



16th International Conference on Greenhouse Gas Control Technologies, GHGT-16
23rd -27th October 2022, Lyon, France

Perspectives on Future CCUS Infrastructure Design

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Abstract

In this paper, we systematically review existing models and identify software tools suitable for the optimal planning and design of large-scale Carbon Capture, Utilisation and Storage (CCUS) infrastructure. We identify key factors, relevant system constraints (and the lack thereof) that need to be considered when optimising CCUS systems. The components of the supply chain considered include CO₂ capture, (re-)conditioning, transport, storage and utilisation, and how spatial, temporal, economic, social, environmental, policy and technical factors have been integrated into models in the literature. Findings showed past works to be saturated with respect to techno-economic factors, but sparse on social, policy, business and other non-technical factors which have been identified to be important for successful large-scale deployment of CCUS infrastructure. Recommendations on future research are then proposed towards a more robust infrastructure design consideration.

Keywords: CCUS industrial clusters, CO₂ transport infrastructure, Optimisation

Abbreviations/Acronyms

CCS	Carbon Capture and Storage
CCU	Carbon Capture and Utilisation
CCUS	Carbon Capture, Utilisation and Storage
CO ₂	Carbon Dioxide
DME	dimethyl ether
DMC	dimethyl carbonate
EOR	Enhanced Oil Recovery
ETS	Emissions Trading Scheme
LCA	Life Cycle Assessment
MI(N)LP	Mixed Integer (Non-)Linear Programming
PSA	Pressure Swing Adsorption
RO	Real Options
VSA	Vacuum Swing Adsorption

1. Introduction

One of the key challenges of implementing Carbon Capture, Utilisation and Storage (CCUS) involves the optimal planning and design of large-scale infrastructure. The type, size, and capacity of CCUS infrastructure should be

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designed to avoid underestimating the mitigated and transported amounts of Carbon Dioxide (CO₂) that could lead to penalties for emitters, or overestimating the capacity that would translate to financial losses due to unjustified capital costs. The demand for and cost of CCUS infrastructure, particularly in industrial clusters, depend on many factors: the number and size of CO₂ emitters, availability of potential CO₂ transport and storage/utilisation options, social and regulatory factors amongst others. As such, finding the optimal solution with appropriate models for CCUS infrastructure requires a whole-system approach that involves cost-benefit analysis, while also accounting for non-economic decision criteria - safety, regulatory, societal factors, etc. (D'Amore et al., 2021, Bjerketvedt et al., 2020, Jakobsen et al., 2014, Lee et al., 2017, Middleton et al., 2012).

Previous works on the optimal design and/or efficient dynamic operation of infrastructures for CCUS projects of various scales vary by type of adopted objective functions, assumed specific scenarios and system constraints (see Fimbres Weihs and Wiley (2012), Knoope (2015), Bui et al. (2018), Middleton and Bielicki (2009), Morbee et al. (2011), Zhang et al. (2018)). As a result, some advanced models for large-scale CO₂ infrastructure design optimisation may not be comprehensive enough, e.g., due to simplified assumptions about considered transport modes, CO₂ stream composition, purity specifications for transport or limitations of CO₂ transport to pipelines only, and the lack of societal and/or regulatory constraints.

Thus, the main objective of this paper is to systematically review the key factors and relevant system constraints that need to be considered when optimising CCUS systems of various scales. We review the key components of the CCUS supply chain examining CO₂ capture, (re-)conditioning, transport, storage, and utilisation options under spatial, temporal, economic and technical conditions. In addition, non-economic/non-technical factors that affect the decision making process are reviewed including the availability of transport routes, social factors, as well as other regional policies in play. Based on the reviewed literature, key model elements are identified towards an integrated systems approach to enable a robust design of CCUS infrastructure, particularly for large-scale projects.

This work is structured as follows: in Section 2, a general overview is given for the CCUS infrastructure, its components and the design considerations in literature. The key design objectives considered are explained in Section 3 alongside model constraints, with some existing software tools explained in Section 4. Concluding remarks and recommendations are then given in Section 5.

2. CCUS Infrastructure

2.1. CO₂ supply chain

Figure 1 shows a CO₂ supply chain detailing the key components that are considered in CCUS infrastructure design - carbon emissions source, its capture facility, compression (or generally, conditioning/reconditioning for transport), transportation to its utilisation and/or storage site, and its actual storage/utilisation.

