# A Suggested Methodological Framework to Enhance Comparability and Reliability for Life Cycle Assessment of CO<sub>2</sub> Adsorption in Energy-Intensive Industries

- 4 Yipeng Yao<sup>1</sup>, Marie-Eve Duprez<sup>1</sup>, Guy De Weireld<sup>1, \*</sup>
- 5 1. Thermodynamics and Mathematical Physics Unit, Faculty of Engineering, University
- 6 of Mons, 20 Place du Parc, Mons, 7000, Belgium
- 7 \*. Corresponding author: Thermodynamics and Mathematical Physics Unit, Faculty of
- 8 Engineering, University of Mons, 20 Place du Parc, Mons, 7000, Belgium
- 9 E-mail address: guy.deweireld@umons.ac.be

### 10 Abstract

11 Among the various  $CO_2$  capture technologies, adsorption capture appears to be an emerging and promising technology characterised by operational flexibility, low 12 13 pollutant emissions, and low energy consumption. It is expected to be crucial in carbon 14 capture and storage systems. Whilst Life Cycle Assessment (LCA) has emerged as the 15 consensus methodology for evaluating the environmental impacts of this technology, 16 methodological heterogeneity in LCA applications has limited the comparability and 17 credibility of research findings. This study systematically reviews 31 LCA studies 18 published between 2006 and 2025, examining methodological commonalities and 19 differences across four aspects: goal and scope definition, inventory analysis, impact 20 assessment and interpretation. Current LCA methodological standards and guidelines 21 were used as benchmarks to analyse the challenges and opportunities in  $CO_2$ 22 adsorption LCA methodology and to propose a methodological framework. The 23 findings reveal that commonalities (e.g., functional unit) and differences (e.g., system 24 boundary, life cycle stages and process stage alignments) exist among LCA 25 methodologies. Moreover, compared to existing standards and guidelines, current 26 methodological applications demonstrate notable gaps (e.g., the lack of data quality 27 evaluation and the classification of significance levels). Consequently, we propose a 28 hierarchical improvement framework comprising three levels based on required 29 additional effort levels - minor, moderate, and major efforts. This framework aims to 30 systematically enhance the comparability and reliability of LCA studies. This work 31 contributes to establishing common LCA application protocols and provides 32 methodological guidance for future environmental assessments of CO<sub>2</sub> adsorption 33 technologies.

34 Keywords: Life cycle assessment; Methodology; Carbon dioxide; Adsorption.

# 35 Abbreviation

| Abbreviation | Full name                                      |  |  |  |  |
|--------------|--|--|--|--|--|
| AC           | Activated Carbon                               |  |  |  |  |
| CC           | Climate Change                                 |  |  |  |  |
| CCS          | Carbon Capture and Storage                     |  |  |  |  |
| CCU          | Carbon Capture and Utilisation                 |  |  |  |  |
| CCUS         | Carbon Capture, Utilisation, and Storage       |  |  |  |  |
| DAC          | Direct Air Capture                             |  |  |  |  |
| DQR          | Data Quality Rating                            |  |  |  |  |
| DQRs         | Data Quality Requirements                      |  |  |  |  |
| ELCD         | European Life Cycle Database                   |  |  |  |  |
| EF           | Environmental Footprint                        |  |  |  |  |
| EPD          | Environmental Product Declaration              |  |  |  |  |
| GHG          | Greenhouse Gas                                 |  |  |  |  |
| IEA          | International Energy Agency                    |  |  |  |  |
| ILCD         | International Reference Life Cycle Data System |  |  |  |  |
| LCA          | Life Cycle Assessment                          |  |  |  |  |
| LCIA         | Life Cycle Impact Assessment                   |  |  |  |  |
| MDEA         | Methyl diethanolamine                          |  |  |  |  |
| MEA          | Monoethanolamine                               |  |  |  |  |
| MOFs         | Metal-Organic Frameworks                       |  |  |  |  |
| NDC          | Nationally Determined Contributions            |  |  |  |  |
| OAT          | One-at-a-time                                  |  |  |  |  |
| OEF          | Organisational Environmental Footprint         |  |  |  |  |
| PEF          | Product Environmental Footprint                |  |  |  |  |
| VSA          | Vacuum Swing Adsorption                        |  |  |  |  |
| PSA          | Pressure Swing Adsorption                      |  |  |  |  |
| VPSA         | Vacuum Pressure Swing Adsorption               |  |  |  |  |
| TSA          | Temperature Swing Adsorption                   |  |  |  |  |

#### 37 **1. Introduction**

38 In the global context of climate change mitigation, limiting warming to 1.5°C (as 39 adopted in the Paris Agreement) or even 2°C requires immediate and drastic 40 reductions in Greenhouse Gas (GHG) emissions across all sectors [1]. Alongside the 41 shift from fossil fuels to renewable energy, enhancing energy efficiency, and reducing 42 consumption, Carbon Capture and Storage (CCS) is recognised as an essential 43 solution—especially in hard-to-abate sectors such as cement, lime, steel production, 44 and petroleum refining, where process-related emissions are important [2]. In this 45 framework, CO<sub>2</sub> adsorption technology has emerged as a promising alternative to 46 amines absorption/regeneration technologies due to its high selectivity, relatively low 47 energy demand, and reliable performance over a broad range of temperatures and 48 pressures, making it especially suitable for deployment in energy-intensive industries 49 such as thermal power generation, cement manufacturing, and steel mills [3-8].

50 Evaluating the environmental performance of CO<sub>2</sub> adsorption technologies 51 through Life Cycle Assessment (LCA) is essential to ensure their sustainable and large-52 scale application [9, 10]. LCA offers a comprehensive tool to: (1) Quantify GHG 53 Reduction - Precisely determine the net  $CO_2$  (equivalent) mitigation attributable to 54 adsorption processes, which is central to their environmental benefit. (2) Identify 55 Environmental Burdens - Detect potential shifting of impacts, such as increased 56 resource use or secondary pollutant emissions, thereby preventing unintended burden 57 transfers. (3) Highlight Life-Cycle Hotspots – Analyse each stage of the technology's 58 life cycle to reveal process inefficiencies and guide improvements in both process flow 59 and adsorbent performance. (4) Facilitate Technology Comparison and Decision-60 Making - Generate comparable environmental impact data across different 61 adsorbents and process configurations to support informed decisions.

62 Despite the guidance provided by ISO 14040 and ISO 14044 for LCA [11, 12], these 63 macro-level standards do not fully address the variability inherent in specific 64 applications, leaving room for methodological interpretation. In the realm of CO2 65 adsorption, variations in system boundary definitions, functional unit selections, and 66 impact category considerations have led to inconsistencies among studies. Such 67 discrepancies complicate direct comparisons—whether a study isolates the adsorption 68 process or extends to cover adsorbent production and disposal, or whether different 69 functional units (e.g., in power industries, CO<sub>2</sub> captured per tonne versus net 70 electricity generated) are used-thereby potentially skewing policy decisions and 71 resource allocation. Against this backdrop, establishing a consensus-based LCA 72 framework tailored to CO<sub>2</sub> adsorption is crucial to ensure comparability and enhance 73 decision reliability.

74 Several related review articles have emerged in recent years on the LCA of CO<sub>2</sub> 75 adsorption [13-19], offering valuable insights into this developing field. Table 1 76 summarises the significant information of these studies. These reviews show several 77 notable properties: (1) In terms of coverage, most works devote only one chapter to 78 LCA, often as a subsection within broader discussions, suggesting that LCA remains a 79 relatively underexplored dimension; (2) Regarding the scale of the reviewed object, 80 these reviews span from adsorbent materials to full CCS systems, yet comprehensive 81 attention to the intermediate scale of "CO2 adsorption technology"-as a process 82 situated between material and system-remains limited; (3) As for content focus, a

substantial number of reviews prioritise LCA results-particularly impact 83 84 assessment—while discussions on the LCA methodological practices are relatively scarce; (4) In terms of methodological coverage, only a few studies have attempted to 85 systematically address all four classical LCA phases (goal and scope definition, 86 87 inventory analysis, impact assessment, and interpretation), with most limiting their 88 scope to selected components. (5) Regarding the solutions for the identified LCA 89 methodological gaps, only one study has addressed this field but without any examples. 90 All in all, these existing works have laid a valuable foundation for our work, indicating 91 the potential contribution of a more holistic, methodology-oriented review focused on 92 CO<sub>2</sub> adsorption technologies at the medium scale and further proposing the potential 93 solutions with examples for the LCA methodological gaps.

