



U.S. DEPARTMENT OF
ENERGY

BEST PRACTICES FOR LIFE CYCLE ASSESSMENT (LCA) OF DIRECT AIR CAPTURE WITH STORAGE (DACs)

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List of Acronyms and Abbreviations

| | |
|------------------|--|
| CDR | Carbon Dioxide Removal |
| CFP | Carbon Footprint for Products |
| CH ₄ | Methane |
| CO _{2e} | Carbon Dioxide Equivalents |
| COP | Conference of Parties |
| DAC | Direct Air Capture |
| DACS | Direct Air Capture with Storage |
| DOE | U.S. Department of Energy |
| EPA | U.S. Environmental Protection Agency |
| EOR | Enhanced Oil Recovery |
| FU | Functional Unit |
| GHG | Greenhouse Gas |
| REET | Greenhouse gases, Regulated Emissions, and Energy use in Technologies Model |
| GWP | Global Warming Potential |
| IPCC | Intergovernmental Panel on Climate Change |
| IEA | International Energy Agency |
| IO | Input-Output |
| ISO | International Organization for Standardization |
| kWh | Kilowatt-hour |
| LCA | Life Cycle Assessment |
| LCI | Life Cycle Inventory |
| LCIA | Life Cycle Impact Assessment |
| MJ | Megajoule |
| MRV | Measurement, Reporting, and Verification |
| NETL | National Energy Technology Laboratory |
| N ₂ O | Nitrous Oxide |
| TEA | Techno-Economic Analysis |
| TRACI | Tool for Reduction and Assessment of Chemicals and Other Environmental Impacts |
| TRL | Technology Readiness Level |

Executive Summary

As the one of the performance elements of the Carbon Negative Shot, robust life cycle greenhouse gas (GHG) accounting is a critical element for Carbon Dioxide Removal (CDR). Life Cycle Analysis/Assessment (LCA) is an existing framework that is well suited to evaluate the environmental implications of CDR. By design, LCA provides a holistic perspective of the potential environmental impacts of a product or process across the different life cycle phases. Not only can LCA be used to help determine the net CO₂e removal of a CDR approach, but it can also help with the assessment of potential tradeoffs with other environmental impacts. Even though the approaches for LCA are codified in the ISO 14040/14044 standards, we recognize the need to establish specific best practices for the subjective elements in those standards to harmonize data and methods to allow for consistent assessments of CDR approaches.

This document is envisioned as a complement to, not a replacement for, the ISO standards to address issues that are specific to applications of those standards to DACS analysis. The goals of these Best Practices are to:

- Foster consistency of LCA of DACS systems to enable more complete understanding of potential impacts of CDR
- Assess sensitivity and uncertainty in results to provide confidence in the study outcomes and potential risk envelopes for technology performance
- Understand potential tradeoffs and co-benefits of DACS systems
- Leverage best practices from the LCA research and practitioner community to account for considerations specific to evaluation of emerging technologies

Each life cycle stage (goal and scope definition, life cycle inventory analysis, life cycle impact assessment, and interpretation) is broken down into the key decisions that must be made in accordance with ISO 14040/14044 framework. For each decision, the specific relevance to the application to DACS is provided along with recommended Best Practices.



BEST PRACTICES FOR LIFE CYCLE ASSESSMENT (LCA) OF DIRECT AIR CAPTURE WITH STORAGE (DACs)

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1. Introduction

At COP26 in November 2021, U.S. Secretary of Energy Jennifer Granholm announced the third target in the DOE's Energy Earthshots Initiative, the Carbon Negative Shot (US DOE, 2021). Carbon Negative Shot is the all-hands-on-deck call for innovation in technologies and approaches that will remove CO₂ from the atmosphere, capturing and durably storing it at meaningful scales for less than \$100/net metric ton of CO₂-equivalent (CO₂e). This effort is being deployed to achieve a net-zero carbon economy and eventually remove legacy carbon pollution to help address the climate crisis, with a dedicated focus on doing so in a just and sustainable manner.

Four performance elements will define the technologies DOE will advance through this initiative. This document aims to support the second performance element.

1. Less than \$100/net metric ton CO₂e for both capture and storage.
2. **Robust accounting of full life cycle greenhouse gas emissions.**
3. High-quality, durable storage with costs demonstrated for monitoring, reporting and verification for at least 100 years.
4. Enables necessary gigaton-scale removal. To put this into perspective, one gigaton of CO₂ is equivalent to the annual emissions from the U.S. light-duty vehicle fleet. This is equal to approximately 250 million vehicles driven in one year.

1.1 Motivations

To tackle the world's climate crisis and achieve net-zero emissions by 2050, we need a dual strategy: we must both minimize the emissions reaching the atmosphere and compensate for any residual emissions by permanently removing accumulated carbon dioxide (CO₂) from the atmosphere. Carbon dioxide removal (CDR) is a key part of this strategy, as well as any future strategy to go beyond net-zero to address legacy emissions. Nearly all climate model scenarios that achieve international climate goals suggest the need for a near-term focus on CDR development and deployment. As the second performance element of the Carbon Negative Shot, robust life cycle GHG accounting is a critical element for CDR. Not only can accounting help with the evaluation of different CDR approaches and measurement of progress and potential for climate benefit, but it also serves as the foundation for quantifying and establishing equivalency for comparison across approaches for CDR that facilitate CDR's uptake in regulatory, market, and other settings.

Life Cycle Analysis/Assessment (LCA) is an existing framework that is well suited to evaluate the environmental implications of CDR. By design, LCA provides a holistic perspective of the potential environmental impacts of a product or process across the different life cycle phases. This includes the extraction of raw materials through the end-of-life. Emissions to the environment (air, water, and land) are translated to a variety of potential impacts ranging from climate change to human health. Two International Organization for Standardization (ISO) standards provide the principles and framework (14040) and requirements and guidelines (14044) for conducting LCA (ISO, 2006a, 2006b). A separate standard, ISO 14067, focuses

specifically on the reporting of the carbon footprint for products (CFPs) (ISO, 2018). It is largely based on ISO 14040/14044, but with a narrower focus on potential impacts related to climate change.

Not only can LCA be used to help determine the net CO₂e removal of a CDR approach, but it can also help with the assessment of potential tradeoffs with other environmental impacts. Even though the approaches for LCA are codified in the ISO standards, we recognize the need to establish specific best practices for the subjective elements in those standards to harmonize data and methods to allow for consistent assessments of CDR approaches. This document focuses specifically on one subset of CDR approaches, Direct Air Capture with Storage (DACs).

1.2 Purpose

Direct air capture with storage (DACs) is gaining significant interest as a carbon dioxide removal technology that could be deployed, in addition to aggressive decarbonization efforts, to limit warming levels to 1.5 or 2.0 degrees Celsius relative to pre-industrial periods.

Generically, DAC involves the capture of carbon dioxide from ambient air (at a concentration of 0.04%) via chemical means. The two predominant technical pathways being considered are the use of a solid sorbent or a liquid solvent to bind to the carbon dioxide (McQueen & Wilcox, 2021; National Academies of Sciences, Engineering, and Medicine, 2019). Following capture, the sorbent or solvent is regenerated for future cycles. The product of the operation is purified and compressed carbon dioxide. There are multiple possible dispositions for the purified carbon dioxide, including subsurface sequestration as well as utilization/conversion. DACs and other mechanisms that combine DAC with CO₂ disposition that results in the permanent sequestration of CO₂ out of the atmosphere are carbon dioxide removal. When DAC is coupled to nonpermanent CO₂ storage, it is not CDR. Similarly, the quantity of CO₂ removed by a DACs process could be less than that captured by the DAC unit if any downstream leakage occurs in the transportation, injection, and storage of the CO₂.

Due to the potential disparate uses for utilization and conversion, this document focuses specifically on permanent geologic storage as the final disposition for captured carbon dioxide as a CDR strategy. The best practices that are discussed herein for specific unit processes can be applied to the capture stage regardless of disposition, but additional guidance and decisions are required to assess the end use of the utilization/conversion product(s).

While this document mentions examples based on the sorbent and solvent pathways, it is not intended to be exclusively applicable to those pathways. The principles discussed could be generically applied to any engineered DACs system that provides the same function. The carbon removal efficacy of DACs technologies is a function of the greenhouse gas intensity of energy and material requirements for each unit of carbon dioxide that is captured and sequestered from the atmosphere. Both technologies are energy intensive, meaning that the source and amounts of required energy/material inputs are critical to determining the overall level of removal.

As an assessment framework, LCA is governed by ISO (14040/14044); however, those standards are generic and do not offer guidance for specific technology applications, nor do they provide

any of the data necessary to complete a study. The purpose of this effort is to provide specific guidance for implementation of the ISO standards to DACS systems to enable consistent and robust LCAs of DACS systems across the four phases of LCA: goal and scope definition, life cycle inventory analysis, life cycle impact assessment, and interpretation.