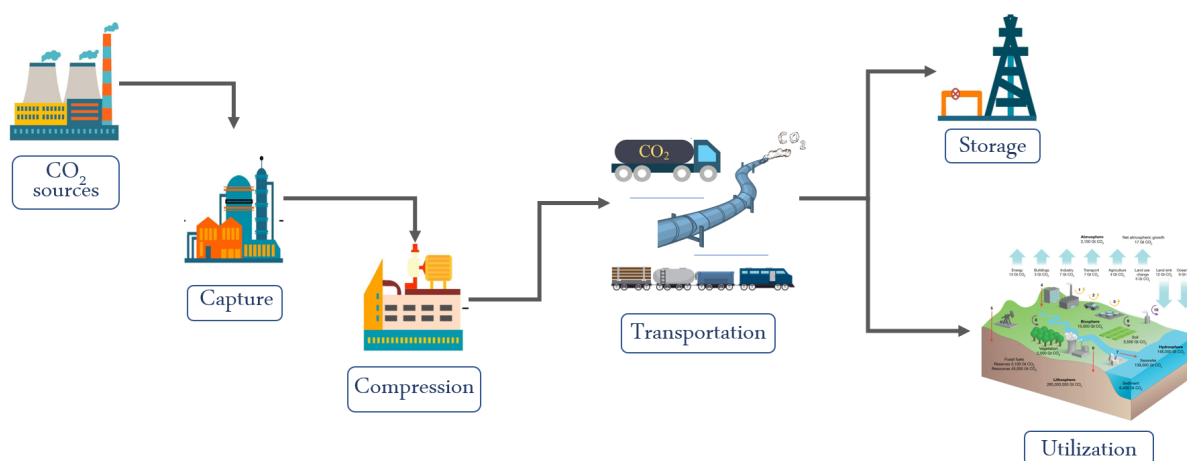


Figure 1: CO₂ supply chain scheme

The capture step refers to all pre-, post- and oxy-fuel combustion process routes, and/or all chemical and physico-chemical processes adopted to produce a CO₂ rich stream from flue gases or other emitting sources (Kuckshinrichs and Hake, 2015). The compression (or conditioning) step refers to all processes, such as dehydration, purification, desulphurisation, ash/particle removal, etc., that alter the physical (and/or chemical) characteristics of the captured stream, making it suitable for transport/storage/utilisation. This step generally depends on the mode(s) of transport adopted: pipeline, ship, motor/rail. The final step involves the storage and/or utilisation of CO₂ for high value chemicals/energy production. Storage sites include geological reservoirs, depleted oil & gas fields, saline aquifers suitable for CO₂ sequestration.

Pipeline transport is the most popular mode of transporting CO₂ considered in literature and in practice. Pipelines present the advantage of being able to cost-effectively transport CO₂ from multiple sources to multiple storage locations over a range of conditions, distances, and terrains, especially for large volumes (Ağralı et al., 2018, Grant et al., 2018, Mechleri et al., 2017, Kalyanarengan Ravi et al., 2017, Zhang et al., 2020, D'Amore et al., 2018, Knoope et al., 2013). Optimising CO₂ transportation cost through pipeline plays an important role for large-scale deployment of CCUS systems (Zhang et al., 2018). Here, a number of factors need to be considered: pipeline size, pipeline material, where to construct the pipeline, pipeline network route, CO₂ pipeline specification, target transportation conditions, location, and size of compression/purification stations.

Pipeline size and material are selected from industry-standard pre-defined nominal pipe options/Nominal Diameter (ND) (BS EN 10208-2, 1997, ISO, 1995) based on the required CO₂ stream conditions in relation to proven correlations available in literature (Mechleri et al., 2017). Operational and capital costs, as well as technical properties of the selected pipe option - pipeline outside/inside diameter, material of construction, yield stress, wall roughness, etc., can further be obtained based on known correlations and existing data (IEA-GHG, 2005).

