

Pinch Analysis targeting for CO₂ Total Site planning

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Received: 14 December 2015 / Accepted: 6 March 2016 / Published online: 6 April 2016
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Abstract Rising CO₂ emissions that have been primarily attributed to fossil fuel utilisation have motivated extensive research on optimal CO₂ reduction planning and management. Carbon (more precisely CO₂) capture and storage (CCS) and carbon capture and utilisation (CCU) have been the potential solutions to control CO₂ emissions. However, mitigating CO₂ emissions via CO₂ storage in geological reservoirs without utilisation is merely a technology transition, and CO₂ utilisation is limited due to the short lifespan of products. The integration of CCS and CCU, described as carbon capture, utilisation and storage (CCUS), has recently been introduced as a better option to mitigate CO₂ emission. This study introduces a new algebraic targeting method for optimal CCUS network based on a Pinch Analysis–Total Site CO₂ integration approach. A new concept of Total Site CO₂ Integration is introduced within the CCS development. The CO₂ captured with a certain quality from the largest

CO₂ emissions sources or plants is injected into a CO₂ pipeline header to match the CO₂ demands for utilising by various industries. The CO₂ sources and demands are matched, and the maximum CCU potential is targeted before the remaining captured CO₂ is injected into a dedicated geological storage. One or more headers are divided into certain composition ranges based on the purity level of the CO₂ sources and demands. The CO₂ header can satisfy the CO₂ demands for various industries located along the headers, which require CO₂ as their raw material. The CO₂ can be further regenerated, and mixed as needed with pure CO₂ generated from one or multiple centralised CO₂ plants if required. The main consideration for the problem is the CO₂ purity composition of targeted sources and demands. The proper estimation of CO₂ integration will reduce the amount of CO₂ emission needed to be stored and introduced to systematic CO₂ planning and management network.

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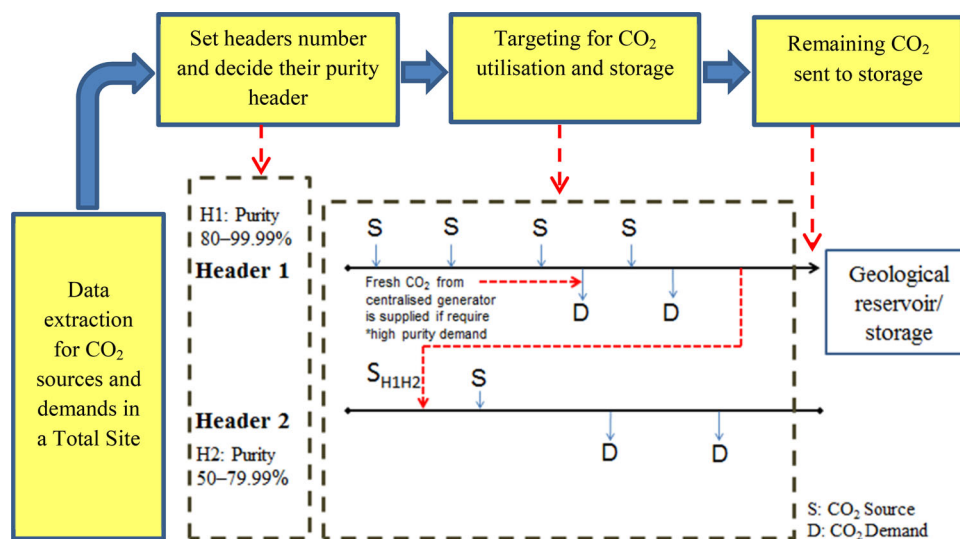
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Graphical Abstract



Keywords CO₂ emission reduction · CO₂ sources and demands · CO₂ management · CO₂ capture, utilisation and storage · CO₂ total site

Introduction

The increase in anthropogenic CO₂ emissions from various energy-intensive industries (e.g. power plant, chemical plants) has initiated an urgent need for effective CO₂ emission mitigation strategies. Global CO₂ emissions from power generation could be reduced by 19 % if countries with high emission levels, such as China and the United States, are able to benchmark their performance with global median emissions (Ang et al. 2011). The key technology to mitigate the increasing CO₂ emission is storage (Diamante et al. 2014) or utilisation (Armstrong and Styring 2015). The CO₂ emissions can be reduced by capturing CO₂ and injecting it into geological storage (CO₂ capture and storage, CCS) or through utilisation (CO₂ capture and utilisation, CCU). This technology involves the capturing of CO₂ from the exhaust gases from large industrial facilities and appropriately storing it in geological storage sites, such as depleted oil and/or gas reservoirs, saline aquifers, coal seams and other similar formations (Diamante et al. 2014). The CCS and CCU are integrated processes made up of three distinct general parts: CO₂ capture, transportation and end-of-pipe solution either being utilised or injected into a geological storage. The capture of CO₂ from large industrial sources is through a variety of capture techniques, such as pre-combustion, post-combustion and oxy-fuel combustion processes to have a relatively pure CO₂ stream (Diamante et al. 2014).

Capture technologies aim to produce a concentrated stream of CO₂ that can be compressed, transported and stored. The concentrated CO₂ specifications are generally based on the requirements for handling large CO₂ streams via pipeline transportation or tanker, which depends on the distance and cost. Meylan et al. (2015), however, have stated that CO₂ storage is a high investment without profitability, low public acceptance and uncertainty in long-term effect, whereas CO₂ utilisation by recycling or as raw material is much more desirable and consistent with industrial ecology principles (Meylan et al. 2015).

In the oil and gas industry, CO₂ has been used as an injected agent to remove the oil trapped in rocks, known as Enhanced Oil Recovery (EOR) agent to increase the oil extraction yield (Cuéllar-Franca and Azapagic 2015). The technology was first tested on a large scale in the 1970s in the Permian Basin of West Texas and South-Eastern New Mexico (Melzer 2012). In the food and drink industry, CO₂ is used as a carbonating agent, preservative, packaging gas, solvent for flavour extraction and decaffeination process. In addition, it is also required in the pharmaceutical industry as an intermediate agent in drug synthesis and is used as a respiratory stimulant. However, applications in the food industry and pharmaceuticals are restricted to sources that produce CO₂ waste streams of high purity. The conversion of CO₂ emissions into valuable products such as chemicals and fuels is also related to CO₂ utilisation alternatives, but chemicals and fuels offer limited storage periods because of their short lifespan (Cuéllar-Franca and Azapagic 2015). The CO₂ is released from the used chemicals and fuels into the atmosphere before the benefits of the capture can be realised. For that reason, future research efforts should focus on the synthesis of materials and products with

longer life spans. The development of CO₂ mineralisation as the means of utilisation was later discovered as the bridge between CO₂ emissions storage and utilisation. Mineral carbonation comprises a chemical reaction between a metal oxide such as magnesium or calcium and CO₂ to form carbonates, which are stable and capable of storing CO₂ for long periods (decades to centuries) (Geerlings and Zevenhoven 2013). However, it has been reviewed as a high-cost investment with high energy penalty for large-scale applications. A life cycle of mineral carbonation in European power generation has resulted in 15–64 % of greenhouse gas (GHG) emission reductions, but has increased the levelised cost of electricity (LCoE) at about 90–370 % on a per kWh (electricity) (Giannoulakis et al. 2014) basis. The statistics on the United States CO₂ utilisation by various sectors is shown in Fig. 1 (US EPA 2011).

