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A Physical Absorption Assessment of a New Alternative Solvent for Carbon Capture

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The reliance of the world economies on the use of fossil fuels (i.e. coal, natural gas and oil) as primary source of energy, have contributes to the high emission of CO_2 in atmosphere. One of the promising way to mitigate the CO_2 emission is by implemented Post Combustion Carbon Capture (PCCC) through absorption process. PCCC by amines based solvent is a method to remove the carbon dioxide from the main stream of escape gases before releasing them to the atmosphere. Using this technology, it is possible to reduce CO_2 emissions rate around 80 % to 95 %. Currently, the commercialise solvent used for carbon capture which is monoethanolamine, (MEA) have some drawbacks such as high energy penalty for regeneration process, solvent degradation issue and not environmental friendly. Therefore it is a need to develop new alternative solvent to improve the current carbon capture process. The objective of this study is to evaluate the absorption and desorption performance of new alternative solvent for carbon capture process. In this study, Aspen Plus software is used to simulate the absorption and desorption process, estimate and evaluate the performance of MEA and all new alternative solvent. Three absorption performance criteria that is assessed in this study are percentage of CO_2 capture by each solvent, energy required for solvent regeneration and percentage of solvent loss through thermal degradation process. This performance assessment is only based on the physical absorption theory. The reaction interaction between CO_2 and solvent will not be assessed in this study due to the limitation of data of new alternatives solvent. The result of this study shows that, all the new alternatives solvent is suitable for PCCC process. Besides, some of the solvent show a good performance (less energy requirement, high capture capacity and low rate of degradation) when compare with MEA.

1. Introduction

Carbon dioxide gas is the gas that contribute the highest amount of greenhouse gas in the atmosphere. As the concentration of this gas in atmosphere increase, it will lead to the rising of Earth temperature and adverse effects on the environment. The emission of CO_2 in atmosphere is mainly comes from the human activities in power generation sector such as the burning of fossil fuels, coal and natural gas. This is due to the limitations of other options in power generation sector. As the results, fossil fuels will continue to become a major sources of future energy worldwide to meet the energy demands, especially in developing countries (IEA, 2013).
Reductions in CO_2 emissions can be realised in the short term approach through the application of carbon capture. The main idea of carbon capture is to achieve Near-Zero emissions from fossil fuels power plants technologies which could be very competitive strategy to mitigate the CO_2 emission in atmosphere. In terms of CO_2 capture, there are different techniques to carry out the process like post-combustion, pre-combustion and oxy-combustion. This study will focus on the application of Post Combustion Carbon Capture (PCCC). PCCC operates by contacting flue gas exiting the power station containing CO_2 with solvent, before it will be released to the atmosphere. As an effective PCCC technology, chemical absorption method is regarded as the most promising one. This method has been used for several years in coal gasification and natural gas processing with successful results. Many absorbents have been applied to this chemical absorption process. For example

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aqueous solutions of alkanolamines, potassium carbonate, and aqueous ammonia, but monoethanolamine (MEA) is the most established solvent for chemical absorption PCCC process.
However, the major challenges is the used of MEA as solvent leads to several disadvantages on the overall performance of carbon capture process such as solvent loss due to thermal degradation, degradation of solvent in the presence of oxygen (Zaman and Lee, 2013), high corrosion rate of pipelines and equipment (Yu et al., 2012), and high energy required to regenerate the solvent (Olajire, 2010). All these disadvantages greatly increase the overall cost of PCCC process (Hasaneen et al., 2014), and thus hindered the large-scale application of PCCC technology (Bandyopadhyay, 2011). Currently, plenty of significant research in absorption of CO_2 field has been done through experimental and computational approach. The studied focus on the properties of desired solvent and try to develop new alternatives solvent for absorption process which can improved the current carbon capture performance. Example of related study are, synthesis and selection of hindered new amine solvents (Chowdhury et al., 2011), design of ionic liquid solvent for enhanced CO_2 Capture (Chong et al., 2014) and development of systematic framework for selection of amines mixture as CO_2 solvent candidate (Zarogiannis et al., 2015).
The main objective of this study is to evaluate the physical absorption and desorption performance of new alternatives solvents based on the CO_2 capture efficiency, total energy requirement for solvent regeneration and amount of solvent loss through thermal degradation process. Then the results is compared with the performance of standard solvent MEA. In this work the PCCC process is simulated using the Aspen Plus simulation software to estimate and evaluate the physical absorption and desorption performance of the solvents. Comparisons of new alternatives solvent and the standard solvent MEA is done through scoring system to screen and determine which solvent is most suitable for PCCC process in terms of high absorption capacity, low energy requirement for regeneration energy and low thermal degradation rate.

