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A New Algebraic Pinch Analysis Tool for Optimising CO_2 Capture, Utilisation and Storage

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Optimal CO_2 reduction planning can curb the rise in environmental emissions due to the increase in energy demand and utilisation. Carbon (more precisely, CO_2) Capture and Storage (CCS) has been one of the proposed solutions to control CO_2 emissions. However, mitigating CO_2 emissions via CO_2 storage in geological reservoirs without utilisation is neither a sustainable solution, nor really a clean technology option. This paper introduces a new algebraic method for targeting the optimum CO_2 capture, utilisation and storage based on the Pinch Analysis approach. A new Total Site CO_2 Integration concept is introduced. The concept is to capture CO_2 with certain quality from various plants on the Total Site and inject it into CO_2 headers. The CO_2 headers are divided into certain composition ranges. The CO_2 headers can satisfy the CO_2 demands for various industries located along the headers, which require CO_2 as its raw material. The CO_2 can be further regenerated, and mixed as needed with pure CO_2 generated from one or multiple centralised CO_2 plant if required. The excess CO_2 is to be sent to geological storage. The proper utilisation of CO_2 will reduce the amount of CO_2 needed to be stored. This will extend the geological carbon storage-life capacity. Aside from estimating CO_2 utilisation, this method also allows an industrial site planner to identify the suitable industries that can act as CO_2 sources or CO_2 demands for a given region.

1. Introduction

The increase of CO_2 emissions induced by use of fossil fuels has initiated an urgent need for proper CO_2 reduction planning that includes CO_2 sequestration, utilisation and storage. Many studies dealt with carbon capture and storage (CCS) to mitigate climate change by capturing CO_2 into geological sequestration (Diamante et al., 2014), biological fixation (Geerlings and Zevenhoven, 2013) or utilisation (Man et al., 2014). CCS is a tool for CO_2 reduction in the atmosphere. It involves the capture of CO_2 from an industrial plant and its storage in secure reservoirs, to enable the usage of fossil fuels while controlling the CO_2 emitted into the atmosphere. CCS is an integrated process made up of three distinct parts; CO_2 capture, transport and storage. Capture technology aims to produce a concentrated stream of CO_2 that can be compressed, transported and stored. Transport of captured CO_2 is mostly by pipeline, however it depends on the distance and cost. The sequestration of the captured carbon is the final part of the process (Oh, 2010).

Earlier work in CCS by Tan et al. (2009) determines the CO_2 emission target while minimising the need of power plant retrofit. The authors used a Pinch Analysis (PA) graphical methodology, which provides useful insights for the planning and optimisation of power generation. A study of CCS using Carbon Constrained Energy Planning (CCEP) was also demonstrated with insight and optimisation based targeting techniques for multi-period scenarios (Ooi et al., 2014). Related to CCS, Soundararajan et al. (2014) studied the carbon capture technology in order to improve the CO_2 capture efficiency. The assessment of the CCS