The composition of the captured CO₂ stream also plays an important role for pipeline transport. Impurities in CO₂ streams have been shown to affect compression power, fluid phase conditions, storage considerations, etc. (Porter et al., 2016; 2021, Wilkes et al., 2021). In addition, countries/regions as well as pipeline operators are known to have fixed CO₂ stream specifications that users must abide by. Wilkes et al. (2021) provided a list of some existing pipeline projects globally and their specifications. It is therefore important that capture, compression and conditioning be tailored towards existing regional specifications during infrastructure design. It is worth noting that due to variations volume and purity of CO₂ streams by reason of the type of emitter, individual financial risks for the investing parties also vary. Thus, larger emitters with less pure streams are expected to invest more. This additional investment may either be in the deployment of capture/purification facilities, or for specialist transport solutions, e.g. corrosion protection and higher compression costs.

Although pipelines are the most popular means of transport owing to the aforementioned advantages, ships are now seen as key for early deployment of CCS due to their low-cost, low investment and flexibility to reach offshore storage sites (D'Amore et al., 2018). D'Amore et al. (2018) considered shipping as a transport option. Transport costs were simply scaled based on the distance and quantity of CO₂ being transported. However, much more detail is required for adequate infrastructure design using ships as a mode of transport.

One of such design considerations is the conditioning and re-conditioning of CO₂ before and after shipping respectively. Gaseous/Dense phase CO₂ (which is the state received from capture processes and most pipeline transport) needs to be pressurised to about 30 bar, cooled and expanded to ensure liquid CO₂ is obtained for ship transport. This is a more expensive process than pipeline conditioning (Bjerketvedt et al., 2020). Furthermore the ship size, number of ships, sailing speeds, and the fuelling costs also need to be taken into consideration. Geske et al. (2015a) proposed an optimisation model for ship sizing in a fleet scheduling context - size of vessel, size of fleet, and the schedule of operation given transport volumes, distance, and the times for travelling and (un-)loading. As shipping is a non-continuous transport medium, there is also the need for buffer storage at shipping nodes, the size of which can depend on uncertainties in demand, weather factors, available ships and their performance. Bjerketvedt et al. (2020) investigated a number of these uncertainties and other operational fluctuations on the design and expected cost of ship-based CO₂ transport. Karjunen et al. (2017) also showed that the scale and operational mode of CO₂ emission sources determine the size of the intermediate storage required for Carbon Capture and Utilisation (CCU) projects.

Studies have further shown that it costs more for smaller emitters (in terms of conditioning power requirements) to adopt a mode of transport via pipelines (Wilkes et al., 2021), and based on regional policies and end-utilisation locations, pipeline/ship transport is infeasible and/or uneconomical - owing to the unavailability of waterways, short distances between nodes, higher subsidies for alternative transport modes, etc. - hence the need for motor/rail options.

2.2. CO₂ transport networks

Apart from the actual size of the pipeline being used and its cost, infrastructure design also encompasses the efficient routing of the pipeline from source to sink (Figure 2). This may be a point-to-point (PTP) pipeline or trunk line depending on the number of source/sink nodes (Peletiri et al., 2018). PTP pipelines connect a single source to a single sink node, while trunk lines connect multiple sources to a single or multiple sink nodes. The cost effectiveness of both pipeline route design depend on the distance and angle between nodes (Peletiri et al., 2018). Middleton and Bielicki (2009) further proposed a routing algorithm (deployed in the SimCCS tool) that first generates a 1-km raster grid cost surface with estimated pipeline construction costs for each grid cell. Geographical features of each grid cell are factored into the construction costs using a weighted factor. The total construction cost between two network nodes can then be calculated using a modified Dijkstra's (1959) shortest path algorithm.

Geske et al. (2015b) applied a piecewise linear cost model to optimally design a multi-modal (pipeline and shipping) CO₂ transport network and applied it to case studies across the West Mediterranean region. MILP models were used as a basis for the design optimisation of multi-modal European CO₂ transport networks in the studies by D'Amore et al. (2021) and Becattini et al. (2022).