2. New alternatives solvent candidates

The use of alternative solvents has gained more attention during the recent years to overcome the drawbacks of the current commercialised solvents. In this study, 25 new alternatives solvent candidates from amines functional group is used for physical absorption and desorption performance study. Out of 25 alternatives solvent, 21 are categorised as primary and secondary amines solvents and 4 are categorised as tertiary amines solvents. The list of new alternative solvents used in this study is showed in the Table 3 (Primary and secondary amines solvents are from 1 to 21 while tertiary amine solvent from 22 to 25). All these new alternative solvents are taken from a previous study conducted by Ahmad et al. (2015).
These new alternative solvents are generated by using CAMD approach where the target properties of the desired solvent are specified first, then the solvent that match the target properties are identified and generated for the CO_2 capture. The physical target properties that are considered in the generation of these alternatives solvents are solubility parameter, normal boiling point, normal melting point, flash point surface tension, density, vapour pressure and viscosity. The detailed explanation on the generation of this new alternatives solvent can be found in Ahmad et al. (2015).

3. Methodology for assessment of physical absorption and desorption performance

This section describes the methodology to evaluate the physical absorption and desorption performance of MEA and all new alternatives solvent. A case study is carried out to know the suitability of new alternatives solvents for PCCC process and to compare its performance with standard solvent, MEA. In order to estimate the physical absorption and desorption performance of MEA and the new alternatives solvents, a simulation model using the Aspen Plus software is developed for PCCC process. The step by step methodology of this study is shown below.

a. First the Aspen Plus simulation model which consist of absorption column, desorption column and other unit operation is developed as shown by process flow diagram in Figure 1.
b. Next, the Aspen Plus simulation model is tested using MEA as the standard solvent. As validation step of the simulation model, the result of simulation model using MEA solvent is compared with the result of previous study from literature. For this purpose, flow-rate data for the inlet flue gas and operation conditions in the absorption and stripper columns are taken from similar projects where MEA is used as the main solvent.
c. After the simulation model has been validated, various parameters such as solvent flowrate, inlet flue gas flowrate, temperature and pressure of input streams as well as the operating condition of the absorber column, stripper columns and other unit operation are recorded and kept as constant variable.
d. Then the validated Aspen Plus simulation model is used to evaluate all the new alternatives solvent.

The process performance of all new alternative solvent and MEA are evaluated based on the result of Aspen plus simulation model. Three process performance criteria that are assessed in this study are:

a. CO_2 absorption efficiency (The result is based on percentage of CO_2 capture in absorber column).
b. Energy required for solvent regeneration (The result is based on reboiler heat duty in stripper column).
c. Percentage of solvent loss through thermal degradation process (The result is based on the percentage of solvent exit at the top of absorber and stripper column).

The next section will describe in detail the description of PCCC process and the development of Aspen Plus simulation model for PCCC process.

3.1 PCCC process description

PCCC process is based on the standard absorption-desorption concept as showed in the process flow diagram in Figure 1. In this process, the flue-gas from the power plant enters the absorption column at the bottom while the solvent solution (lean solvent stream) enters at the top of the absorption column. The temperature inside the absorber column is basically between 40 °C to 60 °C. Absorption column is place where both CO_2 and solvent come in contact and the absorption process takes place through interaction between solute (CO_2) and solvent. From the top of the column, the scrubbed gas containing mostly nitrogen gas (N_2) and part of the remaining CO_2 are vented to the atmosphere. On the other hand, the rich solvent exit from the bottom of the column is pumped to the top of a stripper going through a heat exchanger and heater reaching 120 ºC before entering the stripper column. In the stripper column, solvent is regenerated at a pressure 1.2 bar. Heat is supplied in the stripper column using the re-boiler. This heat is required to separate CO_2 from solvent. This process contributes to a major energy penalty of the PCCC process. The pure CO_2 gas leaves the stripper column at the top of the stripper column. Meanwhile lean solvent leaves the system at the bottom of the stripper and then pumped back to the absorber through the heat exchanger and cooler to reduce the temperature of lean solvent before entering back the absorption column. Solvent and water are added to the lean solvent stream using a mixer to balance the composition of lean solvent before the recycling process enters the absorption column.