We envision the audiences for this document to include technology developers, federal funding awardees, state- and federal-level policymakers and regulators, entities (companies, organizations, individuals) interested in evaluating CDR procurement, and potential host communities for CDR technologies.

1.3 Document goals and objectives

This document is envisioned as a complement to the ISO LCA standards (14040/14044) to address issues that are specific to applications of those standards to DACS analysis.

Goal 1: Foster consistency of LCA of DACS systems to enable more complete understanding of potential impacts of CDR

- 1.1 Provide definition to key goal and scope elements in the LCA framework (functional unit, analysis scope, system boundaries, etc.)
- 1.2 Include technical/physical flows as key outputs in addition to the LCA impacts to facilitate future updates and harmonization
- 1.3 Define the required elements for the life cycle inventory data collection
- 1.4 Recommend background data sources for the life cycle inventory data collection stage

Goal 2: Assess sensitivity and uncertainty in results to provide confidence in the study outcomes and potential risk envelopes for technology performance

- 2.1 Establish uniform modeling scenarios for key energy inputs
- 2.2 Identify key parameter sensitivities and co-benefits of DACS systems

Goal 3: Understand potential tradeoffs and co-benefits of DACS systems

- 3.1 Assessment of full suite of environmental impacts in addition to global warming
- 3.2 Separate ledger accounting for potential co-benefits and co-products to accurately differentiate between avoided and removed emissions

Goal 4: Leverage best practices from LCA research and practitioner community to account for considerations specific to evaluation of emerging technologies

- 4.1 Coordination and integration of TEA and LCA efforts for better understanding of potential operating envelope and corresponding impacts
- 4.2 Suggest best practices unique to these applications that is not included in ISO 14040/14044

The goals and objectives above provide the perspective from which this document was developed. It should be noted that this document is not a replacement for ISO 14040/14044 and does not do the following:

1. Instruct users exactly how to conduct and document an LCA – those requirements are well defined in the ISO 14040/14044 standards and other established LCA practices and guidelines
2. Require the use of specific data sources and/or modeling platforms
3. Provide a specific report template or reporting requirement
4. Attempt to resolve general methodological issues that have been debated in the LCA research and practitioner community

1.4 Emerging technologies and LCA

As a framework, LCA can be deployed across the entire product development spectrum from concept through commercialization. The benefits to integrating LCA into the early stages of a technology include early identification of potential hotspots or burden shifting. Responding to these sorts of findings is much easier and more cost-effective at an early stage while the design, materials, and processes are still fluid (Bergerson et al., 2020). While there is benefit in performing LCA earlier in the development cycle, it is also more challenging because there is inherently more uncertainty across all phases of the assessment as it is an entirely prospective evaluation of potential impacts as opposed to a retrospective look at legacy impacts.

According to the IEA, liquid solvent and solid sorbent DAC are both classified at a Technology Readiness Level (TRL) of 6 as of 2021, which corresponds to large prototype demonstration (IEA, 2021). Multiple government agencies, including the DOE, use the TRL scale to define where a particular application is in the development cycle (US Government Accountability Office, 2020). The TRL can also be used to help guide and scope the requirements of an LCA across different phases of development (Moni et al., 2020).

Below is a high-level summary of some of the additional factors that need to be considered in each phase of a study when applying LCA to technologies that are not commercially mature:

- Goal and scope definition:
 - Functional unit – At early stages, there may be multiple possible functions that evolve over the development and integration of a product or process into a larger system
 - System boundary – While a cradle-to-grave assessment is always preferred, in some cases, the end use and end-of-life may be unknown or uncertain, the appropriate unit processes corresponding to the boundaries should be included
 - Competitive products – Due to the fluidity of the defined function or deployment into a new market, it may be difficult to define a functionally equivalent product system for comparison
- Life cycle inventory (LCI):
 - Data collection – At early stages, the full extent of the system may be unknown, including sources and types of material and energy inputs from the technosphere

- Temporal and geographic representation – The potential location of an operation and the timing of deployment may both change over the development cycle and both items can have significant impacts on the background system data that is used in the system
- Scale up impacts – The required material and energy inputs for a process per unit product change through scale-up
- Life cycle impact assessment (LCIA):
 - Environmental impact categories – Truly novel products may have impacts that are yet to be understood, nor characterized in existing impact assessment methods
- Interpretation:
 - Uncertainty and sensitivity – The results of LCA must appropriately correspond to the development stage and convey the corresponding uncertainty in data, process parameters, and modeling choices.

These issues do not preclude the performance and interpretation of high quality LCA at early stages. Rather, there are additional steps and approaches that can be leveraged to attempt to mitigate them. These principles are embedded throughout the remainder of this document in each of the stages of the LCA:

1. Clarity in goal – representation of current stage vs. future deployed stage
2. LCA should be conducted multiple times throughout the development cycle to appropriately capture design choices, refinement, and technology improvements
3. Full documentation and communication of assumptions and datasets throughout all phases of the LCA
4. Robust selection of modeling scenarios to reflect potential operating envelope and associated uncertainties – baseline, optimistic, and pessimistic
5. Sensitivity testing of key parameters

1.5 TEA and LCA

Like LCA, Technoeconomic analysis (TEA) is a common analytical framework that is also used to assess emerging technologies. The focus of the TEA is on the technical and economic viability of a product or process. Whereas the primary outputs of an LCA are the potential environmental impacts associated with a system, the primary output of a TEA is the estimated cost of production. This differs from Life Cycle Cost (LCC), which assesses the total cost over the life of a functional unit (e.g., an asset or service), including capital, maintenance, and end-of-life elements. There are many parallels between TEA and LCA and they are often performed in tandem. The outputs of a TEA process model can be used to directly inform the modeling of the primary process of interest in an LCA. For instance, the TEA model can provide amounts and specifications for the material and energy inputs, estimated emissions, and capital materials and equipment for a potential production site based on a modeled facility output.

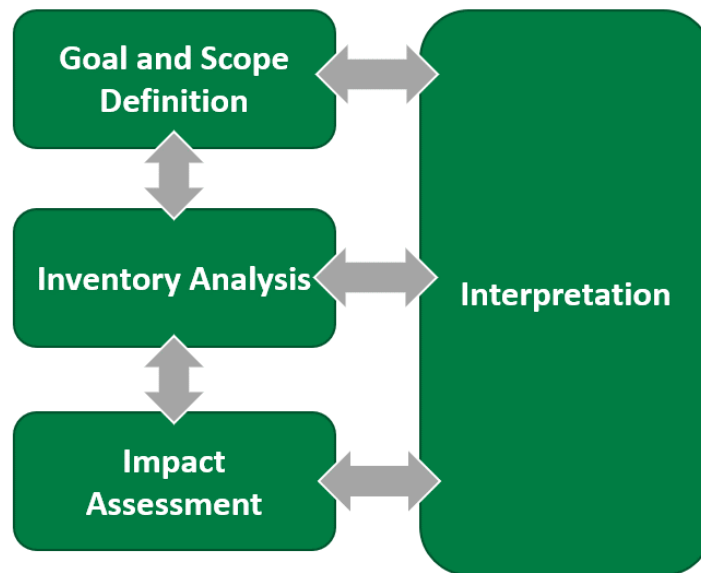
TEA can be useful when applied to emerging technologies, but like LCA, the same sorts of uncertainties exist. It is important that when a TEA is used to inform an LCA that there is a clear discussion of the goal, scope, and assumptions of the study. One way that analysts performing a TEA might address uncertainty is by running a set of scenarios to cover a variety of potential operating conditions. To the extent feasible, the same scenarios should be considered when designing and conducting the LCA. Both LCA and TEA are iterative frameworks and ideally, there is iteration and coordination between the entities performing both to develop the most robust assessment of a technology.

1.6 Document structure

This document is organized into chapters according to the four primary stages of LCA as illustrated in Figure 1:

1. Goal and scope definition
2. Life cycle inventory analysis
3. Life cycle impact assessment
4. Interpretation

Figure 1. LCA Stages; adapted from (ISO, 2006a)



Each life cycle stage is broken down into the key decisions that must be made in accordance with ISO 14040/14044 framework. Note, this document is not intended as a replacement for ISO 14040/14044, nor does it specifically address each of the items addressed in those standards. Rather it should be viewed as a companion document when evaluating DACS.

This is not a legal document and thus the recommendations included are provided as best practices based on the experience of the U.S. Department of Energy Office of Carbon Management.

Within each of the chapters aligning to the LCA stages, subsections are presented to address the key decision areas in that stage. Each subsection is organized as follows:

- Brief background discussion of the key decisions that must be made within the life cycle stage
- Relevance of those decisions to the application of LCA to DACS
- Recommended best practices for those decisions

The final chapter summarizes all the best practice recommendations across all the LCA stages.

2 Goal and scope definition

The goal of an LCA is critical in framing all the future decisions and structure of an LCA. According to Section 4.2.2 of ISO 14044, the goal should state the following:

- “the intended application;”
- “the reasons for carrying out the study:”
- “the intended audience, i.e., to whom the results of the study are intended to be communicated”
- “whether the results are intended to be used in comparative assertions intended to be disclosed to the public.”

