Verification of a Solvent Optimization Approach for Postcombustion CO₂ Capture Using Commercial Alkanolamines

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ABSTRACT

This paper verified a phase equilibrium approach for optimization of conceptual solvents by using process simulations of commercial solvents, N-methyl-diethanolamine (MDEA) and 2-amino-2-methyl-1-propanol (AMP) aqueous solution, for a conventional absorption/desorption based postcombustion CO₂ capture process. The simulated total heat/total equivalent work for the investigated tertiary/hindered amines has the same trends as those based on the phase equilibrium approach for conceptual solvents with the same heat of reactions. Moreover, the simulated CO₂ working capacities for the commercial solvents agree well with those obtained with the phase equilibrium approach for the corresponding conceptual solvents, verifying the phase equilibrium approach. Results of parametric tests using the AMP aqueous solution illustrate that there is an optimal lean loading for the lean solution and an optimal temperature for the stripper inlet solvent to achieve the least total equivalent work/total heat.

Keywords: CO₂ capture; solvent optimization; approach verification; alkanolamine; postcombustion flue gas; conventional absorption/desorption process.

1. INTRODUCTION

Amine scrubbing is currently the leading technology for postcombustion CO₂ capture.¹ However, high energy consumption in solvent-based CO₂ capture continues to be a major hurdle for commercialization. The U.S. Department of Energy (DOE)/National Energy Technology Laboratory (NETL)² estimates that the deployment of current postcombustion CO₂ capture technology, aqueous monoethanolamine (MEA) solution based chemical absorption process, in a new pulverized coal power plant would decrease the plant efficiency by 30%. Clearly, an economical and energy efficient CO₂ capture process is a prerequisite for global CO₂ emission control from fossil energy sources to mitigate global warming. However, through optimization of solvent properties and the absorption/desorption process, it may be possible to reduce the energy penalty from CO₂ capture.^{3,4}

Energy consumption for solvent regeneration, represented by reboiler heat duty, is an important parameter for design and operation of a cost-effective CO₂ capture process. Some commonly used solvents are aqueous solutions of alkanolamines, such as MEA, diethanolamine (DEA), and methyl-diethanolamine (MDEA).⁵ MEA is the most widely used because it has a fast rate of reaction with CO₂, reasonable degradation resistance, and low solvent cost. However, high desorption energy consumption,

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vaporization losses and equipment corrosion issue are disadvantages of MEA. Sterically hindered and tertiary amines, 2-amino-2-methyl-1-propanol (AMP) and MDEA are receiving increased attention recently due to their loading up to 1 mol of CO₂/mol of amine and relatively low energy consumption for solvent regeneration, leading to significant savings in process costs.⁶ MEA solvent requires high reboiler heat duty, from 3,800 to 5,400 kJ/kg CO₂.⁷ The AMP with DEA activated solvent has a modest heat requirement of 3030 kJ/kg CO₂.⁸ To compare among the CO₂ capture processes, Oyeneke and Rochelle³ applied the concept of “equivalent work,” which is the equivalent loss of electricity in the power plant due to the steam extraction and the required power demand due to the CO₂ compression.

Effects of various stripper configurations on energy consumption have been studied^{3,9-10} and both reboiler duty and the total equivalent work were reduced compared to a simple stripper by using configurations including multipressure stripping, vacuum stripping or stripping with vapor recompression. Because the reboiler heat duty relates inversely to lean-CO₂ loading/rich-CO₂ loading and alkanolamine concentration,⁷ the reboiler energy saving can be also achieved by optimizing the lean solvent loading, the solvent concentration and the stripper operating pressure for MEA-based CO₂ capture process but the optimal heat duty is still 3000 kJ/kg CO₂.¹¹

Heat of reaction has been identified as a key property for optimization of the CO₂ capture process.^{4,12} A phase equilibrium approach¹² was developed to describe a conceptual solvent, which is characterized by the heat of reaction between CO₂ and the solvent. Optimization of a conceptual solvent is achieved through quantification of the impact of heat of reaction on the sensible and stripping heat. The conceptual solvent was optimized for the least total equivalent work for a conventional absorption based post-combustion CO₂ capture process. Results show that the least total equivalent work is about 0.1034 kWh/kg CO₂ with a heat of reaction of 71 kJ/mol CO₂ for tertiary or sterically hindered amines under typical solvent regeneration conditions of 2 atm operating pressure.