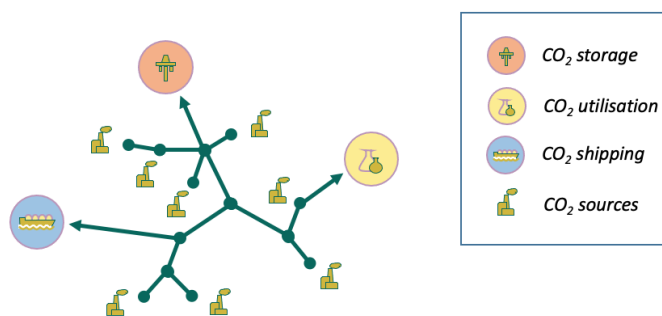


Figure 2: Multi-source multi-sink transport network

2.3. System operation and dynamics

Another consideration worth exploring in current CCUS infrastructure project are temporal factors. Traditionally, pipeline networks of a fixed optimal size are designed to last the entire project lifetime. However, owing to the dynamic nature of CCUS projects, changing regional policies and long project life times, it is also important to design projects that will grow over a long time period, or shrink. This is due to the ongoing transition to renewable energy sources and the decarbonisation targets across developing nations. Thus, the amount of CO₂ emitted from industrial sources may significantly change in the long run. Some industries will cut their CO₂ emissions as part of decarbonisation efforts, e.g. by electrification and/or transition to hydrogen, while the hydrogen producers will likely increase their capacities resulting in larger amounts of CO₂ produced as a by-product (blue-hydrogen) (Dawood et al., 2020a). The development of hydrogen/CO₂ infrastructure may also overlap in time and/or location (Leguijt, 2020). These changes in carbon demand/emission and/or CCUS policies over time may be captured in the infrastructure design by optimising over discrete intervals over the entire lifespan as done by Kim et al. (2018) and Mechleri et al. (2017). Each discrete time interval should have unique conditions of CO₂ demand, emission limits, a decision to invest in carbon capture now, or in the future, as well as other dynamic conditions over the project lifetime.

Fimbres Weihs and Wiley (2012) applied a genetic algorithm to optimise a CO₂ network topology considering non-linear cost models describing the effect of economies of scale, as part of a general modelling framework for optimisation of the network upon transient design constraints. Jensen et al. (2013) proposed using a phased approach to design a CO₂ transport network respecting the changes in the sinks and sources capacities with time. The SimCCS tool by Middleton et al. (2020b) also enables decision support for CCS infrastructure projects via the optimisation of the costs, routing, sources, sinks, and transport pipelines capacities, along with other criteria including policies and trade-off between capture, transport, and storage, over several periods of the CCS infrastructure deployment. Becattini et al. (2022) optimised the CCUS infrastructure rollout for different emission reduction pathways considering economic and environmental factors, showing that ships and barges can be competitive to pipeline transportation, while using road and rail transport can be cost-effective for smaller CO₂ transport capacities and shorter duration projects. Karjunen et al. (2017) also developed a node-base tool for assessment of the cost, capacity and infrastructure requirements for CCU projects considering the effects of scale and temporal variations in CO₂ emission by industrial sources and consumption by CCU plants.

3. Design Objectives

Table 1 summarises key literature on CCUS infrastructure design, their model type, objective and constraints considered. Each of these works deal with a (sub-)set of the CCUS infrastructure components discussed above under differing objectives and level of detail for constraints. Some of these objectives and constraints are discussed below.

3.1. Cost

Total cost has been considered as the primary objective in CCUS infrastructure design. However, the composition of these costs vary in each research endeavour - capture, compression, dehydration, transportation, and storage injection costs, as well as utilisation revenue streams (Middleton and Bielicki, 2009, Zhang et al., 2018) - all depending on the mode of transportation being considered. Each of these cost components comprise both the capital/investment, as well as the operating and maintenance aspects reported over a fixed period, usually annually. The total investment cost can however be significantly offset by re-using existing infrastructure for CO₂ transport and storage (Brownsort et al., 2016).

CO₂ capture costs have been shown to contribute around 70-80% of the overall CCUS infrastructure (Zhang et al., 2018) with capture plants mainly located at the source of CO₂ (Leonzio et al., 2019, Zhang et al., 2020). CO₂ capture cost depends on flue gas characteristics such as its composition, flow rate, emission source type, and the CO₂ capture

