Contents lists available at ScienceDirect

Sustainable Production and Consumption

journal homepage: www.elsevier.com/locate/spc

Review article

A review of optimization and decision-making models for the planning of CO_2 capture, utilization and storage (CCUS) systems

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A B S T R A C T

Carbon capture, utilization and storage (CCUS) is considered as one of the key strategies for mitigating climate change. This technology involves CO_2 capture from stationary sources, followed by distribution of CO_2 to different intermediate utilization and/or final storage options. CO_2 *capture and utilization* (CCU) by itself offers resource conservation benefits by displacing the need for extracted CO_2 from natural sources. On the other hand, CO_2 *capture and storage* (CCS) provides CO_2 emissions reduction by sequestration of captured CO_2 for long-term storage. Combining CCS and CCU can potentially result in valuable symbiosis, but remains debatable due to gaps between the roles of these technologies in energy engineering. Such gaps have resulted in slower commercial deployment of CO_2 "-capture. Some important issues resulting from these technologies have been addressed in previous studies through *process systems engineering* (PSE) methodologies, which are able to provide rigorous decision support during CCUS planning. This review paper provides an in-depth discussion of the state-of-the-art of these tools, and also discusses recent developments on integrating CCUS components in large-scale planning. While recent literature in this area reveals the availability of tools for planning and policy-making, further research opportunities are identified through the bibliometric trends that show how CCUS research can develop further.

Keywords: Carbon management; CO_2 capture; Utilization and storage (CCUS); Optimization; Decision support; Process systems engineering (PSE)

Contents

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Received 1 April 2017; Received in revised form 16 September 2017; Accepted 15 October 2017; Published online 3 November 2017.

https://doi.org/10.1016/j.spc.2017.10.001
2352-5509/

1. Introduction

Energy-related CO_2 emissions have become a major concern due to the adverse climatic effects of greenhouse gases (GHGs). As of 2016, worldwide CO_2 emissions amounted to approximately 32.3 Gt, of which a major portion comes from the combustion of fossil fuels (EIA, 2016). The emission level will continue to increase in the coming decades in the business-as-usual (BAU) scenario of economic and population growth trends (IEA, 2016). The continued dependence on fossil fuel combustion for many energy applications leads to the need for the development of different low-carbon technologies for emissions reduction. Thus, the 21st Conference of Parties (COP21), also known as the Paris Agreement, sets a reduction target of 60% for CO_2 emissions (UNFCCC, 2016). Cumulative contributions of low-carbon technologies can result in a 39% reduction in annual CO_2 emissions by 2035 (IEA, 2013). Achieving such reductions will be possible only through decoupling of economic growth and CO_2 emissions (Obama, 2017). Key strategies for reducing CO_2 emissions include measures such as (1) improving efficiency on both the demand side (efficient energy use) and the supply side (efficient electricity generation); (2) using low-carbon energy sources (e.g., nuclear and renewable energy) as an alternative to fossil fuel sources; and (3) capturing CO_2 from fossil fuel combustion. In the case of the electricity generation sector, current economic and social issues still hinder the widespread deployment of nuclear power and renewable energy. Thus, conventional fossil fuel-based power generation systems will still play a significant role in the foreseeable future (Williams et al., 2012). This trend makes it imperative to use technologies that will allow utilization of fossil fuels in a carbon-constrained world.

One of the potentially scalable technologies for managing GHG emissions is *CO_2 capture and storage* (CCS) (Pires et al., 2011). CCS can contribute about 19% of the required emissions reductions by 2050 (IEA, 2016). CCS involves capturing CO_2 from industrial flue gases, and then transporting it for injection into secure geological reservoirs (Maroto-Valer, 2010). Capture technologies include post-combustion capture (Gibbins and Chalmers, 2008), pre-combustion capture (Røkke and Langørgen, 2009), oxy-fuel combustion (Wall et al., 2009), and chemical looping combustion (Shahrestani and Rahimi, 2014). Storage options include geological formations such as depleted oil or gas reservoirs, inaccessible coal deposits, and saline aquifers (Davison et al., 2001). Unlike other low-carbon options, CCS can be retrofitted to existing fossil fuel-fired power plants, thus reducing CO_2 emissions from flue gas by as much as 90% (Gibbins and Chalmers, 2008). CCS can hence play an important role in carbon management to aid the transition to a global low-carbon energy economy (Jägemann et al., 2013). However, despite its potential for mitigating the effects of climate change, CCS is expected to incur additional costs for capture, transportation and injection of CO_2 (de Coninck and Benson, 2014). Use of CCS will increase the cost of electricity due to parasitic power losses (for CO_2 capture and compression) as well as the requisite capital investments. Because of these economic drawbacks, out of 275 projects (most of which are in the power sector), 26 (9%) have been cancelled or delayed (Global CCS Institute, 2016).

Due to the high cost of CCS, economic incentives and carbon taxes will be needed to encourage the deployment of CCS especially in the power generation sector (Grimaud and Rouge, 2014). Alternatively, instead of treating captured CO_2 as having negative economic value, it can be used for various positive-value applications. This strategy is known as *CO_2 capture and utilization* (CCU) (Aresta and Dibenedetto, 2010; Li et al., 2016a, b). Such uses can allow reduction of the costs incurred in installing CCS infrastructure. CCU can then be coupled with CCS to reduce the cost for unified *CO_2 capture, transport and storage* (CCUS) systems. This integrated carbon management strategy enables fossil fuel-based power generation, CO_2 emissions reduction and revenue generation simultaneously. Major options for CO_2 utilization can be classified into two main categories, i.e. the use of CO_2 as chemical feedstock, and use as injection fluid. For the former, the captured CO_2 can be used for fuel synthesis (e.g. methanol production) or for material synthesis (e.g. polymer production) (Aresta and Dibenedetto, 2010). From a carbon balance standpoint, the use of CO_2 as a feedstock does not result in permanent sequestration; thus, CO_2 utilization in this manner should be treated as a resource conservation strategy, where the captured CO_2 displaces fresh CO_2 that would otherwise have to be extracted from natural sources (Bruhn et al., 2016). In such cases, there is minimal direct benefit from the use of CO_2 itself, which, only results in a neutral carbon balance (von der Assen et al., 2014). CO_2 can be utilized for enhanced material recover (EMR) by injection into depleted oil reservoirs, inaccessible coal beds and shale formations for enhanced oil recovery (EOR), enhanced coal bed methane (ECBM) recovery and enhanced shale gas recovery (ESGR), respectively (Li et al., 2016a, b). These options are capable of partially sequestering CO_2 permanently into geological formations when the useful products are recovered. However, CO_2 streams used for certain utilization options (e.g. food and beverage applications) require certain impurity limits or other quality specifications (Mohd Nawi et al., 2016a, b). Thus, natural CO_2 sources and CO_2 from non-combustion industrial processes are often used to meet the requirements (Middleton et al., 2015). Given the diverse characteristics of the component technologies, the

