.86-0.86	0.86	1.12·10 ⁻³
H ₂ , CG-CCS	1.66-1.98	1.79	2.34·10 ⁻³
H ₂ , SMR	0.96-0.96	0.96	1.25·10 ⁻³
H ₂ , SMR-CCS	1.42-1.73	1.61	2.10·10 ⁻³
H ₂ , WE-Grid mix	2.10-6.73	4.46	5.82·10 ⁻³
H ₂ , WE-Hydropower	6.30-6.30	6.30	8.22·10 ⁻³
H ₂ , WE-Solar	13.37-13.37	13.37	17.44·10 ⁻³
H ₂ , WE-Wind	7.41-7.41	7.41	9.67·10 ⁻³
H ₂ , WSCL	NA	<u>0.92</u>	<u>1.20·10⁻³</u>
NH ₃ , SMR	1.11-1.96	1.53	2.50·10 ⁻³
NH ₃ , SMR-CCS	1.21-2.09	1.65	2.70·10 ⁻³
NH ₃ , WE-Grid mix	NA	<u>3.47</u>	<u>5.67·10⁻³</u>
NH ₃ , WE-Hydropower	NA	<u>4.5</u>	<u>7.36·10⁻³</u>
NH ₃ , WE-Solar	NA	<u>8.42</u>	<u>13.77·10⁻³</u>
NH ₃ , WE-Wind	NA	<u>5.11</u>	<u>8.36·10⁻³</u>
NH ₃ , WSCL	<u>1.09-1.93</u>	<u>1.51</u>	<u>2.50·10⁻³</u>

¹Refer to section 4.8.1 for guidance on how these values are estimated.

²FTEJ: Full Time Equivalent Jobs.

8.2.7 Technology readiness level (TRL)

Table (B.12). Technology readiness level (TRL) of fast-response technologies

Technologies	TRL	Ref.
Flywheel	7.5	[36]
SMES	7	[36]
FB-VR	6.5	[36]
FB-ZB	5.5	[36]
LA	8.5	[36]
Li-ion	8	[36, 37]
Li-Fe-Ph	8	[36]
Li-Ni-Mn-Co	8	[36]
Na-Ni-Cl	6	[38]
Na-S	6.5	[36]
Ni-Cd	8.5	[36]

Table (B.13). Technology readiness level (TRL) of long-term energy storage alternatives

Storage options	Reported TRL	Used TRL	Ref.
H ₂ , CG	8-9	8.5	[39]
H ₂ , CG-CCS	6-8	7	[39]
H ₂ , SMR	8-9	8.5	[39]
H ₂ , SMR-CCS	6-8	7	[39]
H ₂ , WE-Grid mix ¹	NA	7.75	-
H ₂ , WE-Hydropower ²	NA	2	-
H ₂ , WE-Solar	1-3	2	[39]
H ₂ , WE-Wind ²	NA	2	-
H ₂ , WSCL ¹	NA	7.75	-
NH ₃ , SMR ³	NA	8.5	-
NH ₃ , SMR-CCS ⁴	NA	7	-
NH ₃ , WE-Grid mix ⁵	NA	7.75	-
NH ₃ , WE-Hydropower ⁶	NA	2	-
NH ₃ , WE-Solar ⁷	NA	2	-
NH ₃ , WE-Wind ⁸	NA	2	-
NH ₃ , WSCL ⁹	NA	7.75	-

¹Average of the reported value for hydrogen produced using coal gasification (H₂, CG), hydrogen produced using coal gasification with CCS (H₂, CG-CCS), hydrogen produced using steam methane reforming (H₂, SMR), and hydrogen produced using steam methane reforming with CCS (H₂, SMR-CCS) is used.

²Is considered the same as hydrogen based on water electrolysis using solar energy (H₂, WE-Solar)

³Considered the same as hydrogen produced based on the steam methane reforming

⁴Considered the same as hydrogen produced based on the steam methane reforming with CCS

⁵Considered the same as hydrogen produced based on the water electrolysis using grid mix energy

⁶Considered the same as hydrogen produced based on the water electrolysis using hydropower

⁷Considered the same as hydrogen produced based on the water electrolysis using solar

⁸Considered the same as hydrogen produced based on the water electrolysis using wind

⁹Considered the same as hydrogen produced based on the water-splitting by chemical looping

8.2.8 Monetization transforming coefficients

Table B.14. Monetization transforming coefficients for the used indicators in DEA

Indicators	Coefficient	References
LCOE ¹	-	-
Energy consumption	6.6 €/GJ	[40]
Energy density ^{2,3}	0.68 €/kg Sb-eq	[40]
Water used	0.045 €/m ³	[40]
GWP	0.15 €/kg CO ₂ -eq	[40]
Employment ⁴	3157308 €	[41]

¹This indicator is initially expressed in [€/GJ] and does not need any transformation.

²Reported coefficient is related to resource use, minerals, and metals. It is per kg of antimony (kg Sb-eq). Acknowledging that the energy density is influenced by various materials used in the structure of technologies, we assume that kg of storage technology is equal to kg of antimony. Since this is the only value we found regarding material use, we use it to monetize the energy density. It is supposed that no technology is significantly benefited or harmed by using this coefficient.

³This indicator is used only for the fast-response cluster.

