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ENERGY AND MATERIAL MINIMIZATION DURING CO_2 CAPTURE USING A COMBINED HEAT AND MASS INTEGRATION TECHNIQUE

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Abstract

Heat and mass exchange occur concurrently during CO_2 capture. Therefore, the application of a combined heat and mass exchanger network (CHAMEN) could be a very good option to reduce energy and material consumption simultaneously during CO_2 capture. In this study, a systematic technique for the synthesis of combined heat and mass exchanger networks (CHAMENs) was introduced to concurrently minimize the use of external utilities and mass separating agents (MSA) during adsorptive CO_2 capture. The method proposed in this study is based on an innovative approach that integrates a mathematical programming technique for the heat exchanger networks (HENs) synthesis and a sequentially-based composition interval technique for mass exchanger networks (MENs) synthesis with regeneration. A combined optimization approach was used to minimize the total annualized cost of the synthesized CHAMEN. An example was solved to test the efficacy of the proposed method. The cost of mass separating agents, as well as hot and cold utilities which form the total annualized costs (TAC) for the combined heat and mass exchangers, was minimized. The total annualized cost (TAC) of the synthesized CHAMEN obtained in this study (TAC=$199800/yr) showed significant improvement over the TAC reported in the literature using other synthesis techniques. Results obtained in this study confirmed that the integration of a combined heat and mass exchanger with regeneration network is an effective way to minimize heat and mass during adsorptive CO_2 capture. The combined heat and mass exchanger networks adequately satisfied the heat and mass balance of the process with a lower total annualized cost.

Keywords: *Adsorption, CO_2 capture, Combined heat and mass exchanger network, Energy minimization, Mass separating agent, Process optimization*

1. Introduction

Most CO_2 capture techniques (e.g. absorption, adsorption and membrane separation) are material and energy-intensive in nature. So far, sorbent blending and scrubbing; the use of phase change solvents; and extra external utilities such as steam and cooling water have been proposed as ways to reduce energy consumption during CO_2 capture [1]. Although these strategies have helped in dropping down energy requirement to some extent, it has in turn increased process cost thereby rendering carbon capture an expensive technology. To ensure the economic advantage of the available CO_2 capture techniques, this study proposed the application of process synthesis techniques through the synthesis of heat exchanger networks (HENs) and mass exchanger networks (MENs) to minimize both energy and material consumption. Heat and mass exchanger network synthesis has been a major research topic in the field of process system engineering and environmental sustainability because heat and mass are very important resources in many industrial applications [1], [2]. Industrial applications like the separation of CO_2 from flue gas streams using sorbents account for high consumption of energy and other resources such as sorbents, steam and cooling water [3]. The excessive use of these important but expensive resources must be minimized to make CO_2 capture technology affordable in developing countries, especially in sub-Saharan Africa [4]. So far, It has been documented in the literature that the application of heat and mass exchanger networks or a combination of both in CO_2 capture studies could be a promising technique for integrating processes with a potential of providing meaningful improvements over the synthesis of the individual heat and mass exchanger networks [1, 5–7]. Since the use of heat and mass is typically intertwined in most CO_2 capture techniques, it is important to account for such interactions in this study. Furthermore, heat and mass exchanger network synthesis has been a key area of research that has significantly contributed to industrial energy-saving, improved plant efficiency and material minimization since the past four decades [8].

Until now, researchers have attempted the synthesis of heat and mass exchanger networks separately without combining them with a regeneration network [9-11]. Furthermore, the majority of HENs synthesis techniques reported in open literature applied pure mathematical programming approaches based on the stage-wise superstructure model proposed by Yee and Grossmann [12]. The superstructure-based SYNHEAT model allows for a large number of likely stream matches into a superstructure, while fully considering stream splitting and isothermal mixing [13], [14]. According to Furman and Sahinidis [15], the superstructure-based method is very effective when used to determine potential networks. However, its complex non-linear formulation makes it challenging to solve with current solvers. Also, most superstructure-based formulations do not consider some important details for heat exchanger design, such as fluctuating heat transfer coefficients, pumping costs, number of baffles, tube passes, and number of shells. In addition, the formulation of Yee and Grossman [12] cannot be extended to consider the aforementioned details for heat exchanger design because its already complex combinatorial nature with increased non-linearity will not yield optimal solutions. Other reports in this field that did not apply the super-structure based approach used pinch analysis-based concepts [15].

As far as could be ascertained, most CHAMEN synthesis techniques reported so far in the literature applied mathematical programming or pinch analysis techniques separately. No methodology has effectively combined a pinch technology-based technique with a mathematical programming technique to synthesize a combined heat and mass exchanger network while considering sorbent regeneration. This study presents an overview of combined heat and mass exchanger networks synthesis (CHAMENS) in relation to energy and resource minimization while considering sorbent regeneration. It also discusses a hybrid simultaneous-sequentially based methodology to design and operate CHAMENs with a focus on applying it to reduce the high energy requirement associated with sorbent-based CO_2 capture methods. This hybrid technique is new and its application in the field of CO_2 capture has not been reported before now.