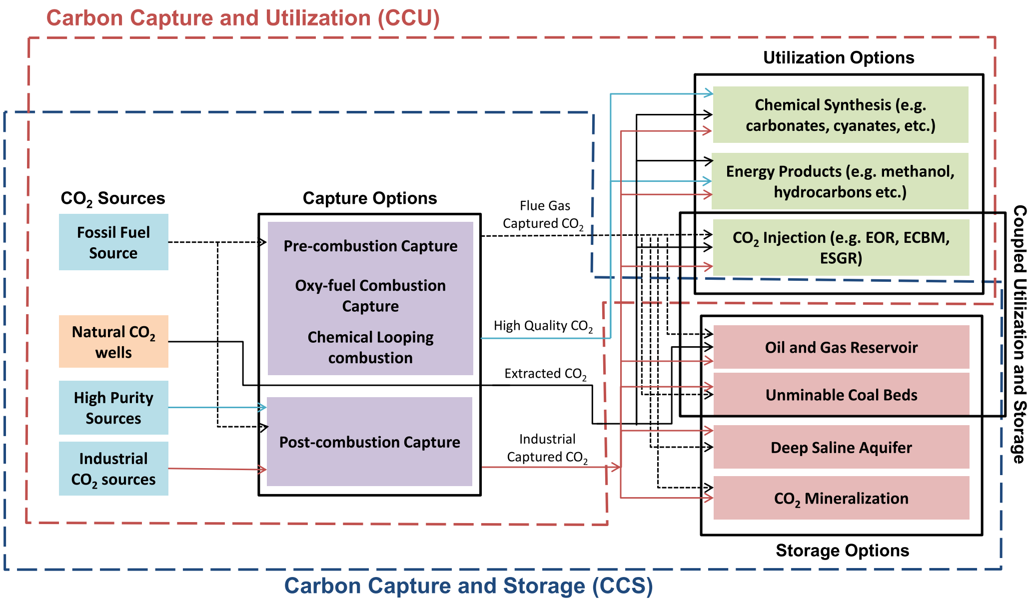

Fig. 1 – CCUS Superstructure with different options for each component.

systematic planning of large-scale CCUS systems becomes a complex task that requires consideration of economic, spatial, temporal, and other technology-specific issues.

There are a number of review papers that provide a synopsis of specific aspects of CCUS literature. For example, these papers focus on the impacts of CCU options (Cuéllar-Franca and Azapagic, 2015), the integration of CCU into the CCS context (Bruhn et al., 2016) and techno-economic analysis and planning of CCS alone (Huang et al., 2013; Foo and Tan, 2016). A review on CO_2 utilization options for climate change mitigation has been done by Aresta and Dibenedetto (2010). Cuéllar-Franca and Azapagic (2015) surveyed the state-of-the-art in the life cycle assessment (LCA) of CCUS systems, while Bruhn et al. (2016) differentiate between the carbon management benefits that accrue from CCU and CCS. A survey of the modeling of CO_2 utilization, options such as EOR and ECBM, was done by Tian et al. (2016). This paper focuses more on how each component of CCUS can be modeled than on how optimization tools aided CCUS planning. Other papers have discussed recent technological advances in capture (Wang et al., 2017), utilization (Alper and Orhan, 2017) and storage (Cantucci et al., 2016). Monitoring and verification techniques were discussed further by Li et al. (2016a, b). These review articles focus on technological developments of system components. Other review papers focused on techno-economic analysis of CCS through mathematical programming approaches (Huang et al., 2013) and process integration techniques (Foo and Tan, 2016). However, none of these previously published review papers cover developments in techniques for the systematic planning of CCUS for purposes of policy development and decision making. In the recent IEA Expert Workshop on "*The Role of Process Integration for Greenhouse Gas Mitigation in Industry*", the use of tools such as mathematical programming and pinch analysis has contributed to planning energy systems with carbon constraints. This review paper differs from previously published works by focusing on the development of decision support methods for macroscale CCUS planning. This review also includes a bibliometric analysis to identify research gaps that require further study.

In the planning of CCS and CCUS systems, it is necessary to consider multiple factors to both maximize economic benefits and minimize CO_2 emissions. Relevant factors include grid-wide energy balance implications of retrofitting power plants for CO_2 capture, risks associated with injecting CO_2 into geological reservoirs, and system-level techno-economic feasibility. This review paper surveys recent developments in the planning of CCUS systems, focusing specifically on process systems engineering (PSE) tools that aid decision-makers to consider the issues mentioned previously. Bibliometric trends in the CCUS literature are also analyzed. The rest of this paper is organized as follows. The next section presents an overview of CCUS systems, including technology options for each system component. Then, scalability issues in these components, as well as prospects for CCUS development, are discussed. An in-depth discussion of various tools for planning and decision support is then given. These tools include mathematical programming, pinch analysis, automated targeting and other computational techniques. Next, bibliometric trends in CCUS literature are presented. Future directions for research on the planning of CCUS are also recommended.

2. CCUS technology overview

Fig. 1 shows an integrated CO_2 chain involving CCUS technologies. CO_2 sources (e.g. industrial plants) can be retrofitted with different capture technologies in order to produce CO_2 supply of different quality levels. For instance, power plant sources (fossil-fuel based) can be retrofitted with any of the given capture options, producing CO_2 with traces of other gases resulting from combustion (Aresta and Dibenedetto, 2010). Unless a CO_2 purification process is available, the captured CO_2 from flue gases cannot be used in food processing and chemical synthesis due to the presence of undesirable impurities such as SO_x and NO_x. Extracted CO_2 from natural wells is often used for injection into depleted oil reservoirs for EOR (Middleton et al., 2011; Godec et al., 2011). However, use of extracted CO_2 results in net positive CO_2 footprint (Naims, 2016). Use of captured CO_2 can thus potentially reduce the demand for extracted CO_2 to give net reduction in system-level GHG emissions (Bruhn et al., 2016).

After selection of CO_2 sources with appropriate capture options, CO_2 streams of different quality can be distributed to different options for utilization and storage (Cuéllar-Franca and Azapagic, 2015). These utilization options include chemical synthesis of polymers, carbonates and cyanates (Mikkelsen et al., 2010), methanol and hydrocarbon production (von Der Assen et al., 2015) and CO_2 injection for EMR (Li et al., 2016a, b). The latter option results in partial permanent CO_2 sequestration in depleted oil and gas reservoirs, inaccessible coal seams, and deep saline aquifers; in other words, utilization and storage can be coupled through simultaneous EMR and geological sequestration. Additional materials such as oil and gas can then be recovered from underground reservoirs through displacement by CO_2 injection and storage (Rehman and Meribout, 2012). In such cases, additional revenue from enhanced recovery of valuable products can potentially offset some of the costs of capturing and handling CO_2, which currently is one of the major obstacles to large-scale deployment.