There are currently 13 large-scale CCUS integrated projects in China, which are currently in the early stage of identification (six projects), evaluation (three projects) and definition (four projects) towards developing commercial use of CCUS (Li et al. 2015a) to mitigate CO₂ emissions in China. Planning for systematic management in CCUS technology (Li et al. 2015b) could play an important role in mitigating climate change. The optimal integrated CCUS is the potential strategy to utilise the captured CO₂ or stored in secure reservoirs (Li et al. 2015a) or geological sites, which enable the use of fossil fuels (major contributor to CO₂ emissions) while controlling CO₂ emitted into the atmosphere. The CO₂ emissions management involves reducing energy-consuming services (Bandyopadhyay 2015), increasing the efficiency of energy conversion or utilisation, fuel switching, enhanced potential CO₂ demands, utilising renewable energy sources and enhanced CO₂ sequestered either via mineral carbonation, forestation, ocean fertilisation or direct artificial CO₂

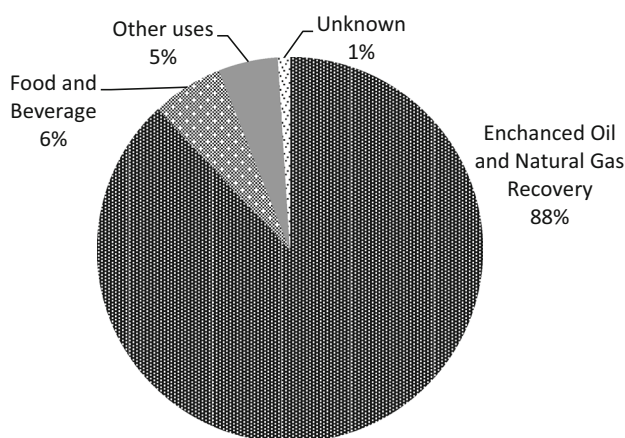


Fig. 1 The United States CO₂ utilisation by sectors in 2011 (US EPA 2011)

sequestration (i.e. injection into the ocean and geological formations (Ghorbani et al. 2014).

Systematic planning and management of CO₂ emissions is a sustainable potential alternative to address the increasing in anthropogenic CO₂ emissions from various major industries, including power plants, chemical plants, refineries, cement production, iron and steel industries (Kravanja et al. 2015). This issue has led to extensive research into proper planning and policy formulation for the past decades and remains a need for effective approaches that can systematically plan CO₂ emission reduction through Process Integration (PI)–Pinch technology. Pinch Analysis (PA) was first developed for the optimal design of heat exchange networks (HEN) by Hohmann (1971) and further developed by Linnhoff and Flower (1978)—see (Klemeš et al. 2014) for detail description. The Composite Curves (CCs) are one of the most widely used techniques for utility targeting in Heat Pinch Analysis (Linnhoff and Flower 1978). PI is a family of methodologies for combining several parts of processes or whole processes to reduce consumption of resources or harmful emissions into the environment. Its methodology has successfully developed over the years into better utilisation and savings regarding energy, water and other resources (Klemeš et al. 2014). PA has successfully emerged as an effective design tool for various resource conservation systems, such as optimal hydrogen systems (Alves and Towler 2002), heat and power (Perry et al. 2008), extended Water Pinch and wastewater minimisation networks (Wan Alwi et al. 2008), design gas network (Wan Alwi et al. 2009), Total Site Heat Integration (Varbanov and Klemeš 2010), biomass supply chain (Lam et al. 2010), solid materials (Klemeš et al. 2012), Power Pinch (Wan Alwi et al. 2012) and mass Pinch Analysis (Martinez-Hernandez et al. 2013). In addition, the PI mathematical programming has been widely explored as an integrated planning tool for bioenergy system footprints (Tan et al. 2009a), multiple plants network involving water integration and hydrogen recovery (Aviso et al. 2011) and for multi-regional biomass production supply chain (Tan et al. 2012). It has also been extended for CO₂ reduction management and planning that included carbon-constrained energy planning (Tan and Foo 2007), electricity (Atkins et al. 2010), energy penalty reduction (Harkin et al. 2010), CO₂ planning in an industrial park (Munir et al. 2012), carbon emission management (Manan et al. 2014), carbon capture and storage (CCS) planning (Ooi et al. 2013a) and waste management Pinch Analysis (Ho et al. 2015).

In Carbon Pinch Analysis, Tan and Foo (2007) introduced a tool for preliminary CO₂ emission planning in the power sector. The graphical Carbon Emission Pinch Analysis (CEPA) approach was introduced to satisfy both energy demand and specified emission limits by the

regions. An extended work on CO₂ constraint planning that was proposed by Tan et al. (2009b) had used the graphical Pinch-based methodology with consideration of CCS retrofit planning in the power generation sector. The use of pinch analysis with a programming optimisation combination is demonstrated to target energy penalty for additional heat and power in CCS implementation (Harkin et al. 2010). The graphical CO₂ emission targeting by Pinch Analysis is addressed for the planning problem of the storage of captured CO₂ in reservoirs. The CO₂ Storage Composite Curves (CSCC) (Ooi et al. 2013a) tool using a targeting method is developed for selection and allocation of CO₂ storage capacity with power plants. A CO₂ Grand Composite Curve (GCC) (Ooi et al. 2013a) is used for scheduling the storage capacity surplus or deficit to ensure adequate CO₂ storage support in CCS networks (Ooi et al. 2013a). Consideration of the capacity and injectivity constraints of the geological demand is proposed for matching CO₂ sources and storage demands within a predefined geographical region as the alternative procedure in CCS planning (Diamante et al. 2013). This work is extended using either graphical or numerical techniques with multi-region systems to overcome the limitation of previous Pinch Analysis approaches in planning (Diamante et al. 2014). A study of CCS using CO₂-constrained energy planning (CCEP) was demonstrated with insight and optimisation-based targeting techniques. In their work, an extended graphical approach and optimisation framework of a targeting method (ATM) (Ooi et al. 2013b) model in the CCS planning problem is developed for solving the multi-period scenarios. There are several works on CO₂ emission reduction that look into the potential of CO₂ reduction planning and management methods using the PA approach. Munir et al. (2012) have introduced a holistic minimum CO₂ emission target within CO₂ demand planning and CO₂ exchange using modified sources and demand curves (SDC). The work considered the CO₂ management hierarchy (CMH) in minimising CO₂ emissions. The maximum CO₂ exchange potential and the minimum CO₂ targets are established by prioritising options via CMH using a graphical Source and Demand Curve. This study has provided a systematic and user-friendly visualisation tool planning for holistic minimum CO₂ targets in industrial parks. An algorithmic method called the generic CO₂ cascade analysis (GCCA) was introduced by Manan et al. (2014) to analyse systematically the CO₂ minimisation options. It includes direct reuse, source and demand manipulations, regeneration reuse and CO₂ sequestration using a numerical approach. The GCCA was developed to complement the generic graphical SDC in terms of efficiency, accuracy and the ability to handle cases involving a large number of stationary CO₂ emission sources and demands in an industrial