This paper verifies the phase equilibrium approach for optimization of conceptual solvents using commercial solvents, including a tertiary amine (MDEA aqueous solvent), and a sterically hindered amine (AMP aqueous solvent). In this study, the energy performance of the absorption/desorption process using MDEA or AMP was obtained through process simulations. The thermal performance of MEA aqueous solvent was also simulated using a similar optimization approach as a reference case. The findings obtained from this work provide new insights and guidance for identifying energy efficient solvents and develop a strategy for cost-effective postcombustion CO₂ capture.

2. METHODOLOGY

2.1. Overview. The verification of the phase equilibrium approach was conducted with process simulations.¹² Specifically, the thermal performance of a conventional absorption/desorption based CO₂ capture process was simulated using ProTreat[®] software.¹³ ProTreat was developed for simulating processes for acid gas removal from a variety of high and low pressure gas streams by absorption into solutions including single/blended amines or physical solvents. The ProTreat simulator is a mass and heat transfer rate based model for both absorption and regeneration columns. The software was validated by comparison of vapor-liquid-equilibrium data from simulation and experimental data for various amines and at various concentrations under various temperatures.

2.2. Phase Equilibrium Approach. The phase equilibrium approach was developed for optimizing a conceptual solvent by minimizing the total equivalent work for absorption/stripping based post-combustion CO₂ capture.¹² The conceptual solvent was characterized according to its heat of reaction, which was further used to estimate sensible and stripping heat through a phase equilibrium model that links equilibrium CO₂ partial pressure with solvent properties (such as heat of reaction and working capacity) and operating conditions (such as temperature). For hindered/tertiary amines, the phase equilibrium model can be described by,¹²

$$P_{CO_2}^* = e^{17.163 + 0.1035\Delta H_R - \frac{\Delta H_R}{RT}} \cdot \frac{\alpha^2}{(1-\alpha)} \quad (1)$$

where $P_{CO_2}^*$ is CO₂ equilibrium partial pressure with aqueous amine solutions; α is CO₂ loading in the aqueous amine solution, expressed as moles of chemically combined CO₂ per mole of amine; ΔH_R is the heat of reaction between the solvent and CO₂; R is the ideal gas constant; T is absolute temperature.

In absorption/stripping-based CO₂ capture processes, the total heat consumption (Q_T) includes three components: heat of reaction or heat of absorption (Q_R), sensible heat (Q_S), and stripping heat (Q_W):

$$Q_T = Q_R + Q_S + Q_W \quad (2)$$

In the phase equilibrium approach, the heat of reaction is known, which refers to the total heat released when CO₂ is absorbed from a low CO₂ loading (0-0.4 mole CO₂/mole amine) at 40°C with typical amine concentrations. The sensible heat refers to the additional energy required after the heat recovery to achieve the desired regeneration temperature. This additional energy is quantified by a temperature approach (ΔT), which is usually known for commercial heat exchangers. The sensible heat is estimated by,

$$Q_s = \frac{C_p \Delta T}{x \Delta \alpha} \quad (3)$$

where C_p is the specific heat of the aqueous solvent; ΔT is the heat exchanger's temperature approach; x is the mole fraction of a solvent in aqueous solution; $\Delta \alpha$ is the working capacity of the conceptual solvent, defined by $\Delta \alpha = \alpha_2 - \alpha_1$, where α_1 and α_2 are the CO₂ loading (mol CO₂/mol amine) in the lean and rich solution, respectively.

In the phase equilibrium approach, gas-liquid phase equilibrium for CO₂ is assumed to be achieved for both lean and rich solution in both absorber and stripper. Therefore, both lean and rich CO₂ loadings can be estimated using Equation 1 where CO₂ partial pressures in the flue gas and operating temperatures in the absorber are known, thus sensible heat can be estimated.