For climate change mitigation, the objective of the planning of CCUS systems is to maximize the use of the captured CO_2. Due to the energy and economic penalties of CO_2 capture, it is then necessary to establish an incentive scheme (Lambert et al., 2016), or a CO_2 pricing mechanism (Li et al., 2016a, b) to encourage implementation. On the other hand, the increase in the number of available options for CO_2 utilization or storage can accelerate the deployment of CCUS for climate change mitigation. On the other hand, public perception and lack of a legal framework on geological storage limit the use of geological sequestration for carbon management. Thus, the integration of utilization and storage is difficult, since utilization is hardly considered in the CO_2 storage context. Planning tools focusing on these issues of both CCU and CCS aim to optimize the deployment of both strategies on a regional or global scale. The development of large-scale CCS projects is discussed in the next section, along with initiatives to demonstration CCU for climate change mitigation. These projects suggest the potential for CCU and CCS to be integrated as CCUS.

3. Global status of CCUS

Numerous projects have been implemented to demonstrate the capabilities of CCUS as a climate change mitigation option and to identify operational issues during scale-up. Two major components are considered in this section: the contribution of CCS to the reduction of GHG emissions, and the development of utilization projects to speed up CCS development. Data given here were obtained from the project database in the Global CCS Institute Project Database (2016).

Demonstration projects for CCS and CCUS are being developed to gain information about the scalability of the technology. There are currently 21 industrial-scale CCS projects that have been conceptualized, developed and operated since 1970's (Global CCS Institute, 2016). In the early stages of CCS demonstration, emphasis is on the use of CO_2 for EOR (Bruhn et al., 2016). CO_2 sources involved in the demonstration projects are mainly from natural wells and small- to medium-scale industrial plants (e.g. fertilizer plants, natural gas sweetening, etc.). Only a few projects, such as Boundary Dam (Lanktree, 2014) and Kemper County (Hunter, 2014), use captured CO_2 from power plants as the CO_2 source. Efforts are being made to increase the number of large-scale CCS projects, especially in the power generation sector. As of the present time, 11 projects in the global power generation sector are in the planning stages of development (Global CCS Institute, 2016). It is expected that these projects will commence operation in the next decade. Based on this data, a projection can be made on the global availability of captured CO_2 capture in the future. Fig. 2 shows that approximately 200 Mt of CO_2 can be captured (and utilized or stored) by the end of 2040 if the projects identified are executed successfully. However, this figure accounts for only 5% of the needed 4 Gt/y of CO_2 reduction towards transition to clean energy (Global CCS Institute, 2016). To achieve the necessary emissions cuts, the growth rate of CCS deployment will need to be 32.2% annually (Global CCS Institute, 2016). Furthermore, these projects involve only one source to be connected to a single CO_2 storage option; in the future, regional-scale CCS and CCUS systems with multiple CO_2 sources and sinks using shared distribution infrastructure will need to be developed. Furthermore, planning for energy systems in the future will require integration of different projects to accelerate CO_2 reduction through CCUS, coupled with other carbon management strategies.

Based on the Global CCS Institute Report (2016), there are currently 17 identified non-EOR CO_2 utilization projects, of which 15 are operational. Certain utilization options that do not rely on CO_2 injection include food and beverage applications, mineralization and carbonation treatment. Although these options are capable of temporarily storing CO_2 at different temporal scales, the main purpose of these options is to replace the conventional processes with more efficient ones. The projects identified handle 0.15 Mt of CO_2 annually. Some of these projects have used coal-fired power plants as the CO_2 source for food and beverage applications, with additional processes being used to remove traces of unwanted impurities. Examples of these projects include Huaneng Gaobeidian Pilot Project (Hester and Harrison, 2010) and AES Shady Point and Warrior Run CO_2 recovery (US EPA, 2015). Huaneng Gaobeidian Power Plant is a demonstration project where 3 kt/y of CO_2 is captured and purified. On the other hand, AES Shady Point project captures 0.13 Mt/y of CO_2 from two power stations. Although these projects demonstrate the technological feasibility to utilize CO_2 from coal-fired power plants, only a small percentage of the total CO_2 output can be processed for utilization due to the difference in scale of the downstream utilization processes. These demonstration projects are used primarily to gain information on CO_2 utilization economics. The increasing number of CCU projects globally shows greater opportunities to deploy CCUS on a large scale as part of an integrated global carbon management strategy (Quadrelli et al., 2014). Despite its naturally limited scale, CCU is still an important climate change mitigation strategy due to its capability to partially offset CCS costs. Thus, in the absence of policy incentives such as a carbon tax, positive revenues from CCU can stimulate investment in CO_2 capture, transportation and distribution facilities, which in turn can facilitate subsequent entry of CCS as a more scalable carbon management strategy.

The development of CCUS globally remains slow, and based on current trends, substantial contributions to the 70% emissions cut target set in the Paris Agreement cannot be met. However, with the increase in the start-up of new CCU projects, it is possible to accelerate the growth of CCUS to meet the desired level of reduction. Note that the successful

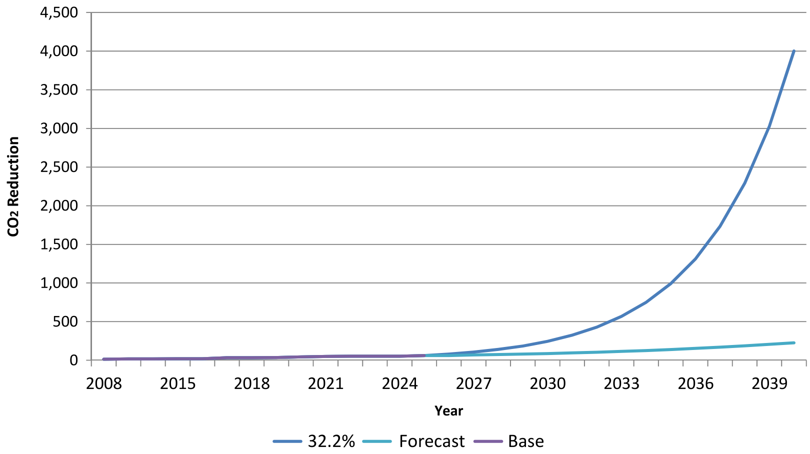

Fig. 2 – Annual CO_2 emissions reduction in Mt attributed to CCS projects.
***Source:* Data from Project Database in Global CCUS Institute, 2016.**

integration of CCU and CCS depends on whether CCU can provide the necessary revenue to offset the cost of CCS. The lessons drawn from these demonstration projects can thus be used to accelerate CCS deployment by integrating it with utilization options. However, as previously pointed out, success of CCS projects depends on different scalability issues. Several obstacles, such as lack of economic incentives, are the main causes of project failure. Many of these issues can be resolved by various planning tools using PSE approaches.