With regards to DACS, potential study goals could include:

- Evaluation of a single DACS pathway to identify potential environmental impact hot spots and the impact of uncertainty in key operating and design parameters
- Comparison of different DACS technological approaches
- Comparison of DACS to different types of CDR approaches

The primary focus of this document is on the first goal; however, the results of that analysis can be used to inform studies that focus on the latter two goals. These Best Practices will help ensure that the assessment of any individual technology is robust so as to help facilitate a comprehensive comparison.

2.1 Functional unit

Background

As noted in ISO 14044, “the scope of an LCA shall clearly specify the functions (performance characteristics) of the system being studied.” The choice of the functional unit is linked directly to the goal and scope of the LCA. In the context of an LCA, the functional unit has multiple uses. First, it must clearly describe what the product or service does and the corresponding characteristics that define it. This allows the functional unit to serve as a consistent basis for comparison for multiple alternatives. Systems that do not yield the same function are incomparable unless the constituent systems are modified such that they provide a consistent function. Second, the functional unit services a practical role as the primary reference flow in the LCA model to which all inputs and outputs are quantitatively related and scaled.

The functional unit and system boundary are also linked. The expansion (or contraction) of the boundary to include (exclude) additional elements of the life cycle directly affects the functional unit.

Relevance to DACS

The function for DACS is untraditional in the sense that it provides an environmental good, that is, the functional unit is in the same units as one of the evaluated impact categories (i.e., climate change) and thus represents a circular analytical requirement. The overall goal of the LCA should also be considered when selecting a functional unit. Example functional units that could be (or have been) used to evaluate DACS systems include:

1. Mass of CO₂ captured
2. Mass of CO₂ captured from the atmosphere
3. Mass of CO₂ captured from the atmosphere and permanently stored
4. Mass of net CO₂e captured from the atmosphere and permanently stored

While the above functional unit options appear similar, there are nuances that make them unique and potentially uncomparable. The 'mass of CO₂ captured' functional unit could include captured on-site fossil emissions in addition to CO₂ captured from the atmosphere. More specificity is required to make this functional unit less ambiguous. The 'mass of CO₂ captured from the atmosphere' is more specific and establishes a different basis for comparison that is more relevant for Carbon Dioxide Removal. The 'mass of CO₂ captured from the atmosphere and permanently stored' functional unit adds expands the boundary downstream to include the storage of the captured CO₂, resulting in CO₂ removal.

The final functional unit, 'mass of net CO₂e captured from the atmosphere and permanently stored,' incorporates two additional components beyond the others considered. First, the term 'net' implies that the final amount should subtract any positive emissions that occur throughout the life cycle relative to a baseline, e.g., atmospheric concentration assuming a baseline effectiveness of the relevant CO₂ sink. Second, the addition of the 'e' in 'CO₂e' denotes that this functional unit would include the impacts of all GHGs in the life cycle. It should be noted that this functional unit would be iterative as the scaling of the intermediate flows in the model would depend on the outputs of the LCA itself. There are other analogous functional units, for example busbar vs. delivered electricity where the difference between the two is a scaling factor to account for any losses of the product (electricity) and emissions that occur during transmission and distribution; however, in those cases, only technical flows change and scale the individual unit processes. The results of an analysis using the 'mass of CO₂ captured from the atmosphere and permanently stored' functional unit could be scaled to account for the net impacts of all GHGs.

Figure 2 and Table 1 provide a simple example of a DACS system to illustrate the differences in LCA results for a single impact category (global warming) based upon the choice of different functional units. Note, the values used for the calculation are notional and not intended to represent any specific design or scenario. In addition to atmospheric capture, this example system also includes the capture of on-site fossil emissions associated with fossil energy combustion. Two distinct types of flows are depicted in the figure: process flows and emissions flows. Process flows include materials, energy, and captured CO₂, whereas emissions flows are supply chain or process emissions related to the operation represented in each block.

The first two functional units correspond with a cradle-to-gate system boundary since the disposition of the captured CO₂ is not specified. Note, in both cases, the system operates in the same way. The only difference is the denominator – CO₂ captured (which includes atmospheric and fossil) versus only CO₂ captured from the atmosphere. Numerically, these different functions, manifested as different denominators for scaling system impacts, yield different results and different interpretations about the system. With the first functional unit, the impacts associated with the capture of 1 kg CO₂ from the atmosphere are normalized to the total CO₂ captured, in this case 1.5 kg. This could potentially lead to misinterpretation regarding the CDR benefits. With the second functional unit, the same 1 kg of CO₂ is captured from the atmosphere, but since the basis is specific to that flow, the net result is higher in magnitude.

When the management of the captured atmospheric CO₂ is included in the third and fourth functional units, the system boundary is expanded downstream to include the full life cycle (i.e., ‘cradle to grave’). In this example, there is a minor numerical difference for the results between the second and third functional units when re-emissions of captured CO₂ associated with storage are low, but the interpretation implications are different because the second functional unit leaves unaddressed life cycle impacts (cradle-to-gate, which notably cannot be defined as removal because the atmospheric fate of the CO₂ is unknown), whereas the third represents the full life cycle (cradle-to-grave). Finally, the fourth functional unit relies upon a scaling of the results of the LCA based on the third functional unit. In this example, to achieve a net removal of 1 kg CO₂e from the atmosphere, the DACS system must capture and store 1.85 kg of atmospheric CO₂.

As illustrated by this example, different functional units for an identical system can result in different interpretations and understanding. It is important that functional units are descriptive and precise. For example, it is possible that the “captured CO₂” in the first functional unit could be implied to mean “capture of atmospheric CO₂.” However, without sufficient definition, the use of imprecise terms could result in the inaccurate interpretation of results and inappropriate comparisons with other systems. For the purposes of the assessment of DACS, it is recommended that LCAs utilize the mass of CO₂ captured from the atmosphere and permanently stored’ functional unit. This avoids the ambiguity inherent with the first two examples and avoids the iterative requirements of the fourth example and establishes a consistent comparison basis that could be used not only across DACS systems, but also broadly with other CDR approaches. Overall, this functional unit effectively allows the interpretation of the net removal impact (i.e., net kg CO₂e removed per functional unit), which is the key metric of interest when assessing CDR pathways, not just the functional unit itself.

For consistency, the captured CO₂ stream at the exit of the DAC facility should be pressurized to 2,200 psig and contain a minimum of 95% CO₂ by volume and not exceed any of the other established component limits established in the National Energy Technology Laboratory’s CO₂ Impurity Design Parameters (IPCC, 2005; NETL, 2019). While this document focuses on DACS, in the broad application of DAC, the disposition of the CO₂ also affects the selection of the functional unit, so it is worth discussing here. When the captured CO₂ is utilized for enhanced oil recovery (EOR) or is transformed to another product via a conversion process, the function of the system must also consider the service provided by the product of that activity in addition

to the removal of CO₂ from the atmosphere. Depending on the product, the storage of the captured CO₂ may have less permanence, and this should be reflected accordingly in the functional unit.