| Ref. | Year | Author                      | Length          | Review Object                                | The scale<br>of Review<br>Object | Content and<br>Proportion                                     | Coverage of LCA<br>Methodology   | Solution for the<br>LCA<br>methodological<br>gaps? | Example |
|------|------|-----------------------------|-----------------|--|----------------------------------|---|--|--|---------|
| [13] | 2022 | Wang et<br>al.              | One<br>chapter  | CO₂ capture                                  | Large                            | LCA<br>methodology  | All four phases  | No   | No      |
| [14] | 2022 | Yuan et<br>al.              | One<br>chapter  | Solid waste-<br>derived<br>porous<br>carbons | Small                            | Half of the LCA<br>results, half of<br>the LCA<br>methodology | Functional unit,<br>system boundary,<br>impact categories,<br>database, software                   | No   | No      |
| [17] | 2023 | Karimi et<br>al.            | One<br>chapter  | CO₂<br>adsorption                            | Medium                           | LCA case studies  | No   | No   | No      |
| [16] | 2023 | Jiang et<br>al.             | Half<br>chapter | Adsorption-<br>based DAC                     | Medium                           | Focus on LCIA<br>results                                      | No   | No   | No      |
| [15] | 2023 | Duval-<br>Dachary<br>et al. | Full text       | Bioenergy with<br>CCS                        | Large                            | Focused on<br>inventory<br>methodology                        | Inventory phase  | Yes  | No      |
| [18] | 2024 | Jia et al.                  | One<br>chapter  | Engineered<br>biochar-based<br>CO2 adsorbent | Small                            | Mostly LCIA<br>results, less on<br>methodology                | Functional unit,<br>system boundary,<br>inventory data,<br>impact categories,<br>impact assessment | No   | No      |
| [19] | 2025 | Umar et<br>al.              | One<br>chapter  | Biomass-<br>derived carbon<br>adsorbents     | Small                            | LCIA results only   | No   | No   | No      |
| This | 2025 | Yao et al.                  | Full text       | CO2  | Medium                           | LCA   | All four phases  | Yes  | Yes     |

# 94 Table 1. Summary of related review literature on LCA of CO<sub>2</sub> adsorption

| work adsorption methodology |  |
|-----------------------------|--|
|-----------------------------|--|

96 Given the promising prospects of  $CO_2$  adsorption in energy-intensive industries 97 and the ambiguities in its LCA methodologies, this study seeks to address these gaps 98 by proposing a comparable and reliable LCA framework explicitly tailored for  $CO_2$ 99 adsorption technologies. As depicted in Figure 1, the study focuses on three key 100 aspects: (1) Systematically identifying commonalities and differences in LCA 101 applications across published studies by examining the four phases—goal and scope 102 definition, inventory analysis, impact assessment and interpretation—to distil typical paradigms and key differences; (2) Highlighting the gaps and opportunities between 103 104 current practices and an ideal state, using the latest international standards (ISO 14040 105 [12] and its 2020 amendment [20]), European standards (ILCD handbook series [21-24]) and authoritative books (e.g., Environmental Life Cycle Assessment [25]) as 106 107 references, while also identifying effective methods not explicitly covered by these 108 requirements; (3) Developing a consensus-driven LCA methodological framework that 109 enhances both comparability and reliability. This framework is intended to contribute 110 to standardising LCA practices for CO<sub>2</sub> adsorption technologies, thereby providing 111 researchers with a suggested evaluation basis and offering more robust scientific evidence for decision-makers to select optimal technological solutions and formulate 112 113 effective environmental policies.



The application of methodology in current research

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#### Figure 1. Research contents in this work

#### 116 **2. Method**

117 The full process of this literature review and framework development is illustrated in Figure 2, which follows the principles and structure of the PRISMA guidelines [26, 118 119 27], with customised modifications to suit the specific objectives of this work. The 120 process follows a top-to-bottom sequence along the left side of the flowchart, 121 encompassing the following steps: Research questions, Search strategy, Identification, 122 Screening, Included, Metadata analysis, Refinement, Alignment, and Framework roll-123 out. This approach ensures a systematic definition of research questions, a rigorous 124 design of search strategies, transparent and efficient literature screening, and 125 scientifically robust metadata analysis and synthesis, thereby providing a solid

126 theoretical basis for LCA studies in the context of CO<sub>2</sub> adsorption.

127 During the literature retrieval phase, keywords such as "CO<sub>2</sub> adsorption" and 128 "LCA" were used to search two academic scientific and technical databases—Scopus and Web of Science<sup>™</sup>—on 10 April 2025, yielding 287 records from Scopus and 452 129 records from Web of Science<sup>™</sup>, for a total of 739 records. In the subsequent screening 130 phase, studies were excluded based on criteria including duplicate, language, article 131 132 type, and relevance to the scope. This rigorous filtering process resulted in 28 eligible 133 studies; additionally, 28-based citation tracking contributed 3 further relevant records, 134 leading to a final total of 31 studies for subsequent metadata analysis.

135 Based on the included studies, a comprehensive metadata analysis and 136 methodological refinement were performed, focusing on the four key phases of the LCA methodology (goal and scope definition, inventory analysis, impact assessment, 137 138 and interpretation). Alignment with the last today's international standards and 139 guidelines facilitated the identification of common gaps and potential opportunities in 140 the current research landscape, ultimately culminating in developing a tailored LCA 141 methodological framework to enhance compatibility and reliability for the CO<sub>2</sub> 142 adsorption domain, with representative case examples illustrating its practical 143 applicability.



# 145Figure 2. The integrated process of conducting a literature review and developing a146suggested LCA methodological framework

# 147 **3. Results**

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According to ISO 14040, LCA is divided into four phases: goal and scope definition, inventory analysis, impact assessment, and interpretation [12]. This section is structured based on these four phases, with each subsection elaborating on the commonalities and differences in the methodological applications observed in existing studies. Subsequently, the gaps between the actual and ideal states are analysed, and potential opportunities for improvement are discussed. The fifth subsection builds upon the preceding four to propose a suggested methodological framework. 155 A total of 31 eligible publications were analysed in this study. Detailed information 156 about these publications, including their identification numbers, titles, authors, and 157 publication years, can be found in the "Supplementary Document 1 Metadata of 158 Methodology". The numbering system follows a chronological order from the earliest 159 to the most recent publications. Additionally, the Supplementary Document 160 1 Metadata of Methodology also contains detailed information on the specific 161 methodological elements extracted from the four phases of the eligible publications. 162 It includes the following phases: (I). Goal and scope definition (goal, type of 163 comparison, type of LCA, system boundary, process or stage breakdown, functional 164 unit, software or tool); (II). Inventory analysis (foreground data, background data, 165 allocation criteria, inventory visibility); (III). Impact assessment (method, type/number of impact categories, final score); (IV). Interpretation (significance 166 167 analysis type, uncertainty analysis object, uncertainty analysis type, uncertainty 168 analysis method, sensitivity analysis object, sensitivity analysis type, sensitivity 169 analysis method).

# 170 **3.1. Goal and Scope Definition**

171 In the goal and scope definition phase, the core elements that should be 172 addressed include the goal, type of LCA, system boundary, life cycle stage and process 173 breakdown, functional unit, cut-off rules, Data Quality Requirements (DQRs), and the 174 software or tool used.

#### 175 **3.1.1. Goal definition and its type**

176 The original description of the goal varies significantly due to differences in 177 research subjects and the authors' writing styles, making it difficult to directly 178 summarise a unified definition paradigm. However, as LCA is typically comparative and 179 is conducted to analyse the environmental impact differences between various 180 options [21], this study extracts and clusters the research objectives of existing 181 publications based on the objects compared in comparative LCA. The complete results are presented in the "goal" column of the supplementary document 1. Furthermore, 182 183 the objects of comparison are hierarchically arranged from broadest to narrowest, as 184 shown in Figure 3.

Figure 3 illustrates that the comparative LCA of CO<sub>2</sub> adsorption can be categorised
 into five levels, corresponding to eight types. Specifically:

187 188 ♦ Level 1 compares two options: with and without CCS systems, i.e., the differences before and after installing a CCS system.

- 193 
   Level 3.1 compares different carbon capture technologies under the same capture route. For instance, carbon capture technologies in post-combustion capture include adsorption, absorption, membrane separation, and CaO looping.
- 197 
   ↓ Level 3.2 compares different storage technologies under the same capture
   198 route. For example, storage technologies include geological storage,
   199 ocean storage, and others.

- Level 4.1 and Level 4.2 are two parallel sub-levels:
   Level 4.1 examines the differences between various adsorbent materials
   used in CO₂ separation via adsorption technology. Examples include
   activated carbon (AC), zeolites, and metal-organic frameworks (MOFs).
   Level 4.2 compares different regeneration modes under CO₂ absorption.
  - For instance, pressure swing adsorption (PSA), temperature swing adsorption (TSA), and hybrid mode.

207 Level 5.1 and level 5.2 are two parallel sub-levels:

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- ♦ Level 5.1 compares different synthesis (manufacturing) methods for the same CO₂ adsorbent. For instance, MOFs can be synthesised via mechanochemical, solvothermal, and other methods.
- 211 212

214 In summary, from Level 1 to Level 5, the scope of the objects being compared 215 becomes progressively narrower, and the scale of investigation becomes increasingly 216 detailed, transitioning from a macro to a micro perspective. Additionally, Level 4 and 217 Level 5 represent internal comparisons of CO<sub>2</sub> adsorbents, with the research focus 218 entirely within the scope of adsorption technology. In contrast, Level 1 to Level 3 219 represents external comparisons of CO<sub>2</sub> adsorption. While CO<sub>2</sub> adsorption may be a significant subject in comparative LCA, other options (e.g., without CCS, capture routes, 220 221 and capture technologies) are also critical objects of investigation. Therefore, in the 222 hierarchical structure of comparative LCA, Level 4 and Level 5 treat CO<sub>2</sub> adsorption as 223 the primary research subject, whereas in Level 1 to Level 3, CO<sub>2</sub> adsorption is more of 224 an important branch within the broader CO<sub>2</sub> capture and storage chain.