4. Scalability issues in CCUS

Integrating CO_2 sources, capture technologies, utilization options and storage sites is one of the major challenges in deploying CCUS on a large scale. Major issues include reduction of the high energy requirement for capture, selection of appropriate CO_2 utilization technologies, and dealing with uncertainties in the geophysical characteristics of storage sites. There are other problems that arise when integrating CCUS components. For example, there can be a mismatch of the temporal and spatial characteristics of the components of CCUS. For example, the operating lives of multiple sources and sinks will generally not coincide perfectly, and their CO_2 flowrates may span a range of several orders of magnitude. Since the system components will generally be plants operated by different companies, there needs to be a means to facilitate cooperation with respect to the use of shared facilities such as pipelines., The lack of legal framework for assigning liability of storage sites also needs to be dealt with. In this review, PSE tools such as mathematical programming and pinch-based methods are discussed in the context of addressing such issues.

A large component of CCUS economics is attributable to the cost of CO_2 capture. For climate change mitigation, power plants should be prioritized for CO_2 capture. However, additional power generation capacity will be needed to compensate for the power used for capture processes. For instance, additional power generation costs are estimated at 40% for integrated gasification combined cycle (IGCC) and natural gas combined cycle (NGCC), and 50%–80% for coal-fired power plants (Abellera and Short, 2011). Decision support tools for planning CO_2 capture systems focusing on this issue are discussed in the following sections.

The selection of CO_2 sources for utilization is important in assessing the deployment of technologies in the future (von der Assen et al., 2016). Several technologies for converting CO_2 into high-value end products such as methanol and carbonates have been developed (Mac Dowell et al., 2017). In addition, CCU presents different profitable options to delay CO_2 emissions, and is thus only considered primary for resource security (Zhang et al., 2014). CCU can be considered as a way to offset the cost of developing CCS systems. This can achieved through CO_2 injection for EMR, and especially for EOR, which is a relatively mature technology. Planning tools are necessary in order to balance cost-effective production of CO_2-derived products and long-term sequestration of CO_2.

One of the most important issues of CCUS to be addressed is the characterization of storage sites. An important assessment methodology for storage site development is the estimation of storage capacity and injectivity limits. Storage capacity is based on the porosity of the formation (i.e. void space in geological formations), while the injectivity limit, which determines the maximum flow rate for injection, is based on permeability (i.e. pore connectivity) (Holloway, 2007). Estimates can be done using seismic surveys, which also characterize the rock formation. Computational methodologies have been proposed by Bachu et al. (2007) for different storage options. Bradshaw et al. (2007) developed a "techno-resource pyramid" approach to systematically organize the levels of storage capacity, depending on the assumptions made. Their approach addresses estimation errors starting from the total pore volume of the reservoir (theoretical capacity) up to the most economical volume for injection (viable capacity). Uncertainties arise with estimating the best parameters for CO_2 storage based on different techno-economic aspects. Characterization of storage sites also includes storage security (Bourne et al., 2014), economics of CO_2 injection (Carneiro et al., 2015) and technical and health risks due to CO_2 flow behavior in the reservoir (Kopp et al., 2010). Integrated CCUS planning should take into account these aspects.

Integrating components of CCUS also entails scalability issues. Various review papers (Huang et al., 2013; Foo and Tan, 2016) identify the following decision questions for planning CCUS systems:

- How should CO_2 sources and sinks be matched?
- How can the total CCUS network cost be minimized?
- How can total CO_2 emissions reduction be minimized?

The first decision question involves *source–sink matching* based on the characteristics of the CO_2 sources and sinks. These

Table 1 – Scalability Issues in CCUS (de Coninck and Benson, 2014; Bruhn et al., 2016).

Source	Capture
• Compatibility of CO_2 source for utilization options	• High energy requirement for CO_2 capture. • High cost for CO_2 capture. • Compatibility of CO_2 capture with CO_2 source
Utilization	**Storage**
• Additional processes to meet requirement in utilization options. • Energy requirement for utilization may result to net positive CO_2 footprint. • Conventional CO_2 source (i.e. underground extracted CO_2) dominates captured CO_2 from power generation in most processes • Most technology not designed for long term climate change mitigation purpose. • Comingling to climate change mitigation is debatable: issues arise with the conflict of CCU with energy decarbonization goals	• Storage security issues such as induced seismicity and groundwater contamination. • Uncertainty in CO_2 capacity and injection limits affects long term planning • Public resistance to geological sequestration impedes CCS deployment. • Legal framework for storage liabilities is not yet established.

include their availability, location, and CO_2 stream and storage characteristics. The second question includes how many power plants can be retrofitted with capture facilities, how the pipeline network be designed for minimal cost, and how much CO_2 is allocated for utilization to generate revenues. The third question addresses the climate change mitigation benefits that result from direct CO_2 sequestration coupled with offsets from displacement of extracted CO_2. As in many industrial systems, there may be an inherent conflict between these economic and environmental goals. Thus, mathematical tools are necessary to aid planning based on these scalability issues involved in integrating components of CCUS system.

These issues hinder the development of CCUS as a carbon management strategy for climate change mitigation. Table 1 summarizes these issues, which can be addressed at different technological scales (Floudas et al., 2016). Micro-scale research in CCUS allows the development of new technological pathways for CO_2 utilization (Huang and Tan, 2014) and the development of new processes to efficiently capture CO_2. Meso- to macro-scale approaches include the development of cost effective ways to design CO_2 capture, utilization and storage techniques, and planning and decision making for regional CCUS systems (Chen et al., 2016). This review focuses on the tools for the macro-scale deployment of CCUS. Planning methods and tools are directly involved in policy-making for CCUS (Bryngelsson and Hansson, 2009). This study discusses the past literature on planning models for decision makers, policy makers and CCUS experts. The next section provides an in-depth discussion of the planning tools used for CCUS.

5. PSE for planning CCUS systems

Techniques such as pinch analysis and mathematical programming can be used to aid in planning for large-scale deployment of CCUS. Recent literature on the use of pinch analysis for the planning of CCS systems considers different temporal and spatial factors. On the other hand, mathematical programming techniques are capable of handling a wide variety of issues in CCUS, and are widely used in literature. These different methods are discussed in their respective subsections. Table 2 summarizes the general features and capabilities of these tools. Mathematical programming provides a flexible, high-resolution framework to handle detailed aspects in the planning of CCUS systems, while pinch analysis methods can be used to provide high-level insights for the CCUS planning. Other techniques can also be used in this context. For example, numerical simulations can be used to create a virtual environment to test different strategies and scenarios. P-graph (process graph) methodology provides an alternative to mathematical programming which can determine multiple optimal and near-optimal solutions in CCUS network planning problems. Graphical techniques (e.g. pinch analysis) are limited to the analogy that can be derived from the problem structure. On the other hand, simulations and mathematical programming may provide wider options for CCUS but the drawback may be on the computational effort needed.