Figure 2. DACS Functional Unit GHG Accounting Example: System

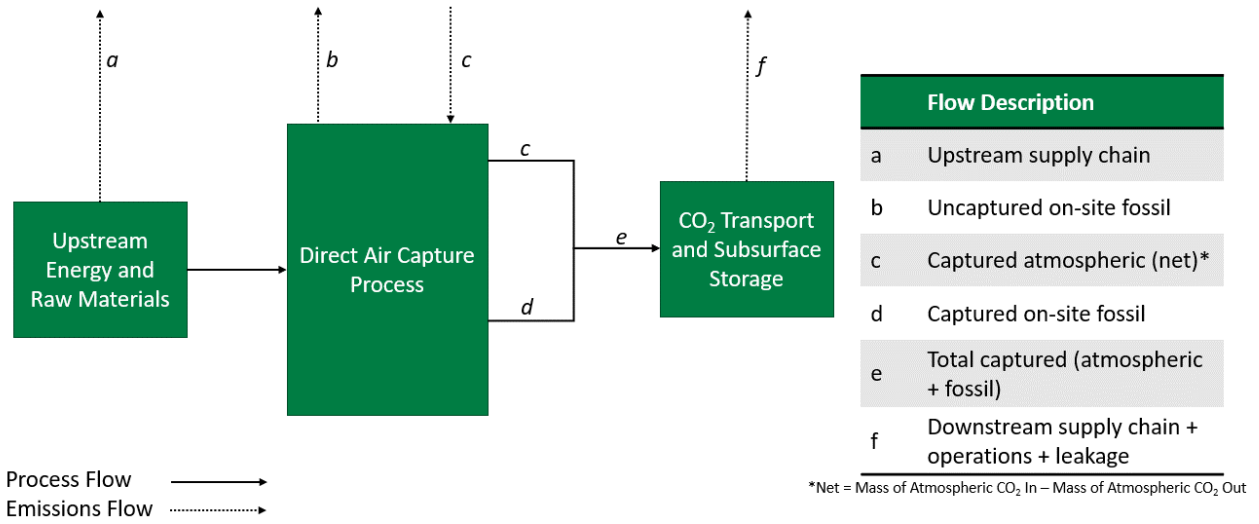


Table 1. DACS Functional Unit GHG Accounting Example: Results

| Functional Unit | System Boundary | Calculation (kg CO ₂ e/FU) |
|--|-----------------|--|
| 1 kg CO ₂ captured | Cradle-to-gate | $c = 1$ $kg\ CO_2e = \frac{a+b-c}{c+d} = \frac{0.40+0.05-1.00}{1.00+0.50} = -0.37$ |
| kg CO ₂ captured from the atmosphere | Cradle-to-gate | $c = 1$ $kg\ CO_2e = \frac{a+b-c}{c} = \frac{0.40+0.05-1.00}{1.00} = -0.55$ |
| kg CO ₂ captured from the atmosphere and permanently stored | Cradle-to-grave | $c = 1$ $kg\ CO_2e = \frac{a+b-c+f}{c} = \frac{0.40+0.05-1.00+0.01}{1.00} = -0.54$ |
| net kg CO ₂ e captured from the atmosphere and permanently stored | Cradle-to-grave | Scale up factor $c' = \frac{-1}{FU\ 3\ Result} = \frac{-1}{-0.54} = 1.85$ $kg\ CO_2e = \frac{c'(a+b+f)-c'}{1} = \frac{0.85-1.85}{1} = -1$ |

*Notional values used for calculation example: a = 0.40; b = 0.01; c = 1.00; d = 0.50; e = 1.50; f = 0.01; all measured in units of kg CO₂e

Best Practices

- Analyze DACS using this functional unit: Mass of CO₂ captured from the atmosphere and permanently stored
- Report CO₂ removal via DACS as net mass of CO_{2e} captured from the atmosphere and permanently stored
- At the downstream gate of the DAC facility, CO₂ should be compressed to 15.3 MPa (2,200 psig) and contain a minimum of 95% CO₂ by volume (IPCC, 2005; NETL, 2019)

2.2 System boundary

Background

The system boundary for an LCA defines which processes are included and excluded from the assessment. Like the functional unit, the choice of the system boundary is directly linked to the goal of the study. According to ISO, processes can be excluded to the extent that they do not significantly change the outcome of the study. All exclusions should be noted and justified.

When evaluating a comparison of two LCA studies, consistency in boundaries is just as important as consistency in functional unit. While two studies with equivalent function can be compared, if there are differences in the system boundaries, the result of the comparison will be misleading.

While boundaries for each system are often unique, there are a set of generic terms that are used to refer to which processes are included or excluded:

- Gate-to-Gate: This boundary only encompasses the operations at the DAC facility. The technical and intermediate flows cross the boundary, but the resulting supply chain impacts associated with the upstream and downstream processes create or transform those flows are not accounted for. Only emissions directly from the process of interest are accounted for with this boundary.
- Cradle-to-Gate: a modification of the gate-to-gate boundary, in which all processes upstream of the process of interest are included back to the extraction of the required raw materials from the Earth. None of the processes downstream from the DAC facility are included.
- Cradle-to-Grave: This is the most comprehensive set of boundaries and includes all the activities associated with the functional unit from extraction of raw materials through CO₂ disposition as the end-of-life.

Relevance to DACS

As noted above, the system boundary is linked to the goal of the study. DACS systems necessarily require a cradle-to-grave boundary to achieve the stated function of CO₂ removal. This boundary represents a complete accounting throughout the life cycle that is useful for markets and considerations in a policy context (e.g., evaluating different CDR approaches or different CO₂ dispositions). When evaluating DAC technologies, a truncated cradle-to-gate

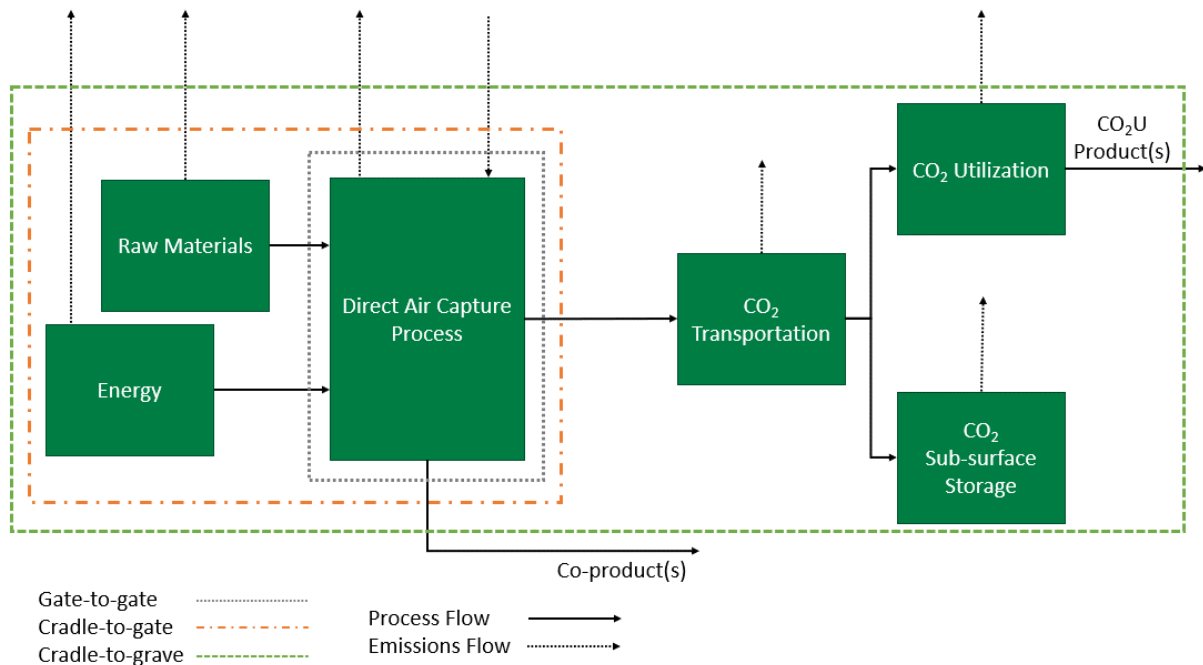
boundary may be used for consistent technology comparison with the same final CO₂ disposition (i.e., different variations of DAC). In application, the difference between these two boundaries in practice is the exclusion or the inclusion of the transportation and disposition of the captured carbon dioxide.

For cradle-to-gate boundaries, the system should include any on-site CO₂ compression to 2,200 psig and contain a minimum of 95% CO₂ by volume, but not transportation in a pipeline (IPCC, 2005; NETL, 2019). For cradle-to-grave boundaries, the system should include CO₂ transportation and final disposition:

- Sub-surface storage: inclusive of CO₂ injection, ongoing site monitoring activities, disposal well construction, etc.
- Carbon dioxide utilization/conversion: raw material and energy requirements for conversion operations, product use and end-of-life
- Enhanced Oil Recovery (EOR): injection, re-emission of produced CO₂, oil field support activities, crude oil transport, refining, end use

Carbon dioxide utilization/conversion and EOR further complicate the system because they result in additional co-products from the system and could require the analysis to be reframed with a different functional unit. Additional discussion of these approaches is provided in Section 6.

Figure 3. System Boundary Examples for DAC



Best Practices

- Evaluate DACS with a cradle-to-grave boundary to fully account for the function of the system
- For all dispositions of the captured CO₂, which include utilization/conversion or EOR, the system boundary should encompass the downstream fate of the captured CO₂ as well as any associated activities
- Depict the system boundary graphically using a process flow diagram to depict processes included within the analysis scope

2.3 Defining comparison systems

Background

One of the purposes for convening an LCA may be to compare potential alternatives. According to ISO 14044, a comparative assertion is an “environmental claim regarding the superiority or equivalence of one product versus a competing product that performs the same function.”

The decision to make a comparative assessment should be documented as part of the goal of the study. ISO stipulates that all the data quality requirements must be fully specified, documented, and addressed as part of the comparative LCA. Prior to interpreting the results, the equivalence of the systems under study must be evaluated according to the following elements:

- Functional unit
- System performance
- System boundary
- Data Quality (e.g., temporal, geographical, and technological representation (Edelen & Ingwersen, 2016))
- Allocation Procedures (see Section 3.5)
- Impact assessment (see Section 4)

Relevance to DACS

As DACS technology continues to develop, it may be desirable to make comparisons for different pathways and vendors (e.g., solid sorbent vs. liquid solvent). Further, as the suite of potential CDR approaches emerges, there will likely be comparisons made to DACS.

There are potential challenges when using LCA to compare emerging technologies at different stages of development. For early-stage technologies, the performance of the system will change as it moves closer to demonstration or commercialization (e.g., from increased process or material efficiency due to economies of scale). There is also temporal uncertainty regarding when the emerging technology in question will deploy at scale and what the market and technology landscape will be at that future point.