⁴The estimation method is described before the table.

8.3 Uncertainty analysis

Using Eq. (C.1), we estimate the standard deviation (σ) of the lognormal distribution of an uncertain life cycle impact.

$$\sigma = \ln\left(\sqrt{e^{\sqrt{\sigma_1^2 + \sigma_2^2 + \sigma_3^2 + \sigma_4^2 + \sigma_5^2 + \sigma_b^2}}}\right)^2 \quad (C.1)$$

Here, σ_1^2 to σ_5^2 are values related to the scores of the Pedigree Matrix. In essence, the practitioner needs to characterize the quality of the corresponding dataset by assigning a score in the 1 to 5 range for each of the categories provided in Table (C.1), i.e., reliability (related to σ_1), completeness (σ_2), temporal correlation (σ_3), geographical correlation (σ_4), and future technical correlation (σ_5) [42]. With these scores at hand, Table (C.2) translates them into the values of parameters σ_1 to σ_5 appearing in Eq. (C.1) [43]. Note that these values depend on the Ecoinvent dataset rather than on individual life cycle inventories or impacts.

Table (C.1). The Pedigree matrix used to assess the quality of data sources [42].

Indicator score	1	2	3	4	5 (default)
Reliability	Verified data based on measurements	Verified data partly based on assumptions or non-verified data based on measurements	Non-verified data partly based on qualified estimates	Qualified estimate (e.g., by industrial ex-pert)	Non-qualified estimate
Completeness	Representative data from all sites relevant for the market considered, over an adequate period to even out normal fluctuations	Representative data from >50% of the sites relevant for the market considered, over an adequate period to even out normal fluctuations	Representative data from only some sites (<50%) relevant for the market considered or >50% of sites but from shorter periods	Representative data from only one site relevant for the market considered or some sites but from shorter periods	Representativeness unknown or data from a small number of sites and from shorter periods
Temporal correlation	Less than 3 years of difference to the time period of the dataset	Less than 6 years of difference to the time period of the dataset	Less than 10 years of difference to the time period of the dataset	Less than 15 years of difference to the time period of the dataset	Age of data unknown or more than 15 years of difference to the time period of the dataset
Geographical correlation	Data from area under study	Average data from larger area in which the area under study is included	Data from area with similar production conditions	Data from area with slightly similar production conditions	Data from unknown or distinctly different area (North America in-stead of Middle East, OECD-Europe instead of Russia)
Further technological correlation	Data from enterprises, processes and materials under study	Data from processes and materials under study (i.e., identical technology) but from different enterprises	Data from processes and materials under study but from different technology	Data on related processes or materials	Data on related processes on laboratory scale or from different technology

Table (C.2). Uncertainty factors (variances of the underlying normal distributions) used to convert the data quality indicators of the pedigree matrix in Table (C.1) into additional uncertainty [43].

	1	2	3	4	5
Reliability	0.000	0.0006	0.002	0.008	0.04
Completeness	0.000	0.0001	0.0006	0.002	0.008
Temporal correlation	0.000	0.0002	0.002	0.008	0.04
Geographical correlation	0.000	0.000025	0.0001	0.0006	0.002
Further technological correlation	0.000	0.0006	0.008	0.04	0.12

The last parameter in Eq. (C.1) is σ_b^2 , corresponding to the so-called basic uncertainty. This parameter depends on particular the life cycle inventory entry [43]. In a traditional approach, one would have a different σ_b value for each life cycle inventory contributing towards a certain impact. Note, however, that in this contribution, we aim to characterize the uncertainty on the final impact (GWP) based only on its most significant stressor (CO₂ emissions), so only one value of σ_b is needed (i.e., $\sigma_b = 0.0006$ for CO₂ emitted to air).

Finally, the median of the lognormal distribution is computed from the nominal value provided in Ecoinvent, as shown in Eq. (C.2).

$$\mu = \ln(\text{nominal value}) \quad (\text{C.2})$$

8.4 References

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Clean Energy Transition: Requirements, Realities, and Consequences

The production and utilization of fossil fuels have long been criticized for their wide-ranging impacts on the environment, health, and social equity. Clean energy technologies are often seen as a solution to these issues, promising reduced greenhouse gas emissions, diversification of the energy basket, and enhanced energy security. However, the requirements and implications of transitioning to CETs have not been thoroughly evaluated – until now.

This thesis addressed the gap by examining the comprehensive requirements and consequences of developing clean energy infrastructures. It highlighted initial apprehensions regarding the impacts on human rights, inequalities, and transition justice, underscoring the need for a balanced analysis of CET development.

This research estimated the requirements for widespread CET adoption, assessed realistic capabilities, and analyzed the socio-economic, environmental, and technical impacts and aspects. It also evaluated the geopolitical ramifications of shifting energy paradigms. It revealed, based on evidence rather than mere suggestions, that a crucial aspect of this transition is understanding the equitable distribution of its benefits and burdens, ensuring that the clean energy system is accessible and beneficial to all.

In summary, this thesis contributed to the discourse on clean energy by providing a holistic evaluation of the transition's implications for sustainable development. It aimed to inform policymakers, stakeholders, and the global community about the necessary steps to ensure that the shift towards clean energy is not only technologically and economically feasible but also socially just and inclusive. May it be a small light on this way.