5.1. *Mathematical programming models*

Mathematical programming models are a useful family of techniques for planning CCS systems. Such models have been a fundamental part of PSE for many decades (Stephanopoulos and Reklaitis, 2011). The application of mathematical programming to CCUS dates back to the late 80's, when an integer programming model was proposed for CO_2 allocation for EOR (Turk et al., 1987). A review by Huang et al. (2013) presents some of the optimization models for dealing with techno-economic aspects of CCS. Approaches in developing mathematical techniques for CCUS were classified according to different methods of designing the large-scale CCUS systems. These methods covered energy models, pipeline infrastructure design and source–sink matching. Energy models focus on the energy balance aspects of CCUS systems, particularly to account for power losses incurred during capture. On the other hand, pipeline infrastructure design models focus on the economics of building and operating CO_2 distribution networks. Lastly, source–sink matching focus only on high-level identification of which CO_2 sources should be matched with different utilization or storage options, without necessarily delving into detailed engineering of the pipeline networks. Some models consider more than one of these aspects.

Table 2 – Different planning approaches used for CCUS.

Source: **Adapted from Tapia et al. (2016a)**

Approach	Advantages	Limitations
Pinch analysis	• Quick insights may readily be obtained. • Little computational effort is required.	• Solutions are difficult for larger problems. • Limited factors can be taken simultaneously.
Mathematical programming	• Multiple factors can then be simultaneously be addressed through constraints expressed as inequalities	• Guaranteed global optimum may not be obtained from non-linear program. • Problems with multiple dimensions (sets) may take longer time for larger problems. • Multi-objective models generate infinitely equally important solution. Insights are then harder to obtain.
Numerical simulation	• Tools work on different scales considered. This works best for determining effects of unit simulations in large-scale system.	• Larger problem may be difficult to solve. • Optimality may not be guaranteed.
P-graph	• Provide multiple with different configurations. Process of eliminating less suitable solutions is not difficult. • Scaling factors are optimal for each configuration.	• Method is limited to the structure of the mathematical model present.

However, having a single mathematical model to address all of these issues at once may result in excessive complexity and undue computing effort (Biegler and Grossmann, 2004). Instead, a multi-stage approach can be used such that the results of each phase can be used to customize and simplify the formulation of subsequent models.

Multi-objective optimization approaches have also been developed considering energy constraints; such models have been applied to the Taiwan (Bai and Wei, 1996) and Greece (Mavrotas et al., 1999) electricity sectors. These models were developed to determine the effect of CO_2 capture options to power generation considering both costs and CO_2 emissions reduction. On the other hand, a mixed integer linear program (MILP) was developed by Tekiner et al. (2010) using energy scenarios generated by Monte Carlo simulation under different energy demands. Since parasitic energy loss is one of the factors that hinder large-scale CCS deployment, research and development of planning techniques are focused on considering such energy penalties and the associated costs. Case studies were presented for Alberta power generation sector (Ordorica-Garcia et al., 2009) and Ontario power generation (Elkamel et al., 2009) addressing these issues in CCS deployment. A review of Nakata et al. (2011) considers different energy models for a low carbon society. On the other hand, van den Broek et al. (2008) provided an energy plan for the Netherlands using the MARKAL-NL-UU model. An integer linear program (ILP) by Tan et al. (2010) enables retrofit selection having CO_2 emissions minimization as the objective and power demand as target constraints. A similar MILP model was also developed by Pękala et al. (2010). Planning approaches using the automated targeting formulation were developed to generate CCS retrofitting strategies with storage constraints (Ooi et al., 2013a) and with changing power demands (Ooi et al., 2014). Power capacity expansion with CCS has also been addressed in recent papers using particle swarm optimization (Saboori and Hemmati, 2016). CCS was also considered in a model for future low-carbon power generation considering operational flexibility of current power plants (Brouwer et al., 2015). Certain models also consider specific low carbon alternatives as part of the decision scenarios. Such models include biofuel consideration for bi-criterion optimization (Öztürk and Turkay, 2016) and nuclear power phase-out scenario for Switzerland (Pattupara and Kannan, 2016). These energy models provide insights for carbon-constrained planning, which present a systematic means to integrate CCS into the power sector consisting of old and new plants. These models also assess the suitability of CCS in a given geographic system as part of a mix of low-carbon options. However, capture costs and energy penalties are not the only economic issues in CCUS. Transportation, injection and storage costs have also been addressed through infrastructure models developed using mathematical programming.

Source–sink matching is an important aspect of planning CCS systems. It provides a high-level means to estimate the economic feasibility of regional deployment of the technology, prior to detailed engineering design. It involves selection of source–sink matches based on the characteristics of the sources and sinks. Factors that affect source–sink matching include CO_2 balances, scheduling, and geographical constraints. A MILP continuous-time optimization model was developed by Tan et al. (2012) but without the capability of addressing injectivity limits. An improved version of this model was then proposed by Lee and Chen (2012). A discrete-time model was later developed that also accounted for reservoir injectivity limits (Tan et al., 2013). Storage reservoir uncertainties have also been addressed via fuzzy optimization (Tapia and Tan, 2014) and robust programming (He et al., 2014) approaches. These tools give insights into how CO_2 emissions reduction can be compromised to minimize technical risks such as errors in estimating storage site characteristics. These models also enabled CO_2 emissions reduction potential to be determined even under conditions of data uncertainty. A unified MILP model capable of simultaneously handling both energy penalty issues and source–sink matching was then proposed by Lee et al. (2014). Other recent works on scheduling for CCUS systems include a discrete-time model for EOR operations (Tapia et al., 2016a) and a strip-packing model for both utilization and storage operations (Tapia et al., 2016b). A production scheduling model for ECBM operations was developed without considering the source–sink matching aspect (Huang and Tan, 2014). Optimal revamp approach was developed using two-step mathematical optimization to address unexpected changes in CCUS systems, such as the discovery of reservoir leaks (Tapia and Tan, 2014).

Pipeline infrastructure design is also important in CCUS planning. Transportation of captured CO_2 through pipelines accounts for about 10% of the total cost in CCUS systems (Rubin et al., 2015). Models using geographical information systems (GIS) in conjunction with mathematical programming have been developed to determine pipeline network layout. Examples include *SimCCS* (Middleton and Bielicki, 2009) and *SimCCS*^{TIME} (Middleton et al., 2012) for static and dynamic scenarios, respectively. These models considered spatial constraints to determine network configuration. Single-stage (Sun and Chen, 2015) and multi-stage (Sun and Chen, 2017) models have also been developed for CCUS pipeline networks in China. These works show that minimizing CO_2 transportation cost through pipeline network optimization is important for the successful large-scale deployment of CCUS technology. However, in addition to economic issues, technical aspects such as uncertainties in operating conditions also need to be accounted for (Tian et al., 2016). Furthermore, storage site selection is affected by the characteristics of pipeline design (e.g., pipeline size and distance) in both onshore (Wang et al., 2016) and offshore (Sanchez Fernandez et al., 2016) infrastructure.