park. The work resulted in a potential tool to set the minimum CO₂ emission target and maximum CO₂ recovery.

The concept of Total Site was introduced by Dhole and Linnhoff (1993). The Grand Composite Curve (GCC), first introduced by Linnhoff et al. (1982), was modified for the Total Site (TS) targeting of fuel, cogeneration, emissions and cooling by integrating the heating and cooling system with the site utility system. Klemeš et al. (1997) later developed a Site Utility Grand Composite Curve (SUGCC) targeting method for reduction of fuel, power and CO₂ emissions in TS. Perry et al. (2008) applied TS targeting in Locally Integrated Energy Sectors (LIES) to design both heat and power integration and consequently reduce the carbon footprint. Total Site Heat Integration (TSHI) involved the integration of heating and cooling systems, heat recovery and utilities among multiple processes and/or plants interconnected on an industrial site. A comprehensive overview on the method developments in TSHI can be obtained from Klemeš et al. (2013). TS concept has also been introduced for interplant water integration (Chew and Foo 2009) and interplant hydrogen networks (Deng et al. 2014). In this paper, a new Total Site CO₂ Integration (TSCI) concept with sources and demands incorporating CO₂ purity considerations has been developed in this study, which is innovated from Total Site concept. Throughout the TSCI concept, all CO₂ sources and demands are interconnected by a CO₂ pipeline system on the TS. As CO₂ utilisation technologies begin to mature, and as more industries, which require different purity of CO₂ as their demands are constructed; it will be possible to tap the CO₂ from the constructed headers. This would subsequently reduce the amount of CO₂ stored in the geological reservoirs. Some large-scale CCS projects and CO₂ header pipes have been planned in many regions to channel captured CO₂ from industries to dedicated geological reservoirs. For example, the Global CCS Institute (Global CCS Institute 2014) reported that in China, CO₂ sources from various industries located in potential areas are identified to send their captured CO₂ and sequestration to the dedicated geological storage via pipeline transport.

The TSCI concept proposed in this paper differs from the concept of interplant Hydrogen Integration (Alves and Towler 2002) from several aspects. Firstly, cascading of the CO₂ sources and demands is based on the locations of CO₂ sources and demands along the header and not based on their purities. In addition, the newly proposed TSCI method also includes the targeting of CO₂ purity at each location of the header, targeting the minimum flow rate of fresh CO₂ supply needed for the demands, and screening the appropriate CO₂ sources to enable CCU to be fully utilised and the minimum amount of high-purity CO₂ sent

to the CO₂ storage or reservoir. This is because, the main challenge of CCUS is the need for CO₂ transfer across distances and the cost to integrate the CO₂ sources, sinks and storage. Integration of the existing CCS network with CO₂ utilisation or conversion into value-added products, such as solvents, chemicals and pharmaceuticals (also known CCUS network), has the potential to generate additional revenue and compensate part of the cost of implementing the CO₂ emission reduction strategy (e.g. cost of CO₂ capture technology, transportation, etc.). There are the two example scenarios of TSCI studies are considered to establish the TSCI tool development. In this study, a new numerical technique in TSCI and a procedure to obtain the target of CO₂ emission sources and demands through a centralised header system are developed. The key aspect of this study is to develop a targeting methodology for maximising the recovery of CO₂ to be utilised and minimising CO₂ to be sent for sequestration through centralised CO₂ headers.

Problem statement

Total Site CO₂ Integration (TSCI) involves the integration of CO₂ capture and utilisation across industries and/or plants that are linked by gas headers before the CO₂ sources are permanently stored. The TSCI planning problem can be stated as follows:

Given a set of CO₂ sources (S) and CO₂ demands (D) at different purities (P) along CO₂ capture, utilisation and storage (CCUS) headers, it is desired to develop a planning tool to maximise the utilisation of CO₂ sources to satisfy CO₂ demands across total site, and minimise the amount of CO₂ sent to storage. TSCI consists of one high-purity header and one low-purity header that accept CO₂ sources at different purities, to be used to satisfy CO₂ demands. A stream of fresh CO₂ is available to be mixed with the CO₂ source headers to satisfy a targeted CO₂ demand purity requirement.

The issues derived for the Total Site CO₂ Integration (TSCI) planning are given as

- Can different CO₂ purity headers be created based on the various industry carbon capture technologies? Companies can be charged differently based on their CO₂ purity injected into the header and this can be used as a guideline for policy makers.
- How will the different purity CO₂ (sources) injected into the headers affect the overall purity of CO₂ inside the header?
- How can the amount of CO₂ purity required by industries (demands) be satisfied?

- Can a centralised pure CO₂ generator plant be built to balance the CO₂ purity required by the demands? And what should the capacity be?
- How much CO₂ would be finally stored in the geological reservoirs after it has been utilised by the demands along the headers?

The CO₂ Total Site Problem Table Algorithm (CTS-PTA) has been developed to address all of these issues. The tool can be used for CCUS planners to design future CO₂ headers and develop proper CCUS policies and mechanisms to maximise the CO₂ utilised and minimise the CO₂ stored.

Methodology for Total Site CO₂ Integration (TSCI)

A methodology development of the TSCI targeting technique for optimal carbon target of CO₂ capture, utilisation and storage is described in this section, and new definition for the role of TSCI is illustrated in Fig. 2. The CO₂ Total Site Problem Table Analysis (CTS-PTA) is a developed numerical method for planning and managing the CO₂ sources and demands using centralised headers. Figure 3 shows the overall flowchart of the TSCI methodology.

