Sequential Synthesis of Mass Exchanger Networks for CO_2 Capture

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***Abstract*— Most of the current research in process synthesis focus on heat exchanger network synthesis. Reports on mass exchanger network synthesis mostly discussed single-component problems using simultaneous approaches. However, less attention has been given to mass exchanger network synthesis with multi-component problems using the sequential technique. Till date, it has not been easy to systematically choose between the process and available external mass separating agents (MSA) in mass exchanger network synthesis during the adsorption of CO_2. In this paper, we set out a technique for targeting external mass separating agent and its network design. The technique was applied to a CO_2 adsorption process involving two mass separating agents (process and external MSAs) that overlap. A thermodynamic analysis of the CO_2 adsorption process was outlined in this study using the composition interval method. Feasible structures were formulated and the synthesis task was expressed in a two-stage targeting procedure as an optimization task. Unlike previous studies reported in the past for mass exchanger network synthesis, this contribution considers a trade-off between the process MSA S_1 and external MSA S_2 to determine the minimum amount of external MSA required for the CO_2 capture process. A case study was adapted from open literature to demonstrate the effectiveness of the synthesized mass exchanger network during a typical CO_2 capture process. Outcomes from this study indicate that mass integration via process synthesis is an effective strategy that can minimize the quantity of external utilities required during the adsorption of CO_2 from a rich stream of flue gas.**

***Index Terms*— Adsorption, CO_2 capture, Composition interval method, Mass exchanger networks, Network design**

I. INTRODUCTION

ABSORPTION and adsorption are known technologies for CO_2 capture [1], [2]. However, these technologies are highly material intensive and also require high energy input during sorbent regeneration thereby making the technologies for CO_2 capture expensive. To tackle this challenge and address the need to minimize waste in industrial processes, there is a need to synthesize and design optimal mass exchanger networks. In the field of chemical engineering, process integration is a tool for analyzing the process mass and energy flows for reducing the use of raw materials, external utilities and waste discharge as well as maximizing the internal heat and mass exchange. Synthesis of optimal mass exchanger networks for the CO_2 adsorption process could minimize the use of external utilities and provide a lasting solution to the problem of excessive use of external utility associated with most adsorption processes. Synthesis of optimal mass exchanger networks (MENs) using simultaneous approach (mathematical programming) has been rather well established in literature [3]–[5]. Hence, we are considering a sequential approach in this study.

Mass exchangers are direct contact mass-transfer components that utilize mass separating agents (MSAs) to preferentially separate certain components (example; impurities, pollutants and by-products) from a certain rich stream into a lean stream. Mass exchange units are commonly used in separation operations in process industries. Popular mass exchange operations include adsorption, stripping, absorption, ion exchange, and solvent extraction. Fig. 1 shows a typical mass exchanger with flow streams in countercurrent directions.

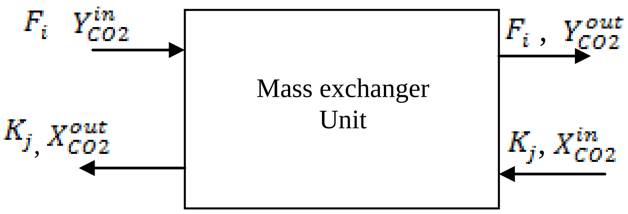

Fig. 1. A mass exchanger for CO_2 absorption

Literature is rich in different methods and approaches for synthesis of mass exchanger networks [3], [6]–[12]. For instance, the synthesis of separation sequences for mass exchanger networks was first reported by Siirola et al. [13] using heuristic approach. This was the first attempt to synthesize mass exchanger networks for separation systems reported by researchers in the early 70's. The authors reported that it might not be possible to apply heuristic approach to most systems at all times due to thermodynamic limitations. In view of this, Thompson and King [14] introduced a technique that combined heuristics with algorithmic programming in order to determine types of separation processes alongside their sequences. In another study, an evolutionary approach for the synthesis of multicomponent separation sequences involving mass