The stripping heat refers to the latent heat of water vapor carried away per unit of product gas (CO₂) at the top of the stripper. Under conventional low operating pressure, both water and CO₂ can be taken as ideal gas. Then, stripping heat can be simply estimated by the ratio of water and CO₂ partial pressures, given by,

$$Q_w = \frac{P_{H_2O}}{P_{CO_2}} \Delta H_w \quad (4)$$

1 where P_{H_2O} and P_{CO_2} are the water and CO₂ partial pressures at the top of a stripper; ΔH_w is the latent heat
2 of water vaporization.

3 In the phase equilibrium approach, the stripper operating pressure is a known constant (2 atm) and is
4 assumed as the sum of CO₂ and pure water saturated vapor pressures. The CO₂ partial pressure as a
5 function of temperature is estimated with Equation 1 and pure water saturated vapor pressure as a
6 function of temperature is also available from references.¹⁴ Therefore, the temperature T of the rich
7 solvent on top of the stripper can be estimated numerically. When the rich solvent temperature is obtained,
8 water vapor and CO₂ partial pressures can be determined accordingly and the stripping heat can be
9 calculated with Equation 4.

10 **2.3. Configuration of CO₂ Capture Process.** This paper investigates postcombustion CO₂ capture
11 from coal-fired power plant flue gas with 90% CO₂ removal. The flue gas is assumed to be at atmospheric
12 pressure and to contain 14% CO₂ with the balance of the stream being N₂, H₂O, and O₂. Because solvent
13 optimization depends on the CO₂ capture process and associated operating conditions, a conventional
14 absorption/stripping process was used. The process flow diagram is shown in Figure 1. After initial
15 cooling, the raw flue gas flows from the bottom of the absorber upwards against a countercurrent stream
16 of a selected amine solution. The gaseous CO₂ is absorbed into the solution, and the clean flue gas exits
17 from the top of the absorber. Two sets of inter-stage cooling are applied to avoid high temperature in the
18 absorber and to enhance mass transfer efficiency.

19 The CO₂ rich solution exits from the bottom of the absorber and is heated by the hot lean solution from
20 the stripper through a lean-rich cross heat exchanger. Then, it enters the top of the stripper. The rich
21 solution flows downward against a countercurrent flow of water vapor generated in a bottom reboiler
22 until the CO₂ concentration in the solution is reduced to the inlet level (lean loading) for the absorber. The
23 CO₂ product is separated from the gaseous mixture by passing it through a condenser where water vapor
24 is condensed and removed. The lean solution from the bottom of the stripper provides heat to the rich
25 solution through an internal heat exchanger located at two meters from the top of packing within the
26 column and an external cross heat exchanger in order to improve CO₂ stripping efficiency and heat
27 recovery. CO₂ stripping efficiency herein is defined as the total mass of CO₂ stripped out from the rich
28 solution to the gaseous phase over the total mass of CO₂ in the rich solution brought into the stripper. The
29 temperature approach at cold end of internal heat exchanger is assumed to be operated at least 5°C.
30 Finally, the lean solution passes through a cooler to achieve a designated temperature and returns to the
31 top of the absorber.

32 It should be pointed out that the focus of this study is to verify a approach of solvent optimization for
33 CO₂ capture from post-combustion flue gases.¹² The verification was conducted from the standpoint of
34 thermal performance instead of engineering economics. However, in a commercial process the
35 minimization of cost may be a more desirable optimization target than the minimization of energy
36 consumed.

37 **2.4. Operating Conditions.** The operating conditions for the process in Figure 1 and the composition
38 of flue gas are summarized in Table 1. The flue gas data are adopted from the DOE/NETL report (Case
39 12) for a supercritical pulverized coal plant after flue gas desulfurization.¹⁵ The solvents used in this study
40 include a tertiary amine (50 wt% MDEA aqueous solvent), and a sterically hindered amine (30 wt% AMP

aqueous solvent). For thermal performance comparison with a widely used commercial amine, 30 wt% MEA aqueous solvent was also used.