CCS models extended to CCUS problems have been considered in the recent literature. Hasan et al. (2014) developed a multi-scale approach for cost-effective CCUS systems, focusing on the adjustments to the technical aspects of CO_2 capture. An integrated process model for an EOR system was developed by Rahmawati et al. (2015) considering both operating parameters and economic benefits from the system. CO_2 emissions have also been considered in the design of heat integration system (Hassiba et al., 2016). A cost minimization approach has been proposed by Al-Mohannadi and Linke (2016) for CO_2 networks, which was then extended to multi-period problems (Al-Mohannadi et al., 2015). Mathematical programming tools have also been used for oil field development, which can be considered as a special case of CCUS (Foo et al., 2016; Tavallali et al., 2016). Table 3 summarizes these mathematical programming tools. Models developed in the past can be integrated into a systematic framework to guide planning of future projects. In particular, it will be necessary for these models to address uncertainties that arise from the decades-long time horizons involved in planning CCUS systems. Examples of potential uncertainties include climatic conditions, geophysical properties of storage reservoirs, economic parameters (e.g., energy costs) and environmental policies (e.g., future carbon taxes).

5.2. *Pinch analysis-based methods*

Pinch analysis can give useful insights for CCUS system planning. The method was applied to planning CCS systems involving multiple CO_2 sources, CO_2 capture technologies available and CO_2 storage sinks (Tan et al., 2010). Recently, this method has been extended to CCUS application in which selection also utilization sinks requiring certain CO_2 streams (Mohd Nawi et al., 2016a). Pinch analysis-based tools for CCUS are based on three objectives: to determine the best CCS retrofit for an energy grid, to determine the optimal CO_2 source–sink matching, and to maximize CO_2 utilization of captured CO_2.

Early application of pinch analysis for CCS planning involves determining the target minimal retrofit to meet a CO_2 emission limit (Tan et al., 2009). In this case, a composite curve is created based from increasing carbon intensity of the available energy sources and the retrofit target is determined by the required reduction. Insight gained from this method is the required compensatory power due to the retrofit. Shenoy and Shenoy (2012) used limiting composite curves to determine targets for CCS retrofit and include the method for cost optimization. However, this work lacks the consideration of power loss during CCS retrofit. In the approach developed by Tan et al. (2009), the compensatory power was assumed to have negligible CO_2 emissions. Sahu et al. (2014) developed an algebraic approach for CCS retrofit considering emission targets with significant emissions from compensatory power. A multi-period retrofit strategy was developed by Ooi et al. (2014) which involves the minimum extent of retrofit and the compensatory power requirement. These approaches presented can determine the amount of power for retrofit considering only the CO_2 intensities of the energy sources. Uncertainties such as changes in power demand may be considered for retrofitting strategy.

Other tools based on pinch analysis were developed for source–sink matching. These tools provide solution for single-period (Diamante et al., 2013) source–sink matching in CCS subject to capacity and injection rate limit constraints. The method also includes sensitivity analysis to determine the changes in the optimal solution with respect to the change in capacity and injectivity limits. It was later extended to multi-period time setting by Ooi et al. (2013b). However, the lack of taking into account the injectivity constraint is the limitation of this approach. A unified pinch analysis approach was developed by Diamante et al. (2014) to address injectivity constraint into the graphical technique. A recent review by Foo and Tan (2016) discusses these techniques for energy planning in CCS systems. The method is limited to considering two factors at a time. In the case of energy planning with CCS, pinch analysis-based technique is based on energy and CO_2 emissions. On the other hand, CCS source–sink matching takes into account CO_2 flow rate and quantity only. However, these provide quick insights into how much CO_2 capacity is utilized optimally for CO_2 emissions reduction.

Pinch analysis-based tools have also been extended to CCUS applications. The general problem statement is also based on source–sink matching with additional CO_2 purity constraints. One of these tools for CCUS is a targeting approach developed by Mohd Nawi et al. (2016a) considering geological storage as least prioritized CO_2 sink. A generic carbon cascade approach (GCCA) technique was also developed to achieve minimum extracted CO_2 (fresh CO_2 feed) requirement (Manan et al., 2014). This involves matching CO_2 sources with CO_2 utilization options as demands subject to purity constraints (Abdul Aziz et al., 2016). Pinch analysis has been applied in this system having geological reservoirs as back-up CO_2 sink options (Mohd Nawi et al., 2015). Pressure drop and pipeline infrastructure planning have been addressed using the same methodology in regional planning (Mohd Nawi et al., 2016b).

These pinch analysis-based tools have developed from CCS planning to CCUS planning considering retrofitting of CO_2 sources for both utilization and storage. Table 4 summarizes the tools discussed in this section. Pinch analysis methods are good for gaining quick insights and better understanding of the CCUS scenario. Even if limited factors can be considered for each tool, new developments can still be made by considering strategies for the future direction of CO_2 in CCUS systems as a valuable raw material rather than a waste material.

Table 3 – Summary of mathematical programming tools.

Tools focused on CO_2 capture	Tools focused in CO_2 transportation
• Early approach for CO_2 capture integration in power generation: Taiwan (Bai and Wei, 1996) and Greece Cases (Mavrotas et al., 1999) • Uncertainty analysis based on energy demand (Tekiner et al., 2010) • Hybrid methods in energy planning (van den Broek et al., 2008) • ILP model for retrofit selection (Tan et al., 2010) • Integration of CO_2 capture with other low carbon options: biofuels (Öztürk and Turkay, 2016), nuclear energy (Pattupara and Kannan, 2016)	• Early approach for CO_2 allocation (Turk et al., 1987) • Pipeline Infrastructure Models: *SimCCS* (Middleton and Bielicki, 2009) and *SimCCS*^{TIME} (Middleton et al., 2012). • Decision support tools for assessing economics of CO_2 transportation: Single-stage (Sun and Chen, 2015) and multi-stage (Sun and Chen, 2016) decision frameworks. • Determining of the effects of different parameters in CO_2 transportation design: pipeline sizing (Wang et al., 2016) and operating conditions (Tian et al., 2016)
Tools focused on CO_2 Utilization	**Tools focused in CO_2 Storage**
• EOR scheduling using discrete-time approach (Tapia et al., 2016a) • ECBM injection allocation and scheduling (Huang and Tan, 2014) • Gas field development considering CO_2 quality constraint (Foo et al., 2016) • Oil field development (Tavallali et al., 2016)	• Source–sink matching models considering temporal constraints: discrete-time (Tan et al., 2013) and continuous-time (Tan et al., 2012; Lee and Chen, 2012) scheduling of storage operations. • Accounting for uncertainties in CCS systems: storage uncertainties (Tapia and Tan, 2014) and temporal uncertainties (He et al., 2014)
Integrated tools	
• Revamp framework for CCUS systems (Tapia and Tan, 2015) • Integrated framework for CCUS considering technical improvements (Hasan et al., 2014) • Integrated process model specifically designed for EOR operations (Rahmawati et al., 2015) • Carbon integration analogous to water network design in static (Al-Mohannadi and Linke, 2016) and multi-period (Al-Mohannadi and Linke, 2016) settings. • CO_2 utilization with heat integration (Hassiba et al., 2016)	

Table 4 – Summary of pinch analysis tools.