technology-material combination. Hasan et al. (2014) presented a rigorous simulation-based cost model for investment and operation of capture (of at least 90%) and compression (to 150 bar) processes for a range of technologies. These models have been adopted by other authors (Leonzio et al., 2019). Zhang et al. (2018; 2020) also considered the selection of the optimal capture technology out of four alternative classes in a mixed integer linear programming (MILP) model - absorption (using MEA and Piperazine), membranes (POE-1, POE-2 and poly vinylamine), PSA and VSA (using 4 zeolites). A linearised model was presented which calculated the capture and compression (to 15MPa) investment and operating cost for each technology. The model allowed for the free selection of the CO₂ capture rate as opposed to a constant assumed value. Middleton and Bielicki (2009) used CO₂ capture cost derived from literature in (IPCC, 2005). These costs assumed that as much as 90% of the total amount of CO₂ produced from a source node can be captured. Kalyanarengan Ravi et al. (2017) explored the possibility of a central CO₂ capture unit amongst multiple emitters as studies show compression and capture costs to be the largest cost contributors which decrease with increased flue gas flow rate. However, results showed that cost savings were not enough to justify its adoption.

Dehydration is a step which is mostly carried out as part of the conditioning of the CO₂ stream. It avoids the formation of free water in the pipeline (Serpa et al., 2011) which leads to corrosion and hydrate formation, amongst other problems (Kolster et al., 2017). Wilkes et al. (2021) cited an optimal moisture content of between 250-350 ppm for pipeline transport. Most literature quote dehydration costs for flue gas using triethylene glycol (TEG) absorption process to be \$10.22/tCO₂ according to Hasan et al. (2014) for flue gas from a power plant. Apart from water, other impurities such as non-condensable gases may also be required to meet acceptable levels in the CO₂ stream. These impurities may increase the likelihood of propagating fractures in pipelines, reduce storage capacities, etc. (Kolster et al., 2017, Mahgerefteh et al., 2012). Porter et al. (2021) outlines some of these purification steps suitable for CO₂ streams to meet pipeline specifications.

With respect to compression and for high volume, high pressure CO₂ applications, multi-stage centrifugal compressors constructed largely of stainless steel are the norm (IEAGHG, 2014). Wilkes et al. (2021) developed process models to investigate the effects of stream impurities and pipeline operating conditions on compression train power requirements, specifically for CO₂ conditioning for pipeline transportation. This may further be paired with known correlations to estimate the cost of compression for known CO₂ stream input/output conditions, as opposed to using reported cost curves.

Actual CO₂ transportation costs depend on the mode of transport being adopted, geographical locations of the emitters, and not just on the amount of CO₂ produced/captured. Zhang et al. (2018) used the cost model proposed by Serpa et al. (2011) which is a piecewise linear approximation of available CO₂ cost estimates for construction, operation and maintenance of pipelines combined with publicly available estimates from large natural gas pipeline projects. This model expressed these costs as a function of the amount of CO₂ transported, the terrain factor and the length of pipe segments. A similar modelling approach was proposed by Knoope et al. (2013) and adopted by Leonzio et al. (2019). The pipeline operating cost is typically taken as a fraction of the capital/investment cost in the range 1.5 - 4% (Serpa et al., 2011). It has been noted, however, that these cost models based on natural gas pipeline estimates greatly underestimate the actual costs for CO₂ pipelines owing to the difference in physicochemical properties of both fluids (Kim et al., 2018).

CO₂ storage costs may be grouped into injection investment and operating costs (Zhang et al., 2018). Storage injection costs are reasonably highly dependent on the reservoir type - offshore/onshore, depleted fields or deep saline formations, and characteristics - porosity, permeability and depth (Zhang et al., 2018). Zhang et al. (2018), Leonzio et al. (2019) adopted a model which factored in the depth of the well, the number of wells which need to be built, as opposed to only injection rates used by some other authors. The operating costs for storage was taken as 4% of the investment cost.

In addition to cost terms, some authors have considered utilisation revenues within their minimum total cost objectives. A popular revenue source associated with CO₂ utilisation in literature is enhanced oil recovery (EOR) (Zhang et al., 2018, Elahi et al., 2017, Ağralı et al., 2018, Nie et al., 2017, Wang et al., 2020). CO₂ may also be utilised in various chemicals production as well e.g. syngas, methanol (Leonzio et al., 2019). Leonzio et al. (2019) considered CO₂ utilisation options for methanol production via an indirect route - methane dry reforming. Zhang et al. (2020) further explored 15 conversion routes for CO₂ utilisation in an MILP model obtaining additional products such as synthetic gasoline, diesel, acetic acid, dimethyl ether (DME), dimethyl carbonate (DMC), and several by-products. However, it should be noted that for most chemicals production routes the source, possible transportation, associated costs and emissions of accompanying reacting species and utilities need to be factored into the design, as was done by Leonzio et al. (2019) and Zhang et al. (2020).