Best Practices

- Ensure functional equivalence between systems, including the management and provision of co-products for all systems under evaluation
- Document assumptions regarding the future landscape into which an emerging technology might deploy, including identifying which system dynamics are included
- Use consistent assumptions and data quality requirements for background data for all systems to ensure equivalent comparability
- Represent the system boundaries for the different systems visually to communicate consistency when comparing two or more DACS or CDR systems

3 Life cycle inventory analysis

The LCI stage involves gathering all the key inputs and outputs associated with all unit processes within the established system boundary, including both technical and elementary flows. Unit processes represent the smallest portion of a system for data collection and relate inputs to outputs via an established relationship. Data collection for the LCI includes both the physical flows between processes (e.g., a process demands X kWh of electricity), but also the associated emissions in the value chain for that flow (e.g., Y kg CO₂ per kWh of electricity).

When collecting data for the purposes of an LCA, it is sometimes helpful to differentiate between the foreground and background of a system. The foreground represents the direct operations of the primary process or technology of interest and which the commissioner of an LCA can have direct impact, whereas the background includes all the supporting upstream and downstream processes (i.e., value chain) where the commissioner has limited impact. Thus, the representation of the foreground system should be more detailed and sophisticated than the background system, in terms of representation in the model, results, and sensitivity/uncertainty assessment.

To determine common themes in those flows, a review of the recent TEA and LCA DAC literature was conducted, looking at both solvent- and sorbent-based designs (de Jonge et al., 2019; Deutz & Bardow, 2021; Keith et al., 2018; Liu et al., 2020; Terlouw, Treyer, et al., 2021). From these studies, it was clear that the key LCI data inputs could be binned into the following groups: DAC operations, energy, construction, process chemicals, captured CO₂ management, waste management, decommissioning, and land use.

The common theme across all the studies is the relationship between the amount and carbon intensity of the energy that is used to run the process, both as electricity and heat, and the net storage of CO₂ that the facility achieves. The authors found that the other inputs had very minor effects on the net storage factor, most of the time contributing positive emissions on the scale of grams for a functional unit of 1 kg of CO₂ stored. Nonetheless, they should be considered for completeness and periodically reevaluated as DACS systems mature. In some cases, the choices between alternatives did have significance on other environmental impacts evaluated (Deutz & Bardow, 2021; Terlouw, Treyer, et al., 2021).

This section separates data collection into two groups: non-consumables (those occur on a one-time basis) and consumables (those that occur routinely)

3.1 Data collection: facility operation

Background

The plant operation includes the activities and processes that would be included in a gate-to-gate system boundary. It is also generally referred to as the foreground system. Depending on the study, the representation of plant operations can range from a black box depiction to a detailed dynamic process model that is linked to the LCA. During this data collection activity, it is important to gather all information about the physical flows of inputs and outputs from this boundary, inclusive of raw materials, energy, emissions, products, wastes. This information will

then link to the modeling of background system impacts associated with the consumables required by the facility.

For mature systems, the facility of interest is usually operational meaning that the required information is readily accessible. With earlier stage technologies, the information that is used to represent the system comes from process engineering models that use fundamental engineering relationships to characterize the system.

Relevance to DACS

Due to the early nature of the technology, most of the key data to represent the facility operation will be based on engineering simulations. These models are utilized to characterize costs of operation and include the key inputs and outputs to the extent that they affect these costs. It should be noted that the scope of these models is variable and additional estimates or data sources may be required to fully characterize the facility operations (e.g., emissions species not tracked by the engineering model). As technologies are materialized and introduced to the market for potential future regulatory compliance and policy incentive, MRV (measurement, reporting, and verification) of foreground data will become increasing important and necessary.

Best Practices

- Separately report and account for any captured fossil or other non-atmospheric CO₂ (e.g., from on-site fossil fuel combustion) from the captured atmospheric CO₂ for consistency with the functional unit
- Define LCA scenarios with a direct tie to process and cost engineering model (i.e., TEA) scenarios such that they characterize the underlying facility operating envelope (see Section 5.2)
- Coordinate with process and cost engineering modeling (e.g., TEA) team to capture data necessary for LCA
- Report physical quantities for process inputs and outputs (e.g., MJ energy, kg materials) in addition to the associated inventory of emissions (e.g., kg emission)
- Clearly identify degree of uncertainty and variability, particularly for modeled rather than empirical inputs

3.2 Data collection: non-consumables

Background

The processes included in this category generally occur prior to operation, and the corresponding emissions are often approximated as one-time impacts. These include a combination of non-routine plant inputs as well as manufacturing of capital equipment and site construction. The amounts of these materials do not change as a function of variability in the production of a facility (e.g., a facility that operates full-time versus part-time). Since these emissions associated with these activities are not directly tied to ongoing operations, they are

amortized over the expected life of the operation so that they can be normalized to the functional unit:

$$\frac{\textit{Total emissions from activity}}{\textit{Integrated facility design capacity} * \textit{Capacity factor} * \textit{Operational lifetime}} = \frac{\textit{mass of emissions}}{\textit{functional unit}}$$

*Units for equation terms:

- Total emissions from activity = mass of emissions
- Total plant design capacity = mass atmospheric CO₂ removed per year
- Capacity factor = percentage time plant is operational over the course of one year
- Operational lifetime = years

Some non-consumables may also need to be replaced multiple times throughout the lifetime of a facility (e.g., sorbent materials). The emissions associated with those replacements should also be considered and amortized to the functional unit as follows:

$$\frac{\textit{Total Emissions per Replacement} * \frac{\textit{Number of Replacements}}{\textit{year}} * \textit{Operational lifetime}}{\textit{Total plant design capacity} * \textit{Capacity factor} * \textit{Operational lifetime}} = \frac{\textit{mass of emissions}}{\textit{functional unit}}$$

There are several different approaches that can be used for developing inventory data to represent these activities:

- Material/equipment list from a TEA and translation to the base material inventories developed by process LCA methods (e.g., structural steel, concrete, etc.)
- Economic input-output (IO) modeling is an approach that maps expenditures to different economic sectors, which are then tied to emissions associated with those sectors (Carnegie Mellon University Green Design Institute, 2018; US EPA, 2020)

It should be noted that there may often be uncertainty in these processes, especially for emerging technologies. The effect of this uncertainty on the overall results should be explored by using reasonable proxies and ranges for the process in question. Also, multiple approaches can be utilized as necessary to best provide a complete representation of these materials. Depending on the stage in development, some approaches may be more reasonable than others (e.g., use of IO methods at low TRL prior to the completion of a comprehensive TEA).

Relevance to DACS

Like other industrial processes, the relevant processes for DACS likely include the following:

- Manufacturing of capital equipment
- Site construction

- Initial system charging and replacement of process materials, chemicals, and catalysts (e.g., sorbent or solvent)
- Working fluids

Best Practices

- Utilize a modeling approach that provides the best data that is available to represent these activities corresponding to the stage of development
- Update representation of design and underlying LCI data as technology matures and nears deployment
- Test sensitivity of the assumed facility lifetime and any non-consumables that require replacement during the facility operating life (see Section 5.2 for additional recommendations)

3.3 Data collection: consumables

Background

Consumables vary by application, but generally include routine inputs for a facility such as, raw materials, energy, ancillary inputs, water, and waste processing. The amounts of consumables generally scale according to the amount of output from a process.

Relevance to DACS

For DACS, the following consumables should be included in the LCI:

- Energy:
 - Heat (e.g., embodied in steam)
 - Electricity
- Process chemicals/materials:
 - Solid sorbent replacement
 - Solvent makeup
 - Others
- Water (including water required for steam)

Best Practices

- Model specific pathways/technologies for producing the input based on best available information
- When multiple potential sources/types are being evaluated as part of the design, develop separate LCA scenarios for each
- Report physical quantities for inputs and outputs in addition to the associated inventory of emissions
- Review Section 3.4 for recommended data sources for representing the emissions associated with these inputs

3.4 Data collection: key processes and potential data sources

A variety of LCI data sources exist, both public and commercial (e.g., ecoinvent, GaBi, etc.). Public data sources from the DOE and Federal Government are provided below:

- National Energy Technology Laboratory (NETL)
 - Natural gas model
 - Gate-to-gate saline aquifer storage model
 - U.S. Electricity Baseline
 - Grid Mix Explorer Excel tool
 - openLCA Unit Processes
 - Unit Process Library
- Argonne National Laboratory (ANL) The Greenhouse gases, Regulated Emissions and Energy use in Technologies (GREET) model
 - [LCI of energy inputs](#)
 - [LCI of materials inputs](#)
- U.S. Federal LCA Commons
 - NREL U.S. Life Cycle Inventory (USLCI) database
- U.S. EPA Environmentally-Extended Input-Output (USEEIO) Models

The table below provides an overview of the key process inputs that would likely need to be gathered as part of the LCI. U.S. DOE and other federal resources are provided for each.