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however revealed that the technology not only demands major capital investments, it is also not suitable for ocean territories and when there is limited land for geological storage. CCS has merely been adopted as a transitional technology (Câmara et al., 2013).
A derivative of CCS, namely CO_2 capture, utilisation and storage (CCUS) is the potential technology to utilise captured CO_2 as an alternative to mitigate climate change (Pérez-Fortes et al., 2014). Utilisation or conversion of the captured CO_2 into value-added products, such as solvent and pharmaceutical products, has the potential to generate additional revenue and compensate part of the high cost of implementing the CCS technology. A new plant with CCS technology has an incremental cost of about 7 % for 25 % of CO_2 avoidance (Lee and Hashim, 2014). Many challenges consequently exist in achieving the successful CO_2 utilisation, including the development of technologies capable of economically fixing CO_2 in stable products for indirect storage. The technological investigation to discover new applications and reaction, which do not use energy that exceed the CO_2 utilised are needed to reduce the net CO_2 emission (US DOE, 2014). Carbon capture and utilisation (CCU) on a coal gasification process has resulted in increased process carbon element efficiency and in carbon footprint reduction (Man et al., 2014). There are recent works on CO_2 emission reduction that look into the potential CO_2 reduction planning and management methods. Munir et al. (2012) have introduced Carbon Pinch Analysis (CPA) to target the minimum fresh carbon and carbon emission for stationary point sources in a refinery industrial park. The paper considered Carbon Management Hierarchy (CMH) in minimising the CO_2 emissions. An algorithmic method called Generic Carbon Cascade Analysis (GCCA) technique was introduced by Manan et al. (2014) to systematically analyse the carbon minimisation options including direct reuse, source and demand manipulations, regeneration reuse and carbon sequestration. The work resulted in an accurate tool to set the minimum carbon emission target and maximum carbon recovery. The papers however do not consider the utilisation of specific CO_2 headers or integration with the existing CCS planning and development.
This paper presents a new algebraic technique and a procedure to obtain the total site target for the CO_2 utilisation and storage integration. Total Site (TS) heat inetgration involves the integration of heat recovery among multiple processes and/or plants interconnected by common utilities on an industrial site. The method was introduced by Dhole and Linnhoff (1993) and further developed into TS heat recovery targeting by Klemeš et al. (1997). A comprehensive overview on the method developments in Total Site Heat Integration (TSHI) can be referred to Klemeš et al. (2013). The concept of TSHI has been adapted to the new Total Site Carbon Integration (TSCI) concept introduced in this work. Currently, there are CO_2 header pipes being planned to be constructed in many regions to channel captured CO_2 from industries to geological reservoirs. For example in China, CO_2 sources from various industries located in different districts or provinces are identified to send their captured CO_2 and sequester to the dedicated geological storage via pipe line transport (Global CCS Institute, 2014). The idea is, as CO_2 utilisation technologies begins to mature, and as more industries which require different purity of CO_2 as their demands are constructed, it will be possible for these industries to tap the CO_2 from the constructed headers. This will subsequently reduce the amount of CO_2 stored in the geological reservoirs and lengthen the reservoirs life time. Several questions remain to be addressed such as: 1) Can different CO_2 purity headers be created based on the various industry carbon capture technologies? The charge for the industries to inject their CO_2 into the higher purity headers will be less than the lower purity headers. (2) How will the different purity CO_2 (sources) injected into the headers affect the overall purity of CO_2 inside the header? (3) How can the amount of CO_2 purity required by the industries (demands) be satisfied? Can a centralised pure CO_2 generator plant be built to balance the CO_2 purity required by the demands? And what shall the capacity be? (4) How much CO_2 will be finally stored in the geological reservoirs after it has been utilised by the demands along the headers? The Carbon Total Site Problem Table Algorithm (CTS-PTA) has been developed to address all these issues. The tool can be used for CCUS planners to design future CO_2 headers and develop proper CCUS policies and mechanisms to maximise the CO_2 utilised and minimise the CO_2 stored.

2. Methodology

Following is the developed methodology for TSCI.

2.1 Step 1: Set the number of CCUS header for the region and decide its header CO_2 purity

Decide on the number of CCUS header for the region and the flue gas CO_2 purity which needs to be transported along the pipe lines. For example, the first header (H1) can be set to only accept flue gas with CO_2 purity which a geological sequestration (the final destination) can accept e.g. 80 to 100 %. The second header (H2) can be set at a lower purity for demands which do not need a high purity CO_2. For example it can transport flue gas between 50 to 79.99 % CO_2 purity. Since Header 2 flue gas cannot be sent to a geological sequestration as the final destination (since its purity is lower than 80 %), the flue gas within this line must be fully consumed by the last demand at the end of its pipeline. This can be controlled by allowing only limited amount of sources to be injected into this header.