Figure 1. Schematic of the absorption/stripping based CO₂ capture process.

Table 1. CO₂ capture process operating conditions.

Parameter	Unit	Value
Absorption column		
Nominal CO ₂ removal	%	90
Lean solution feed temperature	°C	40
Operating pressure	atm	1
Flue gas flow rate	kg/hr	3,122,000
Flue gas composition		
N ₂	vol%	67.7
O ₂	vol%	2.3
CO ₂	vol%	13.3
H ₂ O	vol%	16.7
Stripping column		
Rich solution feed temperature	°C	Varies
Operating pressure	atm	2
Heat exchanger		
Minimum of temperature approach	°C	5

2.5. Evaluation of Thermal Performance. In simulation of the CO₂ capture process in Figure 1, the total heat consumption is determined by the known reboiler duty in the stripper. If the heat loss in the process is neglected, the sensible heat is the heat consumed to heat up the lean solvent for the temperature difference between the lean solution exiting from the cross heat exchanger and the rich solution entering the cross heat exchanger, given by

$$Q_s = L \cdot C_p (T_2 - T_1) / Y_{CO_2} \quad (5)$$

where L is the solvent flow rate; C_p is the specific heat; T_2 is the temperature of the lean solvent exiting from the cross heat exchanger; T_1 is the temperature of the rich solvent entering the cross heat exchanger; Y_{CO_2} is the CO_2 product yield. All parameters for an amine solvent in the right-hand-side of Equation 2 are known from ProTreat simulations.

The stripping heat can be estimated with Equation 4. The water and CO_2 partial pressures at the top of a stripper are also known from ProTreat simulations.

Because the heat of reaction generally changes with reaction temperature and CO_2 loading, the real heat of reaction is estimated by the difference between the total heat consumption and the sum of sensible heat and stripping heat based on Equation 2.

Since the temperature in the reboiler differs for different amines, the direct comparison of total heat consumption does not reflect the effect of the reboiler temperature on the work value of the steam. The concept of equivalent work introduced by Oyenekan and Rochelle³ was applied in this study, which converts the total heat to total equivalent work, defined by,

$$W_T = 0.0002778 Q_T \cdot \eta \quad (6)$$

where W_T is total equivalent work in kWh; η is Carnot cycle efficiency, defined by $\eta = 1 - 313.15 / (T_L + 10)$. Herein, T_L is the temperature in K for the lean solution exiting from the reboiler. Because the practical heat efficiency usually cannot achieve Carnot cycle efficiency, Equation (6) may not be accurate for converting heat to work, but it provides a useful estimate for our purpose.

3. RESULTS AND DISCUSSION

3.1. Energy Performance. In the simulation of the energy performance for the CO_2 capture process depicted in Figure 1, process conditions were established to be consistent with the assumptions made in the phase equilibrium approach.¹² First, the CO_2 loading for the lean solution (the inflow to the absorber) was set as high as possible to allow its CO_2 equilibrium pressure to approach the CO_2 partial pressure in the flue gas at the top of absorber. Second, the solvent circulation flow rate is set as low as possible to let the CO_2 equilibrium pressure of the rich solution at the bottom of absorber to approach the CO_2 partial pressure in the flue gas. To achieve 90% CO_2 removal from the flue gas, however, higher CO_2 lean loading usually leads to larger solvent circulation flow rate, which will go against the second assumption by reducing the rich loading due to increased circulation flow rate. The tradeoff is adjust the lean loading and solvent circulation flow rate by try-and-error method to achieve close differences between the CO_2 partial pressure in gas phase and the CO_2 equilibrium pressure in the corresponding liquid phase along the absorber depth. Next, the temperature of the rich solution entering the stripper was set as low as possible unless CO_2 re-absorption occurs at top of the stripper. Finally, the minimum temperature approach for both the cross and internal heat exchangers is 5 °C.