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exchanger networks was proposed by Stephanopoulos and Westerberg [15]. This evolutionary approach was further developed into a combined heuristic and evolutionary strategy for the synthesis of mass exchanger networks. El-Halwagi and Manousiouthakis [16] proposed a procedure for optimal synthesis of MENs using sequential method (pinch analysis). The authors established that by using a composition interval method, a composition pinch point could be set on the mass transfer composite curves and the minimum allowable composition difference 'ε' can be ascertained. The minimum utility targets (minimum MSA consumed) can also be obtained from the mass transfer composite curves before any network design using this approach. The use of P-graph theory to solve problems involving mass exchanger networks (MENs) was introduced by Friedler et al. [17]. The work of Friedler et al. [17] was later improved by combining the P-graph theory with non-linear mathematical programs of Cabezas et al. [18] to determine the network structure and its operating conditions. It is worthy to note that most of the methods highlighted applied mathematical programming (Simultaneous techniques). The main disadvantage of the aforementioned methods is the difficulty faced while setting up and understanding the mathematical formulations involved. In response to this, a pinch-based methodology for synthesis of mass exchanger networks (MENs) considering the capital cost target was presented by Hallale and Fraser [19]. The authors dealt with a special case of mass exchanger networks involving water minimization in which both utility and the capital costs were targeted before network design.

In the present study, an optimal network of mass exchangers is synthesized for cost-effective adsorption of CO_2 from a rich flue gas stream with 'Polyaspartamide' (adsorbent) as the mass separating agent that must be minimized while the packed-bed adsorption column is the mass exchange unit. In the sequential approach developed for this study, the overall synthesis problem is decomposed within a sequence of smaller problems that are easier to solve. However, this approach cannot explore the interactions between sub-systems to obtain an improved solution. The sequential procedure in this study can further be used to target optimal loads and levels for multiple utilities by using the process grand composite curve on a direct numerically-based technique. It can also be used to determine the consumption target of each utility by maximizing the use of the cheapest utilities (process MSA) and minimizing the loads of expensive ones (external MSA).

This study differs from previous studies on mass exchanger networks synthesis in that the minimum mass of CO_2 to be captured by the external mass separating agent (MSA) is first determined before network design. Thermodynamic constraints and cost of MSAs (sorbents) are also incorporated into the synthesis task in this study to generate a cost-effective and thermodynamically feasible network. Although this study mainly deals with material minimization during gas-solid adsorption, the principles and techniques can easily be applied to any mass exchanger network with other solid and liquid sorbents as MSAs. In addition, it is the purpose of this work to also determine the maximum amounts of process and external MSAs (adsorbent) that can be used to remove CO_2 from a CO_2-rich process stream with little operating costs.

II. PROBLEM STATEMENT

The problem investigated in this study is the preferential adsorption of CO_2 from a CO_2/N_2 stream using a solid sorbent and it is presented in this way:

'Given a set of rich streams 'R' and a set of lean streams 'L', The task is to synthesize an optimal network of mass exchanger units which can preferentially separate CO_2 'C' from a rich mixture of CO_2 and N_2 to a set of lean streams at a minimum cost. The flow rate for each rich stream is represented as 'F'. The rich stream flows from a stream composition Y_i to a target composition Y_t while each lean stream has a supply composition of X_i and a target composition X_t. The flow rate of the lean stream is denoted as 'K' and it is not known but restrained by a definite maximum flow rate expressed in Equation (1).

$$K_j \leq K_L \qquad (1)$$

The lean streams can be classified as process or external MSA respectively (S1 and S2). The process MSA is virtually free and already exists in the adsorption plant site. The mas flow rate of the process MSA (S1) is already known and obtained by dividing its available mass with the total adsorption time. The external MSA (S2) can be purchased and its flow rate can be determined by economic considerations using the constraint in Equation (1).

To solve the aforementioned problem in this study, the following major assumptions have been made;

1. The flow pattern in the mass exchanger unit is considered to be counter current.
2. Throughout the network, the mass flow rate of each stream is constant.
3. In order to attain a single equilibrium relation, temperature and pressure do not change throughout the network of each stream
4. Exchange of mass between rich-rich and lean-lean streams is not allowed.

