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A systematic procedure for process energy evaluation for post combustion CO_2 capture: Case study of two novel strong bicarbonate-forming solvents

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HIGHLIGHTS

- Energy evaluation of two strong bicarbonate-forming solvents applicable for post combustion CO_2 capture.
- A novel procedure for overall energy evaluation of CO_2 capture plants.
- Simulation to find optimum operation for CO_2 capture plants.

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ABSTRACT

Process simulation is used for energetic evaluation of two novel strong bicarbonate forming solvents for post combustion CO_2 capture, intended for coal- and natural gas based exhaust streams. An evaluation framework has been developed where process energy sinks are coupled to process energy balances based on the basic principles of a thermal heat engine. This procedure enables coupling of detailed solvent properties, such as reaction enthalpy, VLE, and kinetics, with the overall process operation, while accounting for the magnitude of the energy sinks in the process. The method identifies areas where there may be room for potential improvement, shows how the fundamental chemical properties of the solvents give rise to the overall capture potential, and highlights interdependencies between major energy sinks in the process. This framework is then used to clarify where heat is spent in the process for two novel solvent systems: activated 2-Piperidineethanol (2-PPE) and 1-(2-Hydroxyethyl)pyrrolidine (1-(2HE)PRLD). These novel solvents are compared with a base case of MEA and Cesar1. Activated 2-Piperidineethanol showed the best performance for the process setup evaluated in this work. The regenerative efficiency parameter for this solvent is 66% with an optimum specific reboiler duty of 2.78 MJ/kg CO_2 removed; a 22% reduction compared to MEA in the coal case. Furthermore, the solvent seems to be sufficiently fast to be used in an industrial absorber and is a promising system for post combustion CO_2 capture. This results in a power plant specific energy penalty for avoided CO_2 of 0.27 $kWh_{el}/kg\ CO_2$. The evaluation framework can also identify the potential for additional energy improvements by economizing configurations for improved internal heat distribution.

1. Introduction

1.1. Background

The increased focus on carbon capture and storage (CCS) stems from the need to reduce CO_2 emissions from fossil fuel combustion as described by the IPCC [1] and the IEA [2]. CO_2 reduction pathways consistent with the Paris Agreement of limiting global temperature rise “well below 2 °C” [3] requires implementation of large-scale CCS globally. This means that CO_2 must be captured from a wide range of sources in power generation and industry, and transported to suitable storage sites.

Post combustion capture with solvents is a robust technology and viable for large scale CO_2 capture from point sources such as power plants and industrial flue gases. In the past decade, with the increased focus on climate change, significant reductions in energy requirements have been realized in post combustion CO_2 capture technology. This has been accomplished by developing more energy efficient solvents as well as more energetically efficient process configurations for an overall improved capture process [4–10].

Specifically, recent research has focussed on reducing the waste heat released by the CO_2 capture process and using the heat added to the process in a most efficient manner. State-of-the-art research on CO_2

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Nomenclature

α	CO_2 loading (mol CO_2/mol amine)
β_{CO_2}	CO_2 capture ratio (–)
C_{P_l}	specific heat capacity liquid(MJ/kg K)
C_i	molar concentration component i (mol/m^3)
$\Delta h_{Vap,H_2O}$	molar heat of vaporization for water (J/mol)
$\Delta h_{Abs,CO_2}$	molar solvent heat of absorption CO_2 (J/mol)
$H_{g,in}$	enthalpy flow gas, into control volume (J/s)
ΔH_{Abs}	solvent heat of absorption CO_2 (MJ_{Th}/kg CO_2)
$\Delta H_{Vap,H_2O}$	heat of vaporization for water (MJ/kg)
$\mathrm{H_A}$	enthalpy at state A (or B) normalized to captured CO_2 (MJ/kg)
$\mathrm{H_{CO2}}$	enthalpy ideal gas CO_2 (MJ/kg)
$\frac{L}{G}$	liquid-to-gas ratio (kg/kg)
M_i	molecular weight for component i (kg/mol)
n_{eff}	solvent regeneration efficiency (–)
ρ_l	liquid density (kg/m^3)
Q_{Reb}	reboiler duty (MJ_{Th}/kg CO_2)
Q_{Abs}	absorption heat loss to surroundings (MJ_{Th}/kg CO_2)
Q_{Sens}	solvent sensible heat loss to surroundings (MJ_{Th}/kg CO_2)
Q_{Strip}	stripping heat loss to surroundings (MJ_{Th}/kg CO_2)
Q_{Ideal}	thermodynamic ideal heat limit for regeneration (J/s)
Q_{Real}	the real heat requirement for regeneration (J/s)
R	gas constant (J/mol K)
SRD	specific reboiler heat duty (MJ_{Th}/kg CO_2)
T	temperature (°C)
w_i	weight fraction component i (–)
W_{Fan}	fan work (MJ_e/ kg CO_2)
y_i	molar fraction of component i, gas phase

Subscript

$\wedge$	indicating additional cooling sinks within control volume
Am	amine
L	lean solvent stream
R	rich solvent stream
Sol	solvent

capture with amines primarily follows two pathways: solvent development and more energetically efficient process configurations.