Nomenclature

A	Heat transfer area
B	Exponent in cost equation of heat exchanger
C	Unit cost for MSA/lean stream/utility
CF	Fixed cost for heat exchanger
Cp	Heat capacity
cu	Cold utility
C_{CU}	Hot utility unit cost
C_e	Heat exchanger area cost coefficient
CF_{CU}	Unit charge of cooler (fixed)
CF_e	Heat exchanger unit's fixed charge
CF_{HU}	Heater unit's fixed charge
C_{HU}	Area cost coefficient for the heater
C_{HU}	Unit cost of hot utility
C_j	Final CO_2 adsorbed by MSA
FC	Annualized capital cost
F_{CP}	Heat capacity flow rate of main stream
G_i	Mass flow rate of the rich main stream
hu	Hot utility
i	i^th rich stream
j	j^th MSA/lean stream
k	k^th stage in MEN
L	Mass flow rate of the MSA/lean main stream
MEN	Mass exchanger network
MSA	Mass separating agent/lean stream
N	Number of mass exchanger trays
Q	Heat load
Qcu	Heat load of cold utility
Qhu	Heat load of hot utility
R	Rich stream
TAC	Total annual cost
T_j^{LB}	Inlet temperature to MSA
T_j^{UB}	Outlet temperature from MSA
x_j^s	Supply composition of CO_2 in the MSA
x_j^t	Target composition of CO_2 in the MSA
x	Concentration of MSA/lean stream
y	Concentration of rich stream

1.1 Advances in the synthesis of CHAMENs

The recent work of Yoro et al. [1] reported an extensive review on the application of heat and mass integration techniques for energy and material minimization during CO_2 capture via HENs and MENs synthesis. The authors discussed the prospects of introducing heat and mass integration techniques via the application of individual HENs, MENs and a combined heat and mass exchanger network for energy and material saving. However, the techniques proposed in the review were not tested in any case study. Srinivas and El-Halwagi [16] were the first group of researchers to present a methodology for the synthesis of a combined heat and mass exchanger network. The researchers formulated a technique that focused on optimizing individual mass-exchange temperatures in a constant-temperature unit, which was used to simultaneously isolate a certain pollutant from a set of rich streams to a physical and reactive lean stream (mass-separating agents) while also accomplishing a specific heat transfer task in a cost-effective manner. In spite of the results obtained by Srinivas and El-Halwagi [16], their proposed technique is only effective with reactive mass exchangers without considering the annualized capital cost of the absorbers and the regenerating units.

Papalexandri and Pistikopoulos [17] suggested a hyperstructure-based mixed integer non-linear programme based mathematical model to tackle the problem of combined heat and mass integration. However, the major drawback with their methodology is that the model formulation for the hyperstructure was observed to be extremely non-linear and non-convex in nature. This is due to the introduction of many binary variables to the problem; hence, it became very difficult to get better results than the one reported by Srinivas and El-Halwagi [16]. Furthermore, Prakotpol and Srinophakun [18] developed a genetic algorithm in MATLAB to minimize energy and material consumption in a wastewater minimization problem. The researchers formulated an optimization model for both single and multiple contaminants as an MINLP. Although the proposed algorithm was useful for the synthesis problem, it had similar limitations as the hyperstructure-based MINLP model of Papalexandri and Pistikopoulos [17]. Soywiset et al. [19] presented a simultaneous technique for heat and mass exchanger network synthesis using an ASPEN process simulator. The authors applied their technique to the synthesis of HENs and MENs separately and then CHAMENs. However, they concluded that CHAMEN synthesis was not suitable for all industrial applications. This simply means that by using their proposed methodology, synthesizing HENs and MENs separately possibly offers a reduced total annualized cost than combining them in a network.

In another contribution, Isafiade and Fraser [2] suggested a methodology based on pinch technology, where the sub-HEN and sub-MEN were combined via heat and mass pinch approach to investigate the effect of mass exchange temperature on the annual operating cost and how the annualized capital cost affects CHAMENs. Further findings from the work of Isafiade and Fraser [2] revealed that depending on the methodology used, assumptions and process considered, synthesizing a combined heat and mass exchanger network yields better results than an individual synthesis of HENs and MENs, in contrast to the claims of Soywiset et al. [19]. Furthermore, Liu et al. [20] suggested a new methodology for the simultaneous generation of CHAMENs with multi-dimensional optimization problems. The methodology was a blend of the mass pinch technology for mass exchanger network (MEN) synthesis and a quasi T-H diagram technique for the heat exchanger network (HEN) synthesis which are both sequential in nature. The authors introduced a lean by-pass stream to a combined network structure to decrease its associated costs. The authors then suggested a mathematical model and a cross-genetic algorithm annealing-based method to achieve a synchronized minimization for the total cost of the MEN and the HEN separately. However, the technique was ineffective when tested for a combined heat and mass exchanger network in a multi-period situation. Additionally, Liu et al. [21] and Velázquez-Guevara et al. [22] developed a superstructure for the synthesis of mass exchanger networks by modelling the superstructure through general disjunctive mathematical programming and then re-formulated it as a mixed integer non-linear program. The proposed superstructure allowed for mixing and splitting of process streams thereby increasing the number of possible exchangers in the superstructure. In this study, the technique introduced is quite different from the one proposed by Liu et al. [20] because here, we hybridized a simultaneous-sequential based approach to achieve an optimal CHAMEN with remarkable energy and material saving during adsorptive CO_2 capture.