III. SYNTHESIS PROCEDURE

The synthesis task was carried out in a two-stage targeting technique with change in composition as the driving force. First, the minimum amount of mass separating agents for CO_2 adsorption was determined through thermodynamic analysis before designing the network configuration. Flow rates of the external MSA was also determined and potential mass exchange operations were screened according to the procedure of Kaguei and Wakao [20]. In the next phase of the synthesis task, a composition interval for each feasible pair of rich-lean stream was used in a generalized procedure to minimize the total annual cost of the synthesized network and integrate thermodynamic limitations into the synthesis method. A case study involving CO_2 adsorption was used in order to show the application of MEN synthesis concepts to a typical CO_2 capture problem and minimum utility target networks were generated by merging any rich-end design with any corresponding lean-end design.

IV. THE SEQUENTIAL CONCEPT

The concept of pinch analysis was applied in this study to formulate a composition interval table to locate the pinch bottleneck (pinch point) at a specified minimum allowable composition difference (ε = 0.0001). This value of ε was chosen to avoid infinite sizes of mass exchanger which could make the generated network design expensive. The minimum utility requirement of the capture process was also determined using the same approach. Equilibrium equation for the transferable component (CO_2) is in a linear relationship between the process MSA and the rich stream concentration as expressed in Equation (2).

$$Y = mX^* + b \tag{2}$$

X^* is the maximum equilibrium composition of the lean stream theoretically attainable. The minimum allowable composition difference 'ε' if included in the equilibrium relation expressed in Equation (2) can be used to avoid infinite sizes of mass exchangers. The new equilibrium equation is thus presented in Equation (3).

$$Y = m\,(X^* + \varepsilon) + b \tag{3}$$

The corresponding composition scales of components in the lean and rich streams can also be obtained from Equation (3). In the composition interval table presented in this study, composition intervals correspond to the supply or target composition of components in each stream. The composition interval diagram for both rich and lean stream is shown in Table II. Excess capacity of the external MSAs needed for the capture process can also be obtained from the composition intervals presented in Table II while the molar flow rates of the lean and rich streams are shown in Table I. The composition interval diagrams (CID) constructed in this study can be used to calculate the minimum mass flow rates of MSA (adsorbent) required for the capture process; this could be modelled into a non-linear program to optimize the total annualized cost for the process in a simultaneous approach. The material balance on CO_2 that is moved from stream i to stream j is obtainable using Equation (4).

$$F_i \quad (Y^{in}_{CO2} - Y^{out}_{CO2}) \quad = \quad K_j \quad (X^{out}_{CO2} - X^{in}_{CO2}) \tag{4}$$

Where F_i is the flow rate of the rich stream, K_j lean stream flow rate, Y^{in}_{CO2} and Y^{out}_{CO2} are the inlet and outlet composition of CO_2 in the rich stream, X^{out}_{CO2} and X^{in}_{CO2} are the outlet and inlet composition of CO_2 in the lean stream respectively.

A. Case Study: Adsorption of CO_2 using polyaspartamide

This example considers two rich and two lean streams. It is adapted from Yoro [21] which involves the preferential adsorption of CO_2 onto polyaspartamide from two gas streams. The gas compositions given in Yoro [21] was provided in weight percentages; hence, it was modified in this study by making appropriate molar and mass flow rate conversions where necessary. The problem data is presented in Tables I and II. In this case study, the supply composition of CO_2 in the gas mixture was 15 wt. % and the desirable target composition was 6 wt. %. The main reason why the adsorption of CO_2 was considered in this example is to capture CO_2 from a mixture of gases. The removal of CO_2 is necessary because CO_2 is a greenhouse gas that has negative impact on the atmosphere if allowed to be emitted. For this adsorption process, two mass separating agents (process and external MSAs) were considered with a minimum approach composition specified as 0.0001. The value of the minimum approach composition chosen in this study will prevent the infinite sizes of the mass exchangers during design. This is very vital because it reduces the overall design cost of the CO_2 capture process.