Step 1: CCUS header for allocation of CO₂ sources and demands

The number of CCUS headers is decided based on the flue gas purity of CO₂ sources and demand in a potential area. The flue gas CO₂ flow rate and purity are determined based on the requirements of the demands. For example, the first header (H1) can be set to only accept flue gas with CO₂ purity that a geological storage (the final destination) can accept, e.g. 80–100 %. The high-purity CO₂ is preferred as impurities in the flue gases have significant impacts on the reservoir system of geological storage (Pearce et al. 2015). The second header (H2) can be set at a lower purity than H1 to satisfy other lower purity demands. For example, it can accept flue gas between 50 and 79.99 % CO₂ purity. Because H1 is designed for reservoir storage as the final destination, the flue gas within H2 must be fully consumed by the last demand at the end of its pipeline. This can be controlled by allowing only a limited amount of sources to inject into this header.

Step 2: identification of CO₂ sources and demands

The CO₂ flowrate of flue gas emissions from various sources can be identified using the following equations:

Fig. 2 Illustration of the TSCI network

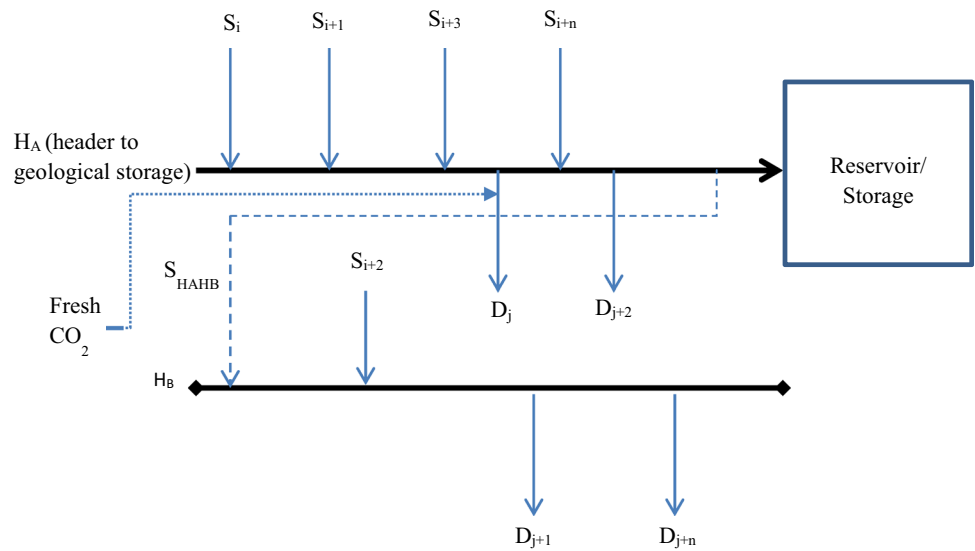
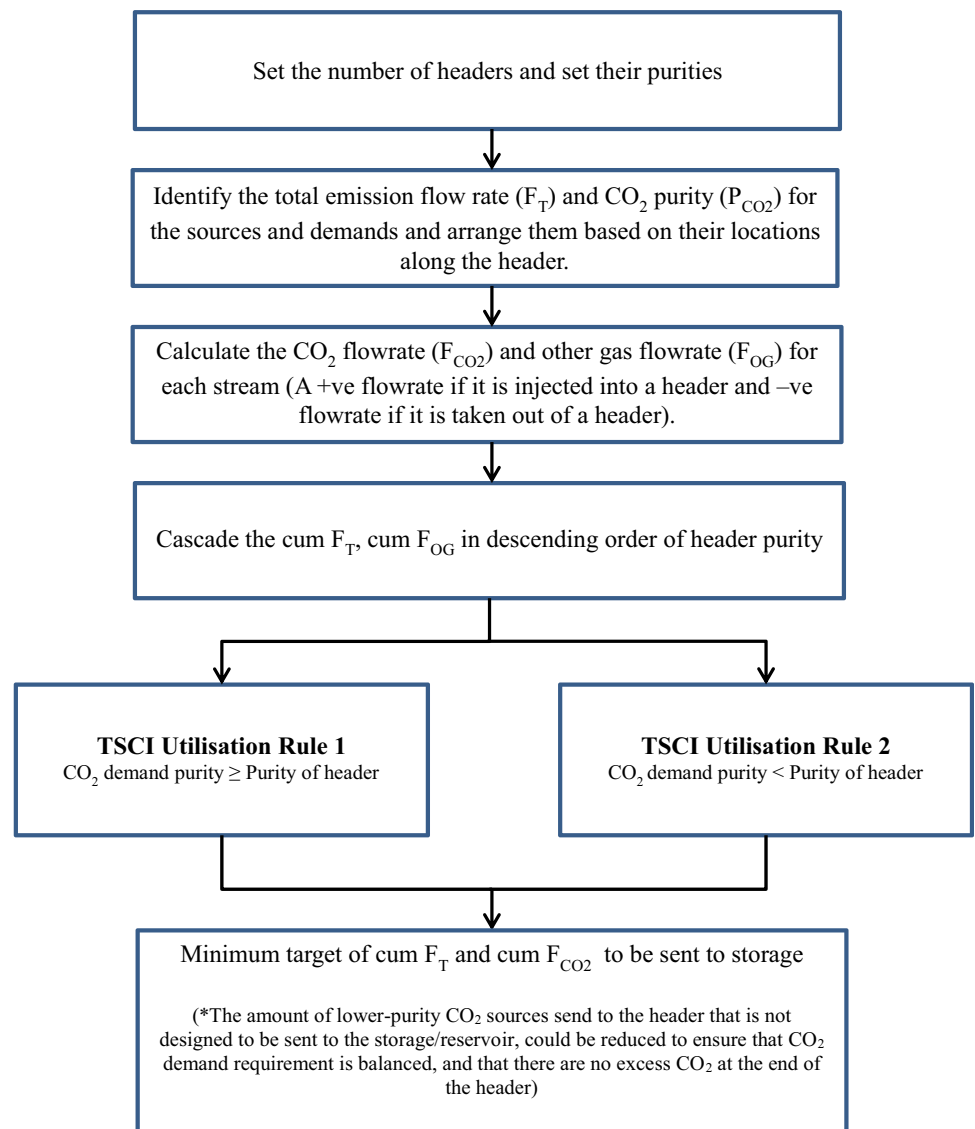