Table 2. Key LCI data collection processes, parameters, and data sources

| LCI Data Category | Parameters | DOE and Other Federal Resources |
|--|--|---|
| DAC Operation | Inputs and outputs associated with the facility operations, including any on-site emissions | Unique to each project – user input based on engineering model |
| Consumables – Electricity | <ul style="list-style-type: none"> • Consumption mix technology contributions by generation type • Inclusive not only of generation facility emissions, but also fuel and material supply chains, where applicable • Future grid mixes based on proposed year of deployment using data provided in EIA’s Annual Energy Outlook ‘Reference Case’ | <ul style="list-style-type: none"> • U.S. Electricity Baseline (NETL) – regionalized consumption mixes with options to customize technological representation • ANL GREET |
| Consumables – Heat | <ul style="list-style-type: none"> • For onsite combustion: direct emissions should be included in DAC operation, but fuel supply chain (e.g., natural gas) accounted for separately • For offsite combustion: both fuel combustion and fuel supply chain should be accounted | <ul style="list-style-type: none"> • NETL • ANL GREET • Federal LCA Commons |
| Non Consumables – Construction/Capital | Amounts (mass or dollars) of key materials (e.g., steel, concrete, aluminum, copper, | <ul style="list-style-type: none"> • Process-based LCA could be conducted material LCI data |

| LCI Data Category | Parameters | DOE and Other Federal Resources |
|--|---|---|
| Activities | plastics) for process equipment and site infrastructure | from NETL, GREET, Federal LCA Commons <ul style="list-style-type: none"> Alternatively, to estimate data based on purchasing, could leverage U.S. EEIO approach |
| Consumables – Process Chemicals and Water | Inclusive of initial system charges as well as any required routine makeup over the life of the facility (solvents, sorbents, etc.) | <ul style="list-style-type: none"> Highly dependent on the chemical – some data are available from NETL, GREET, and U.S. LCI Alternatively, to estimate data based on purchasing, could leverage U.S. EEIO approach |
| CO ₂ compression, transport, injection, MRV | Initial on-site compression of the captured CO ₂ should be included the DAC site electricity consumption, but required boost compression and transport are included here Storage site activities include site prep, well construction, injection, brine management – these are all variable by site and could be parameterized if desired to evaluate geographic/geologic variability | NETL gate-to-grave assessment of saline aquifer storage of CO ₂ |
| Waste management | Handling, transport, and management of any process wastes from DAC operations | U.S. LCI for landfilling or incineration; GREET or NETL for transport |
| Land use change | Site disturbance/clearing to facilitate DACS operations and infrastructure | GREET and NETL have land use change/conversion factors |
| Decommissioning | Deconstruction, waste disposal, material recycling | Proxy industrial facility for these impacts (e.g., power plant decommissioning is included in some of the NETL LCAs) |

3.5 Co-product management

Background

Co-product management is a broad term used to encompass the approaches to handling systems with multiple products leaving the system boundary. In these systems, it is often desirable to produce results on the basis of a single product. ISO 14044 prescribes the following hierarchical approach for managing co-products:

1. Avoid allocation by
 - a. Subdividing the system into sub-processes with individual products and model those sub-process inputs and outputs accordingly
 - b. Expansion of the system to include the functions of all products leaving the system boundary

2. Partition (allocate) the inputs and outputs of the system “in a way that reflects the underlying physical relationships between them.” Typical bases for the physical relationship include mass and energy value.
3. Use an alternative allocation basis when a physical relationship cannot be established – e.g., economic value.

While subdivision is the preferred approach in ISO 14044, for complex and heavily integrated systems, it is often infeasible due to data limitations. The next preferred approach, system expansion, essentially solves the issues of co-products by including them in the functional unit. This approach removes any of the potential subjectivity introduced in the subsequent approaches, but with the drawback that it renders comparison with other systems more difficult because the system in question no longer produces a single product, but multiple products. Any comparison in LCA must be based in principle on equivalence in function. For this reason, some practitioners have added a subsequent step to the system expansion process and take a credit for the avoided production via conventional means of the system’s co-products. This approach is often referred to as system expansion with displacement. It is also referred to as ‘substitution’ or ‘avoided burden.’ An alternative approach when using system expansion is to modify the comparison system to include the additional processes necessary to ensure equivalent function with the system under study.

It should be noted that the use of system expansion with displacement can result in net negative flows of emissions in the life cycle inventory. These negative values do not imply uptake of emissions (e.g., carbon dioxide) from the environment, but rather that evaluated system for producing the primary output is environmentally preferred to the comparison approach for the impacts evaluated. Baselines should be clearly identified, and displacive impacts should be identified as such.

Relevance to DACS

While the primary purpose of DACS is the removal of carbon dioxide from the atmosphere, some of the evolving designs may include co-products. These can include, but are not limited to, potable water, oxygen, and low-grade heat. In addition, DACS may also result in additional environmental goods as co-benefits, including the removal of some criteria air pollutants (e.g., particulate matter, SO₂, and NO_x). Similar to the removal of atmospheric CO₂, the removals of other pollutants are part of the functional unit of the system and will be in the same units as one of the evaluative impact categories and thus represents a circular analytical requirement. Since these products and services have functional value that would otherwise require alternative interventions, they must be addressed in the context of a multifunctional system. In the DAC system, the removal of CO₂ would be defined as the determining product, whereas the co-products would be defined as dependent. In other words, the amount of CO₂ removed would not be scaled based on the increase in demand for any of the dependent co-products.

By necessity, co-products are managed throughout LCI databases to provide LCI data on the basis of a single product that may be used as an input to another process. Where different

options exist, a consistent approach should be considered for both the foreground and background data to the maximum extent feasible.

Best Practices

- Follow the established co-product management hierarchy in ISO 14044 Section 4.3.4
- If sub-division is not possible, use system expansion with a multiproduct functional unit
- Avoidance and removals should always be accounted for separately, not combined with each other
- Maintain a record of the physical system depicting the impacts with and without management of co-products
- Test multiple co-product management approaches, including allocation. This can help determine how robust conclusions are across multiple approaches.

4 Life cycle impact assessment

Background

The Life Cycle Impact Assessment (LCIA) Phase pertains to the translation of LCI emissions into potential environmental impacts based on the selection of a particular set of categories and characterization factors. According to ISO 14044, “the selection of impact categories shall reflect a comprehensive set of environmental issues related to the product system being studied, taking the goal and scope into consideration.”

The results of the LCIA stage depend heavily upon the decisions and data collection in the earlier stages of the LCA. The choice of system boundary, availability, and representativeness of the LCI data, and the characterization methods used all affect how meaningful and comparable a set of LCIA results are. There may also be significant geospatial variability that is not accounted for in the impact assessment methods.

Relevance to DACS

While the primary focus in evaluating DACS and other CDR systems in an LCA context is the quantification of the net carbon dioxide (equivalents) removed from the atmosphere, LCA provides a basis for evaluating other potential environmental impacts allowing for an assessment of the potential tradeoffs between them. This more holistic view is how LCA differs from carbon footprinting.

Best Practices

- Utilize the EPA’s Tool for Reduction and Assessment of Chemicals and Other Environmental Impacts (TRACI) version 2.1 method for LCIA (US EPA, 2021) to characterize the following impact categories (additional impact methods and impact categories may also be reported): ozone depletion, acidification, eutrophication, smog formation, human health particulate, human health cancer, human health noncancer, ecotoxicity.
- TRACI 2.1 was last updated in 2012 and thus does not reflect the latest global warming potential characterization factors from the Intergovernmental Panel on Climate Change (IPCC) Sixth Assessment Report (AR6). It thus recommended to utilize the IPCC AR6 GWP characterization factors for translation of GHG emissions to Global Warming Potential impacts as a replacement for the factors in TRACI (IPCC, 2021), and adopt future IPCC GWP characterization factors as they are released.

Table 3. Excerpt of IPCC AR6 GWP Characterization Factors

| GHG | 20-Year | 100-Year |
|------------------|---------|----------|
| CO ₂ | 1 | 1 |
| CH ₄ | 82.5 | 29.8 |
| N ₂ O | 273 | 273 |

5 Interpretation

According to ISO 14044, the life cycle interpretation phase includes:

- Identification of significant issues based on the results of the LCI and LCIA phases
- Evaluation of completeness, sensitivity, and consistency
- Conclusions, limitations, and recommendations

These Best Practices focus primarily on the second item in the following sections, though the others are of critical importance and are addressed thoroughly in the ISO 14040/14044 standards.

5.1 Negative emissions accounting

Background

In LCA, negative emissions generally arise from one of two situations:

1. Removal of the emission species from an environmental compartment (e.g., biomass uptake of atmospheric CO₂ during photosynthesis). Note the removal of an emission from one compartment does not imply permanence of storage or avoidance of future re-emission. Those attributes, along with shifts to other environmental compartments, should be accounted for in separate processes within the system boundary.
2. Avoided emissions associated with the production of a product by another means (e.g., when using system expansion with displacement to manage co-products)

The interpretation of these two situations is quite different (Tanzer & Ramírez, 2019). In the first scenario, the emission of interest is physically removed from an environmental compartment. The exact amount is defined by the functional unit for the system of study. If the functional unit is scaled up, the corresponding physical removal is also scaled up along with any downstream fate of the emission.