TABLE I
RICH AND LEAN STREAMS DATA FOR CASE 1

Rich Streams	**F (kmol/h)**	**Y_{in} (kmol/kmol)**	**Y_{out} (kmol/kmol)**	**Density (kg/m^3)**
R1	1.51	0.15	0.06	1.98
R2	1.23	0.15	0.08	1.98
Lean Streams	**K (kmol/h)**	**X_{in} (kmol/kmol)**	**X_{out} (kmol/kmol)**	**Density (kg/m^3)**
S1	1.33	0.10	0.05	1.25
S2	∞	0.10	0.07	1.25

Considering the minimum allowable composition interval ε which is an optimizable parameter, it is practically possible to transfer CO_2 from a rich stream for any value of Y to a lean stream X as given by Equation (5).

$$X_{CO2,j} = \frac{Y_{CO2,i} - b_{CO2,j}}{m_{CO2,j}} - \varepsilon_{CO2,j} \tag{5}$$

The cost of mass separating agents (sorbents) used will be at a minimum value at this point (ε= 0.0001) but when $\varepsilon_{CO2,j}$ is increased, operating cost of the capture process increases. Considering the assumptions highlighted for this study, Equation (5) can be used to create the corresponding composition scales for CO_2 in the lean process streams S_1 and S_2.

TABLE II
COMPOSITION INTERVALS FOR CO_2 ADSORPTION

Intervals	**Rich stream Y**		**Lean stream X**	A **Input** (kg/s)		B **Output** (kg/s)	C **Excess** (kg/s)
	0.150	R1	0.130				
1				0.000		0.070	0.070
	0.147	R2`	0.110	0.070		0.085	0.015
2							
	0.144		0.080	0.085		0.098	0.013
3							
	0.142		0.060	0.098		0.100	0.002
4							
	0.140		0.050	0.100		0.170	0.070
5							
	0.139		0.040	0.170		0.188	0.018
6					S1		
	0.139		0.000	0.188		-	-

Data on Table II represent the composition mass flows of CO_2 available for capture while the intervals correspond to the head and tail for the case study 1 illustrated. It is assumed here that each lean process stream leaves the network at a specified outlet composition constrained by Equation (1). The composition interval table comprises 3 columns labeled A, B and C excluding the stream representations. Column A and B represent the input and output flows of CO_2 in the streams while column C represents the excess mass of CO_2 available for capture in each interval. The process stream is represented with an arrow on the composition interval table. The rich process streams are denoted as R1 and R2 while lean process streams are S1 and S2. The target composition of the rich stream or the constrained outlet composition of the lean stream is represented by the arrow head while the tail corresponds to the supply composition of respective streams.

It is noted from literature that it is thermodynamically impossible to transfer a negative output of mass between intervals in a composition interval table El-Halwagi and Manousiouthakis [16]. Such negative mass flows in the columns (if any) must be modified by increasing the input to the first interval. In the data presented on Table II, no negative mass was recorded; hence, the case study 1 is thermodynamically feasible without any further modification. Since the thermodynamic constraints are guaranteed to be satisfied from the data in Table II, it is possible to transfer CO_2 from rich to lean streams.

In column C, it is noted that the excess CO_2 removal capacity is 0.070 kg/s .Based on the guaranteed thermodynamic constraints in this case study, this excess can be used to remove CO_2 from the rich streams. The last value in column C (0.018 kg/s) is the minimum mass of CO_2 that is capturable by the external mass separating agent (polyaspartamide) from which the minimum flow is determined. This also implies that for the CO_2 adsorption study in Yoro [21] which lasted for 1200 seconds, about 21.6 kg of CO_2 can be captured per gramme of adsorbent using this method. Another important information that could be obtained from the composition interval table presented here is the pinch point (a point at which the mass flow of CO_2 available for capture vanishes). From the information provided on Table II, the pinch point exists between interval 5 and 6 with a minimum mass flow of 0.170 kg/s. This interval represents the most constrained region of the mass exchanger network design because all matches between the rich and lean streams will be subject to a minimum allowable composition difference at the pinch point.