Tools focused on CO_2 Capture	Tools focused in CO_2 Transportation
• Retrofit selection for power generation (Tan et al., 2009) • Automated targeting based on minimum compensatory power requirement (Sahu et al., 2014)	• Total site targeting considering pipeline infrastructure and pressure drop (Mohd Nawi et al., 2016b)
Tools focused on CO_2 Utilization	**Tools focused in CO_2 Storage**
• Novel pinch analysis technique for total site carbon planning (Mohd Nawi et al., 2015). • Total site targeting for CO_2utilization (Mohd Nawi et al., 2016a) • Generic carbon cascade analysis (GCCA) for planning CCUS systems analogous to water network synthesis (Manan et al., 2014)	• Single period source–sink matching (Diamante et al., 2013) • Multi-period source–sink matching (Diamante et al., 2014)

5.3. *Miscellaneous methods*

Numerical simulations and metaheuristics have been used to characterize the flow characteristics of reservoirs, or to optimize injection schemes to generate best case-scenarios. In particular, numerous papers in the literature suggest methods on deploying CCS simultaneously with EOR operations. For instance, a non-dominated sorting genetic algorithm (NSGA) has been applied to determine the best CO_2 injection scheme to deploy CCS with EOR (Safarzadeh and Motahhari, 2014). Ettehad (2014) developed a model for meeting storage requirements using deep saline aquifers as back-up storage. Leach et al. (2011) provided an extended dynamic model for optimum CO_2 injection scheduling. Genetic algorithm (GA) approaches have been applied to storage development (Biagi et al., 2016) and for CCS deployment (Fimbres-Weihs et al., 2011).

P-graph methodology has been applied to CCS source–sink matching (Chong et al., 2014) and CO_2 management networks (Tan et al., 2017). The advantage of the P-graph approach is the ability to provide robust network configurations by generating both optimal and near-optimal networks. These solutions can then be selected using multi-criterion decision analysis (MCDA) tools such as the analytic network process (ANP) (Promentilla et al., 2013). Applications include site selection (Hsu et al., 2012) and simultaneous source–sink selection under geographic constraints (Promentilla et al., 2013). Applications of these tools to CCUS planning may increase in the future, especially for future issues that cannot be solved using conventional models.

6. Bibliometric analysis of CCUS literature

This section discusses progress in CCUS research as indicated by global publication trends in recent years. The publication list was generated from Scopus database. Three important trends are analyzed:

- Research on CCUS as a low carbon technology
- Development of techniques for planning large-scale CCUS systems
- Global distribution of CCUS publications in comparison with global CCUS projects deployed.

Table 5 shows the keywords used to search the Scopus database for relevant publications. The publication titles having the largest number of documents are also listed. The most frequent title publishing new results in CCS is *Energy Procedia*, which consists of proceedings of different conferences The source with the highest number of peer-reviewed publications on CCS is the *International Journal of Greenhouse Gas Control,* with 807 publications out of a total of 12,932. Aside from keywords related to CCS/CCUS, top keywords from CCS/CCUS search include “coal combustion”, “fossil fuel power plant”, and “costs”. This shows research emphasis on CCS deployment in power plants. Also, CO_2 capture is mentioned almost as much as CO_2 sequestration in the keyword search. In the publication search related to planning techniques, “optimization” is the most frequently used keyword, with “emission control” and “costs” ranked next. The keyword search for planning techniques includes specific methods, such as mathematical programming and pinch analysis.

The increase in publication output related to CCUS shows the growing interest of the global research community in this technology. Fig. 3 shows the yearly Scopus-indexed publications related CCUS compared to low-carbon technologies in general. The number of CCUS publications is significantly lower than those of solar and wind energy due to its relatively young age as a carbon management strategy. In addition, early publications from the start of the 21st Century may have used alternative terminology, which make them less visible via keyword search. On the other hand, there is an increase in the number of publications on CCUS as compared to hydroelectric and nuclear energy. Also, the average growth in publications on CCUS is the highest (42%) among low carbon technologies. This trend indicates an interest in CCUS as a transitional low-carbon technology (Endres et al., 2016).

Research trends on CCUS planning tools were also analyzed. Fig. 4 shows the Scopus-indexed publications on planning tools for CCUS in comparison with other aspects of CCUS. The number of publications on planning tools accounts for less than 5% of the total CCUS publications. This small number indicates limited current interest by the scientific community, but also suggests an opportunity for future growth. Such research will be essential to support the growing number of demonstration projects being identified and executed globally.

The large scale deployment of CCUS can also be compared to the research productivity. Fig. 5 shows the number of publications per region in comparison with the number of projects each region has identified and operated. The number of projects is based on the Global CCS Institute Report (2016). The European Union (EU) produced the highest number of publications but only ranks third in terms of projects. On the other hand, the USA has the most projects among these regions due to its active deployment of CCS through EOR. South East Asia has also shows interest in CCUS publications, even though actual projects have not yet been initiated in this region. China has shown interest in CCUS in terms of both demonstration projects and research publications. This data shows active interest in CCUS as a carbon management strategy throughout the world, but the extent of contribution is subject to geographic variations.

In summary, general bibliometric trends indicate that CCUS research is not yet as intensive as research on other low-carbon technologies. This does not mean that CCUS is not a viable option for carbon management; it may simply reveal lack of maturity compared to other technologies. This decade, the global publication rate on CCUS planning has been at about 300–400 papers per year. Given the current status of CCUS, research and development is still needed for it to achieve technological maturity and become competitive with other low-carbon technologies. Decision support tools will then be needed so that large-scale CCUS systems can be planned effectively.

7. Assessment of tools for planning CCUS systems

This section presents a critical assessment of how computational tools are applied to planning CCUS systems. The methods are divided into three broad categories: mathematical programming tools, pinch-analysis techniques, and other miscellaneous methods.

Mathematical programming is capable of addressing detailed issues that need to be integrated into one model. Models presented are capable of providing insights on parasitic energy losses from CO_2 capture and can develop networks between sources and sinks. Unifying multiple factors into one model may give insights on how each component of CCUS affects the others. The main disadvantage of this approach is the general lack of transparency of using an equation-based approach for complex problems. This drawback may result in some difficulty in communicating model solutions to decision-makers in real-life applications, particularly when the optimal solutions are counterintuitive. On the other hand, pinch analysis-based techniques are helpful for providing better insights for simplified or stylized problems with lower resolution. Key issues addressed by these methods include energy planning and CO_2 target identification. The method enables decision makers to determine main targets for CO_2 reduction and energy demand. For some pinch analysis-based tools, equivalent mathematical programming model have been developed, which indicates that these techniques are fundamentally compatible. The relative advantages of these two approaches can also be utilized through a two-stage approach. Pinch analysis can be used to draw broad, high-level insights, while mathematical programming can subsequently be applied to solve a more detailed, high-resolution version of the planning problem. In such cases, the pinch analysis step can be used to simplify the subsequent model formulation to reduce computational effort.