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Figure 3. A hierarchical framework of comparative LCA for  $CO_2$  adsorption

Figure 4 further illustrates the frequency of investigation for different types of comparative LCA. Overall, four types of comparisons are frequently conducted, including Level 1: With or without CCS (6 times), Level 3.1: Capture Technique (13 230 times), Level 4.1: Adsorption Material (8 times), and Level 5.1: Synthesis Method (9 231 times). In contrast, four comparisons are rarely conducted, including Level 2: Capture 232 Route, Level 3.2: Storage Technique, Level 4.2 Regeneration mode, and Level 5.2: 233 Disposal Method, each of which has only been investigated once. Additionally, two of 234 the 31 LCA studies on CO<sub>2</sub> adsorption are non-comparative. These studies evaluate the 235 environmental impacts of synthesising activated carbon from waste polyethene 236 terephthalate plastics [28] and food waste [29] for application in CO<sub>2</sub> adsorption 237 without comparing them to other alternatives.



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Type of Comparative LCA

#### 239 Figure 4. Statistics on types of comparative LCA focused on CO<sub>2</sub> adsorption

#### 240 **3.1.2. Type of LCA**

LCA can be categorised into two types based on the temporal nature of its investigation: Retrospective and Prospective [30]. The term retrospective LCA is defined as: "LCA that models the product system at a recent or distant past point in time relative to the time at which the study is conducted" [31]. In contrast, prospective LCA is defined as: "LCA that models the product system at a future point in time relative to the time at which the study is conducted" [31, 32].

Figure 5 illustrates the frequency and proportion of the two types of LCA investigated in  $CO_2$  adsorption. Among the 31 studies, 27 employed retrospective LCA, while only 4 adopted prospective LCA, accounting for 87% and 13%, respectively. Results suggest that researchers focus more on conducting LCA investigations of  $CO_2$ adsorption technologies relevant to the present or the recent past, probably due to data availability.



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# Figure 5. Types, frequency and percentage of temporal LCA in CO<sub>2</sub> adsorption studies

#### 256 **3.1.3. System boundary and life cycle stage breakdown**

Typically, based on the scope of LCA stages covered, studies can be categorised into two typical types: cradle-to-gate and cradle-to-grave [12]. Among the 31 studies analysed, as shown in Figure 6, 21 (68%) clearly defined their system boundaries, while 10 (32%) did not specify their boundaries.

For those with clearly defined system boundaries, 10 studies (32%) adopted a cradle-to-gate approach [33-40]; 8 studies (26%) followed a cradle-to-grave approach [28, 41-45]; 1 study (3%) employed a cradle-to-use approach [46]; 2 study (6%) used a gate-to-gate approach [39]. Additionally, one study conducted both cradle-to-gate and cradle-to-grave analyses [29].

In summary, most studies have reported system boundaries, with cradle-to-gate and cradle-to-grave approaches being equally prevalent. Other types of system boundaries are relatively less common. However, a significant proportion of studies failed to explicitly clarify their system boundaries, which may impact the comparability and reliability of their findings.



# Figure 6. Types, frequency and percentage of system boundaries in LCA studies of CO<sub>2</sub> adsorption

However, potential inconsistencies and conflicts become apparent upon further examination of the 21 studies with clearly defined system boundaries, particularly through a comparative analysis of system boundaries and technical process stages. Specifically, even when studies claim to adopt the same system boundary, the associated scope of technical processes often differs. Two typical cases are outlined below, accompanied by illustrative examples:

280 Case (i): For cradle-to-gate studies on CO<sub>2</sub> adsorption, the scope of technical 281 processes varies significantly. In the study by Grande et al., the process chain includes 282 Mixing, Synthesis, Cleaning, and Drying [35]. In the study by Zakuciová et al., the 283 process chain covers Turbomachinery, Combustion, Flue Gas Treatment, CO<sub>2</sub> Capture, 284 and Water Consumption [36]. In the study by Luo et al., the process chain encompasses 285 a Pulverized Coal Boiler, Steam Turbine, CO<sub>2</sub> Capture, and CO<sub>2</sub> Compression [34]. It is 286 evident that Grande et al. focused on the synthesis of adsorbents, Zakuciová et al. 287 considered the CO<sub>2</sub> capture process, while Luo et al. extended their scope to include 288 both CO<sub>2</sub> capture and compression. Thus, although all three studies are categorised as 289 "cradle-to-gate", the coverage of technical processes differs significantly.

290 Case (ii): For cradle-to-grave studies on CO<sub>2</sub> adsorption, the technical process 291 scope also varies: Sathre and Masanet's study includes Coal Mining and Transport, 292 Plant Infrastructure, Capture Media Production, Plant Stack Emissions, and CO<sub>2</sub> 293 Transport and Storage [43]. Wang et al.'s study covers Polyethylene Terephthalate 294 Bottle Production and Collection, activated carbon (AC) Production, CO<sub>2</sub> Capture, and 295 AC Disposal [47]. Tao and Brander's study involves Raw Materials Extraction and 296 manufacturing, Power Plants and use, Transportation, Recycling and disposal, with 297 some scenarios considering, e.g., a 13% recycling rate for MOFs. For instance, Sathre 298 and Masanet included CO<sub>2</sub> transport and storage, Wang et al. incorporated AC disposal, 299 and Tao and Brander considered MOF recycling in specific scenarios. Therefore, even 300 though all three studies aim to achieve CO<sub>2</sub> adsorption under a cradle-to-grave 301 framework, the corresponding technical processes mapped by each study are not 302 entirely consistent.

#### 303 3.1.4. Functional unit

304 An essential step in defining the goal and scope of an LCA study is identifying the 305 functional unit, which quantifies the function of a product or service to enable 306 comparisons across different systems or similar studies [11, 12]. However, in practical 307 contexts, the functional unit may refer to the product's function and the product itself 308 [48]. For functional units related to CO<sub>2</sub> adsorption, among the 31 published studies 309 reviewed, one study did not specify any functional unit [42], and another employed 310 two functional units [47]. The remaining 31 functional units can be categorised into 311 three types, as illustrated in Figure 7:

(i) Function-based CO<sub>2</sub> adsorption: CO<sub>2</sub> adsorption is the core function; thus, the
specified amount of CO<sub>2</sub> adsorbed is often set as the functional unit. For example, 1 kg
of CO<sub>2</sub> [39, 45], 1 tonne of CO<sub>2</sub> [33, 49], and 40 mg of CO<sub>2</sub> [50].

(ii) Function-based factory product: Since CO<sub>2</sub> adsorption and storage are often
 employed as decarbonisation technologies for energy-intensive factories, some

studies use the factory's product as the functional unit. For instance, 1 kWh of net
power for power plants [51, 52], 1 kWh of electricity [53], and 1 kg of clinker for
cement plants [40].

(iii) Product-based CO<sub>2</sub> adsorbent: While function-oriented functional units are
the first choice, in cases where the system boundary is cradle-to-gate and does not
account for the product's use or subsequent stages—thus not fully realise the
product's intended function—it may be more appropriate to set the functional unit
based on the production of an equivalent amount of the product. Examples include
1 kg of ZIF-8 [38], 1 kg of AC [28], 1 kg of MIL-53(AI) [54], 1 kg of porous carbon [55],
and 1 kg of UiO-66-NH<sub>2</sub> [34].

327 As shown in Figure 7, the occurrence and the frequency of the three categories— 328 (i) Function-based CO<sub>2</sub> adsorption, (ii) Function-based factory product, and (iii) 329 Product-based  $CO_2$  adsorbent—are 12 (38%), 10 (31%), and 9 (28%), respectively. 330 Results indicate that the occurrence and the frequency of function-oriented and 331 product-oriented functional units are 22 (69%) and 9 (28%), respectively. Therefore, 332 functional units based on service functions remain the dominant choice, while a 333 smaller proportion are product-based, typically associated with cradle-to-gate 334 analyses from the perspective of CO<sub>2</sub> adsorbents.



#### 335

Figure 7. Types, frequency and percentage of function units in LCA studies of CO<sub>2</sub>
 adsorption

#### 338 3.1.5. Software

The software or tools utilised in the 31 studies are summarised in Figure 8. The most widely used software is SimaPro, appearing in 16 instances (52%), significantly exceeding the combined usage of other software or tools (GaBi, eFootprint, Excel, NTNU-owned MATLAB-based routine, OpenLCA, and Umberto), which collectively account for ten instances (31%). Additionally, five studies (16%) did not disclose the software they employed.