To remove 90% of CO_2 from flue gas under the condition prescribed in Table 1, the energy performance obtained from simulations with ProTreat software for the selected amines is summarized in Table 2. Table 3 provides the reference energy performance estimated with phase equilibrium approach for the optimal solvent¹² and conceptual solvents having the equivalent heat of reaction as the selected amines. Because the heat of reaction changes with reaction temperature and CO_2 loading, the second

column of Table 2 lists reference heat of reactions, which are based on total heat released when CO₂ is absorbed from a low CO₂ loading (0–0.4 mol CO₂/mol amine) at 40 °C. Comparing to the reference heat of reaction, the estimated average heat of reaction over the entire range of CO₂ loading encountered in the stripper reduces by 7.2% for MDEA, 4.6% for AMP and 11.9% for MEA.

The CO₂ working capacity are 0.17 mole CO₂/mole amine for MDEA and 0.33 mole CO₂/mole amine for AMP, which are close to the corresponding values estimated with the phase equilibrium approach for a conceptual solvent with the same reference heat of reaction,¹² i.e., 0.16 mole CO₂/mole amine for MDEA equivalent and 0.37 mole CO₂/mole amine for AMP equivalent. The CO₂ working capacity for MEA is 0.20 mole CO₂/mole amine. The larger working capacity of AMP results in less sensible heat than that of MDEA. However, the *Protreat* simulated sensible heats of the investigated amines are obviously higher than those estimated with the phase equilibrium approach for equivalent amines. The reason for such difference is not only the differences in CO₂ working capacity, but also the temperature approach accounting for the sensible heat. Evaporation of a fraction of CO₂ from the rich solution at high temperature during the heat exchange results in the point with minimum temperature approach exists between the cold end and hot end of the heat exchangers. To meet the minimum of 5 °C temperature approach for the exchangers, the cold end temperature approach of the cross exchanger must be larger than 5 °C, which is also the temperature approach account for the sensible heat. The quantity of the fraction evaporated depends on the solvent characteristics. As a result, the temperature approach accounting for sensible heat is different for different amines. Simulation results shows that the temperature approach is 9 °C for MDEA, 6.5 °C for AMP and 13°C for MEA while the temperature approach for the optimal conceptual solvent is 5 °C. Both CO₂ working capacity and temperature approach dominate the sensible heat. Therefore, the rank of sensible heat from large to small is MEA, MDEA, AMP, and the optimal conceptual solvent.

Similar to the results in literature,¹⁶ the stripping heat decreases with increasing reference heat of reaction. However, even for the process using MEA, which has a higher reference heat of reaction than the optimal solvent, the simulated stripping heat is higher than that of the corresponding conceptual optimal solvent. This result implies that the CO₂ partial pressure does not reach its equilibrium pressure in the real process and therefore a relatively higher portion of water is evaporated in the real process.

Because of higher sensible and stripping heat for commercial amines than those for the equivalent conceptual solvents, the total heats are 2493 kJ/kg CO₂ for MDEA and 2295 kJ/kg CO₂ for AMP, which are 9.3% and 10.1% higher than the corresponding total heat estimated for the equivalent conceptual solvents.¹² However, the difference of total heat between MDEA and AMP is 198 kJ/kg CO₂, similar to the corresponding difference for the equivalent conceptual solvents, 195 kJ/kg CO₂. Similarly, MDEA's total equivalent work is 23.8% higher than AMP, close to the difference for the MDEA equivalent that is 20.2% higher than the AMP equivalent. These results indicate that either the total heat or the total equivalent work based on commercial tertiary/hindered amines has the same trends as the equivalent conceptual solvents that were determined by the phase equilibrium approach. Furthermore, the simulated total heat for MEA is quite close to that of optimized MEA processes in the literature,¹¹ which indicates that the configuration of the conventional absorption/desorption process is advanced and reliable.

Table 2. Energy performance by ProTreat simulation for the selected amines.