3.2 Aspen Plus simulation model development

The Aspen Plus simulation model is developed and implement for PCCC process to estimate, evaluate and compare the effectiveness of process performance of new solvents with standard solvent MEA. The overall process flow diagram for PCCC process simulated using Aspen Plus software is shown in Figure 1. The process is modelled to capture CO_2 from coal-fired power plants. Radfrac model which is an equilibrium stage column model is used for both absorption and desorption column. The thermodynamic properties and activity coefficients are estimated with an electrolyte- NRTL (ELECNRTL) model. This model is used to correlate mean ionic activity coefficients of mixed solvent electrolyte systems.

All the input parameters data for the process simulation model are showed in the Table 1. The inlet data of the flue-gas stream for coal-fired power plant (500 MW) used in this study were taken from the studied carried out by P. R. Arachchige et al. (2012). For the flue-gas stream, the H_2O and H_2S chemical were not taken on account in this study. Besides, no after-processing of separated CO_2 or pre-processing and cooling of flue gas is implemented in this simulation. Flue gas is assumed to enter into the absorber column at the desired temperature and is also free from undesired gases and other impurities. Meanwhile, the input parameter data introduced in the process simulation model for absorption and desorption column have been taken from the previous study (Léonard and Heyen, 2011). The absorber was simulated to work at 1.1 bar and modelled with 17 stages and the stripper column works at 1.2 bar and 23 stages.

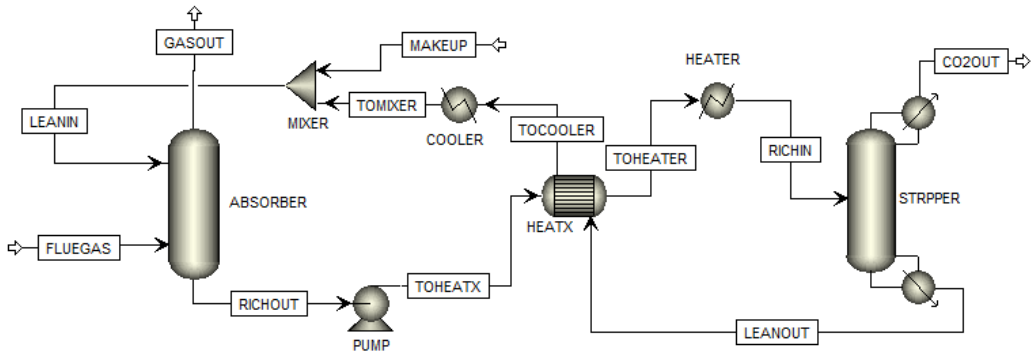

Figure 1: Aspen Plus process flow diagram for absorption and desorption of PCCC process

Table 1: Input parameter for Aspen Plus simulation model of PCCC process.

Input Parameter	Value
Inlet Flue gas:	
Flow rate (kg/h)	600
Temperature (ºC)	40
Pressure (bar)	1.1
Composition (Mol %)	
N_2	0.800
CO_2	0.135
O_2	0.065
Inlet Lean Solvent	
Flow rate (kg/h)	6,000
Temperature (ºC)	40
Pressure (bar)	1.1
Composition (mass %)	
MEA	0.30
H_2O	0.70
Absorber Column	
Temperature (ºC)	40
Pressure (bar)	1.1
Number of stages	17
Stripper Column	
Temperature (ºC)	120
Pressure (bar)	1.2
Number of stages	23

4. Result and discussion

4.1 Result of simulation using MEA

In first part of the study, the developed Aspen Plus Simulation model is used to estimate and evaluate the performance of MEA solvent. Results of the simulation shows that the MEA solvent is able to capture 52.52 % of CO_2 from coal power plants. The percentage of MEA solvent loss throughout the process is around 0.37 %. Meanwhile, the total energy required to regenerate the MEA solvent is 17.94 GJ/t CO_2 capture. The result show a deviation from previous study which is 90 % of CO_2 capture and the total energy required is around 4.0 to 6.0 GJ/t CO_2 capture (P. R. Arachchige et al., 2012). The difference of this result is due to the driving force consider in the simulation of absorption and desorption process. In the previous study conducted by P. R. Arachchige et al. (2012), the reaction interaction between MEA and CO_2 and the physical aspect of the absorption process is considered. Meanwhile, this study only focused on the physical aspects of the absorption and desorption process to capture CO_2 (e.g. solubility and diffusion of CO_2 in solvent).