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Figure 8. Types, frequency and percentage of software in LCA studies of CO<sub>2</sub>
 adsorption

#### 348 **3.1.6. Gaps and opportunities**

#### 349 **3.1.6.1.** Goal definition and common comparative reference

350 As mentioned in Section 3.1.1: Goal Definition and Its Type, although most LCA 351 studies are inherently comparative—aiming to distinguish the environmental 352 advantages and disadvantages of different options—the definition of the goal often 353 varies significantly depending on the research context and the researchers' expression 354 style. This variability makes it challenging to assess the comparability of different 355 studies, potentially leading to a loss of comparability. Furthermore, it somewhat 356 weakens the transferability and mutual validation of research findings. The excessive 357 heterogeneity in goal definitions also obscures the positioning of the studied subjects 358 within the overall CO<sub>2</sub> adsorption system, posing a challenge to the research's 359 readability and comprehensibility.

Based on the above analysis, this study proposes the following recommendations: (i) Clarify the positioning of the subjects in comparative LCA studies: While considering the contextual differences of the studied subjects, it is advisable to integrate the hierarchical framework presented in Figure 3 to refine the research objectives further and clearly articulate the positioning of the compared subjects within the system. For instance, does the comparison between capture technologies, adsorbents, or a hybrid comparison involve multiple approaches?

367 (ii) Establish a common benchmark for comparable LCA studies: Systematic and 368 high-confidence LCA results are among the key pursuits of consensus-driven research. 369 Achieving this requires collaborative efforts to build robust and systematic results 370 across multiple studies. A critical prerequisite for this is establishing a set of consensusbased comparative benchmarks. Such benchmarks would leverage the collective 371 372 strengths of group research findings, thereby advancing the development of a more 373 robust system. The proposed benchmarks should centre around CO<sub>2</sub> adsorption and 374 adopt the most generalised options as the standard. For example:

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♦ Level 1: Factories without CCS equipment,

- - Level 3.1: MEA-based CO<sub>2</sub> scrubbing technology,
- - Level 4.1: Activated carbon or zeolite,
- - Level 5.1: Physical activation of activated carbon,
  - ♦ Level 5.2: Landfilling of activated carbon.

These interconnected yet stratified benchmarks serve as the "trunk," other options can be referenced as "branches" extending from the trunk. Together, they form an interconnected and multidimensional "network" of comparability.

### 386 **3.1.6.2.** Type of LCA

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387 Statistical analysis in Section 3.1.2 indicates that most current LCA studies on CO<sub>2</sub> 388 adsorption technologies adopt a retrospective type, while prospective LCAs remain 389 comparatively scarce. As a result, the outcomes tend to be static and may lack 390 sufficient responsiveness to technological dynamics. Given the rapid pace of 391 development in  $CO_2$  adsorption — particularly under the urgent demand for climate 392 change mitigation — static assessments are increasingly inadequate in capturing the 393 environmental relevance of emerging technologies. Therefore, enhancing the use of 394 prospective LCA is of notable value. For instance, patent-based prospective analysis 395 can offer unique advantages in supplementing life cycle inventory data, modelling 396 future scenarios, and improving the predictive capacity of LCA results [56, 57].

### 397 **3.1.6.3.** System boundary, life cycle stage breakdown and cut-off rules

398 Based on the analysis in Section 3.1.3 regarding system boundary and life cycle 399 stage breakdown, certain variability exists in the correspondence between system 400 boundary types and the coverage of actual technical processes and unit processes 401 across different studies. To mitigate the implicit inconsistency in the correspondence 402 amongst system boundaries, life cycle stages, and technical process stages, this study 403 builds upon existing research practices and integrates the theoretical frameworks of 404 ISO 14040 and the European Union guidelines. We propose a schematic diagram, as 405 shown in Figure 9, which illustrates the system boundary, default LCA stages, detailed 406 technical process chain for CO<sub>2</sub> adsorption, and their corresponding relationships. This 407 diagram aims to enhance consistency and comparability in future research.

408 According to ISO 14040, the life cycle stages are categorised as: (1) Raw material 409 acquisition, (2) Production, (3) Transport, (4) Use, Recycling/Reuse, and (5) Waste 410 treatment [12]. ISO 14020 defines the life cycle stages as: (1) Raw material acquisition, 411 (2) Production, (3) Distribution, (4) Use, and (5) End-of-life [58]. Meanwhile, the 412 Product Environmental Footprint (PEF) framework specifies the default life cycle stages 413 as: (1) Raw material acquisition and pre-processing, (2) Manufacturing, (3) Distribution, 414 (4) Use, and (5) End-of-life [59]. Although the terminologies used in these two 415 international standards and the latest methodological framework proposed by the 416 European Commission are not entirely identical, their underlying meanings are (almost) 417 consistent. Since PEF is the most recently published framework, this study adopts its 418 terminology to guide the precise classification and alignment of system boundaries 419 and technical processes in CO<sub>2</sub> adsorption.

The three subtypes of system boundaries mentioned earlier are (i) Cradle-to-gate,
(ii) Cradle-to-use, and (iii) Cradle-to-grave, as shown in Figure 6. Additionally, a unique

subtype, (iv) Cradle-to-cradle, needs to be included in the diagram. This subtype
involves recovery or recycling during the "E. End-of-Life" stage, where waste is
processed for reuse. For instance, the reactivation of activated carbon, as discussed in
Figure 3, allows the reactivated carbon to enter a new life cycle.

426 For the complete technical process chain serving CO<sub>2</sub> adsorption, there are two 427 subtypes with slight differences, corresponding to the CO<sub>2</sub> adsorption perspective, and 428  $CO_2$  adsorption and storage perspective, (3) and (4), respectively, in Figure 9. The core 429 distinction between the two lies in their scope: Studies focusing on the LCA of CO<sub>2</sub> 430 adsorbents centre on the entire process related to the adsorbent itself, excluding B2. CCS system construction, the subsequent handling of the adsorbed CO<sub>2</sub> (D2. CO<sub>2</sub> 431 432 process, D3. CO<sub>2</sub> transportation, and D4. CO<sub>2</sub> storage), and E2. Construction dismantling waste disposal. In contrast, studies on the LCA of CCS based on CO2 433 434 adsorption encompass the entire CCS value chain, which is broader in scope than the 435 adsorbent-focused studies. These typically include B2. CCS system construction, the 436 subsequent handling of the adsorbed CO<sub>2</sub> (D2. CO<sub>2</sub> process, D3. CO<sub>2</sub> transportation, 437 and D4. CO<sub>2</sub> storage), as well as E2. Construction dismantling waste disposal.



438

Figure 9. A schematic diagram showing the system boundary, default LCA stage and
 technological process chain (two sub-types: CO<sub>2</sub> adsorbent and CO<sub>2</sub> adsorption and
 storage) for CO<sub>2</sub> adsorption, as well as the matching relationships among these
 three elements

When defining system boundaries, an essential aspect that must not be overlooked is the explicit description of the criteria for including or excluding initial inputs and outputs. Unfortunately, only one study by Wang et.al [49] of the 31 studies reviewed clearly explained this point. The cause may be related to the widespread use of a default cut-off value of 1%. According to the European Union's PEF guidelines, "Processes and elementary flows may be excluded up to 3.0% (cumulatively) based on material and energy flows and the level of environmental significance (single overall
score)" [59]. Therefore, this paper recommends that future studies briefly report the
cut-off values applied to improve the transparency and comparability of research.

#### 452 **3.1.6.4. Data quality requirements (DQRs)**

453 According to investigations, published studies typically disclose their data sources (In section 3.2.1) but rarely explain the requirements for data quality. Following ISO 454 455 14040 and ISO 14044 standards, specifications for data quality should include 456 temporal coverage, geographical scope, technological representativeness, accuracy, 457 completeness, representativeness, consistency, reproducibility, data sources, and 458 uncertainty of the information [11, 12]. In addition, the Product Environmental 459 Footprint (PEF) and the Organisational Environmental Footprint (OEF) also specified 460 the Data Quality Requirements (DQRs) as follows:

- 461 462
- There are two minimum requirements: completeness, methodological appropriateness, and consistency.
- 463
- 464 465
- Four quality criteria: technical, geographical, temporal representativeness, and precision.
- $\diamond$  Three quality aspects: documentation, nomenclature, and review [59].

Although different organisations may have slightly different DQRs, spelling out as clearly as possible the rules governing the DQRs to which the study adheres, facilitates subsequent Data Quality Assessment (DQA) and the implementation of uncertainty analyses.

#### 470 **3.1.6.5. Software**

471 Research has shown that different software tools can yield varying LCA results 472 [60-63], making software comparison both an intriguing and contentious topic [64-66]. 473 In the context of CO<sub>2</sub> adsorption, the current dominance of SimaPro in LCA studies 474 highlights its importance but may also constrain the diversity of methodological 475 development. Although the software is merely a tool for conducting LCA and seems to 476 have no strong correlation with the development of LCA methodologies, its 477 implementation relies on these software platforms. Different software, each with 478 varying degrees of maturity, offers differing functionalities-one of which aims to 479 effectively realise LCA methodologies. For instance, the support for uncertainty analysis varies among software: For characterising LCI data uncertainty, SimaPro (v.8.4) 480 481 supports four types of probability distributions, GaBi (v.8.5) supports two types, 482 Umberto LCA+ supports none, while Brightway2 supports eleven types [67]. Therefore, 483 depending too heavily on a single software package may lead to methodological 484 homogenisation and possibly limit the practice and advancement of diverse 485 methodologies due to the market dominance of one software. Thus, adopting a variety 486 of software could foster innovation and diversify the implementation of 487 methodologies to some extent.