Another cost term worth considering in CCUS infrastructure design is that associated with the emissions trading system (ETS). ETS allow for the purchase/sale of carbon credits between emitters which are evaluated based on prevailing regulatory constraints such as the emission limits/cap and/or size of the emitters. In order to meet emission targets, an emitter may invest in CCUS technologies/options and/or purchase carbon credits. Ağralı et al. (2018) carried out such analysis for a scenario in Turkey determining the carbon price value beyond which carbon capture becomes preferable to trading in the ETS.

3.2. Policy/regulatory factors

Regulatory and political factors directly and indirectly affect conditions such as the prevailing and projected policies on carbon prices (Ağrali et al., 2018), affinity for a CO₂ capture technology and/or transport mode adoption amongst others. These have a knock-on effect on CCUS infrastructure design in order to avoid scenarios of over-specification in light of future policies, or the adoption of unfavourable technologies.

One technique adopted in the literature to account for these factors is via a stochastic multi-stage multi-scenario mathematical approach. Also used to explore future uncertainties, this technique investigates the evolution of uncertainties through a set of scenarios while still keeping the decision criteria constant. Elahi et al. (2017) adopted this technique to investigate the effect of policies (as obtained from scenarios from the Zephyr model) on carbon price trajectories in the United Kingdom, showing the conditions where CCS is worth adopting under carbon mitigation targets. Another technique is via a real options (RO) decision making framework. The RO methodology is a tool for investment decision making which offers flexibility in the timing of investment decisions in relation to uncertain parameters. Nie et al. (2017) used this methodology to analyse uncertain parameters in CCUS infrastructure design such as the CO₂ market price, geological storage site uncertainty as well as other policy and market uncertainties. Such analysis provides a robust set of results for policy formulation and/or storage and transport investments decisions as a range of risks can be incorporated. Kim et al. (2018) also analysed the effect of policy changes by considering a discrete set of scenarios with fixed time intervals over the entire project time to understand the implications on the CCUS infrastructure design.

3.3. Environmental factors

Although the primary and inherent goal of CCUS projects is the reduction of harmful carbon emissions through capture, utilisation and/or storage. It is still quite important to specifically include environmental constraints within a modelling framework. One reason is that the key objective for most, if not all, emitters will be to obtain a minimum cost design. Further hard constraints need to be included to meet environmental requirements. These environmental factors have mostly been considered as additional constraints (to total cost objective models) in the literature, often to enforce a minimum CO₂ reduction target by emitters (Leonzio et al., 2019, Wang et al., 2020). As emission quotas, carbon prices and other policies change with time, a multi-period infrastructure model will present a robust design for CCUS projects.

Lee et al. (2017) also used the Eco-indicator 99 method of Life Cycle Assessment (LCA) within an MILP model to ascertain the environmental impacts of CCUS projects. The Eco99 score was calculated as the environmental damage scaled by a weighing factor determined subjectively by the decision maker. The environmental damage was evaluated as the normalised sum of the installation and operation impact of CO₂ captured, transported and sequestered.

3.4. Social/Societal and safety factors

It is well known that CO₂ presents major environmental concerns, hence the need for its abatement. It also generates adverse effects on health dependent on its concentration and the duration of exposure. This may result in irreversible damage and possibly death (D'Amore et al., 2018), and can occur at any point along the CO₂ supply chain (Figure 1), becoming an important consideration in infrastructure design. D'Amore et al. (2018) incorporated societal risk assessment within a minimum-cost spatially-explicit modelling framework. It was estimated as the risk of leakage (and its associated set of hazardous incidents) during transport and its societal consequences on the local population, ensuring that risk levels are kept below pre-set thresholds. Risk mitigation options were also included to reduce the probability of consequences on a local population.

3.5. Financing and business factors

In addition to all the previously mentioned factors, the nature of existing (or the development of) business models is also a key enabler for a successful deployment of CCUS infrastructure especially for industrial clusters. In Europe, key business model options for transmission and storage infrastructure include a regulated asset base model, a public ownership model or a public private partnership model (Moe et al., 2020). The choice of business model affects infrastructure ownership, costs/revenues allocation, etc., and is a necessary consideration in the design and subsequent deployment of CCUS infrastructure as it affects who along the CCUS value chain bears what costs, the speed of infrastructure rollout, and market uncertainties. Readers may refer to Moe et al. (2020) for more detail on these models and the current challenges regarding these considerations.