Fig. 3 The flowchart for the TSCI methodology



$$F_{CO_2} = F_T \cdot (P_{CO_2}/100), \quad (1)$$

$$F_{OG} = F_T - F_{CO_2}. \quad (2)$$

Step 3: Problem Table Algorithm construction

The CO₂ Total Site Problem Table Algorithm (CTS-PTA) is constructed to determine the amount of CO₂ target based on the CO₂ TS concept. Available CO₂ sources and demands that have been identified in a region are arranged, based on their location along the headers from the beginning of the pipeline until the identified end. The source gas flow rates (F_T) and the gas CO₂ purity (P_{CO_2}) are obtained from the data. Other industries that can utilise CO₂ (demands) and the minimum P_{CO_2} they can accept are also determined. The amount of CO₂ (F_{CO_2}) within the gas can be calculated using Eq. 1, and other gas flow rates (F_{OG}) such as N₂, O₂, CO, NO_x and SO_x can be calculated using Eq. 2 (Munir et al. 2012) for the pipeline. The numbers of sources and demands and the header that CO₂ can be injected into or taken out for utilisation are listed in Columns 1 and 2. After the end of the H1 line, the remaining gas within H1 will be sent to the geological reservoir for longer term storage. Each source and demand of P_{CO_2} and F_T are arranged in Columns 3 and 4. In Column 4, the source flow rate value is indicated as a positive value as it is adding more flue gas to the header, while the demands flow rate is indicated as a negative value, given that the flue gas is being extracted from the header. The calculated F_{CO_2} and F_{OG} using Eqs. 1 and 2 are listed in Columns 5 and 6. The next key step is cascading sources and demands for H1 first. The sources and demands are required to match by performing F_T and F_{CO_2} cascade. At the sources' locations, F_T and F_{CO_2} for H1 are accumulated from the top to the bottom row starting from zero, as shown in Columns 7 and 8 using Eqs. 3 and 4. The header CO₂ purity (P_{H1}) after accumulating all of the sources can be calculated using Eq. 5 and listed in Column 9 of CTS-PTA:

$$\text{Cum } F_{T,H1,i} = \text{Cum } F_{T,H1,i-1} + F_{T,i}, \quad (3)$$

$$\text{Cum } F_{CO_2,H1,i} = \text{Cum } F_{CO_2,H1,i-1} + F_{CO_2,i}, \quad (4)$$

$$P_{H1,i} = \frac{\text{Cum } F_{CO_2,H1,i}}{\text{Cum } F_{T,H1,i}}. \quad (5)$$

At the demands' locations, F_T and F_{CO_2} are accumulated from the top to the bottom row with $F_{T,H1-D}$, $F_{T,H2-D}$, $F_{CO_2,H1-D}$ and $F_{CO_2,H2-D}$ values considered, as given in Eqs. 6 and 7. The $F_{T,H2-D}$ and $F_{CO_2,H2-D}$ calculations that are indicated for H2 will be explained in the next section. The $F_{T,H1-D}$ and $F_{CO_2,H1-D}$ values are derived from utilisation rules 1 or 2 to satisfy the CO₂ demands. These equations are described as follows:

$$\text{Cum } F_{CO_2,H1,i} = \text{Cum } F_{CO_2,H1,i-1} + F_{CO_2,H1-D,i} + F_{CO_2,H2-D,i}, \quad (6)$$

$$\text{Cum } F_{T,H1,i} = \text{Cum } F_{T,H1,i-1} + F_{T,H1-D,i} + F_{T,H2-D,i}. \quad (7)$$

TSCI utilisation rule 1

The demand requires a higher CO₂ purity ($P_{CO_2,D,i}$) (e.g. 95 %) than the accumulated CO₂ purity in H1 ($P_{CO_2,H1,i-1}$) (e.g. 87 %). To satisfy the requirement, a mixture of pure CO₂ from the centralised CO₂ generator is needed to blend with the header gas. Equations 8 and 9 determine the amount of $F_{CO_2,H1-D}$ (Column 10) and $F_{T,H1-D}$ (Column 11) that are required to supply from H1 to the demand. Equation 10 estimates the flow rate of pure CO₂ ($F_{CO_2,FC-D}$) needed to satisfy the demand purity for H1 (Column 12). If $P_{CO_2,D,i} > P_{CO_2,H1,i-1}$,

$$F_{CO_2,H1-D,i} = F_{OG,D,i} \times P_{H1,i-1} / (1 - P_{H1,i-1}), \quad (8)$$

$$F_{T,H1-D,i} = F_{CO_2,H1-D,i} / P_{H1,i-1}, \quad (9)$$

$$F_{CO_2,FC-D,i} = F_{CO_2,H1-D,i} - F_{CO_2,D,i}. \quad (10)$$

TSCI utilisation rule 2

The demand requires equal or lower CO₂ purity ($P_{CO_2,D,i}$) (e.g. 85 %) than the accumulated CO₂ purity in H1 ($P_{CO_2,H1,i-1}$) (e.g. 87 %). In this case, F_T from H1 is directly supplied to demand, $F_{T,H1-D}$ (Column 11) as the purity demand requirement is fulfilled, Eq. 11. This assumes that the demand can accept equal or higher purity sources. $F_{CO_2,H1-D}$ (Column 10) can be calculated using Eq. 12. If $P_{CO_2,D,i} \leq P_{CO_2,H1,i-1}$,

$$F_{T,H1-D,i} = F_{T,D,i}, \quad (11)$$

$$F_{CO_2,H1-D,i} = F_{T,H1-D,i} \cdot P_{H1,i-1}. \quad (12)$$

The last row for Column 7 (Cum F_T) and Column 8 (Cum F_{CO_2}) gives the minimum target of F_T and F_{CO_2} to be sent to geological storage for the carbon mitigation initiative. The summation of Column 12 gives the total amount of pure CO₂ supplied by the centralised pure CO₂ generator ($F_{CO_2,FC}$) that needs to be blended with H1 to satisfy the high-purity demand as given in Eq. 13:

$$F_{CO_2,FC} = \sum_{i=0}^n F_{CO_2,FC-D}. \quad (13)$$

Next, the same procedures are applied to the other header if required (e.g. H2). Requirements of the sources and demands in H2 are addressed by performing F_T and F_{CO_2} cascading using Eqs. 14 and 15. The Cum $F_{T,H2}$ and Cum $F_{CO_2,H2}$ are shown in Columns 13 and 14. The utilisation rules are followed to satisfy CO₂ demands. However, the cleaner flue gas from H1 has the potential to be

utilised instead of using pure CO₂ to satisfy higher CO₂ purity demands for Utilisation Rule 1. The amounts of F_T taken from H2 ($F_{T,H2-D}$) and H1 ($F_{T,H1-D}$) to satisfy demand at H2 can be calculated using Eqs. 16 and 17. Other equations are similar by replacing H1 with H2.

$$\text{Cum}F_{\text{CO}_2,\text{H}_2,i} = \text{Cum}F_{\text{CO}_2,\text{H}_2,i-1} + F_{\text{CO}_2,\text{H}_2-D,i}, \quad (14)$$

$$\text{Cum}F_{T,\text{H}_2,i} = \text{Cum}F_{T,\text{H}_2,i-1} + F_{T,\text{H}_2-D,i}, \quad (15)$$

$$F_{T,\text{H}_2-D,i} = (F_{T,D,i} \times P_{\text{H}_1,i}) - \left[\frac{F_{T,D,i} \times P_{\text{H}_1,i}}{P_{\text{H}_2,i} - P_{\text{H}_1,i}} \right], \quad (16)$$

$$F_{T,\text{H}_1-D,i} = F_{T,D,i} - F_{T,\text{H}_2-D,i}. \quad (17)$$

As H2 is designed to not send to the geological storage, the last row of Cum F_{T,H_2} (Column 13) and Cum $F_{\text{CO}_2,\text{H}_2}$ (Column 14) should not give any access where the surplus value of F_T and F_{CO_2} should be reduced by part of the sources (preferably the one with lower purity) into H2 until the last row of Cum F_{T,H_2} and Cum $F_{\text{CO}_2,\text{H}_2}$ gives a zero value, which is also the pinch point of this TSCI system.