4.2 Result of simulation using new alternatives solvents

In second part of the study, 25 new alternative solvents are introduced in the simulation. The simulation result for all new alternatives solvents is shown in Table 3. In terms of percentage of CO_2 captured, 1,2-Ethanediamine, N-methyl- is the highest one (55.44 %) among all the alternative solvents and the lowest value belongs to the 1,3-Propanediamine, N-(3-aminopropyl)- (53.99 %) being remarkable that the difference between all the solvents is very small. The highest percentage value of solvent loss throughout the process belongs to 1-butamine, N-ethyl-, reaching values such a 7.12 %. On the other hand, the lowest and best value for percentage of solvent loss belongs to1,3-Propanediamine, N-(3-aminopropyl)- with 0.103 %. Result for the third performance criteria which is energy required for solvent regeneration shows that, the lowest value of energy required belongs to1-butamine, N-ethyl- (9.129 GJ/t CO_2), and the highest one is reached by the 5-Aminopentanol (15.096 GJ/t CO_2).

4.3 Comparison of the performance between MEA and new alternatives solvents

After running the simulation model with MEA and all the new alternative solvents, a comparison study was carried out focused on the performance of MEA and new alternatives solvents. In order to choose the most suitable solvent for PCCC process, all the performance criteria are assigned with weightage and rating score. The weighting factor for each performance criteria is defined based on the impact of each performance criteria on the cost of PCCC process. In this case, energy required for solvent regeneration is given the highest

weightage which is 12.5 since it lead to the highest cost impact on PCCC process (Hopkinson et al., 2014). The weightage for percentage of carbon capture and percentage of solvent loss are set as 5 and 7.5. The rating score in this study represent the performance of each solvent based on the simulation result. The rating score is given from 1 to 4 as shown in Table 2 (1 represent the worst performance and 4 represent the best performance). The total score for each solvent tested in this study including MEA is calculated based on the given weightage and rating score. The results of the total score for each solvent is shown in Table 3.

Table 2: Rating score for each absorption and desorption performance criteria.

Percentage of CO_2 Capture (%)	Percentage of Solvent Loss (%)	Energy Required (GJ/t CO_2)	Rating
52.0 – 53.0	4.5 – 7.5	14.0 – 18.0	1
53.0 – 54.0	2.0 – 4.5	12.0 – 14.0	2
54.0 – 55.0	0.5 – 2.0	10.0 – 12.0	3
55.0 – 55.5	0.0 – 0.5	9.0 – 10.0	4

Table 3: Summary of the result of physical absorption performance assessment for all new alternative solvents and MEA solvent.