In this study, it was observed that during of CO_2 capture and storage, heat and mass exchange operations are usually multi-period in nature and are also affected by heating and cooling demands as speculated by other researchers [23],[24]. As such, synthesizing a HEN and MEN as two independent processes will not yield high energy and material saving compared to combining them in a single network [25],[26]. Additionally, most synthesis methodologies reported in the past did not consider the interactions between heat and mass exchange concomitantly [27]. Another research gap identified in this study is that most of the energy conservation tasks in the area of environmental sustainability suggest the use of external utilities (e.g. cooling water, additives) to minimize energy and material usage during CO_2 capture despite its high cost. But in this study, it is proposed that combined energy and mass integration could be an effective and sustainable approach for energy and resource minimization in many energy-intensive industrial processes. Hence, the use of internal process heat and mass for resource minimization via combined heat and mass exchanger network synthesis is proposed. The process synthesis approach presented in this study is new to the field of CO_2 capture, and we envisage that if the proposed technique is fully harnessed with optimized capital cost functions during CO_2 capture operations in large point-sources (for example coal-fired power plants), the emission of CO_2 during power generation will be considerably minimized and significant amounts of energy, as well as material (sorbents) used during CO_2 capture, will be saved.

Against this background, this study was dedicated to synthesizing a combined heat and mass exchanger network with regeneration that can minimize the excessive consumption of energy and mass (material) concurrently while decreasing the levels of CO_2 emission to the atmosphere. The study introduces a new CHAMEN synthesis technique that combines both sequential and simultaneous based principles. This study also discusses multi-period formulations for the first time in a combined heat and mass exchanger network (CHAMEN) with sorbent regeneration. Finally, this study confirms whether the combination of sequential and simultaneous concepts in a single methodology for CHAMENs can yield results with better total annualized cost (TAC).

2. Synthesis of the combined heat and mass exchanger network

The major challenge observed with most synthesis techniques for combined heat and mass exchanger network (CHAMEN) lies in the combinatorial approach as well as the optimization approach between the sub-MEN and sub-HEN. To proffer solution to this challenge, Srinivas and El-Halwagi [16] proposed a MEN–HEN combination technique, in which the heat exchanged finds a pre- and post-MEN with the lean streams flowing through the MEN at fixed stream temperatures. Although this technique yielded results, it is only applicable to single-period CHAMENs where parameters are fixed and do not fluctuate. It cannot be extended to multi-period scenarios where stream temperatures, flow rates and gas composition fluctuate as seen in a typical CO_2 separation study where sorbent regeneration is paramount. As a result, this paper modified the methodology of Srinivas and El-Halwagi [16] to specifically address a CHAMEN synthesis problem with regeneration and fluctuating process parameters. The thermodynamic feasibility of the heat exchanged in this work was ensured by using a lower value of the minimum approach temperature (ΔT_{min}).

In addition, the body of knowledge in this field is rich in different approaches for the synthesis of both reactive and non-reactive CHAMENs [2],[16],[20],[28,29]. However, due to the interaction of heat and mass during adsorptive CO_2 capture, this study reports the synthesis of CHAMENs for adsorptive CO_2 capture alongside the regeneration network. As far as could be ascertained, this has not been reported before now. Furthermore, to improve on the work of Srivinas and El-Halwagi [16], this study was extended beyond optimizing just the outlet gas composition to introduce a more rigorous optimization-based method for the synthesis of CHAMENs to include the coupling of sub-networks as well as simultaneous integration, and the optimization of CHAMENs.

The following assumptions were made for the mass exchangers synthesized in this study;

1) Individual rich and lean stream have a fluctuating mass flow rates throughout the network.

2) The mass exchangers operate at non-isothermal conditions.

3) Mass exchange temperatures are generated only from the temperatures of the lean streams.

4) Equilibrium relations are assumed to be monotonic functions of the sorbent temperature and compositions as described by Henry's law.

3. Problem statement

The combined heat and mass-exchanger network (CHAMEN) synthesis problem in this study is presented as follows;

'Given are a number of rich streams 'NR' and a number of lean streams 'NS' (physical MSAs). The task is to synthesize a cost-effective network of combined heat and mass exchangers that can satisfactorily transfer a certain undesirable pollutant (CO_2) from rich flue gas streams to the MSA (in this case, the sorbent). The flow rate of each rich stream, G_i; the supply (inlet) composition, y_{si}; and the target/outlet composition, y_{ti} are known and specified in the problem. The supply and target compositions of the MSA (sorbent) during absorptive CO_2 capture are given as x_{sj} and x_{tj} respectively. In addition, hot and cold process and utility streams are available to optimize mass exchange temperatures. Important problem data for this study such as gas flow rate, concentration and temperature intervals were adapted from the previous work of Yoro [30] and extended to tackle a combined heat and mass exchanger network synthesis problem to achieve a reduced energy and material usage during adsorptive CO_2 capture.

4. Methodology

A systematic combination of both pinch technology and mathematical programming concepts is employed in this study to synthesize a CHAMEN. The step-wise procedure presented in Figure 1 was used to set the formulation for the synthesis of a combined heat and mass exchanger network (CHAMEN) in this study.