Example scenario 1

The new CTS-PTA method case study in Texas is adapted from Hasan et al. (2014) and Munir et al. (2012) to demonstrate the developed tool. The identification data of CO₂ sources and demands are listed in Table 1 (sources) and Table 2 (demands). Eight sources of potential CO₂ captures and four potential points of CO₂ demands are identified to be sent to dedicated CO₂ geological storage.

Referring to Tables 1 and 2, two headers were set with a purity range between 80 and 99.99 % for Header 1 (H1) and between 50 and 79.99 % for Header 2 (H2). Headers are based on the purity data range. Equations 1 to 5 determine the flow rate and purity of CO₂ sources and demands. The CO₂ sources and demands are arranged accordingly into significant headers purity. S1, S3, S4, S6, S7 and S8 sources can supply CO₂ to H1, while S2 and S5 supply to H2. The same concept is applicable to the demands that are applied to CO₂ supply. The D1 and D2

demands can extract CO₂ from H1, while D3 and D4 can extract from the lower purity range, which is H2, to satisfy their needs. The arrangement of the sources and demands along the header is assumed as shown in Table 3. Positive values indicate CO₂ input flow rate into the header, and negative values are output flow rate from the header.

CO₂ header refers to the CO₂ pipeline system, which is heading to CO₂ storage as the end-of-pipe solution for captured CO₂ emission. The locations of sources and demands are important in a region to perform the targeting CO₂ supplied and amount required sent to geological storage. As explained in the methodology section, CTS-PTA is performed to optimise CO₂ capture, utilisation and storage. The results are indicated as shown in Tables 4 and 5 for TSCI Scenario 1.

In Table 4, the minimum amount of remaining CO₂ in Column 7 (H1) after cascading is 1582.5 t/h, which needs to be sent to geological reservoirs ($F_{T,\text{ST}}$) for CO₂ storage, and CO₂ purity in the stream is accumulated to 84 %. Table 5 shows the continuing CTS-PTA performed for H2. It can be seen that there is excess CO₂ in the last row in Column 13 (Cum F_{T,H_2}), about 375 t/h of CO₂. As H2 does not have access to storage, this value needs to be deducted with a source from H2 (i.e. S2), the largest source in H2. Instead of sending the entire 608.5 t/h of S2 which is the largest CO₂ source to H2, only 233.45 t/h of S2 is supplied into H2 to ensure that CO₂ demand requirement is balanced, and that there is no excess CO₂ at the end of header H2. This is also the pinch point of the system, and noted that prior to considering TSCI, the CO₂ (e.g. S₂ with $F_{T,\text{S}_2} = 375$ t/h) from header H2, which cannot be stored, might still be emitted to the environment. Prior to satisfying the high-purity demand of CO₂, fresh CO₂ from the centralised pure CO₂ generator is requested. An amount of 46.5 t/h of $F_{\text{CO}_2,\text{FC-D}}$ is injected to satisfy the D1 demand and no fresh CO₂ is supplied to H2 as the purity demands in H2 are lower than for the supply stream. Note that H1 is capable of supplying CO₂ to H2 whenever it is required (e.g. S_{H1-H2}) by following TSCI utilisation rules; if not required, the remaining CO₂ emissions are injected into storage as the final destination (Fig. 4).

Table 1 Data for CO₂ sources

Source (S)	Description	P_{CO_2} (%)	F_T (t/h)	F_{CO_2} (t/h)	F_{OG} (t/h)
S1	Cement	90	138.8	124.9	13.9
S2	Refineries/chemical	70	608.5	425.9	182.5
S3	Power (coal based)	85	1174.3	998.2	176.1
S4	Power (NG based)	88	101.5	89.3	12.2
S5	Agricultural	65	69.9	45.4	24.4
S6	Petrochemical	80	615.4	492.3	123.1
S7	Gas processing	90	36.5	32.8	3.6
S8	Iron & steel (corex)	95	27.9	26.5	1.4

Table 2 Data for CO₂ demands

Demand (D)	Description	P_{CO_2} (%)	F_T (t/h)	F_{CO_2} (t/h)	F_{OG} (t/h)
D1	Beverage plant	99	50.0	49.5	0.5
D2	Enhance oil recovery	80	208.3	166.6	41.7
D3	Methanol production	50	83.3	41.7	41.7
D4	Micro algae production	10	220.0	22.0	198.0

Table 3 CO₂ sources and demands header

1 S/D	2 Header	Description	3 P_{CO_2} (%)	4 F_T (t/h)	5 F_{CO_2} (t/h)	6 F_{OG} (t/h)
S1	H1	Cement	90	138.8	124.9	13.9
S2	H2	Refinery/chemical	70	608.5	425.9	182.5
S3	H1	Power (coal)	85	1174.3	998.2	176.2
D1	H1	Beverage plant	99	-50.0	-49.5	-0.50
S4	H1	Power (natural gas)	88	101.5	89.3	12.2
S5	H2	Agricultural	65	69.9	45.4	24.5
D2	H1	Enhanced oil recovery (EOR)	80	-208.3	-166.6	-41.7
S6	H1	Petrochemical	80	615.4	492.3	123.1
S7	H1	Gas processing	90	36.5	32.8	3.7
S8	H1	Iron & steel	95	27.9	26.5	1.4
D3	H2	Methanol production	50	-83.3	-41.7	-41.7
D4	H2	Micro algae production	10	-220.0	-22.0	-198.0