2.2 Step 2: Identify the CO_2 sources and demands

Identify the industries along the header which can capture CO_2 (Sources). Obtain the sources gas flowrate (F_T) and the gas CO_2 purity (P_{CO2}). Identify also the industries which can utilise CO_2 (Demands). Obtain the demands F_T and the minimum P_{CO2} it can accept. The amount of CO_2 (F_{CO2}) within the gas can be calculated by using Eq(1) as described by Munir et al. (2012). Other gases flowrate (F_{OG}) such as N_2, O_2, CO, NO_x and SO_x can be calculated using Eq(2).

$$F_{CO2}=F_T.\ (P_{CO2}\ /100) \quad (1)$$

$$F_{OG}= F_T - F_{CO2} \quad (2)$$

2.3 Step 3: Construct CO_2 Total Site-Problem Table Algorithm (CTS-PTA)

Construct the CTS-PTA to determine the amount of CO_2 target based on TS concept. The procedure is as follows:

i. Sources and demands are arranged based on its location along Header 1 and 2 from the beginning of the pipe line until the end of the pipe line. After the end of the Header 1 line, the remaining gas within Header 1 will be sent to the geological reservoir. The sources and demands number and the header the CO_2 will be injected into or taken out for utilisation are listed in Columns 1 and 2.
ii. P_{CO2} and F_T from each sources and demands are listed in Columns 3 and 4. The demand flowrate is listed as negative values to indicate it is extracting the flue gas from the header, while the sources flowrate is listed as positive values to indicate it is adding more flue gas into the header.
iii. F_{CO_2} and F_{OG} are determined using Eq(1) and Eq(2) and listed in Columns 5 and 6.
iv. The next key step is to match the sources and sinks requirement by performing F_T and F_{CO2} cascading for Header 1 first.

- At the sources' locations, F_T and F_{CO_2} for H1 are cumulated from the top to the bottom row starting from zero as shown in Columns 7 and 8 using Eq(3) and Eq(4). The header CO_2 purity (P_{H1}) after cumulating all the sources is calculated by using Eq(5) and listed in Column 9.

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

$$\text{Cum } F_{CO2,H1,i} = \text{Cum}F_{CO2,H1,i-1} + F_{CO2,i} \quad (4)$$

$$P_{H1,i} = \frac{\text{Cum}F_{CO2,H1,i}}{\text{Cum}F_{T,H1,i}} \quad (5)$$

- At the demands' locations, F_T and F_{CO2} are cumulated from the top to the bottom row with $F_{T,H1\text{-}D,}$ $F_{T,H2\text{-}D,}$ $F_{CO2,H1\text{-}D}$ and $F_{CO2,H2\text{-}D}$ values as shown in Eq(6) and Eq(7). $F_{T,H2\text{-}D}$ and $F_{CO2,H2\text{-}D}$ calculations will be explained in Step v. The $F_{T,H1\text{-}D}$ and $F_{CO2,H1\text{-}D}$ values are derived from utilisation rule 1 or 2 equations as described next.

$$\text{Cum}F_{CO2,H1,i} = \text{Cum}F_{CO2,H1,i-1} + F_{CO2,H1-D,i} + F_{CO2,H2-D,i} \quad (6)$$

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

Utilisation Rule 1: Demand requires a higher CO_2 purity ($P_{CO2,D,i}$) (e.g. 95 %) than the cumulated CO_2 purity in Header 1 ($P_{CO2,H1,i\text{-}1}$) (e.g. 87 %). This indicated the demand need to blend the header gas with pure CO_2 which is taken from the centralised CO_2 generator in order to satisfy the demand requirement. Eq(8) and Eq(9) are used to determine the amount of $F_{CO_2,H1\text{-}D}$ (Column 10) and $F_{T,H1\text{-}D}$ (Column 11) supplied from Header 1 to the demand and Eq 10 is used to estimate the flowrate of pure CO_2 ($F_{CO_2,\ FC\text{-}D}$) needed to satisfy the demand purity for H1 (Column 12).

If $P_{CO2,D,i} > P_{CO2,H1,i-1}$

$$F_{CO2,H1-D,i} = F_{OG,D,i} * P_{H1,i-1}/(1 - P_{H1,i-1}) \quad (8)$$

$$F_{T,H1-D,i} = F_{CO2,H1-D,i}/P_{H1,i-1} \quad (9)$$

$$F_{CO2,FC-D,i} = F_{CO2,H1-D,i} - F_{CO2,D,i} \quad (10)$$

Utilisation Rule 2: Demand requires equal or lower CO_2 purity ($P_{CO2,D,i}$) (e.g. 85 %) than the cumulated CO_2 purity in Header 1 ($P_{CO2,H1,i\text{-}1}$) (e.g. 87 %). In this case, F_T from header 1 is directly supplied to demand, $F_{T,H1\text{-}D}$ (Column 11) as the purity demand requirement is fulfilled Eq(11). This is with the assumption that the demand can accept equal or higher purity sources. $F_{CO2,H1-D}$ (Column 10) can be calculated from Eq(12).