#### 488 **3.2. Inventory Analysis**

#### 489 **3.2.1. Data source**

- Figure 10 illustrates the types, frequencies, and proportions of foreground and
   background data sources in the inventory of CO<sub>2</sub> adsorption.
- 492 For foreground data, the sources can be roughly categorised as field, laboratory,

simulation, theoretical calculation, literature, estimation, and assumption data. 493 494 Typically, the inventory data in an LCA study is a mixture of these sources. Across 31 495 studies, the frequencies of these sources are as follows: 6, 18, 4, 1, 22, 2, and 7, 496 respectively. Results indicate that laboratory data (e.g., [10, 47]) and literature data 497 (e.g., [45, 51]) are frequently used, while field data (e.g., [29, 68]) and simulation data 498 (e.g., [33, 39]) are also important sources. For the small proportion of missing real-499 world data, estimation (e.g., [43]) and assumptions (e.g., [44]) can serve as 500 compensatory approaches.

For background data, Ecoinvent is the most widely used database, with a 501 502 frequency (and proportion) as high as 22 times (85%). Due to the regional 503 characteristics of background data, other regional databases are also adopted based 504 on the location of the investigated object or as substitutes when the local data is 505 unavailable. For instance, the Chinese Life Cycle Database (CLCD) [28, 29, 51], the 506 European Life Cycle Database (ELCD) [28], and the US Life Cycle Inventory Database 507 (USLCI) [47]. Additionally, three studies did not specify their background databases [10, 508 36, 69].



#### 509

511

#### 510 Figure 10. Types, Frequency and Percentage of Foreground Data Sources and

Background Data Sources in LCA Studies of CO<sub>2</sub> Adsorption

#### 512 **3.2.2. Allocation**

513 In the inventory analysis of the 31 studies, the majority (27 studies) did not 514 involve the issue of functional allocation. However, four studies addressed 515 multifunctional allocation; three studies adopted economic value as the allocation 516 criterion [28, 29, 39], and only one set the mass as the allocation criterion [54].

#### 517 **3.2.3. Inventory visibility**

518 Inventory visibility refers to whether the detailed data from the inventory analysis 519 is published alongside the main text (including supporting documents) for reviewers 520 and readers to access. According to statistics, the majority (25 studies) of the 31 521 studies provided the (at least in part) inventory analysis data, while a minority (6 522 studies) did not visualise their inventory results. Detailed inventory analysis can serve 523 as a valuable reference for future research and enhance the transparency of the study, 524 such as the work from Oreggioni et al. [53].

#### 525 3.2.4. Gaps and opportunities

#### 526 **3.2.4.1.** Data source, characteristics and iterative nature

527 LCA requires extensive data support to be successfully conducted. Section 3.2.1, 528 "Data Source," provides a general overview of the data resources used in the studies 529 and their frequency of use. However, there remains a certain degree of ambiguity 530 regarding the type and quality of data employed at different life cycle stages. This 531 ambiguity largely depends on the visibility of the inventory, the extent to which 532 authors describe their data resources and sense of responsibility.

533 In 2022, the European Commission published the LCA4CCU: Guidelines for Life 534 Cycle Assessment of Carbon Capture and Utilisation, which specifies the types and 535 characteristics of data required for different life cycle stages [70]. A summary is as 536 follows:

(i) For the most critical stages, core data is required. This refers to data describing
the primary activities under consideration, typically derived from the surveyed
entities' internal data. Such data is measured, calculated, and/or sourced from
company reports. This type of data is also referred to as foreground data, primary data,
activity data, or production data.

(ii) For upstream stages, supplier- and resource-oriented data are needed. Those
data are either measured or calculated and may originate from company systems. They
may also include secondary data reflecting specific circumstances or data sourced from
literature and databases. Supplier- and resource-oriented data are often referred to as
raw material data, supplier data, or upstream data.

(iii) For downstream stages, customer-, user-, and end-of-life-oriented data are
required. Those data are typically derived from statistical sources, most commonly
secondary data reflecting average conditions, and are sourced from literature or
databases. Customer-, user-, and end-of-life-oriented data are also referred to as
downstream data, use-phase data, or end-of-life data.

(iv) Background data can be found in LCA databases, such as Ecoinvent and GaBi.
The combination of background and foreground data is crucial and may require
separate validation or processing to adapt to specific scenarios.

555 Additionally, Figure 4 in another detailed guidance document published by the 556 European Commission, illustrates the iterative nature of data adoption across different 557 life cycle stages [21]. This iterative process is essential for achieving the objectives of 558 LCA. For example, in the first iteration, a combination of available specific data and 559 easily accessible secondary data can be used. In the second iteration, better data are 560 required for critical processes, and more specific data are needed for foreground 561 processes. In the third iteration, higher-quality data are necessary for key processes 562 and flows (background and foreground) [21].

In summary, clearly articulating the sources, characteristics, and iterative nature of the data used across different life cycle stages or technical process chains can significantly reduce the ambiguity in current studies regarding dataset descriptions. In turn, it enhances the comprehensibility and credibility of inventory analysis results for readers and reviewers.

#### 568 **3.2.4.2.** Allocation

569 When the allocation is applied, the economic value allocation is a commonly 570 adopted criterion (see section 3.2.2). However, according to ISO 14044, the following 571 order of preference should be applied for allocation: physical properties (e.g., mass), 572 economic value, and the number of subsequent uses of recycled materials [11]. 573 Therefore, physical properties should be prioritised as the allocation criterion 574 whenever allocation is unavoidable to depict real-world processes more accurately.

#### 575 **3.2.4.3. Data Quality Assessment (DQA)**

ISO 14044 includes a "validation of data" step during the inventory analysis phase, emphasising the need to ensure data quality aligns with the intended application. Additionally, during the consistency check in the interpretation phase, it is necessary to confirm whether the data quality meets the requirements of the study's goal and scope [11]. This underscores the importance of DQA. However, none of the 31 existing studies have reported on the data quality they investigated.

582 Given the importance of data quality and the current inadequacy of DQA, this 583 work recommends that future research conduct a formal DQA. Methods for DQA can 584 be divided into qualitative and semi-quantitative approaches [71]. The qualitative 585 approach is represented by the US Department of Agriculture's LCA Digital Commons [72], while the semi-quantitative approach is exemplified by the Data Quality Rating 586 587 (DQR) used in ILCD [21], and the PEF and the OEF [59, 73], and the Pedigree Matrix 588 approach employed by ecoinvent in 2013 [74], which proposed in 1996 [75]. It should 589 be noted that although the PEF and the OEF maintain the fundamental principles of 590 ILCD's DQA methodology, such as the six Data Quality Indicators (DQIs) and five-level 591 rating scale (Excellent, Very Good, Good, Fair, and Poor) [59], whilst exhibiting slight 592 variations in the stringency of methodological approach and data quality requirement 593 [76]. Recently, Carlesso et al. have integrated DQR and Pedigree Matrix into one hybrid 594 DQA approach [77]; the complementary nature of the hybrid approach is also 595 demonstrated in Salemdeeb et al.'s study, and a two-tiered assessment method was 596 developed [78]. Since data quality significantly influences the results of LCIA, this work 597 suggests conducting DQA prior to the impact assessment phase, specifically during the 598 inventory analysis phase, rather than during the interpretation phase.

#### 599 **3.2.4.4.** Inventory visibility

As noted in Section 3.2.3, six studies have yet to disclose their inventory analysis results, which might affect the transparency and credibility of the research. Therefore, it is recommended that at least the activity data (foreground data) of the inventory analysis results be published in the paper (either in the main text or as supplementary materials).

605 **3.3. Impact Assessment** 

#### 606 **3.3.1. Impact assessment Method**

Figure 11 illustrates the frequency with which various LCIA methods have been applied in CO<sub>2</sub> adsorption LCA studies. Analysis of 31 publications reveals that ReCiPe was used in 17 instances—substantially more than IMPACT and CML, each applied 4 times—with other methods (e.g., TRACI, IPCC, EF) being used less frequently. This 611 pattern could be attributed to ReCiPe's ability to provide both detailed evaluations 612 through its 18 midpoint and 3 endpoint categories—offering comprehensive 613 environmental impact capture, which is consistent with Rybaczewska-Błażejowska and 614 Jezierski's finding [79].



615

Life cycle impact assessment method

# Figure 11. Types, frequency and percentage of impact assessment methods in LCA studies of CO<sub>2</sub> adsorption

#### 618 **3.3.2. Type and quantity of impact category**

Figure 12 presents the types and quantities of impact categories corresponding to different LCIA methods in CO<sub>2</sub> adsorption LCA studies. Black dots represent midpoint categories, while red stars represent endpoint categories. The analysis indicates that the types and numbers of impact categories selected vary across studies. Overall, the majority (23 studies) employed only midpoint category indicators, such as [34, 51], while eight studies incorporated both midpoint and endpoint categories, such as [37, 38].