Table 5 – Topics for bibliometric trends associated with CCUS.

Topic	Keywords	Top source results (2000–2017)
Low carbon technologies	• Carbon capture and storage, • Carbon capture utilization and storage, • Nuclear energy, • Solar Energy, • Hydroelectric, • Geothermal, • Wind Power	(1) Renewable energy (2) Transactions geothermal resource council (3) Renewable and sustainable energy reviews
CCS/CCUS	• Carbon capture and storage, • Carbon capture utilization and storage, • CO_2Capture • CO_2Utilization	(1) Energy Procedia (2) International Journal of Greenhouse Gas Control (3) Industrial and Engineering Chemistry Research
Planning techniques on CCS and CCUS	• Carbon capture and storage, • Carbon capture utilization and storage AND • Optimization • Mathematical Programming • Pinch Analysis • Automated Targeting • Multi-criterion Decision Analysis • Planning	(1) Energy Procedia (2) International Journal of Greenhouse Gas Control (3) Applied Energy

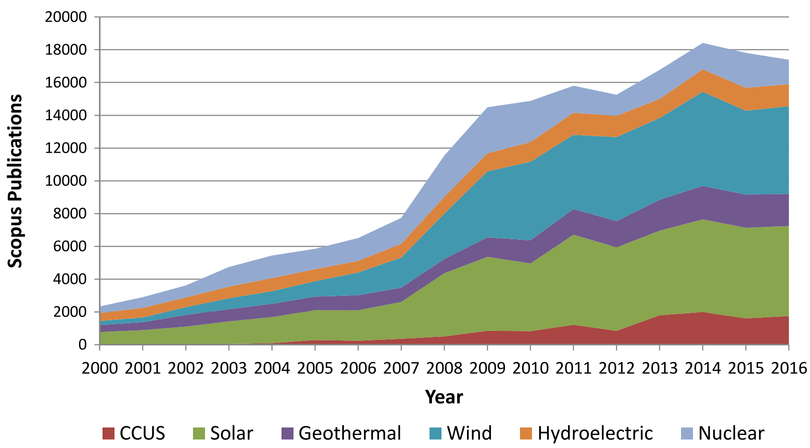

Fig. 3 – Bibliometric trends of CCUS in comparison with other low-carbon technologies.

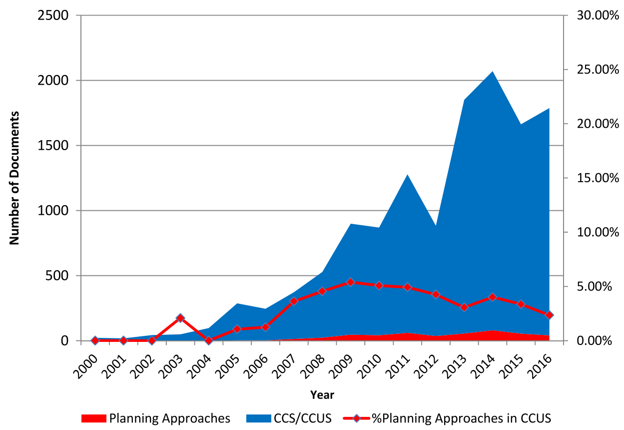

Fig. 4 – Bibliometric trends of CCUS planning in comparison with other research in CCUS.

Recent applications of P-graph methodology for CCS can be readily extended to CCUS. Unlike most mathematical programming tools, this technique can provide alternative pathways for planning CCUS, which is important to manage

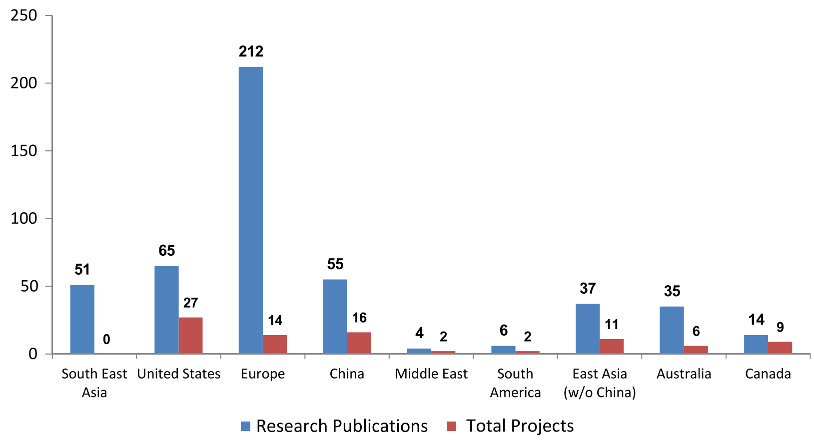

Fig. 5 – Global CCUS projects and publications per region.

uncertainties in the system. Lastly, numerical simulations are very useful in reservoir development. Key issues addressed by these techniques include the characterization of geological reservoirs and flow behavior of CO_2 during injection. These are useful for planning and scheduling injection for utilization options such as EOR and ECBM.

8. Conclusions and research prospects

This review paper has given a state-of-the-art survey of the development of process integration methods for planning CCUS systems as a carbon management strategy. The relatively slow progress of CCUS deployment can in part be attributed to techno-economic risks and uncertainties, which can be mitigated through the availability of robust decision support tools. There is now an extensive body of scientific literature that can eventually address this need. Most of the planning techniques in the literature can be classified as mathematical programming approaches, pinch-based methods, and miscellaneous approaches. These tools can provide valuable insights for decision makers seeking to implement CCUS at scale. Bibliometric trends also reveal gaps in the literature, which also represent opportunities for further research and development to focus on these topics.

Publication trends in CCUS show that the technology is relatively immature compared to other existing low-carbon technologies. Literature suggests that optimization tools would aid planning large-scale CCUS systems addressing different issues, such as integrating CCUS into the energy grid, matching of CO_2 sources and sinks, and developing of pipeline infrastructure. Future direction of CCUS research should focus on the development of better tools for large-scale implementation of the technology. In addition, tools to mitigate the effects of data uncertainty should be developed. Future developments of CCUS planning will involve a wider range of technological options for regional planning. It is also essential to integrate individual methodologies into a unified planning framework that can then be used for large-scale projects. Moreover, future efforts can also address policy development, legal framework and social acceptance. Such developments will allow CCUS to develop into viable and significant carbon management strategy.

Acknowledgments

J.F.D. Tapia would like to acknowledge the Philippine Department of Science and Technology (DOST) through its Engineering Research and Development for Technology (ERDT) program for financial support for his Ph.D. studies. Partial support of the Commission on Higher Education-Philippine Higher Education Research Network (CHED-PHERNet) is also acknowledged.

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