If $P_{CO2,D,i} \leqslant P_{CO2,H1,i-1}$,

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

$$F_{CO2,H1-D,i} = F_{T,H1-D,i} . P_{H1,i-1} \quad (12)$$

The last row for Cum F_T and Cum F_{CO2} gives the minimum target of F_T and F_{CO2} to be sent to geological storage for carbon mitigation initiative. The summation of Column 12 gives the total amount of *pure CO_2 which needs to be supplied by the centralised pure CO_2 generator ($F_{CO2,FC}$) as shown in* Eq(13).

$$F_{CO2,FC} = \sum_{i=0}^{n} F_{CO2,FC-D} \quad (13)$$

v. Next, the same procedures as iv are applied to perform the F_T and F_{CO2} cascading for Header 2. However, the cumulative F_T and F_{CO2} equation for Header 2 is calculated using Eq(14) and 15 as shown in Columns 13 and 14.

$$CumF_{CO2,H2,i} = CumF_{CO2,H2,i-1} + F_{CO2,H2-D,i} \quad (14)$$

$$CumF_{T,H2,i} = CumF_{T,H2,i-1} + F_{T,H2-D,i} \quad (15)$$

For utilisation rule 1, instead of using pure CO_2, the cleaner flue gas from Header 1 will be utilised. The amount of F_T taken from Header 1 and Header 2 for satisfying a demand at Header 2 ($F_{T,H2-D}$, $F_{T,H1-D}$) can be calculated using Eq(16) and Eq(17). The other equations are similar by replacing H1 with H2.

$$F_{T,H2-D,i} = (F_{T,D,i} * P_{H1,i}) - [\frac{F_{T,D,i} * P_{H1,i}}{P_{H2,i} - P_{H1,i}}] \quad (16)$$

$$F_{T,H1-D,i} = F_{T,D,i} - F_{T,H2-D,i} \quad (17)$$

As stated previously, there should not be any excess F_T and F_{CO2} at the last row of Cum $F_{T,H2}$ and Cum $F_{CO2,H2}$. Hence, part of the sources (preferably the one with lower purity) into Header 2 should be reduced until the last row of Cum $F_{T,H2}$ and Cum $F_{CO2,H2}$ gives a zero value.

3. Case study

The new CTS-PTA method is illustrated using a hypothetical case study. The source and demand data for this case study is listed in Table 1.

Table 1: Data for CO_2 sources and demands.

Source (S)/ Demand (D)	Description	P_{CO2}, %	F_T, t/h	F_{CO2}, t/h	F_{OG}, t/h
S1	Natural gas power plant	88	179.9	158.3	21.6
S2	Coal power plant	85	92.9	79.0	13.9
S3	Refinery plant	60	100.0	60.0	40.0
S4	Oil power plant1	80	118.1	94.5	23.6
S5	Oil power plant2	80	118.1	94.5	23.6
D1	Beverage plant	99	50.0	49.5	0.5
D2	Methanol production	50	83.3	41.7	41.7
D3	Enhanced oil recovery (EOR)	80	208.3	166.6	41.7
D4	Chemical Plant	70	20.0	14.0	6.0