626 In terms of the number of impact categories, significant variation exists among 627 studies. For midpoint categories, the range is broad: some studies focus on core 628 environmental impact indicators, with fewer than ten categories, while others consider a more comprehensive set, exceeding ten categories and even covering all 18 629 630 impact indicators. For endpoint categories, the variation is smaller due to the 631 limitation to 3 endpoint categories; IMPACT methodology reduces the number of endpoint categories from 4 to 3 because while climate change was historically 632 633 classified as an endpoint category [80], but is now considered a midpoint category [81].



634

Figure 12. Types and quantity of impact assessment categories in LCA studies of
 CO<sub>2</sub> adsorption

#### 637 3.3.3. Final score

Weighting to obtain an aggregate final score is an optional step in impact assessment [11, 12]. Seven studies (27%) provided final scores for impact categories, facilitating the ranking of different options and decision-making. For instance, Chanchaona and Lau proposed a Total Endpoint Impacts metric based on four endpoint indicators and normalised the results, enabling a straightforward comparison of different adsorbent synthesis routes [50].

#### 644 **3.3.4. Gaps and opportunities**

#### 645 **3.3.4.1. Impact assessment Method**

646 Regarding the impact assessment method, diverse methods have been used in 647 previous studies. However, following LCA4CCU recommendations, the CML method— 648 employing 11 impact categories (basic version)—is endorsed as it harmonises 649 assessments with the Environmental Product Declaration (EPD) system to enhance 650 comparability [70]. Additionally, the Environmental Footprint (EF) method—adopted and recommended by the European Commission [59], which spans 16 impact 651 652 categories and has been notably refined in its update from EF3.0 to EF3.1, with major 653 updates made to key indicators such as Climate Change, Human Toxicity (non-654 carcinogenic) and Freshwater Ecotoxicity, and the weighted impact categories can be 655 summed to obtain the EF single overall score [82]. Overall, we recommend following 656 the latest EU EF method in the future, as its official promotion by European institutions 657 ensures broader international coverage, ongoing updates and enhancements, and 658 ultimately, a robust, transparent, and common approach to assessing the environmental performance of CO<sub>2</sub> adsorption technologies.

#### 660 **3.3.4.2.** Quantity of Impact Assessment Categories

661 As discussed in 3.3.2, Type and Quantity of Impact Categories, most studies still consider fewer than ten impact categories. Since a key value of LCA is the identification 662 663 of trade-offs between categories, and since the environmental impacts of current 664 adsorption technologies are not completely clear, it is recommended that all impact 665 category types be used. If specific categories are excluded, justifications should be 666 provided [70]. Although the core environmental impacts of CO<sub>2</sub> adsorption are often 667 associated with GHG reduction effects (e.g., global warming potential or climate 668 change), it is crucial to identify potential environmental trade-offs arising from CO<sub>2</sub> 669 adsorption implementation to support informed decision-making.

#### 670 3.3.4.3. Final score

671 Seven studies briefly discussed the results of weighting to obtain a final score. However, weighting is based on value choices rather than scientific principles, and 672 different individuals, organisations, and populations may have varying preferences. 673 674 The currently published studies still lack sufficient explanation of weighting factors and 675 methods. According to ISO 14044, it is recommended to provide both the unweighted 676 data and parameter results (or normalised results) alongside the weighted results [11]. 677 Additionally, this paper suggests that future research should include detailed 678 explanations of the selection criteria, values, and methodologies for normalisation 679 benchmarks, weighting factors, and weighting methods to enhance the transparency 680 and credibility of the analysis.

### 681 **3.4. Interpretation**

### 682 **3.4.1. Significant analysis**

683 Significance analysis aids in identifying critical issues in the LCI and LCIA phases. 684 According to the European Commission's "Guide for Interpreting Life Cycle Assessment 685 Results", the objects of significance analysis can be classified as (i) Elementary flow, (ii) 686 Process, (iii) Life cycle stage, and (iv) Impact category [83]. This study adheres to this 687 classification framework while also identifying two additional categories from 31 688 studies, namely: (v) Material and (vi) Mixed (process & material). The frequency of 689 these six types of significance analysis is illustrated in Figure 13. More than half of the 690 reviewed studies (18 papers) conducted significance analysis at the process stage, 691 followed by (vi) Mixed (process & material) and (v) Material, both are 6 studies, 692 respectively. Other types of significance analysis are relatively rare.



Type of significant analysis

# Figure 13. Types and frequency of significance analysis in LCA studies of CO<sub>2</sub> adsorption

#### 696 **3.4.2. Uncertainty analysis**

693

697 It is important to emphasise that sensitivity analysis is not entirely equivalent to 698 uncertainty analysis; these two terms are often used interchangeably but incorrectly 699 [84]. Uncertainty analysis generally consists of four nested and progressive steps: (i) 700 Identification and characterisation of uncertainty, (ii) Uncertainty propagation analysis, 701 (iii) Sensitivity analysis, and (iv) Communication. For a detailed discussion, refer to the 702 work of Igos et al. [67]. Here, we briefly outline the core questions addressed by each 703 step:

(i) Identification and characterisation of uncertainty answer: Where are the
 sources (locations) of uncertainty in the system, and what is their magnitude
 (qualitative or quantitative)?

(ii) Uncertainty propagation analysis answers: How does system uncertainty affectthe results (confidence level)?

(iii) Sensitivity analysis answers: Which part of the uncertainty is more critical(influential)?

(iv) Communication answers: How should the uncertainty content be conveyedto the audience?

Thus, uncertainty analysis encompasses sensitivity analysis. Moreover, the methods used for uncertainty and sensitivity analyses are not identical; for further details, see [67].

716 Uncertainty in LCA can be categorised into three types: Context, quantity (inputs

717 and parameters), and model [67]. Among the 31 studies reviewed, the majority (24 718 studies, 77%) did not conduct uncertainty analysis, while only a minority (7 studies, 719 23%) performed such analysis. As shown in Figure 14, five studies focused on quantity 720 uncertainty, one on context uncertainty, and one did not specify the type of 721 uncertainty. Among the five studies addressing quantity uncertainty, two tried to 722 analyse it but did not specify the methods used; the other three employed Monte 723 Carlo sampling to address quantity uncertainty. Additionally, the study that did not 724 specify the type of uncertainty also used Monte Carlo sampling as an analytical tool. 725 The only study addressing context uncertainty adopted scenario analysis as its method.



# Figure 14. Types of uncertainty objects and analysis methods in LCA studies of CO<sub>2</sub> adsorption

#### 729 **3.4.3. Sensitivity analysis**

726

730 Sensitivity analysis identifies which uncertainties have a significant or negligible 731 impact on the results, thereby enhancing the understanding of result robustness 732 (credibility) [67]. As shown in Figure 15, nearly half (14 studies, 45%) of the 31 studies 733 conducted sensitivity analysis. Among these, the number of investigations targeting 734 quantity and context uncertainties were 11 and 7, respectively. Sensitivity analysis for 735 quantity was uniformly conducted using the one-at-a-time (OAT) method, though the 736 range of variation differed slightly. Most studies set the percentage fluctuation range 737 within ±20%, such as in [34]; one study, however, adopted a more extensive fluctuation 738 range of  $\pm 40\%$  [45]; and Wang et al. set two ranges, i.e.  $\pm 10\%$  and  $\pm 30\%$ , according to 739 the nature of parameters [49]. For context sensitivity, most studies employed scenario 740 analysis, with only one study using marginal analysis [42].



# 741 742

743

# Figure 15. Types of sensitivity objects and analysis methods in LCA studies of CO<sub>2</sub> adsorption

#### 744 3.4.4. Gaps and opportunities

#### 745 **3.4.4.1. Significant analysis of contributor**

746 Section 3.4.1 on significant analysis shows that most studies focused on (ii) 747 process stages as the object of analysis. Additionally, two new variants have emerged: 748 (v) material and (vi) mixed (process & material). While these new forms provide fresh 749 insights into the environmental impacts of CO<sub>2</sub> adsorption from different perspectives, 750 they are not entirely based on an entire life-cycle perspective, particularly true for (vi) 751 mixed (process & material), where the intersection of contributors with different 752 natures makes it challenging to assess whether the consideration of contributors is 753 comprehensive or if omissions exist.

In contrast, the approaches recommended by the European Commission—(i) elementary flow, (iii) life cycle stages, and (iv) impact category—have not been widely adopted despite being more standardised and reliable. Conducting significant analysis on these aspects allows for careful consideration of all contributors of the exact nature from an entire life-cycle perspective, ensuring no omissions and enabling the determination of their respective contribution rates.

Another notable deficiency in the significant analysis of the 31 reviewed studies is the lack of criteria for determining significance levels. Appendix 2 of ISO 14044 provides guidelines for ranking significance and their reference thresholds, as follows:

- 763 764
- A: Most important, significant influence, i.e., contribution > 50%.
   A: Very important, relevant influence, i.e., 25% < contribution < 50%.</li>
- 765
- $\diamond$  B: Very important, relevant influence, i.e., 25% < contribution < 50%.
- 766
- ♦ C: Fairly important, some influence, i.e., 10% < contribution < 25%.</p>
- 766 ≺ 767 ≺
- ♦ D: Little importance, minor influence, i.e., 2.5% < contribution < 10%.</li>
   ♦ E: Not important, negligible influence, i.e., contribution < 2.5% [11].</li>

Additionally, the European Commission advocates for the "most relevant" threshold conditions for (i) elementary flow, (ii) process stages, and (iii) life cycle stages, defined as all elementary flows/process stages/life cycle stages cumulatively 771 contributing more than 80% to any impact category [83].