V. NETWORK DESIGN FOR MINIMUM UTILITY TARGETS

From the composition interval data on Table II, it is possible to generate a network of mass exchangers that use minimum external utility (steam, cooling water and sorbents) by merging any rich-end design with a corresponding lean-end design. In this work, Fig. 4 shows a network for minimum utility targets obtained by combining rich and lean-end designs. Fig. 4 was obtained sequentially but it is worthy to note that when a larger number of streams are involved in minimum utility mass exchanger networks, it will be easier to use a simultaneous approach El-Halwagi and Manousiouthakis [16]. The minimum utility network in this study involved an extra unit more than the target number of units because of the existence of a pinch which decomposed the task into two distinct problems. A rich end network design is first obtained and shown in Fig. 2 while a lean-end design network is shown in Fig. 3.

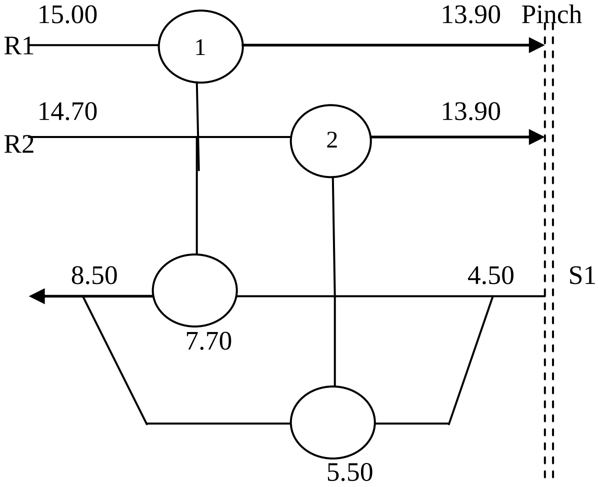

Fig. 2. A Rich-end Network design

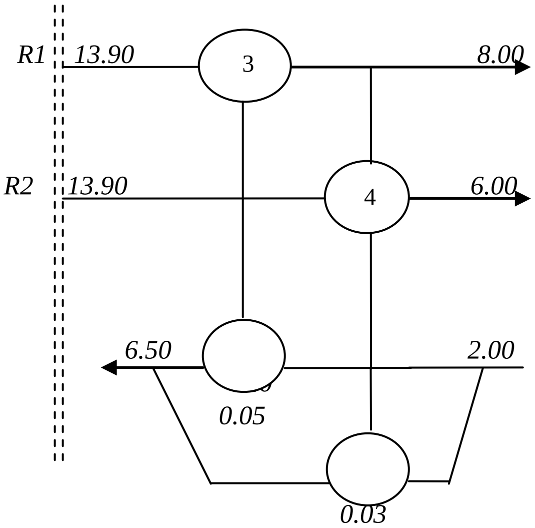

Fig. 3. A lean-end design network

Minimum utility targets can be obtained from the composition interval data by combining the rich-end design in Fig. 2 with a lean-end design in Fig. 3. But according to Linnhoff et al. [22], after merging the rich with lean end design, the minimum-utility pinched network subsequently generated will have one more than the target minimum number of exchanger units. Due to the existence of a pinch which decomposes the task into two distinct sub tasks, the minimum number of units compatible with a minimum-utility design would be obtained by applying the general mathematical expression for minimum number of mass exchangers compatible with a minimum-utility design which is presented in Equation (6). Minimum utility target network for this task is presented in Fig. 4.

$$U = (N_R + N_S) + (N_E - N_i) \tag{6}$$

Where N_R is the number of rich stream, N_S is the number of lean process streams, N_E is the number of external MSAs in the study and N_i is number of independent problem(s) in the