4. Existing Tools for CCUS infrastructure design

This section summarises existing software tools for CCUS infrastructure design which incorporate a number of the previously mentioned considerations without the need for expert modelling know-how by the user.

Table 1: Summary of key literature considerations on CCUS infrastructure design

Source	Model type	Model objective	CO ₂ Capture	Transport Mode	Storage	MS-MS [1]	Multi-period	Environmental	Social	Political/Regulatory	Utilisation
Middleton & Bielicki (2009)	SimCCS (MILP)	Total cost		Pipeline	Geological reservoirs	✓	✓	-	-	-	-
Zhang et al. (2018)	MILP	Total cost	✓ ^[2]	Pipeline		✓	✗	-	Terrain factor	-	EOR
d'Amore et al. (2018)	MILP	Total cost ^[3]	✓	Pipeline; Ships	Geological reservoirs	✓	✗	-	Risk of leakage	-	-
Elahi et al. (2017)	MILP	Expected total costs	✓	Pipeline	Depleted O&G fields, Saline aquifers	✓	✗	-	-	✗CO ₂	EOR
Nie et al. (2017)	MILP+RO	Total cost	✗	Pipeline	Depleted O&G fields, Saline aquifers	✓	✓	-	-	✗CO ₂ , Fiscal Support	EOR
Agrali et al. (2018)	MILP	Total cost	✓	Pipeline		✓	✗	-	-	ETS	EOR
Kim et al. (2018)	MINLP	Total cost	✓	Pipeline	Geological reservoirs	MS-1S	✓	-	-	Set of policy scenarios	-
Leonzio et al. (2019)	MILP	Total cost	✓ ^[2]	Pipeline	Geological reservoirs	MS-1S	✗	CO ₂ reduction target	-	-	Methanol
Grant et al. (2018)	FE/NETL CO ₂ models	Total cost ^[4]	✗	Pipeline	Geological reservoirs	MS-1S	✗	-	-	-	-
Wang et al. (2020)	MILP ^[5]	Total cost	✓	Pipeline	Saline aquifers	4S-1S	✗	CO ₂ reduction target	-	-	EOR
Zhang et al. (2020)	MILP ^[6]	Total cost	✓ ^[2]	Pipeline	Saline aquifers, Coalbeds	✓	✗	CO ₂ reduction target	-	-	15 conversion pathways
Kalyanarangan Ravi et al. (2017)	MILP	Total cost	✓ ^[2]	Pipeline	Depleted O&G fields	MS-1S	✗	-	-	-	-
Bjerketvedt et al. (2020)	MILP	Expected total costs	✗	Ships		✗	✗	-	-	-	-
Lee et al. (2017)	MILP ^[7]	Expected total cost & environmental impact	✓	Pipeline	Geological reservoirs, Saline aquifers	✓	✗	CO ₂ reduction target, LCA (Eco99 score)	-	-	-

^[1] – Multi-source, multi-sink; ^[2] – Multiple capture technologies selected; ^[3] – subject to low societal risks; ^[4] – discrete realizations of hypothetical scenarios; ^[5] – source-sink matching model for planning; ^[6] – superstructure optimization model for discrete pathway sets; ^[7] – multi-objective optimization model

EOR – Enhanced Oil Recovery; ETS – Emissions Trading Scheme; LCA – Life Cycle Assessment; MINLP – Mixed Integer (non-)linear programming; RO – Real Options

4.1. SimCC(U)S

The simCCS model formulation, like any of the MILP problems previously discussed, consists of an objective function (minimise total costs) and a set of constraints that have to be satisfied. For SimCCS, the objective function minimises the sum of fixed and variable costs. Fixed costs for sources, pipelines, and reservoirs approximate the costs to install capture technology; purchase land and construct pipelines; and select, drill, and equip injection sites. Variable costs represent variable CO₂ capture costs (i.e., per tonne of CO₂), maintenance/ pumping through the pipeline network, and the operating costs of the injection process.