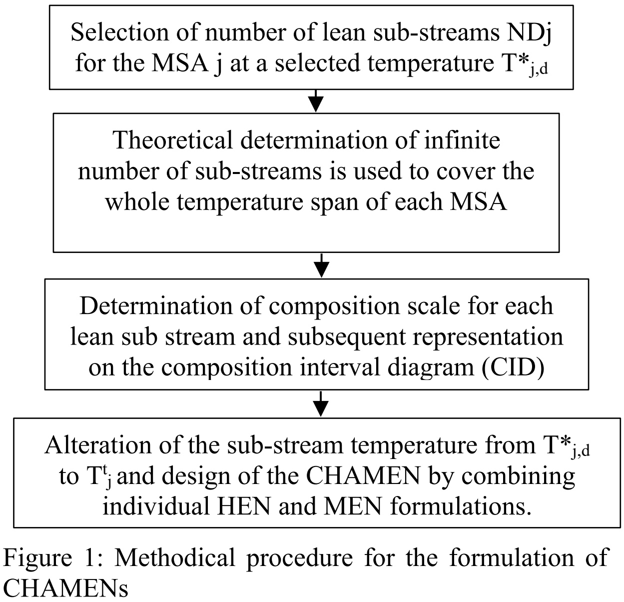

Figure 1: Methodical procedure for the formulation of CHAMENs

The adsorbent (polyaspartamide) for CO_2 capture suffices as the mass transfer agent (MSA) in this study and its cost is determined from Equation (1).

$$\textbf{Cost of MSA} = \sum_{j=1}^{N_s} C_j \sum_{dj=1}^{ND_j} L_j, dj \qquad (1)$$

Material balance around the composition interval is given by;

$$\delta_k - \delta_{k-1} + \sum_j k \sum_{dj\ through\ interval\ K} w^s_{j,k} = W^R_k \qquad (2)$$

Where k = 1, 2 …N_{int}, $L_j, dj \geq 0$, j = 1, 2… N_s

$$\sum_{dj=1}^{ND_j} L_j, dj \leq L^C_j \quad j = 1, 2, \dots N_s \qquad (3)$$

Mass residual constraints for the case study considered in this paper were stated as;

$$\delta_0 = \delta_{N,int} = 0 \qquad (4)$$

$$\delta_k \geq 0,\ k = 1, 2 \dots N_{int} - 1 \qquad (5)$$

Equations (1)-(5) together with the HEN-targeting equations presented by El-Halwagi [31] represent the constraints of the CHAMEN synthesis formulation.

The equilibrium relation for CO_2 scrubbing in water depends on temperature according to Equation (6) which was adapted and modified from Liu et al. [19] to suit this study;

$$y = x_1 (0.053T_1 - 14.5) \qquad (6)$$

Where y refers to the mass fraction of CO_2 in the flue gas stream, T_1 is the temperature of the water in degree Celsius and x_1 is the mass fraction of CO_2 in water after scrubbing.

An objective function was developed in this study to minimize the cost of mass separating agents (MSAs) as well as the heating and cooling utilities. The objective function discussed in this study is a linear programming formulation whose solution determines the optimal flow rate and temperature of each sub-stream as well as its heating/cooling duty. The general methodology used to synthesize the optimal CHAMEN in this study to achieve an improved total annualized cost (TAC) is presented in Figure 2.

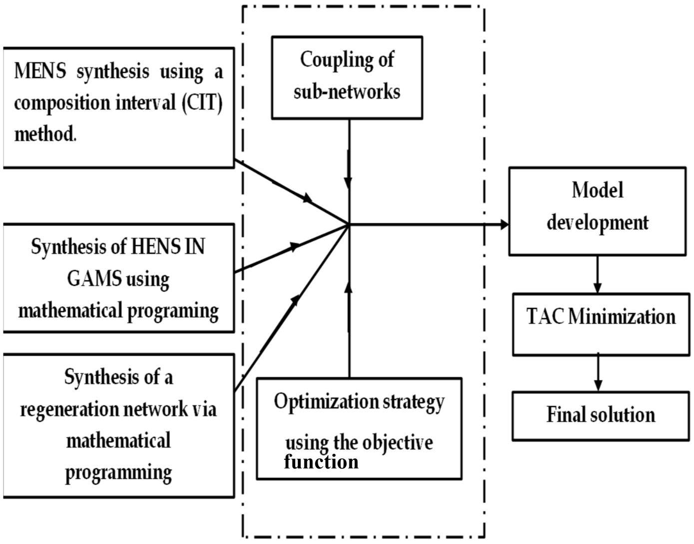

Figure 2: Methodology for the synthesis of a CHAMEN with regeneration network

5. Case study for CHAMEN synthesis

The efficacy of the methodology for synthesizing the CHAMEN with regeneration proposed in this study is tested in this section using a CO_2 adsorption case study from the work of Yoro [30]. The case study has a mass exchanger network (MEN) with mass separating agents (which is the sorbent in this case) integrated with a heat exchanger network (HEN) with the possibility of optimally regenerating the MSAs.

The task: *Adsorption of CO_2 with two MSAs and two cold and hot external utilities*

In this problem, steam and cooling water are the hot and cold utilities added to the process with the aim of heating up and cooling down the mass separating agents (MSAs) for effective adsorption of CO_2. The task is to synthesize a CHAMEN that can adequately transfer CO_2 in the waste streams to the MSA and the energy and material saved determined based on the stream data presented in Table 1-3. The physical meaning of all the symbols used in Table 1-3 and others used elsewhere in this study are already provided in the nomenclature section of this study.