In the second scenario, the negative emissions do not represent a physical removal, but rather an avoidance of emissions by opting for one method of production over another. When an LCA includes a displacement or avoided emissions credit, the implication is that this displacement occurs fully in the market (i.e., the co-product displaces 100% of another product, meaning no additionality occurs). Further, this approach is specific to study goal and scope for the system of interest.

Relevance to DACS

The differentiation of removed and avoided emissions is of critical importance for assessing the efficacy of potential CDR technologies. When evaluating CDR pathways, one of the key metrics will be the amount of net negative emissions relative to an atmospheric rather than technospheric baseline achieved by the technology. Due to the inclusion of material and energy inputs in the LCA, and their associated supply chain emissions, the net portion of the net negative emissions refers to the quantity of CO₂ actually removed after accounting for positive emissions that also occur to support the DACS process. As noted in Section 3.5, DACS systems

may also include co-products. If those co-products are managed using system expansion with a displacement credit for the conventional production of those co-products, the resulting impacts and corresponding interpretation for the DACS system could be distorted (Terlouw, Bauer, et al., 2021).

The example DACS system and corresponding calculations in Figure 4 and Table 4 depict the impacts of different accounting approaches for removed and avoided emissions on the net system GHG emissions. This is an expansion of the example that was used to inform the discussion on functional units in Section 2.1. In this example, the functional unit across all three scenarios is ‘mass of atmospheric CO₂ captured and stored.’ In this example, one or more co-products are produced by the DAC operation. These co-products are managed in accordance with the ISO 14044 hierarchy using system expansion and accounting for full displacement of the conventional production impacts.

Scenario 1 is the base case in which there are no co-products, but 1 kg of atmospheric CO₂ removed from the atmosphere. In Scenario 2, the avoided emissions associated with the co-product allocation are included in the total, implying an increase in removal from the atmosphere over Scenario 1 (-0.74 vs. -0.54). In Scenario 3, these two effects are reported separately. This reporting approach more clearly illustrates what the impacts are associated with removal and avoided emissions.

Figure 4. Direct Air Capture with Co-Product GHG Accounting Example: System

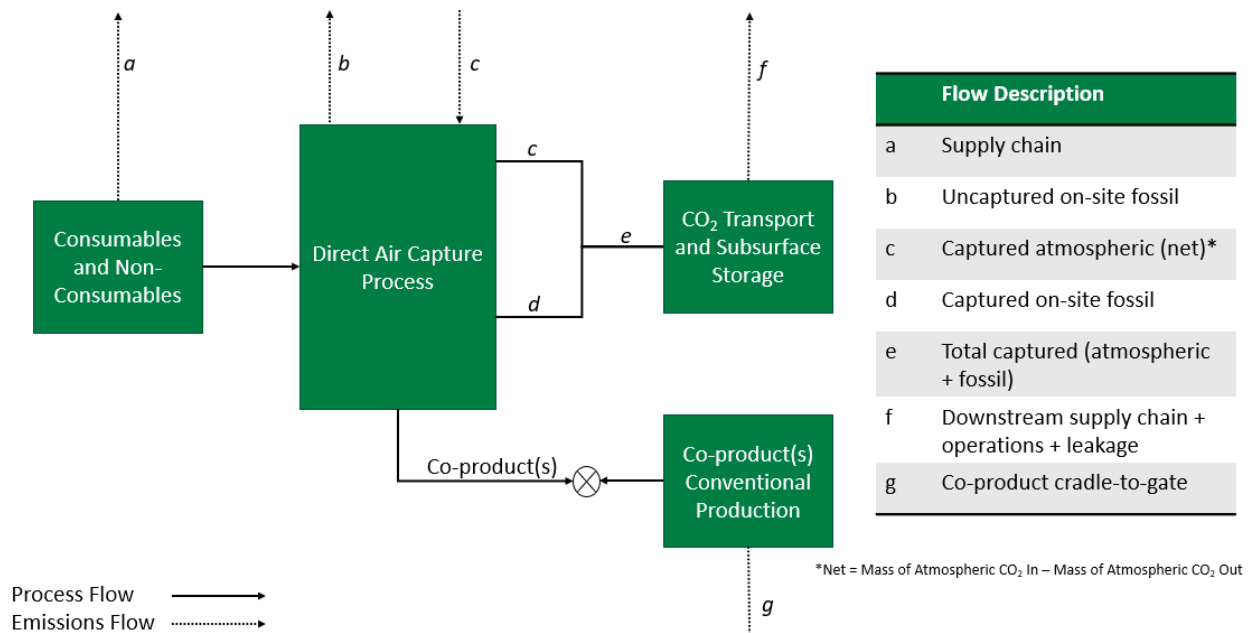


Table 4. Direct Air Capture with Co-Product GHG Accounting Example: Results

| Scenario | Functional Unit | Calculation (kg CO ₂ e/FU) |
|--|--|--|
| 1 No Co-Products | kg atmospheric CO ₂ captured and stored | c = 1; g = 0 $\text{kg CO}_2\text{e} = \frac{a+b-c+f}{c} = \frac{0.40+0.05-1.00+0.01}{1.00} = -0.54$ |
| 2 Co-Product Accounting: Combined avoided and atmospheric removals | kg atmospheric CO ₂ captured and stored | c = 1; g = 0.20 $\text{kg CO}_2\text{e} = \frac{a+b-c+f-g}{c} = \frac{0.40+0.05-1.00+0.01-0.20}{1.00} = -0.74$ |
| 3 Co-Product Accounting: Separate avoided and atmospheric removals | kg atmospheric CO ₂ captured and stored | c = 1; g = 0.20 removed kg CO ₂ e = $\frac{a+b-c+f}{c} = -0.54$ avoided kg CO ₂ e = $\frac{-g}{c} = -0.20$ |

*Notional values used for calculation example: a = 0.40; b = 0.01; c = 1.00; d = 0.50; e = 1.50; f = 0.05; g = 0.20

Best Practices

- For systems with co-products, when system expansion is used to manage multiple outputs, report avoided emissions and atmospheric removals separately in the results (see Scenario 3 in the Table 4 example)
- When a DAC facility includes capture of CO₂ from on-site fossil fuel combustion or other non-atmospheric CO₂, separately report that amount from the atmospheric CO₂ captured

5.2 Sensitivity and uncertainty analysis

Background

LCA is a data-intensive framework, often requiring decisions from the analyst about the representation of the system under study that qualitatively affect results. Uncertainty and variability in these decisions manifest from (1) parameter uncertainty, (2) model uncertainty, and (3) uncertainty due to scenario choices, while variability covers (4) spatial variability, (5) temporal variability, and (6) variability between objects and sources (Huijbregts, 1998). Parameter uncertainty can manifest from variability in the underlying population from which data is sampled, either measured or observed (Bamber et al., 2020). Model uncertainty stems from the mathematical relationships utilized in the LCA model calculations as well as applications of models for producing data for inventories and impacts assessment methods (Bamber et al., 2020). Finally, scenario uncertainty pertains to choices that are made to represent extensions of applications of the system under study, including geographic, technological, and temporal. All LCAs have some combination of these uncertainties, but the importance of each is highly dependent on the application and the system of study.

There are approaches that can be utilized to manage and better understand the implications of the underlying uncertainty and variability in a model:

- Sensitivity analysis: One approach to testing the robustness of the conclusions of an LCA is to alter parameter values and assessing the resulting changes in the model results. The most popular approach, one-at-a-time sensitivity analysis, can highlight the most

important parameters in the model, providing insights for future data collection and representation. More sophisticated approaches, such as moment-independent methods, have been applied to LCA to account for parameter interaction effects that cannot be discerned from a one-at-a-time approach (Cucurachi et al., 2022; Ravikumar et al., 2018).

- Scenario design: Robust scenario design and evaluation can provide insights about how the likely sources of uncertainty will impact the study results over a broad range of assumptions. So-called bounding scenarios can be used to understand the potential best- and worst-case impacts of a potential system. No likelihood is prescribed to either extreme, but they can be used to inform refinement in design as a technology moves towards commercialization.
- Simulation: The overall uncertainty in model results can be evaluated by implementing stochastic simulation of model parameters and data based on the probabilistic distribution of their values. This approach yields a probabilistic representation of the model results. The drawback to this approach is that the interpretation of results, especially for early stage and uncertain technologies where robust underlying parameter distributions do not exist or are not well understood, may imply more certainty than exists. The results are highly dependent upon the underlying distributions chosen to represent the model parameters. Further, informative distributions may not exist for emerging technologies, where data limitations are often significant.