772 Therefore, future research is recommended to strengthen significant analysis for 773 (i) elementary flow, (iii) life cycle stages, and (iv) impact category. On the other hand, 774 clear criteria for contribution levels should be established, and the contribution rates 775 of all significant analyses should be delineated.

#### 776 3.4.4.2. Uncertainty analysis and sensitivity analysis

777 Most studies did not conduct uncertainty propagation analysis, and more than 778 half did not perform sensitivity analysis, which may undermine the credibility of the 779 LCA results. For uncertainty propagation analysis, the focus has primarily been on 780 quantity uncertainty, while propagation analysis for context and model uncertainties 781 remains severely lacking. Similarly, sensitivity analysis for model-related aspects (e.g., 782 characterisation models for impact categories) is also absent.

783 For quantity sensitivity analysis, the OAT method was universally applied. 784 However, OAT is a local sensitivity analysis method that does not account for 785 interactions between two or more variables [85]. For instance, CO<sub>2</sub> capture rate and 786 regeneration energy consumption are strongly correlated [6]. When the  $CO_2$  capture 787 rate is adjusted upward to a certain level, regeneration energy consumption may 788 increase significantly. If sensitivity analysis only considers the CO<sub>2</sub> capture rate without 789 accounting for the correlated changes in regeneration energy consumption, the value 790 of the analysis results is limited.

791

In summary, as far as possible, future research could:

792 (i) Promote the adoption of uncertainty and sensitivity analyses while 793 distinguishing their respective roles.

794

(ii) Address the gaps in context and model uncertainty and sensitivity analyses.

795 (iii) For quantity uncertainty, consider global sensitivity analysis methods (e.g., 796 variance-based methods) to better understand the interactions among strongly 797 correlated uncertainty factors.

#### 798 3.4.4.3. Uncertainty of impact categories and their role in comparative LCA 799 judgments

800 In comparative LCA of different CO<sub>2</sub> adsorption options, discussions often revolve around comparative judgments, i.e., evaluating the advantages and disadvantages of 801 different options based on impact category scores. However, the 31 reviewed studies 802 803 almost universally neglected the differences in uncertainty across impact categories.

- The European Commission classifies impact categories by quality [70, 86]:
- 805 806

811 812

815

816

804

♦ Quality level I: Global warming, Climate change, Ozone depletion, Particulate matter/respiratory inorganics.

- 807  $\diamond$  Quality level II: Ionising radiation (human health and ecosystems), 808 Photochemical ozone formation, Acidification, Eutrophication (terrestrial, 809 freshwater, and marine), Resource depletion (mineral and fossil), Human 810 toxicity (cancer and non-cancer effects), Ecotoxicity (freshwater).
- ♦ Quality level III: Cancer human health effects, Non-cancer human health effects, Ecotoxicity freshwater, Land use, water use, Resource use (water, 813 mineral, metals, and energy carriers).
- 814 The quality levels are defined as:
  - ♦ Quality level I: Recommended and satisfactory.
  - ♦ Quality level II: Recommended but in need of some improvements.

♦ Quality level III: Recommended but to be used with caution.

Jolliet et al. also discussed default rules for determining the significance of 818 819 differences in impact categories across scenarios. For the full version, refer to the 820 original book [25]. Two examples are briefly summarised below:

821 822

817

 $\diamond$  For energy and CO<sub>2</sub>, any difference of at least 10% can be considered as significant.

- 823
- ♦ For toxicity characterisation, impact calculations often involve greater uncertainty, requiring a difference of at least one to two orders of 824 825 magnitude between scenarios to be considered significant.

826 In general, the magnitude of uncertainty varies significantly across impact 827 categories, sometimes differing by orders of magnitude. No universal rule exists for determining the significance of differences across all impact categories. 828

829 Although no universally precise criteria have been established, a cautious and 830 conservative approach is advisable when addressing differences across impact 831 categories in various scenarios. When the differences between two options may fall 832 within the range of uncertainty, it is prudent to avoid making definitive statements that 833 one option is categorically superior to the other in certain impact categories, as such 834 assertions risk leading to overly speculative conclusions. For example, in one study, 835 Gonzalez - Olmos et al. stated in their abstract that "All the key performance indicators studied had better values with 13X-APG than CMS-330" [44], while Jaffar et al. claimed 836 837 that "The novel SPEI-based CCS process showed superior environmental performance 838 compared to the conventional MEA-based CCS process." [40]. However, a more 839 detailed examination of their LCIA results reveals that the scores for some impact 840 categories between the alternatives are very close, even with only negligible 841 differences. Consequently, if impact category uncertainty is not adequately considered, 842 drawing definitive conclusions from LCIA results may be somewhat overoptimistic. 843 Given that some decision-makers are not specialists in LCA, basing decisions solely on 844 such findings could lead to biased outcomes, insufficient robustness, and even 845 erroneous decisions.

846 Generally, two strategies can be adopted to mitigate the challenges posed by 847 impact category uncertainty in comparative LCA:

848 (i) Cross-validation using multiple LCIA methods: By employing several LCIA 849 methods for cross-validation, one can reduce the influence of uncertainty inherent to 850 any single method. This approach enhances the robustness of the comparative LCIA 851 results, the subsequent LCA conclusions, and the reliability of subsequent decisions. 852 For example, Coppola et al. not only utilised the ReCiPe 2016 method but also 853 confirmed their findings using ILCD 2011, with both approaches yielding consistent 854 results [87]. Another study employed ReCiPe 2016, ILCD 2011, CML-IA baseline and 855 IMPACT 2002+ to compare the environmental impacts of the electricity consumption 856 structures across the EU27, Norway, Switzerland and the UK, demonstrating that the 857 ranking of environmental profiles was largely consistent across methods, with 858 discrepancies only in a few impact categories [79].

859 (ii) Sensitivity and uncertainty analysis of characterisation factors and models: 860 given that the uncertainties in LCIA results stem primarily from the underlying 861 characterisation factors and models, and they vary in different LCIA methods [79, 88], 862 performing sensitivity and uncertainty analyses on these components is crucial to 863 establishing the confidence intervals for the results. This way, in turn, provides a robust basis for comparing different scenarios. In addition, if the study needs to draw out the
endpoint impact categories score, normally, their uncertainty level is higher than midpoint impact categories [59, 89]; the normalisation factor and weighting factor could
also be considered in sensitivity and uncertainty analysis.

In summary, both strategies contribute to a deeper understanding of how impact 868 869 category uncertainty affects comparative LCA outcomes. Strategy (i) is more 870 straightforward to implement, whereas strategy (ii) demands a comprehensive 871 understanding of the underlying mechanisms of LCIA methods. The inherent 872 uncertainty in impact categories should not be overlooked, as it can be as significant 873 as the parameter uncertainty that is typically emphasised [88]. Although issues such 874 as the common significance grade of LCIA result differences remain unresolved in the 875 LCA industry, when the differences in certain impact categories between alternatives 876 are minimal, a more cautious approach is warranted to avoid conclusions of 877 insufficient robustness that could adversely affect subsequent decision-making.

#### 878 **3.4.4.4. Differential coping with independent and shared uncertainty in** 879 **comparative LCA**

According to existing 31 surveys, when conducting comparative LCA, although some studies have conducted uncertainty analysis, whether the uncertainties in the comparison options are exclusive (or common) has not been particularly emphasised. However, they are quite different and even determine how to compare different options [25, 85].

885 The above discussion is based on the situation that the uncertainties are 886 independent between different options. However, in the field of CO<sub>2</sub> adsorption, different options may share some of the same uncertainties. For example, when 887 comparing different regeneration processes of the same CO<sub>2</sub> adsorbent, the 888 889 uncertainty of the yield in the adsorbent synthesis stage is consistent because they are 890 in the same production background. It should be noted that if two or more scenarios 891 share common uncertainty, simply comparing through the independent confidence 892 intervals of LCIA results could lead to misleading conclusions; at this time, the 893 researcher should directly co-analyse the probability that option A is higher (or lower) 894 than option B in a certain impact category under the same uncertainty.

895 When addressing shared uncertainties in multi-system analyses, the robustness 896 of joint analysis methods requires consideration of significance levels in comparative 897 LCIA results (as previously discussed). A threshold (e.g., 10%) can be established to 898 determine significant differences: if Option A's result in a given impact category 899 exceeds (or falls below) Option B's result by this fixed percentage (e.g., 10%), the 900 difference is deemed significant. Note that under such stringent criteria, the 901 probability of observing 'significant differences' will inherently be lower than that of 902 detecting 'any numerical differences' between systems.

#### 903 **3.4.4.5. Section Summary**

904 This subsection outlines key uncertainty-related challenges in comparative LCA:

905 (i) Distinguishing uncertainty analysis from sensitivity analysis.