Table 4 CTS-PTA Scenario 1 for H1

i	1	2	3	4	5	6	7	8	9	10	11	12
	S/D	Header	$P_{CO_2, S/D}$ %	$F_{T, S/D}$ t/h	$F_{CO_2, S/D}$ t/h	$F_{OG, S/D}$ t/h	Cum $F_{T, H1}$ t/h	Cum $F_{CO_2, H1}$ t/h	$P_{CO_2, H1}$	$F_{CO_2, H1-D}$ t/h	$F_{T, H1-D}$ t/h	$F_{CO_2, FC-D}$ t/h
1	S1	H1	90	138.8	124.9	13.9	138.8	124.9	0.90			
2	S2	H2	70				138.8	124.9	0.90			
3	S3	H1	85	1,174.3	998.2	176.1	1,313.1	1,123.1	0.86			
4	D1	H1	99	-50.0	-49.5	-0.5	1,309.6	1,120.1	0.86	-3.0	-3.5	46.5
5	S4	H1	88	101.5	89.3	12.2	1,411.1	1,209.4	0.86			
6	S5	H2	65				1,411.1	1,209.4	0.86			
7	D2	H1	80	-208.3	-166.6	-41.7	1,202.8	1,030.9	0.86	-178.5	-208.3	
8	S6	H1	80	615.4	492.3	123.1	1,818.2	1,523.2	0.84			
9	S7	H1	90	36.5	32.8	3.6	1,854.6	1,556.0	0.84			
10	S8	H1	95	27.9	26.5	1.4	1,882.5	1,582.5	0.84			
11	D3	H2	50				1,882.5	1,582.5	0.84			
12	D4	H2	10				1,882.5	1,582.5	0.84			
							$F_{T, ST} = 1,882.5$	$F_{CO_2, ST} = 1,582.5$	$P_{CO_2, ST} = 0.84$			

Fresh CO₂ injected to satisfy purity demand, D1

Table 5 CTS-PTA Scenario 1 for H2

	1	2	3	4	13	14	15	16	17
i	S/D	Header	$P_{CO_2, S/D}$ %	F_T , t/h	Cum $F_{T, H2}$ t/h	Cum $F_{CO_2, H2}$ t/h	$P_{CO_2, H2}$	$F_{CO_2, H2-D}$ t/h	$F_{T, H2-D}$, t/h
1	S1	H1	90		0.0	0.0	0.0		
2	S2	H2	70	608.5	608.5	425.9	0.70		
3	S3	H1	85		608.5	425.9	0.70		
4	D1	H1	99		608.5	425.9	0.70		
5	S4	H1	88		608.5	425.9	0.70		
6	S5	H2	65	69.9	678.3	471.3	0.69		
7	D2	H1	80		678.3	471.3	0.69		
8	S6	H1	80		678.3	471.3	0.69		
9	S7	H1	90		678.3	471.3	0.69		
10	S8	H1	95		678.3	471.3	0.69		
11	D3	H2	50	-83.3	595.0	413.5	0.69	-57.9	-83.3
12	D4	H2	10	-220.0	375.0	260.6	0.69	-152.9	-220.0
					$F_{T, H2} = 375.0$				

Example scenario 2

In this scenario, TSCI will be studied using the proposed method with a one-header approach. There are eight CO₂ sources and four CO₂ demands, as stated in Tables 1 and 2 previously. All of the sources and demands are integrated to estimate the optimal CCUS using a header. Figure 5 shows the illustrated CCUS network in this scenario.

The CTS-PTA is then performed by following the methodology steps for TSCI targeting. As the set header is one, equations for H2 are neglected (Table 6).

The minimum amount of remaining CO₂ in Column 8 after cascading is 1821.2 t/h, which needs to be sent to geological reservoirs ($F_{CO_2, ST}$) for CO₂ storage. The CO₂ purity in the stream header is accumulated to 81 %. An amount of 47.4 t/h of $F_{CO_2, FC-D}$ is injected to satisfy the D1 demand.

The amount of CO₂ sent to geological storage in Scenario 1 is higher than in Scenario 2; however, note that in Scenario 1, an amount of 199.9 t/h of captured CO₂ from

S2 that cannot be stored might still be emitted to the atmosphere as the pinch point of H2 is achieved, while in Scenario 2, there will be no captured CO₂ that might be emitted to the atmosphere as no pinch point is considered, and all excess CO₂ will be sent to storage. The CO₂ purity accumulated in the header that is headed for geological storage is slightly lower, 81 % (Scenario 2), compared with CO₂ purity accumulated in Scenario 1 (84 %). In this study, however, both purity percentages of CO₂ captured are accepted as the geological storage is assumed to accept 80 % and above of CO₂ purity. The comparison results are shown in Table 7. Note that the assumption of this case is in reference to the CCS with no CCUS applied.

Increasing the carbon storage life capacity of sequestration would reduce the potential of CO₂ emissions leaking into the atmosphere. The results indicate that Scenario 1 gives the lowest CO₂ amount to be sent to storage followed by CCS (base case) and Scenario 2. However, the base case has resulted in higher CO₂ emissions emitted into the atmosphere as only some sources are captured and sent

Fig. 4 An optimal TSCI network for Scenario 1

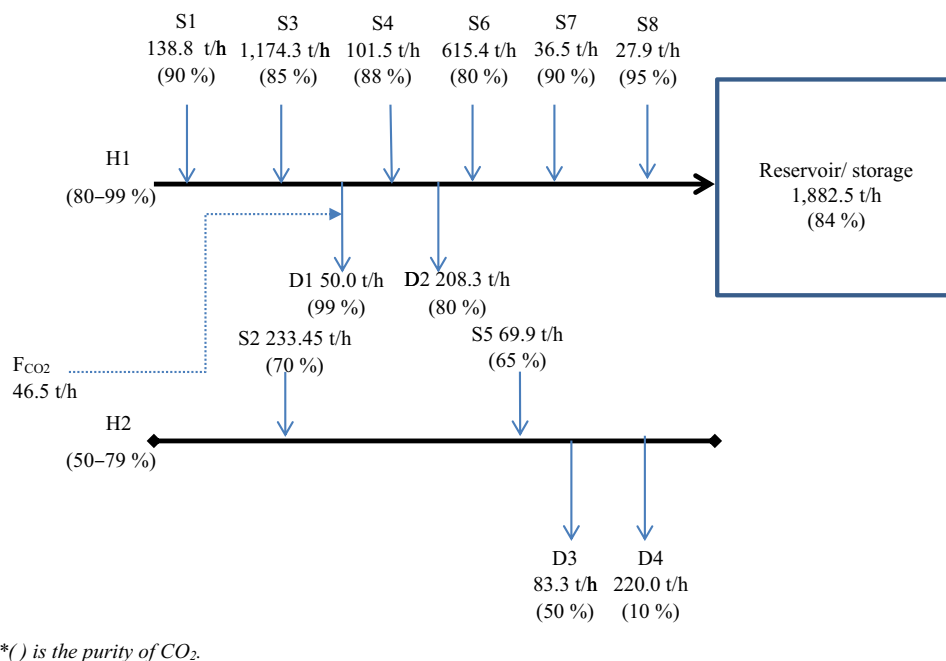
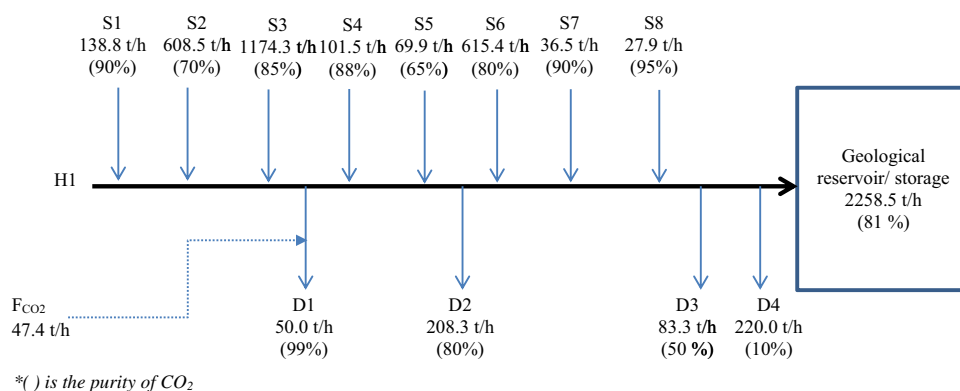