Table 1**:** Waste stream data for CO_2 separation

Stream	Flow rate Gi (kg/s)	Gas Supply comp. y_i^s	Gas target comp. y_i^t
R_1	1.5	0.15	0.05

Table 2**:** Lean stream data

Stream	x_j^s	x_j^t	m_j	ε_j	C_j	T_j^{LB} (˚C)	T_j^{UB} (˚C)
S_1	0.00	0.05	0.10	0.001	0.05	35	50
S_2	0.02	0.09	0.20	0.001	0.01	48	48

Table 3**:** Cold and hot utility stream data

Stream	Supply Temp(˚C)	Target Temp (˚C)	Cost ($/kW.yr)
C_1	15	25	10
C_2	28	35	30
H_1	130	80	120
H_2	120	70	150

Two cooling utilities (cold water) and two hot utilities (steam) are available as shown in Table 3. For this case study, the specific heat capacity is fixed at 4.2 $kJ \cdot kg^{-1} \cdot {}^{\circ}C^{-1}$ (specific heat capacity of water at room temperature) while the minimum approach temperature ΔT_{min} was assumed at 10 ˚C.

The cost of heat exchanger area (A) is expressed in Equation (7) as described by Shenoy [32];

$$\text{Area cost} = 30000 + 750A^{0.81} \qquad (7)$$

The objective function for the mathematical model is presented as Equation (8) and was solved in GAMS (General algebraic modelling system). The objective function comprises of the total annual cost (TAC) of the CHAMEN presented as a combination of the costs associated with the sub-MEN and the sub-HEN. The objective function of the model gives more information on the capital costs of the coolers, heaters and the number of heat exchanger units for all process streams.

$$\text{Min} \sum_{i}\sum_{j}\sum_{k} N_{i,j,k} \,.\, K_{stage} + H_Y \sum_{j} L_j \,.\, C_j^l + \sum CF_{cu,v} + \sum_{v} CF_{hu,w} + \sum_{w}\sum_{u}\sum_{v}\sum_{w} CF_{u,v,w} + \sum_{v} C_{cu,v} \,.\, A_{cu,v}^{Bcu,v} + \sum_{w} Chu_{,w} \,.\, A_{hu,w}^{Bhu,w} + \sum_{u}\sum_{v}\sum_{w} Cv_{w,u} \,.\, A_{v,w,u}^{Bv,w,u} + \sum_{v} C^{cu} \,.\, q_{cu,v} + \sum_{w} C^{hu} \,.\, q_{hu,w} \qquad (8)$$

Hot and cold streams for the networks were determined through optimization using Equation (9).

$T_j^s < T_j^*$, $T_j^* < T_j^t$ = hot stream, j ϵ N_i

$T_j^s > T_j^*$, $T_j^* > T_j^t$ = cold stream, j ϵ N_i (9)

Equations (1)-(9) were coupled with the non-negativity constraints to form a linear program that was modelled and run in GAMS using the DICOPT solver.

Table 4**:** Composition interval diagram for the case study

Interval	Waste stream y 0.15 R1	X_1, 1 at 35 °C	X_1, 1 at 70 °C	Target 0.09
1	0.13			0.08
2	0.12			0.07
3	0.10		0.13	0.06
4	0.09	0.13	0.09	0.05
5	0.08	0.11	0.07	0.04
6	0.07	0.09	0.05	0.03
7	0.06	0.05	0.00	0.03
8	0.05	0.00	$S_{1,2}$	0.02

$S_{1,1}$ S_2

Table 5: Temperature interval diagram

Interval	Hot streams $S_{1,1}$, $S_{1,1}$ T(°C)	Target Temp(˚C)
1	35	130
2	28	120
3	25	80
4	15	70 CU_1

CU_2

6. Regeneration

Since the example considered in this paper involves CO_2 adsorption using a solid sorbent, there is a need to consider the amounts of energy that could be saved during the regeneration of sorbents in the CHAMEN. As a result, a regeneration network was integrated into the CHAMEN in this study. The main MSA target composition during regeneration was determined from the interaction with the stripping column. A complex mathematical problem was solved in GAMS using the DICOPT solver as ΔT_{min} changes and results obtained are presented in Table 6. The superstructure showing expected flows in the combined heat, mass exchanger with regeneration network is shown in Figure 3 while the synthesized CHAMEN alongside its regeneration is presented in Figure 4. To substantiate our claims in this study, the minimum TAC obtained in this study using the proposed technique was compared with other CHAMEN synthesis techniques procedures reported in the past and presented in Table 7. The technique proposed in this study resulted in a slightly superior value of TAC when compared to previously reported techniques as shown in Table 7. The TAC value obtained in this study is closer to that reported by Isafiade et al. [2]. However, the slight difference observed could be attributed to the fact that Isafiade et al. [2] used only a simultaneous approach without considering regeneration while this study used a combined sequential and simultaneous approach with due consideration to sorbent regeneration.

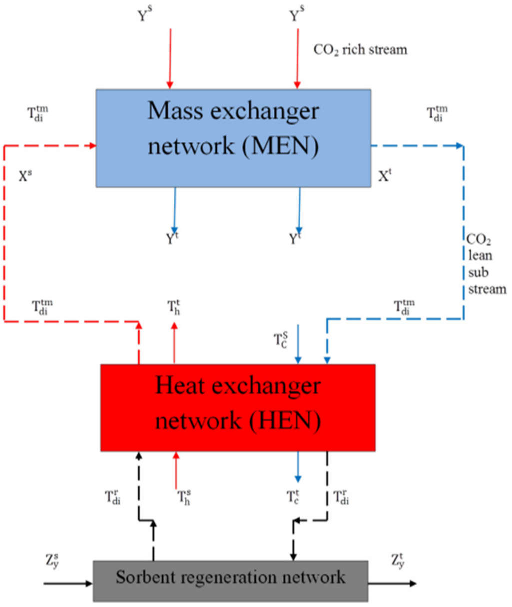

Figure 3: The CHAMEN + regeneration superstructure (Adapted from Yoro et al. [1]).