No.	List of Solvents	Percentage of CO_2 Capture (%)	Percentage of Solvent Loss (%)	Energy Required (GJ/t CO_2)	Total score
1	1,2-Ethanediamine, N-methyl-	55.44	5.80	10.90	65
2	1,3-Propanediamine	55.34	3.08	13.46	60
3	1,2-Ethanediamine, N-ethyl-	54.94	3.93	12.37	55
4	1,2-Ethanediamine,N,N´-dimethyl-	54.98	5.36	11.06	60
5	1,4-Butanediamine	54.85	1.35	14.48	50
6	1,2-Ethanediamine, N,N,N'-trimethyl-	54.45	0.86	14.60	50
7	1,3-Propanediamine, N,N-dimethyl-	54.63	3.63	12.37	55
8	1,5-Pentanediamine	54.51	0.78	14.65	50
9	1,2-Ethanediamine, N,N,-diethyl-	54.33	2.91	12.78	55
10	Diethylenetriamine, N,N-dimethyl-	54.05	0.34	14.55	57.5
11	1,2-Ethanediamine, N'-ethyl-N,N-dimethyl-	54.37	3.51	12.28	55
12	1,3-Propanediamine, N-(3-aminopropyl)-	53.99	0.10	14.71	52.5
13	1-butamine, N-ethyl-	54.75	7.12	9.13	72.5
14	1-Propanamine, N-propyl-	54.74	6.83	9.43	72.5
15	1,6-Hexanediamine	54.24	0.13	14.77	57.5
16	1-Hexanamine	54.65	3.72	12.32	55
17	4-methylpentanamine	54.68	4.64	11.52	60
18	Ethanol, 2-(ethylamino)-	54.67	0.83	14.85	50
19	Ethanol, 2-(propylamino)-	54.35	0.49	14.83	57.5
20	4-Aminobutanol	54.68	0.69	14.94	50
21	5-Aminopentanol	54.29	0.11	15.10	57.5
22	Ethanol, 2-(dimethylamino)	54.92	3.09	13.15	55
23	1-Propanol, 2-(dimethylamino)-	54.51	2.21	13.54	55
24	2-Propanol, 1-(dimethylamino)-	54.61	4.23	11.88	67.5
25	1-Propanol, 3-(dimethylamino)-	54.44	1.13	14.36	50
26	MEA	52.52	0.37	17.94	47.5

Based on the simulation result in Table 3, the first point analysed is the percentage of CO_2 captured. Results show that the percentage of CO_2 captured using MEA is the lowest compared with all the alternative solvents, being 1,2-Ethanediamine, N-methyl- the one with highest value, 55.44 %. The difference between the alternative solvents is not very noticeable. In terms of percentage of solvent loss throughout the process, the percentage of MEA evaporated is minimum which is 0.37 %, but the percentage reached by the 1,3-Propanediamine, N-(3-aminopropyl)-, 0.103 %, is the lowest compare to MEA and others alternative solvents. The last analysis is related to the energy required for solvent regeneration process. In this case, the energy required to regenerate the MEA solvent (17.938 GJ/t CO_2) is the highest one while the lowest value for the energy required belongs to 1-butamine, N-ethyl- (9.129 GJ/t CO_2)..

In term of overall performance, the most suitable solvent for physical absorption and desorption of PCCC process suggested in this study based on scoring system are 1-butamine, N-ethyl- and 1-Propanamine, N-propyl-. This two alternatives solvent recorded the highest total score which is 72.5. This solvents is much more

better than MEA with the total score of 47.5 which is the lowest score compare to all others alternative solvents. This results shows that by using alternatives solvent, the efficiency of physical absorption and desorption performance can be improved.

5. Conclusion

In this study Aspen Plus simulation model is developed to capture CO_2 through absorption and desorption of PCCC process. The developed Aspen Plus simulation model is used to estimate and evaluate the performance of new alternatives solvent and MEA based on the percentage of CO_2 captured, energy required for solvent regeneration and percentage of solvent loss through thermal degradation process. The results of this study show that all the new alternative solvents used are able to capture a minimum amount of 53.9% of CO_2 in the absorber column, making them suitable for the physical absorption of CO_2 through PCCC process.
In terms of capture efficiency of the solvents, results show that the best solvent would be 1,2-Ethanediamine, N-methyl-, capturing the 55.44 % of the CO_2 from the flue-gas stream. Regarding to the percentage of solvent loss, 1,3-Propanediamine, N-(3-aminopropyl)- with 0.103 %, shows the lowest percentage of solvent loss in the process. Significant energy required reduction is achieved by the use of 1-butamine, N-ethyl-, 9.129 GJ/t CO_2, comparing to the MEA results for energy required, 17.93 GJ/t CO_2 captured. In term of overall performance, the most suitable solvent for physical absorption and desorption of PCCC process suggested in this study based on scoring system are 1-butamine, N-ethyl- and 1-Propanamine, N-propyl-. This results shows that the efficiency of the process can be improved and the reduction in the cost of the overall process can be achieved by using new alternative solvents. However, this work is preliminary study which only consider the physical aspect of absorption process. This work will be extended to include the detail reaction interaction between CO_2 and solvent in the performance assessment study of PCCC process in order to improve the accuracy of the result.

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