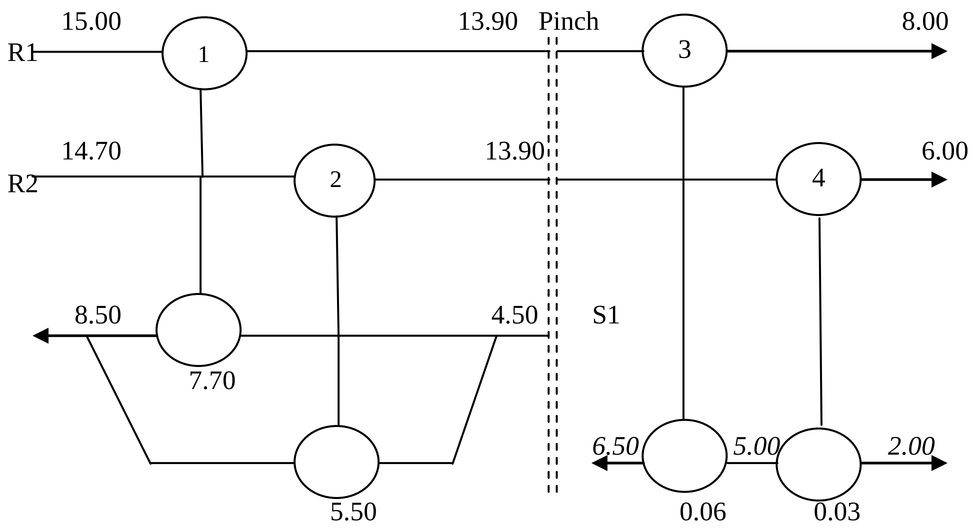

Fig. 4. A minimum-utility network for the adsorption of CO_2 from a CO_2/N_2 gas mixture.

V. CONCLUSION

network. For this work, the minimum utility network of mass exchangers required is:

$$U = (2+1) + (1-1)$$
$$U= 3.$$

Therefore, 3 mass exchangers are required for the synthesis task in this work.

Since any minimum-utility network involves one unit more than the target minimum number of units, it is necessary to develop a method for the systematic reduction in the number of units. This proposed method would involve the use of "mass-load loops" and "mass-load paths as suggested by El-Halwagi and Manousiouthakis [16]. The sequential approach presented in this study is straightforward and can be used to determine the CO_2 avoided, CO_2 capturable and the minimum amount of MSA required for the CO_2 capture process in a detailed study. Nonetheless, it is worthy to note that when larger number of streams are involved in minimum utility mass exchanger networks, a simultaneous approach is preferred to a sequential approach.

In this study, it has been shown that minimum utility targets can be obtained by combining rich and lean-end designs. A systematic procedure that identifies the pinch as the most constrained region of the design procedure which can be used to synthesize a cost-effective and optimal mass exchanger network has also been proposed and tested. It was also established in this study that the minimum quantity of external MSA required for the packed bed CO_2 adsorption process involving 3 mass exchangers is 1.7 kg polyaspartamide. We have also demonstrated that the composition intervals presented in this work offer a two-feasibility criterion that identifies the essential pinch matches and a stream splitting rationale from the case study problem. The most constrained region (pinch point) of the mass exchanger network design in this study lies between the 5th and 6th interval because all matches between the rich and lean streams are subject to minimum allowable composition difference at that point. It should also be noted that although this study focuses mainly on packed bed adsorption columns, the concepts can be readily applied to other stage-wise adsorption and absorption systems. Furthermore, one significant advantage of the sequential technique used in this paper is that, once the optimal targets for the capture process are identified, a pinch design method could be used to automatically synthesize a network. This method could also be extended to cases involving multiple pinch points. However, the limitation of the sequential procedure used in this study is that it cannot consider forbidden stream matches or disallowed mass flows. Finally, the composition interval table presented in this work can be used to calculate minimum flow rates of mass separating agents and gases required for the CO_2 capture process; this could be modelled further into a non-linear program to optimize the total annualized cost for the CO_2 capture process in a simultaneous approach. Future research should consider minimum targeting and sizing of adsorbers required for the CO_2 adsorption process alongside its network design.

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