Solvent	Q_R^0 kJ/kg CO ₂	Q_R kJ/kg CO ₂	Q_S kJ/kg CO ₂	Q_W kJ/kg CO ₂	Q_T kJ/kg CO ₂	η %	W_T kWh/kg CO ₂
MDEA	1336	1240	913	340	2493	21.74	0.151
AMP	1636	1560	474	261	2295	19.11	0.122
MEA	1918	1689	1100	196	2987	21.35	0.177

Note: Q_R^0 are the reference heat of reactions,¹² which are based on total heat released when CO₂ is absorbed from a low CO₂ loading (0–0.4 mol CO₂/mol amine) at 40 °C while Q_R is the average of heat of reaction over the entire range of CO₂ loading encountered in the stripper.

Table 3. Energy performance by phase equilibrium approach for the selected amines equivalent and the optimal conceptual solvent.

Solvent	Q_R^0 kJ/kg CO ₂	Q_S kJ/kg CO ₂	Q_W kJ/kg CO ₂	Q_T kJ/kg CO ₂	η %	W_T kWh/kg CO ₂
MDEA equivalent	1336	695	249	2280	19.68	0.125
AMP equivalent	1636	273	176	2085	17.89	0.104
MEA equivalent	1918	1374	140	3432	16.28	0.155
Optimal	1614	272	180	2065	18.02	0.103

3.2. Parametric Tests. The parameters for the thermal performance analysis include the lean CO₂ loading, the solvent circulation flow, and the temperature of the rich solution entering the stripper. Two criteria for the parametric tests are that the CO₂ removal efficiency from the flue gas must be 90% or higher and the minimum temperature approach for all heat exchangers is 5°C. As a sterically hindered amine, AMP was used for the parametric tests. Parametric test is important to scrutinize the difference of energy performance between a conceptual solvent and a commercial solvent and to provide insight to optimize a conventional absorption/desorption based CO₂ capture process.

The lean loading and solvent circulation flow are interdependent for reaching the 90% CO₂ removal target because the solvent circulation flow rate is usually reduced when CO₂ working capacity is increased by decreasing the lean loading. In the parametric tests for the lean loading, the temperature of the stripper influent solvent flow is constant at 80°C. Figure 2 demonstrates the effect of the CO₂ lean loading on the total energy performance. A least total equivalent work/total heat is identified at an optimal lean loading of 0.365 mole CO₂/mole AMP. The variation of total equivalent work with increasing lean loading becomes less sensitive than that of the total heat because of the reduced Carnot cycle efficiency as shown in Figure 3. Figure 3 also shows that the necessary reboiler temperature and the corresponding Carnot cycle efficiency for the heating steam are inversely proportionally to the lean loading.

Figure 2. Effect of lean loading on energy performance.

Figure 3. Effect of lean loading on reboiler temperature/Carnot efficiency.

When the rich loading is constant at 0.69 mole CO₂/mole AMP, Figure 4 demonstrates the effect of lean loading on stripping heat, sensible heat and the solvent temperature approach accounting for sensible heat. Because the solvent circulation flow rate usually increases with lean loading, slightly more vapor is captured at the top of the stripper by the increased solvent flow, resulting in a slight decrease of the stripping heat. Because of the effect of a fraction of CO₂ vaporization in rich solution during heat exchange, on the other hand, the temperature difference accounting for sensible heat varies with lean loading to meet the requirement of the minimum temperature approach for heat exchange. A least temperature difference accounting for the sensible heat is also identified at a lean loading of 0.365 mole CO₂/mole solvent. Accordingly, a least sensible heat is also identified at the lean loading of 0.365 mole CO₂/mole solvent. When lean loading is less than 0.365 mole CO₂/mole solvent, the temperature difference accounting for the sensible heat offsets the impact of the solvent circulation flow rate on sensible heat. When lean loading is greater than 0.365 mole CO₂/mole solvent, however, the increased circulation flow plays a greater role than the relatively flat temperature difference, resulting in a rapid increase of sensible heat. As a result, there is an optimal lean loading for the conventional amine-based absorption/desorption CO₂ capture process.

Figure 4. Effect of lean loading on heat performance.