Table 6: TAC obtained at different target compositions and ΔT_{min}.

Compositions		ΔT_{min} (°C)	TAC for CHAMEN ($million/yr.)
x^s	x^t		
0.15	0.03	10	0.1998
0.15	0.05	13	0.2156
0.15	0.07	15	0.2800
0.15	0.10	20	0.3763

Table 7: Minimum total annualized cost compared with literature

Reference	Network type	Minimum TAC for CHAMEN ($million/yr.)
This study	CHAMENs	0.1998
Liu et al. [20]	CHAMENs	0.3402
Isafiade et al. [2]	CHAMENs	0.1973
Soywiset et al. [18]	CHAMENs	2. 6731

Table 8: Energy and material saved during CO_2 capture using different energy and material saving techniques

Technique	Energy saved (%)	Sorbent/ material saved (%)	Reference
CHAMEN + Regeneration	30	19	This study
Use of phase change solvents	40	Not reported	Shavalieva et al. [33]
Sorbent blending	17	9	Bachelor and Toochinda [34]
Amine scrubbing	31	Not reported	Pellegrini et al. [35]
Use of extra external utilities	12	0	Bougie and Iliuta [36]

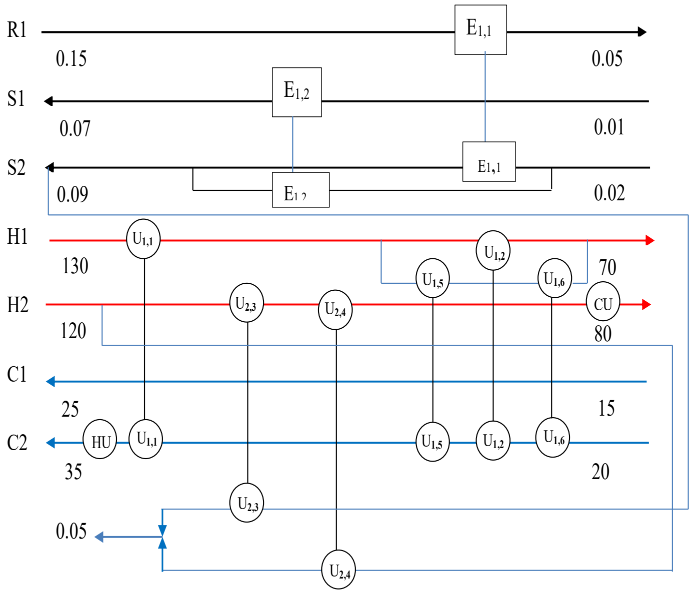

Figure 4: CHAMEN with regeneration for this case study.

7. Discussion of Results

This study attempted using the composition interval method (for MENS), with temperature interval diagram (for HENS) and linear programming to explore the possibility of synthesizing a combined heat and mass exchanger network with a provision for sorbent regeneration. The composition interval diagram presented in this work was used to ensure the thermodynamic feasibility of the mass exchanged during the CO_2 capture process while the temperature intervals catered for the heat exchanged and potential energy saving. The number of intervals represents the number of process streams (both hot and cold) considered in the capture process. The all-positive values in the composition interval diagram (CID) presented in Table 4 established that within any interval, it is thermodynamically feasible to transfer mass from the waste streams to the mass separating agents (sorbents). The solution obtained from the combined network also confirms that the lean stream (sorbent) is actively involved in the adsorption process and a by-pass stream with unequal supply and target temperature is expected. The CHAMENs further illustrates that the incorporation of by-pass streams with the combination of simultaneous and sequential-based synthesis technique yields results with significant improvements over previously reported methodologies that used just mathematical programming or sequential approach.

Another important result presented in this study is the total annualized cost (TAC) of the combined network. A lower value of TAC for the CHAMEN means better operating and capital cost for the network which also translates to higher energy savings and minimization of material in the CO_2 adsorption process. Furthermore, results on Table 6 show that as the target composition of the gas (with respect to mass exchange) and minimum approach temperature (ΔT_{min}) with respect to heat exchanged is increased, the TAC also increases. This means that operating at a lower ΔT_{min} could result in a more efficient combined heat and mass exchanger network with regeneration during CO_2 capture.

The parameters included in the objective function formulated in this study were responsible for the significant decrease in the total annualized cost and energy consumption by the resultant CHAMEN. The value of the minimum approach temperature (10 ^{o}C) adopted in this study impacted positively on energy penalty reduction during adsorptive CO_2 capture which subsequently improves the efficiency of the power plant. The inclusion of a sorbent regeneration network in the CHAMEN presented in this study established that process synthesis techniques can be used to tackle the high energy requirement associated with most CO_2 capture techniques.

The results in Table 7 suggest that the combined methodology introduced in this work is better in terms of the total annualized costs than some methodologies reported in the literature. This makes the combined network generated in this paper more ideal for application in CO_2 capture studies. The amount of energy and material saved during CO_2 capture reported for different energy and material saving techniques is presented in Table 8 and compared with the technique proposed in this study. According to the results in Table 8, the integration of CHAMENs with a regeneration network in a CO_2 capture problem could result in 30 and 19 % energy and material saving respectively. Other techniques that reported a slightly higher value could only account for energy without material saving. Although the use of phase change solvents as proposed by Shavalieva et al. [33] is good and results in a significantly higher energy saving (40%) as shown in Table 8, the technique cannot be extended for material saving. Amine scrubbing technique also resulted in huge energy savings during CO_2 capture, however, it cannot also account for the quantity of materials that could be saved in the process. Thus, it is evident that the integration of a CHAMEN with regeneration as proposed in this study could potentially facilitate and account for a reduction in both energy and material during CO_2 capture.