CO₂ source capture costs are derived from the literature cited in IPCC (2005). CO₂ pressurisation is considered and assumed to occur at the source point. Pipeline construction costs are estimated from 15 years of pipeline construction in the US (1990–2005) as published in the Oil & Gas Journal. The regression uses a Cobb–Douglas function to estimate the non-linear relationship of construction cost on pipeline diameter and length. For the purpose of SimCCS, pipeline construction costs were normalised as a constant amount per unit length, for a 100km pipeline, for each pipeline diameter. This infrastructure design tool has been tested on a number of case studies: for 37 largest CO₂ sources and 14 largest CO₂ capacity oil fields in California (Middleton and Bielicki, 2009) and by other authors in literature.

SimCCS was extended to SimCCUS (Ellett et al., 2017) to account for multiple CO₂ utilisation and storage targets, as well as allowing decision makers to assess the feasibility of business plans. SimCCUS incorporates spatio-temporal considerations in addition to price/tax of CO₂ emissions.

4.2. InfraCCS

JRC's InfraCCS tool enables the optimal network design of pipeline-based (and a limited set of ship-based) inter-country CO₂ transmission for a given set of sources and sinks (Dawood et al., 2020b). This tool is based on a minimum net-present value MILP model which adopts a clustering algorithm for sets of CO₂ sources and sinks (taken from public reports of CO₂ storage), and a routing step with particular considerations of pipeline transport onshore, offshore or over mountainous regions in the European Economic Area (EEA).

4.3. CARSON

The CARbon SOurce Nodal model (CARSON) is a MATLAB-based material balance tool useful for deriving the costs of CO₂ transportation, capture and storage (Karjunen et al., 2017). It adopts a node-based formulation with spatial and temporal detail to calculate transportation costs for each available node pair and transport method - pipe, truck or rail. Capture and storage costs are calculated using data from reference plants and existing literature.

4.4. ArcGIS/MARKAL-based toolbox

van den Broek et al. (2010) proposed the ArcGIS/MARKAL toolbox for spatio-temporal CCS infrastructure planning and design. It integrates ArcGIS - a geographical information system having spatial and routing functions, with the techno-economic MARKet ALlocation (MARKAL) linear optimisation model for energy system analysis over multiple time periods. It assesses which carbon source, sink and transport option should be used over time and to what degree.

4.5. SCO₂PT

Sequestration of CO₂ Tool (SCO₂T) is a software tool for rapid characterisation, sensitivity and uncertainty analysis of saline storage reservoirs (Middleton et al., 2020a). It analyses the impact of reservoir characteristics such as depth, thickness, permeability, porosity, and temperature on sequestration engineering and costs, and is useful in determining the suitability of sites for CO₂ storage needs.

5. Concluding remarks

This paper sought to systematically review relevant system constraints required for large-scale planning and design of CCUS infrastructure. In light of this, past works which proposed optimisation models for CCUS planning, design, and operation were discussed, considering different aspects of the CO₂ supply chain - capture, conditioning, transportation, storage and/or utilisation. These works also adopted varying model objectives, and looked into economic, environmental, technical, social, safety, societal and/or policy factors via integrated models towards optimal decision making.

A key learning from the review was that a great deal of research has focused on techno-economic factors, with multiple sources producing cost models (simulation and optimisation) for transport, capture, conditioning, storage, etc. However, research in optimal decision making for other important non-technical factors are lacking, or basic, such as the effect of societal and policy aspects, business models, on the uptake and costs of CCUS technologies. Most research endeavours were also focused solely on CO₂ transportation via pipelines, and rightly so. CO₂ pipeline transportation is the most popular transport mode for obvious advantages of cost and a range of conditions. However,

other transport modes such as shipping (rail and motor) are now seen as key for the early deployment of CCS. Optimal decision making in the utilisation (on-site or remote) of CO₂ over a wider range of options is also worth considering as it may present new cost-optimal solutions compared to transport and storage in remote sites. How to schedule CCUS infrastructure deployment and the hydrogen transition as two decarbonisation vectors that could work in tandem is also beneficial. Reusing the pipeline infrastructure for transportation of various gases at different times, e.g. reusing the hydrocarbon pipelines for transport of CO₂ and later on hydrogen presents economic advantages that may hasten their deployment.

Acknowledgement

This work has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement no. 884418. The work reflects only the authors' views and the European Union is not liable for any use that may be made of the information contained therein.

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