Fig. 5 An optimal TSCI network for Scenario 2



to storage. The low CO₂ fresh flowrate resulting in Scenario 1 would reduce the overall capital cost of fresh CO₂ generation compared with Scenario 2. Although Scenario 2 has no CO₂ emitted into the atmosphere, it has resulted in the highest amount CO₂ to be stored. In addition, the cumulative CO₂ in Scenario 2 gave the lowest purity (81 %) compared with others, but still within the accepted minimum purity for CO₂ storage, i.e. 80 %. This shows that a single header of CO₂ will create uncertain storage conditions and lead to difficulty in controlling the CO₂ purity from various emission sources. Thus, Scenario 1 has resulted with the optimal CCUS condition with reduction in CO₂ amount to be sent to storage and CO₂ fresh supply to satisfy the demands. Based on the estimation of targeting the CO₂ sources, demands and storage in this study, the carbon storage life capacity has potentially been lengthened by about 10.3 % within the CCUS consideration of

Scenario 1. Furthermore, using this approach may add some specific requirement for pipeline systems, and the numbers of compressors or pump installations will be increased to distribute and transport the CO₂ emissions among the headers.

Conclusion

Total Site CO₂ Integration (TSCI), known as CTS-PTA, has been developed to target the maximum CO₂ being utilised for achieving the minimum CO₂ stored in geological storage. The approach for targeting the CO₂ captured, utilisation and storage for the integrated CCUS network is introduced. This method has been applied to a hypothetical case study to determine the potential CO₂ exchange by using multiple and single CO₂ headers at

Table 6 CTS-PTA Scenario 2

<i>l</i>	1 S/D	2 Header	3 $P_{CO_2,S/D}$ (%)	4 $F_{T,S/D}$ (t/h)	5 $F_{CO_2,S/D}$ (t/h)	6 $F_{OG,S/D}$ (t/h)	7 Cum $F_{T,H}$ (t/h)	8 Cum $F_{CO_2,H}$ (t/h)	9 $P_{CO_2,H}$	10 $F_{CO_2,H-D}$ (t/h)	11 $F_{T,H-D}$ (t/h)	12 $F_{CO_2,FC-D}$ (t/h)
1	S1	H1	90	138.8	124.9	13.9						
							138.8	124.9	0.90			
2	S2	H1	70	608.5	425.9	182.5						
							747.3	550.9	0.74			
3	S3	H1	85	1174.3	998.2	176.1						
							1921.6	1549.0	0.81			
4	D1	H1	99	-50.0	-49.5	-0.5				-2.1	-2.6	47.4
							1919.0	1546.9	0.81			
5	S4	H1	88	101.5	89.3	12.2						
							2020.5	1636.3	0.81			
6	S5	H1	65	69.9	45.4	24.4						
							2090.4	1681.7	0.80			
7	D2	H1	80	-208.3	-166.6	-41.7				-167.6	-208.3	
							1882.1	1514.1	0.80			
8	S6	H1	80	615.4	492.3	123.1						
							2497.5	2006.4	0.80			
9	S7	H1	90	36.5	32.8	3.6						
							2533.9	2039.2	0.80			
10	S8	H1	95	27.9	26.5	1.4						
							2561.8	2065.7	0.81			
11	D3	H1	50	-83.3	-41.7	-41.7				-67.2	-83.3	
							2478.5	1998.5	0.81			
12	D4	H1	10	-220.0	-22.0	-198.0				-177.4	-220.0	
							2258.5	1821.2	0.81			
							$F_{T,ST}$ =2258.5	$F_{CO_2,ST}$ =1821.2	$P_{CO_2,ST}$ =0.81			

Table 7 Summary of results between CCS (base case), Scenario 1 and Scenario 2

	Base case: CCS (without utilisation header)	Scenario 1	Scenario 2
CO ₂ sequestered in storage	1,764 t/h (accepted > 80 % CO ₂ purity from sources)	1,582.5 t/h	1,821.2 t/h
Purity of CO ₂ sequestered	84 %	84 %	81 %
Fresh/Outsource CO ₂ (based on CO ₂ demands)	448.1 t/h	46.5 t/h	47.4 t/h
Potential CO ₂ emissions	346.1 t/h (sources from CO ₂ emission < 80 % purity)	199.9 t/h	-

different purities, and a centralised pure CO₂ generator. With a reduction of 32 and 19 % of carbon storage for different scenarios, this new technique is estimated to plan and manage the CO₂ emission in a sustainable manner and has a lower risk of CO₂ leakage if diluted CO₂ emissions were to continue being utilised. It will simultaneously extend the geological carbon storage life capacity. The targeting technique enables planners to conduct further

analysis and feasibility studies systematically to match the potential sources and demands for a CCUS integrated system. For an optimal CO₂ management and planning strategy in a multi-region system, future studies on a TSCI network should include detailed assessments and considerations of the layout and length of pipelines, availability of CO₂ sources as well as CO₂ demands, and storage locations. In addition, detailed analysis of the energy and

economics of a TSCI network is necessary in order to develop a sustainable CO₂ reduction planning and management system.

Acknowledgments The authors thank the Ministry of Higher Education Malaysia and Universiti Teknologi Malaysia (UTM) for providing the research funds for this project under the research grant votes Q. J130000.2544.07H45, Q. J130000.2409.03G40 and the Pázmány Péter Catholic University (PPKE), Faculty of Information Technology and Bionics, Budapest, Hungary.

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