Figure 5 illustrates the effect of the stripper solvent inlet temperature on energy performance when the CO₂ lean and rich loadings are kept constant at 0.40 and 0.69 mol CO₂/mol AMP, and the solvent circulation rate of the stripper influent is maintained constant at 25 kg/kg product CO₂. For AMP, an optimal of 82 °C will result in the least total equivalent work/total heat. The existence of the optimal inlet temperature results from the effect of the inlet temperature on stripping and sensible heat as shown in Figure 6. The stripping heat increases with increasing stripper influent temperature. The sensible heat, however, is determined by the temperature approach accounting for the sensible heat when the solvent flow is constant. When the inlet temperature is lower than 82°C, the internal exchanger is expected to have a larger heat exchange load but the minimum temperature approach caused by CO₂ evaporation from the rich solution, existed between the cold and hot ends of the internal exchanger, prevents the exchanger to achieve such a desired heat load to meet the required minimum 5 °C temperature approach. As a result, the desired heat exchange load cannot be achieved through heat exchange, which results in a larger sensible heat. Similarly, when the inlet temperature is higher than 82°C, the minimum temperature approach existed in the cross heat exchanger prevents the exchanger to achieve desired heat exchange load, which also results in a larger sensible heat.

4. CONCLUSIONS

This work verified a phase equilibrium approach for optimization of a conceptual solvent by using simulations of commercial solvents, aqueous MDEA and AMP, for a conventional absorption/desorption based postcombustion CO₂ capture process. Simulation results of the energy performance for these solvents indicate the following conclusions:

- The simulated CO₂ working capacities for the commercial solvents agree well with those obtained with the phase equilibrium approach for conceptual solvents with the same reference heat of reaction. However, the simulated sensible heat for a commercial solvent is usually much larger than that of the equivalent conceptual solvent because the temperature approach of a commercial solvent accounting for the sensible heat is usually larger than the minimum temperature approach used to quantify the sensible heat for the conceptual solvent.
- The simulated stripping heat decreases with increasing reference heat of reaction. However, the simulated stripping heat of a commercial solvent is always higher than that of the corresponding conceptual solvent because the CO₂ partial pressure is not able to achieve its equilibrium pressure in the practical process.

- The simulated tertiary/hindered amines has the same trend in total heat/total equivalent work as the conceptual solvent with the same reference heat of reaction, which indicates that the phase equilibrium approach can be used to screen the performance of solvents.
- Results of parametric tests using aqueous AMP illustrate that there is an optimal lean loading for lean solution and an optimal solvent inlet temperature to the stripper to achieve the least total equivalent work/total heat.

Figure 5. Effect of stripper influent temperature on energy performance.

Figure 6. Effect of stripper influent temperature on heat performance.

Notes

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NOMENCLATURE

C_p = specific heat of aqueous solvent [kJ/(kmol·K)]
 ΔH_R = the heat of reaction between the solvent and CO₂ (kJ/mol)
 ΔH_w = latent heat of water vaporization (kJ/mol)
 L = flow rate of the lean solvent exiting from cross heat exchange (kmol/hr)
 P_{H_2O} = water partial pressures (bar)
 P_{CO_2} = CO₂ partial pressures (bar)
 Q_R = heat of reaction (kJ/mol CO₂)
 Q_S = sensible heat (kJ/mol CO₂)
 Q_T = total heat demands (kJ/mol CO₂)
 Q_w = stripping heat (kJ/mol CO₂)
 R = the ideal gas constant; $R = 8.314$ kJ/(kmol·K)
 T_1 = temperature of the rich solvent entering to cross heat exchange (K)
 T_2 = temperature of the lean solvent exiting from cross heat exchange (K)
 ΔT = temperature approach of the cross heat exchanger [K]
 W_T = total equivalent work [kWh]
 x = mole fraction of a solvent in aqueous solution
 Y_{CO_2} = CO₂ product yield (kmol/hr)

Greek Symbols

α = CO₂ loading in the aqueous amine solution [mol/mol amine]
 $\Delta\alpha$ = solvent working capacity [mol/mol amine]
 η = Carnot cycle efficiency

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