8. Conclusions

The benefit of combining heat and mass exchanger networks with a sorbent regeneration network for concurrent minimization of energy and material during CO_2 capture was investigated in this study. It was established from the results obtained in this study that combining heat and mass exchanger with a sorbent regeneration network is an effective way of concurrently minimizing energy and material consumption during CO_2 capture. Results obtained from the case study considered in this work revealed that operating the lean streams at their supply temperatures alone is not the best approach to cut operational cost and simplify CHAMEN network design. Furthermore, It has been demonstrated in this study that it is possible to combine a sequential-based approach (composition interval method) with a simultaneous-based technique (mathematical programming) to achieve optimal results for energy and material saving in a combined heat and mass exchanger network. The combinatorial approach introduced in this study gave insight into how best to combine the heat and mass exchangers with regeneration networks for energy and material minimization. Finally, the total annualized cost obtained in this study (TAC=$million 0.1998 /yr.) showed significant improvement over the TAC previously reported which also mean a significant reduction in energy requirement when compared with previously reported approaches. The CHAMEN synthesized in this study can be extended to minimize energy and material consumption in other CO_2 capture methodologies such as absorption, membrane, and cryogenic separation. Finally, it was established in this study that although other energy-saving techniques for CO_2 capture (for example amine scrubbing, sorbent blending, the use of phase change materials etc.) yielded results in terms of energy-saving, if energy and material minimization is to be accounted for concurrently, the application of a combined heat and mass exchanger network is the better option.

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References

[1] K. O. Yoro, P. T. Sekoai, A. J. Isafiade, and M. O. Daramola, ‘A review on heat and mass integration techniques for energy and material minimization during CO_2 capture', *International Journal of Energy and Environmental Engineering,* vol. 10, pp. 367–387, 2019.

[2] A. Isafiade and D. Fraser, ‘Optimization of combined heat and mass exchanger networks using pinch technology’, *Asia-Pacific Journal of Chemical Engineering*, vol. 2, no. 6, pp. 554–565, 2007.

[3] K. O. Yoro and P. T. Sekoai, ‘The Potential of CO_2 Capture and Storage Technology in South Africa’s Coal-Fired Thermal Power Plants’, *Environments*, vol. 3, no. 3, p. 24, 2016.

[4] K. O. Yoro, M. Singo, J. L. Mulopo, and M. O. Daramola, ‘Modelling and Experimental Study of the CO_2 Adsorption Behaviour of Polyaspartamide as an Adsorbent During Post-Combustion CO_2 Capture’, *Energy Procedia*, vol. 114, pp. 1643–1664, 2017.

[5] M. B. Noureldin, ‘Methods for heat exchanger network energy efficiency assessment and lifetime retrofit’, US8150560B2, 2012.

[6] Y. L. Tan, D. K. S. Ng, D. C. Y. Foo, M. M. El-Halwagi, and Y. Samyudia, ‘Heat integrated resource conservation networks without mixing prior to heat exchanger networks’, *Journal of Cleaner Production*, vol. 71, pp. 128–138, 2014.

[7] F.B. Gabriel and M.M. El-Halwagi, ‘Simultaneous synthesis of waste interception and material reuse networks: Problem reformulation for global optimization’, *Environmental Progress*, vol. 24, no. 2, pp. 171–180, 2005.

[8] K. O. Yoro, A. J. Isafiade, and M. O. Daramola, 'Synthesis of Optimal Heat Exchanger Networks with Quantified Uncertainties and Non-isothermal Mixing', *J. Phys. Conf. Ser.,* vol. 1378, pp. 022018, 2019.

[9] O. S. Azeez, A. J. Isafiade, and D. M. Fraser, ‘Supply-based superstructure synthesis of heat and mass exchange networks’, *Computers & Chemical Engineering*, vol. 56, pp. 184–201, 2013.

[10] S. Ghazouani, A. Zoughaib, and S. Pelloux-Prayer, ‘Simultaneous heat integrated resource allocation network targeting for total annual cost considering non-isothermal mixing’, *Chemical Engineering Science*, vol. 134, pp. 385–398, 2015.

[11] A. Wechsung, A. Aspelund, T. Gundersen, and P. I. Barton, ‘Synthesis of heat exchanger networks at subambient conditions with compression and expansion of process streams’, *AIChE Journal*, vol. 57, no. 8, pp. 2090–2108, 2011.

[12] T. F. Yee and I. E. Grossmann, ‘Simultaneous optimization models for heat integration—II. Heat exchanger network synthesis’, *Computers & Chemical Engineering*, vol. 14, no. 10, pp. 1165–1184, 1990.

[13] K.F. Huang, E.M. Al-mutairi and I. A. Karimi. 'Heat exchanger network synthesis using a stage-wise superstructure with non-isothermal mixing '.*Chemical engineering science,* vol. 73, pp. 30-43, 2012.

[14] J. M. Zamora and I. E. Grossmann, ‘A global MINLP optimization algorithm for the synthesis of heat exchanger networks with no stream splits’, *Computers & Chemical Engineering*, vol. 22, no. 3, pp. 367–384, 1998.