906 (ii) Assessing the significance of LCIA result differences (impact category-specific907 uncertainties).

- 908 (iii) Differentiating independent vs. shared uncertainties in compared systems
- 909 These issues are notoriously complex and error-prone. To mitigate common

910 pitfalls systematically consulting the following progressive checklist after completing a

911 comparative LCA may help mitigate common pitfalls:

- 912 (i) Is this truly a comparative LCA study?
- 913 (ii) Was uncertainty analysis explicitly conducted? (Characterisation, propagation,914 sensitivity analysis, reporting).
  - (iii) Are uncertainty analysis and sensitivity analysis clearly distinguished?
- 916 (iv) Were impact category uncertainties accounted for? (i.e., is the observed LCIA 917 difference significant?)
- 918

915

(v) Do the compared systems share any common uncertainty sources?

# 919 **3.5. A Suggested Methodological Framework**

Building upon the research gaps and opportunities identified in the preceding sections, this part proposes the core elements and develops a hierarchical methodological framework for the LCA of  $CO_2$  adsorption technologies, as illustrated in Figure 16. This framework is based on the baseline of current state-of-the-art identified in this study and aspires towards best practices outlined in ISO 14040, ISO 14044, and the ILCD Handbook. It delineates a suggested pathway from the current status to the aspirational state.

927 The framework qualitatively classifies methodological enhancement efforts into 928 three hierarchical levels, using two progressive discriminative statements based on the 929 degree of additional effort required:

(i) Does the current baseline require further analysis? If not, it is classified as a
minor effort, typically involving supplementary or improved reporting on existing work,
especially aiming to reduce textual ambiguity. If yes, then proceed to the second
criterion:

(ii) Does the new analysis require interdisciplinary knowledge? If not, it
constitutes moderate effort, usually implying that while partial or similar LCA analyses
have been conducted, there is room for methodological refinement, achievable using
conventional LCA expertise. If interdisciplinary knowledge is indeed necessary, it is
classified as a major effort, typically addressing significant methodological gaps or
misapplications that demand mastery of fundamental LCA architecture and supporting
interdisciplinary insights.

The methodological steps described within the framework are not exhaustive; a complete methodological execution must still conform to the latest ISO 14040 and ISO 14044 standards. Rather, this framework serves as an "opportunity checklist", focusing on key points across the four phases of LCA that could significantly enhance comparability and reliability.

946 Specifically, the detailed methodological elements mapped to the three
947 hierarchical levels are shown in Figure 16, while concrete examples supporting these
948 methodologies can be found in "Supplementary Document 2 - Examples".

949 It is crucial to emphasise that this framework is not intended to replace the 950 ISO 14040 standard methodology but acts as a complementary extension tailored to 951 the context of  $CO_2$  adsorption. It offers a conceptual solution for bridging the 952 considerable gap between the current application of LCA methods and the ideal 953 standards in the  $CO_2$  adsorption field.

Compared with standalone ISO 14040 & ISO 14044, this framework offers severalpotential advantages:

(i) Field-specific gap identification: ISO 14040 & 14044 provide the overarching
standards and guidelines for LCA research, treating all four phases with almost equal
importance without explicitly emphasising any specific challenges in a given field. By
contrast, this framework identifies field-specific shortcomings in applying LCA on CO2
adsorption, treating these as an "opportunity checklist" and offering a strategy for
progressive alignment with ISO 14040 & ISO 14044 expectations based on additional
effort levels.

(ii) Focused enhancement of comparability and reliability: While ISO 14040 & ISO
14044 cover broad aspects such as transparency, comparability, reliability,
communicability, and verifiability, this framework particularly targets the
comparability and reliability issues pertinent to the CO<sub>2</sub> adsorption domain, e.g.,
establishing consensus comparability tiers and addressing uncertainty in comparative
impact categories.

969 (iii) Tailored applicability to CO<sub>2</sub> adsorption: ISO 14040 & ISO 14044 offer a generic 970 framework applicable to all products and services without considering the specific 971 characteristics of individual study objects. Conversely, this framework is custom-972 designed for CO<sub>2</sub> adsorption, incorporating field-specific elements like setting 973 functional units for adsorbents and CCS, and proposing consensus-based 974 comparability baselines, thus reducing the trial-and-error process in practice and 975 ensuring a basic quality standard.

976 (iv) Methodological tool recommendations: ISO 14040 & ISO 14044 present
977 general principles without specifying preferred methodological tools, thus allowing
978 diversity but also causing methodological heterogeneity. In contrast, this framework
979 recommends specific methods and tools, such as using the EF 3.1 method for LCIA and
980 global sensitivity analysis for uncertainty assessments.

981 (v) Provision of practical examples: ISO 14040 & ISO 14044 do not provide case-982 specific methodological examples, which can leave practitioners struggling with 983 implementation despite adhering to theoretical principles. This framework is 984 supported by practical examples of methodological elements, offering actionable 985 guidance to practitioners.

However, despite aiming to narrow the gap between practical and ideal LCA
applications and being underpinned by scientific references, the proposed framework
still has several limitations:

(i) Limitations in literature review methodology: Some relevant publications may
have been missed because they did not use standard LCA terms like "life cycle
assessment" but broader descriptors such as "ecological" or "sustainable". Expanding
the search terms would compromise search precision. Thus, a balance between
precision and comprehensiveness inevitably leaves room for omissions.

994 (ii) Cognitive limitations: Some decisions, such as constructing the comparability 995 framework or setting consensus-based baselines for  $CO_2$  adsorption, necessarily relied 996 on the professional judgment of the research team, which might introduce cognitive 997 biases and require further validation or expert evaluation in future work.

(iii) Tension between standardisation and flexibility: While standardisation
promotes comparability and credibility, it may also reduce methodological diversity.
For example, recommending the EF 3.1 method could discourage using alternative
LCIA methodologies. Conversely, despite efforts to refine key elements such as
functional units for CO<sub>2</sub> adsorption, some space for methodological variation remains,

preserving flexibility but also potentially introducing heterogeneity in LCA approachesand results.

1005 In summary, balancing the precision and breadth of the literature review, 1006 overcoming cognitive limitations, and managing the tension between standardisation 1007 and diversity will require ongoing iteration and refinement in future research.



1009 Figure 16. A suggested hierarchical methodological framework to enhance the comparability and reliability for LCA of CO<sub>2</sub> adsorption

## 1010 **4. Conclusion**

1011 This study addresses the methodological ambiguity and inconsistency in 1012 conducting LCA for CO<sub>2</sub> adsorption technologies in energy-intensive industries by 1013 systematically identifying the commonalities and differences in the methodological 1014 elements of 31 existing studies published from 2006 to 2025. It also highlights the gaps 1015 and opportunities for improvement compared to the latest ISO standards, ILCD 1016 guidelines, and other normative documents. Based on these findings, this paper 1017 proposes an LCA methodological framework that considers comparability and 1018 reliability, with the main conclusions summarised as follows:

1019 (i) Existing literature demonstrates certain commonalities in applying LCA 1020 methodologies across the four phases, such as the definition of system boundaries and 1021 functional units. However, certain differences exist simultaneously, such as the 1022 correlation of the system boundary, life cycle stages and processes, and the number of 1023 impact categories considered.

(ii) There remain methodological gaps that require further attention, including
 data quality analysis, reporting on the characteristics and iterative nature of inventory
 data, consideration of uncertainties in impact categories when making comparative
 judgments, and the classification of significance levels in significance analysis results.

1028 (iii) The proposed methodological framework in this paper may enhance the 1029 credibility and comparability of LCA results. The implementation of the framework is 1030 categorised into three Levels of effort:

- 1031
- 1032 1033

1034

- First Level: Minor effort, based on the existing analysis, but adjustments to the format and precision of reporting are needed, such as explicitly defining the hierarchical level of the comparative objects.
- Second Level: Moderate effort, such as completing data quality analysis and adopting a more comprehensive impact assessment categories.
- 1035 1036
- and adopting a more comprehensive impact assessment categories.
   Third Level: Major effort, such as conducting uncertainty and sensitivity analyses for context and models.

analyses for context and models.
 Standardised and comparable LCA results for CO<sub>2</sub> adsorption technologies are a
 critical research objective for LCA practitioners. This study makes a unique contribution
 to the field by improving the consistency and comparability of LCA methodologies. The
 findings provide methodological references for subsequent related studies, reducing
 uncertainty and ambiguity in LCA methodologies applications and encouraging more
 researchers to explore the standardisation of LCA methodologies in greater depth.

# 1044 **Credit authorship contribution statement**

- 1045 **Yipeng Yao**: Conceptualisation, Methodology, Visualisation, Writing original draft.
- 1046 Marie-Eve Duprez: Writing review & editing, Supervision.
- 1047 **Guy De Weireld**: Writing review & editing, Supervision.

# **Declaration of competing interest**

1049 The authors declare that there is no conflict of interest.

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# **Declaration of generative AI and AI-assisted technologies in the**

# 1057 writing process

During the preparation of this work, Yipeng Yao used ChatGPT to improve the manuscript's readability and language. After using this service, Yipeng YAO reviewed and edited the content as needed and took full responsibility for the content of the published article.

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