Header 1 (H1) was set for purity range between 80 to 100 % and Header 2 (H2) was set for purity range between 50 to 79.99 %. From Table 1, S1, S2, S4 and S5 can supply CO_2 gas to H1, while S3 to H2. D1 and D3 can extract CO_2 gas from H1, while D2 and D4 can extract gas from H2 and H1. Table 2 shows the CTS-PTA for the case study. Based on the CTS-PTA, the minimum amount of remaining CO_2 gas to be sent to geological reservoirs ($F_{T,ST}$) is 289.1 t/h. By summing Column 12, the centralised pure CO_2 generator needs to generate 46.7 t/h of CO_2. From Table 2b, it can be seen there are excess Cum $F_{T,H2}$ at the last row. As Header 2 cannot have excess, this value is deducted with a source from H2 i.e. S3. Instead of injecting 100 t/h of S3, only 94.9 t/h is injected to get the last row of Cum $F_{T,H2}$ to be zero. This is

also the pinch point of the system. Note that prior to considering TSCI, the CO_2 (e.g. S3 with $F_{T,S3}$ = 94.9 t/h) from lower purity (less than 80 %), which cannot be stored might still be emitted to the environment. The amount of CO_2 gas sent to geological reservoirs will also be higher at 509.1 t/h if utilisation is not being considered. The new TSCI concept has helped reduce 43 % of CO_2 to be stored.

Table 2a: CTS-PTA for Case Study 1.

	1	2	3	4	5	6	7	8	9	10	11
i	S/D	Header	$P_{CO2,S/D}$ %	$F_{T,S/D}$, t/h	$F_{CO2,S/D}$ t/h	$F_{OG,S/D}$ t/h	Cum $F_{T,H1}$ t/h	Cum $F_{CO2,H1}$ t/h	$P_{CO2,H1}$	$F_{CO2,H1-D}$ t/h	$F_{T,H1-D}$ t/h
1	S1	H1	88	179.9	158.3	21.6					
							179.9	158.3	0.88		
2	S2	H1	85	92.9	79.0	13.9					
							272.9	237.3	0.87		
3	S3	H2	60	100.0	60.0	40.0					
							272.9	237.3	0.87		
4	S4	H1	80	118.1	94.5	23.6					
							391.0	331.8	0.85		
5	D1	H1	99	-50.0	-49.5	-0.5				-2.8	-3.3
							387.7	329.0	0.85		
6	D2	H2	50	-83.3	-41.7	-41.7					
							387.7	329.0	0.85		
7	S5	H1	80	118.1	94.5	23.6					
							505.8	423.5	0.84		
8	D3	H1	80	-208.3	-166.6	-41.7				-174.4	-208.3
							297.5	249.1	0.84		
9	D4	H2	70	-20.0	-14.0	-6.0				-7.1	-8.4
							$F_{T,ST}$ = 289.1	$F_{CO2,ST}$ = 242.01	$P_{CO2,ST}$ = 0.84		

Table 2b: CTS-PTA for Case Study 1 (continue).

	1	4	12	13	14	15	16	17
i	S/D	F_T, t/h	$F_{CO2, FC-D}$ t/h	Cum $F_{T,H2}$ t/h	Cum $F_{CO2,H2}$ t/h	$P_{CO2,H2}$	$F_{CO2,H2-D}$ t/h	$F_{T,H2-D}$, t/h
1	S1	179.9						
				0.0	0.0	0		
2	S2	92.9						
				0.0	0.0	0		
3	S3	100.0	**Reduce to 94.9**					
				100.0	60.0	0.60		
4	S4	118.1						
				100.0	60.0	0.60		
5	D1	-50.0	46.7					
				100.0	60.0	0.60		
6	D2	-83.3					-50.0	-83.3
				16.7	10.0	0.60		
7	S5	118.1						
				16.7	10.0	0.60		
8	D3	-208.3						
				16.7	10.0	0.60		
9	D4	-20.0					-6.9	-11.6
			Excess	**5.1**	**3.0**	**0.60**		

4. Conclusion

A new algebraic targeting method for Total Site Carbon Integration (TSCI) known as CTS-PTA has been developed. A new concept of CO_2 integration which maximises the carbon capture, utilisation and storage have been introduced. The algebraic targeting method has been applied to a hypothetical case study to determine the potential CO_2 exchange by using CO_2 headers at different purities, and a centralised pure CO_2 generator. Application of the new technique has resulted in 43 % reduction of carbon storage. The targeting technique enables planners to conduct further analysis and feasibility studies of CCUS system. Further works can include analysis of more scenarios and techno-economic study.

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