[15] K. C. Furman and N. V. Sahinidis, ‘A Critical Review and Annotated Bibliography for Heat Exchanger Network Synthesis in the 20th Century’, *Ind. Eng. Chem. Res.*, vol. 41, no. 10, pp. 2335–2370, 2002.

[16] B. K. Srinivas and M. M. El-Halwagi, ‘Synthesis of combined heat and reactive mass-exchange networks’, *Chemical Engineering Science*, vol. 49, no. 13, pp. 2059–2074, 1994.

[17] K. P. Papalexandri and E. N. Pistikopoulos, ‘A multiperiod MINLP model for the synthesis of flexible heat and mass exchange networks’, *Computers & Chemical Engineering*, vol. 18, no. 11, pp. 1125–1139, 1994.

[18] D. Prakotpol and T. Srinophakun, ‘GAPinch: genetic algorithm toolbox for water pinch technology’, *Chemical Engineering and Processing: Process Intensification*, vol. 43, no. 2, pp. 203–217, 2004.

[19] S. Soywiset, T. Srinophankun, K. Turnprakiat, and W. Nuengwang, ‘Simultaneous Heat and Mass Exchanger Networks with Process Simulator’, *Journal of Chemical Engineering of Japan*, vol. 46, no. 2, pp. 146–157, 2013.

[20] L. Liu, J. Du, M. M. El-Halwagi, J. M. Ponce-Ortega, and P. Yao, ‘A systematic approach for synthesizing combined mass and heat exchange networks’, *Computers & Chemical Engineering*, vol. 53, pp. 1–13, 2013.

[21] L. Liu, J. Du, and F. Yang, ‘Combined mass and heat exchange network synthesis based on stage-wise superstructure model’, *Chinese Journal of Chemical Engineering*, vol. 23, no. 9, pp. 1502–1508, 2015.

[22] M. Á. Velázquez-Guevara *et al.*, ‘Synthesis of mass exchange networks: A novel mathematical programming approach’, *Computers & Chemical Engineering*, vol. 115, pp. 226–232, 2018.

[23] K. O. Yoro, M. K. Amosa, P. T. Sekoai, J. Mulopo, and M. O. Daramola, ‘Diffusion mechanism and effect of mass transfer limitation during the adsorption of CO_2 by polyaspartamide in a packed-bed unit’, *International Journal of Sustainable Engineering*, 2019. https://doi.org/10.1080/19397038.2019.1592261

[24] K. O. Yoro, M. K. Amosa, P. T. Sekoai, and M. O. Daramola, ‘Modelling and experimental investigation of effects of moisture and operating parameters during the adsorption of CO_2 onto polyaspartamide', *International Journal of Coal Science & Technology*, vol. 6, pp.225-234, 2019.

[25] A. Isafiade, M. Bogataj, D. Fraser, and Z. Kravanja, ‘Optimal synthesis of heat exchanger networks for multi-period operations involving single and multiple utilities’, *Chemical Engineering Science*, vol. 127, pp. 175–188, 2015.

[26] K.O., Yoro, A.J., Isafiade, and M.O., Daramola, 'Sequential synthesis of mass exchanger networks for CO_2 capture'. *In: Lecture notes in engineering and computer science: proceedings of the world congress on engineering and computer science*, San Francisco, USA, vol. 2*,* pp. 503–508, 2018.

[27] K.O., Yoro, A.J., Isafiade, and M.O., Daramola, Multi-period Heat Exchanger Network Synthesis with Temperature Intervals and Uncertain Disturbances, *Chemical Engineering Transactions*, vol. 76, 1039-1044, 2019.

[28] O. S. Azeez, 'Combined heat and mass exchanger network synthesis', PhD thesis, University of Cape Town, 2016.

[29] H. Yeomans and I. E. Grossmann, 'A systematic modelling framework of superstructure optimization in process synthesis', *Computers & Chemical Engineering*, vol. 23, no. 6, pp. 709–731, 1999.

[30] K. O. Yoro, 'Numerical simulation of CO_2 adsorption behaviour of polyaspartamide adsorbent for post-combustion CO_2 capture', MSc. Thesis, University of the Witwatersrand, 2017.

[31] M. M. El-Halwagi, Sustainable Design through Process Integration: Fundamentals and Applications to Industrial Pollution Prevention, Resource Conservation, and Profitability Enhancement. Butterworth-Heinemann, 2017.

[32] U. V. Shenoy, Heat Exchanger Network Synthesis: Process Optimization by Energy and Resource Analysis. *Gulf Professional Publishing,* 1995.

[33] G. Shavalieva, S. Papadokonstantakis, P. Kazepidis, A.I. Papadopoulos, and P. Seferlis, 'Sustainability Analysis of Phase-Change Solvents for Post-Combustion CO_2 Capture', *Chemical Engineering Transactions,* vol. 76, 1045-1050, 2019.

[34] T.T.N. Bachelor, and P. Toochinda, 'Development of low-cost amine-enriched solid sorbent for CO_2 capture'. *Environmental Technology,* vol. 33, 2645-2651, 2012.

[35] L.A. Pellegrini, S. Moioli, and S. Gamba, 'Energy saving in a CO_2 capture plant by MEA scrubbing'. *Chemical Engineering Research and Design*, vol. 89, 1676–1683, 2011.

[36] F. Bougie, and M.C. Iliuta, 'CO_2 absorption in aqueous piperazine solutions: experimental study and modelling'. Journal of Chemical & Engineering Data, 56, 1547-1554, 2011.