Relevance to DACS

Based on a lack of large-scale operating data, there is likely to be uncertainty in the representation of DACS in an LCA. There is significant uncertainty and variability in process parameters, inventory data and modeling choices in early-stage technologies.

Best Practices

The following best practices are made explicit for specific LCI elements of the DACS LCA model in Table 5. It should be noted that every system is different and additional uncertainty scenarios and sensitivity cases should be evaluated beyond the elements included.

- Use of bounding analysis to inform key decision points
- Use of standard modeling scenarios in Table 5
- Use of sensitivity analysis to understand the dependence of key parameters

Table 5. Uncertainty Scenarios and Sensitivity Cases for DACS LCA

| LCI Data Category | Parameter | Scenarios (baseline/upper bound/lower bound) | Sensitivity Cases |
|---|--|--|--|
| DAC Operation | Technical operating performance (TEA case alignment) | <ul style="list-style-type: none"> Alignment to TEA cases: baseline/optimistic/pessimistic Model all relevant TEA scenarios to convey potential range of results Capture efficiency 70%/80%/50% | Capacity Factor: +/- 25% |
| | Co-product management method and displacement value (if applicable) | <ul style="list-style-type: none"> Evaluate different allocation bases as suggested in ISO (e.g., mass, economic value) Model a range of potential technologies that could be displaced by a co-product | Generate LCA results accounting for full substitution (100%) and no substitution (0%) of the conventional pathway for the co-product - |
| Consumables – Electricity | Electricity source | <ul style="list-style-type: none"> Regional grid mix /100% renewables (solar and wind)/ 100% grid-average coal generation Future grid mixes based on proposed year of deployment using data provided in EIA’s Annual Energy Outlook ‘Reference Case’ | Electricity GHG intensity (kg CO _{2e} /MWh) |
| Consumables – Heat | Heat source | <ul style="list-style-type: none"> On-site combustion with capture/waste heat/uncaptured natural gas | Heat GHG intensity (kg CO _{2e} /MJ): 0 to uncaptured natural gas combustion; GWP results |
| Consumables – Natural Gas | Natural gas supply chain – methane intensity | <ul style="list-style-type: none"> Assess results based on impacts of methane leakage in the natural gas supply chain for electricity generation and heat (where applicable) Methane leakage (extraction through delivery)¹: 2%/8%/0.3% | Generate results based on 20- and 100-yr GWP |
| Consumables – Process chemicals and water | Key process material inputs (e.g., solvent makeup, other supporting chemicals) | <ul style="list-style-type: none"> Baseline/Optimistic/Pessimistic assessment process chemical requirements | +/- 50% baseline input amounts |
| Non-Consumables | Capital equipment Process chemicals/catalysts | <ul style="list-style-type: none"> Plant operational lifetime baseline/optimistic/pessimistic | +/- 50% plant operational lifetime |

¹ Emissions of methane throughout the natural gas value chain exhibit significant variability, both geographically and by operator practice. This range attempts to reflect uncertainty and variability in recent measurements and bottom-up estimates (Chen et al., 2021; Rai et al., 2021).

6 Summary and closing

Consistent and robust accounting is imperative for the evaluation of CDR approaches, including DACS. This document builds upon the ISO 14040/14044 standards specifically for the evaluation of DACS. Table 6 includes a summary of all the best practices detailed in this document. While not identified as one of the four phases of LCA, the communication of assumptions and results in the reporting stage is critically important. The qualitative and quantitative portions of each of the Best Practices discussed in this document should be included in the report, in addition to elements described in Section 5 of ISO 14044.

The Best Practices provided in this document apply to DAC with permanent storage (DACS). If evaluation of CO₂ dispositions in addition to storage is of interest, the following DOE LCA resources are recommended:

- Enhanced Oil Recovery: Carbon Dioxide Enhanced Oil Recovery Life Cycle (CELiC) Model (Jamieson, 2019)
- CO₂ Utilization/Conversion: Carbon Dioxide Utilization Life Cycle Analysis Guidance for the U.S. DOE Office of Fossil Energy and Carbon Management Version 2.0 - (Skone, Timothy J. et al., 2022)

Table 6: Summary of Best Practices for DACS LCA

| LCA Stage | LCA Sub-Stage | Best Practices |
|---------------------------|-----------------------------|--|
| Goal and scope definition | Goal | <ul style="list-style-type: none"> Evaluation of a single DACS pathway to identify potential environmental impact hot spots and the impact of uncertainty in key operating and design parameters |
| | Functional unit | <ul style="list-style-type: none"> Analyze DACS using this functional unit: Mass of CO₂ captured from the atmosphere and permanently stored Report CO₂ removal via DACS as net mass of CO₂e captured from the atmosphere and permanently stored At the downstream gate of the DAC facility, CO₂ should be compressed to 15.3 MPa (2,200 psig) and contain a minimum of 95% CO₂ by volume (IPCC, 2005; NETL, 2019) |
| | System boundary | <ul style="list-style-type: none"> Evaluate DACS with a cradle-to-grave boundary to fully account for the function of the system For all dispositions of the captured CO₂, which include utilization/conversion or EOR, the system boundary should encompass the downstream fate of the captured CO₂ as well as any associated activities Depict the system boundary graphically using a process flow diagram to depict processes included within the analysis scope |
| | Defining comparison systems | <ul style="list-style-type: none"> Ensure functional equivalence between systems, including the management and provision of co-products for all systems under evaluation Document assumptions regarding the future landscape into which an emerging technology might deploy, including identifying which system dynamics are included Use consistent assumptions and data quality requirements for background data for all systems to ensure equivalent comparability Represent the system boundaries for the different systems visually to communicate consistency when comparing two or more DACS or CDR systems |

| LCA Stage | LCA Sub-Stage | Best Practices |
|-------------------------------|-----------------------------------|---|
| Life cycle inventory analysis | Data Collection - Facility | <ul style="list-style-type: none"> • Separately report and account for any captured fossil or other non-atmospheric CO₂ (e.g., from on-site fossil fuel combustion) from the captured atmospheric CO₂ for consistency with the functional unit • Define LCA scenarios with a direct tie to process and cost engineering model (i.e., TEA) scenarios such that they characterize the underlying facility operating envelope (see Section 5.2) • Coordinate with process and cost engineering modeling (e.g., TEA) team to capture data necessary for LCA • Report physical quantities for process inputs and outputs (e.g., MJ energy, kg materials) in addition to the associated inventory of emissions (e.g., kg emission) • Clearly identify degree of uncertainty and variability, particularly for modeled rather than empirical inputs |
| | Data Collection – Non-Consumables | <ul style="list-style-type: none"> • Utilize a modeling approach that provides the best data that is available to represent these activities corresponding to the stage of development • Update representation of design and underlying LCI data as technology matures and nears deployment • Test sensitivity of the assumed facility lifetime and any non-consumables that require replacement during the facility operating life (see Section 5.2 for additional recommendations) |
| | Data Collection - Consumables | <ul style="list-style-type: none"> • Model specific pathways/technologies for producing the input based on best available information • When multiple potential sources/types are being evaluated as part of the design, develop separate LCA scenarios for each • Report physical quantities for inputs and outputs in addition to the associated inventory of emissions • Review Section 3.4 for recommended data sources for representing the emissions associated with these inputs |

| LCA Stage | LCA Sub-Stage | Best Practices |
|-------------------------------|--------------------------------------|---|
| Life cycle inventory analysis | Co-Product Management | <ul style="list-style-type: none"> Follow the established co-product management hierarchy in ISO 14044 Section 4.3.4 If sub-division is not possible, use system expansion with a multiproduct functional unit Avoidance and removals should always be accounted for separately, not combined with each other Maintain a record of the physical system depicting the impacts with and without management of co-products Test multiple co-product management approaches, including allocation. This can help determine how robust conclusions are across multiple approaches. |
| Life cycle impact assessment | Impact methods | <ul style="list-style-type: none"> Utilize the EPA’s Tool for Reduction and Assessment of Chemicals and Other Environmental Impacts (TRACI) version 2.1 method for LCIA (US EPA, 2021) (additional impact methods and impact categories may also be reported) Utilize the Intergovernmental Panel on Climate Change (IPCC) Sixth Assessment Report (AR6) Global Warming Potential characterization factors for translation of GHG emissions to Global Warming Potential impacts (IPCC, 2021), and adopt future IPCC GWP characterization factors as they are released. |
| Interpretation | Negative emissions accounting | <ul style="list-style-type: none"> For systems with co-products, when system expansion is used to manage multiple outputs, report avoided emissions and atmospheric removals separately in the results (see Scenario 3 in the Table 4 example) When a DAC facility includes capture of CO₂ from on-site fossil fuel combustion or other non-atmospheric CO₂, separately report that amount from the atmospheric CO₂ captured |
| | Sensitivity and uncertainty analysis | <ul style="list-style-type: none"> Use of bounding analysis to inform key decision points Use of standard modeling scenarios in Table 5 Use of sensitivity analysis to understand the dependence of key parameters |

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