Regarding solvent development, researchers have recently made progress in finding improved solvents for post combustion absorption from flue gases. Key characteristics are higher cyclic capacity, faster reaction rates for CO_2 absorption, and lower heat of absorption, which yields an overall lower thermal energy requirement for regeneration [11]. Several different amine solvents have been investigated, such as blended amines and activated hindered amine systems [12–16]. Hindered amines do not form carbamates due to their steric hindrance around the nitrogen group, thus yielding a potential capacity of one mole CO_2 per mole of amine, contrary to primary and secondary amines, which form carbamates with a maximum capacity of only half a mole CO_2 per mole amine. The drawback is that these hindered amines usually have slow absorption rates or may have unfavorable vapor-liquid equilibrium (VLE) properties for low partial pressure CO_2 gases [17].

Mixed absorbents combine the increased equilibrium capacity of the tertiary bicarbonate forming amines with the higher reaction rate of the primary and secondary carbamate forming amines. Blends of alkanolamines and polyamines may therefore provide tailored properties and, consequently, the ratio of bicarbonate and carbamate is important for optimizing cyclic capacity versus acceptable absorption rates.

Chowdhury et al. [18] screened 24 tertiary amine absorbents, including three synthetic amines, with systematic modification of their chemical structures. They report that seven tertiary amines have the potential to be used for CO_2 capture. Recently, Hartono et al. [19] systematically tested fifteen bicarbonate forming solvents in a screening apparatus for classes of tertiary amines. This resulted in identification of two solvent candidates, 2-Piperidineethanol (2-PPE) and 1-(2-Hydroxyethyl)pyrrolidine (1-(2HE)PRLD), with potential for much higher cyclic capacity than that for monoethanolamine (MEA), but with a significantly lower rate of absorption. For these candidates to be applicable for post combustion CO_2 capture, promotors/activators are needed to improve on the rate of reaction. Following this work, Hartono et al. [20], screened several alkanolamines as possible activators. The promotor, indicated as P4, was selected for further testing for VLE and heat of absorption measurements. These solvents, named HSA1 and HSA2, showed, from preliminary analysis a potential of very large cyclic capacities for both blends. Since the screening tests and experimental data only revealed preliminary information for these solvents, the next phase of work involves model development and simulation against benchmark solvent technologies. To gain further understanding and determine process applicability of HSA1 and HSA2, the present study focuses on a detailed process simulation study of these novel blends.

The second common research pathway has been to develop more energy efficient process configurations. A method often used for estimating thermal energy usage in this regard is to assess and compare the main contributing process heat sinks. To the best of our knowledge, there exists no procedure in the open literature that quantitatively compares rigorous process simulation with a thermal energy sink analysis that can be broken down and compared to simplified heat sink equations directly.

The relationships between fundamental properties of the absorbent and the design of the absorption process, in view of the main process heat sinks, is discussed in Svendsen et al. [21], Oexmann et al. [8] and Neveux et al. [22]. In these studies, simplified equations for the main sinks are given. An elaborate derivation of variants of the Gibbs-Helmholtz equation, applicable to absorption processes, is given in Mathias [23]. It is in this study noted that further process improvements are possible, while staying within the strict bounds imposed by the laws of thermodynamics.

There have been numerous recent papers published on process optimization, simulation and changes in plant design for reducing the energy requirements of a post combustion capture plant. A thorough summary of recent papers up to 2016 is given in Feron [24]. Rochelle et al. [25], uses piperazine (40 wt%) in an energy analysis to assess process reversibility of post combustion capture processes suggesting that absorption with amines is the technology of choice for post combustion capture from coal flue gases. A thermodynamic reversibility analysis is discussed by Lin et al. [26], also for piperazine. In this work, an "advanced flash stripper" configuration is studied, that is claimed to significantly improve process reversibility. Another "superstructure-based" approach using multiple process modifications was carried out by Oh et al. [27]. This study reports improved overall energy efficiencies with different process modifications, such as absorber intercooling and split-flow schemes. Damartzis et al. [28], have recently modelled different plant configurations based on specific characteristics of different solvents. They observed a 22% reduction in reboiler duty by utilization of an intercooled absorber configuration for a 30%wt MEA solvent. This is attributed to the enhanced equilibrium capacity shift towards the absorber bottom. However, it is not stated if the base case operated at an optimum loading level with respect to specific reboiler duty (SRD).

Similarly, Sanpasertparnich et al. [29] report an improvement of 24.4% in SRD by using multiple absorber intercoolers, for quenching the evolving temperature bulge, also for MEA. They report that a rich