CO_2 Vapor Liquid Equilibrium (VLE) Data

TESTING

IN

PARR REACTOR USING SYN-GAS

AT

NATIONAL CARBON CAPTURE CENTER (NCCC)

FINAL REPORT

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CONTENTS

1. PROJET DESCRIPTION

Carbon Clean Solutions Ltd. (CCSL) has developed a solvent to remove CO_2 from acid gases at high pressure. The objective of the project was to measure the Vapor-Liquid Equilibrium (VLE) at several conditions using bottled CO_2 and also using bleed stream from the coal gasification pilot plant at the National Carbon Capture Consortium (NCCC) located near Wilson, AL. There is a PARR reactor at the site which was used to attain the equilibrium conditions. CCS-USA is a wholly owned subsidiary if CCSL.

2. PROJECT GOALS AND ACHIEVMENTS

The goals were to:

1) Use bottled gas and obtain the CO2 VLE at various temperatures
2) Use gasifier bleed stream and obtain the CO2 and H2S VLE at various temperatures

3. HOURS AND CONDITIONS TESTED

Table 1: Test Conditions for Bottled CO_2

Bottled gas – CO_2		
Test	**Temperature in the Parr reactor, C**	**CO_2 mol%**
1	45	20, 40, 60, 80
2	55	20, 40, 60, 80
3	80	20, 40, 60, 80
4	120	20, 40, 60, 80

The test durations were as follows:
Test 1 - 25 minutes
Test 2 - 57 minutes
Test 3 - 106 minutes
Test 4 - 46 minutes
Test 5 - 9 minutes
The tests were run until inlet and outlet CO_2 concentration reached equilibrium.

4. RESULTS AND CONCLUSIONS

4.1 Bottled CO2

Table 2 gives the results while using bottled CO_2.

Table 2: Vapor and Liquid Compositions with Bottled CO_2

Actual Temp C	Actual Press psig	CO_2 Conc %	CO_2 PP psig	CO_2 PP barg	Solvent Volume L	Corrected mol CO_2 /L	Ideal mol CO_2 /L	Solvent Mass g	Corrected mol CO_2/ kg solvent	Ideal mol CO_2/ kg solvent
53.5	332	79.6	264.3	18.0	4.2	5.8	6.5	5135.0	4.7	5.3
46.2	343	58.9	202.0	13.7	4.2	4.9	5.5	5136.0	4.0	4.5
44.9	345	37.5	129.4	8.8	4.2	4.3	4.8	5137.0	3.5	3.9
45.4	347	18	62.5	4.2	4.2	3.4	3.9	5138.0	2.8	3.2
59.8	332	79.2	262.9	17.9	4.4	3.7	4.1	4850.0	3.3	3.7
54.9	343	58.8	201.7	13.7	4.4	2.9	3.3	4850.0	2.6	3.0
54.8	346	37.3	129.1	8.8	4.4	2.3	2.6	4850.0	2.1	2.3
55.3	347	18	62.5	4.2	4.4	1.4	1.6	4850.0	1.3	1.5
81.9	337	79.2	266.9	18.2	4.3	3.1	3.5	5131.0	2.6	2.9
79.7	343	58.9	202.0	13.7	4.3	2.1	2.4	5132.0	1.8	2.0
80.1	346	37.3	129.1	8.8	4.3	1.4	1.6	5133.0	1.2	1.3
80.2	348	18.2	63.3	4.3	4.3	0.6	0.8	5134.0	0.5	0.6
125.1	338	80.0	270.4	18.4	4.6	2.4	2.7	4950.0	2.3	2.6
119.6	347	59.0	204.7	13.9	4.6	1.8	2.0	4950.0	1.7	1.9
120.9	349	37.9	132.3	9.0	4.6	1.3	1.5	4950.0	1.2	1.4
120.2	350	18.2	63.7	4.3	4.6	0.8	0.9	4950.0	0.7	0.9

A: Ideal = Using ideal gas. Corrected= Using compressibility factor for real gas (deviation from ideal ga)

The values of vapor and liquid composition, in equilibrium with each other, at various temperatures, are plotted in Figure 1 below. The CO2 loading was computed using ideal gas law and also with corrections for actual temperature and pressure. The data at 80 C and 120 C are almost identical below the CO_2 loading 1 gmol/L. The reason for this phenomenon is not clear.

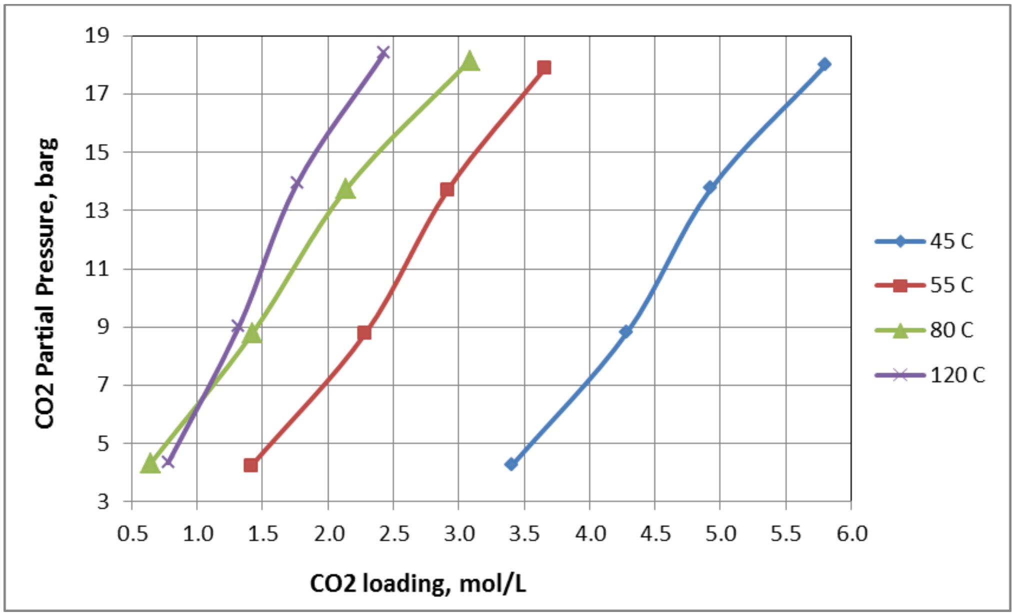

Figure 1: Results from Bottled Gas

The solvents that are widely used in high pressure applications are activated MDEA (35wt% MDEA+5wt% PZ) and Selexol (which is dimethyl ether of polyethylene glycol (DEPG)). The objective of testing was to compare the CCSL solvent with activated MDEA and Selexol. Figure 2 below gives the VLE for CCSL solvent, activated MDEA, and DEPG. Data for CCSL solvent obtained at TNO, an European lab, is also plotted. The data shows that CCSL solvent outperforms the existing solvents prevalent in the industry for high pressure applications at 40 C.

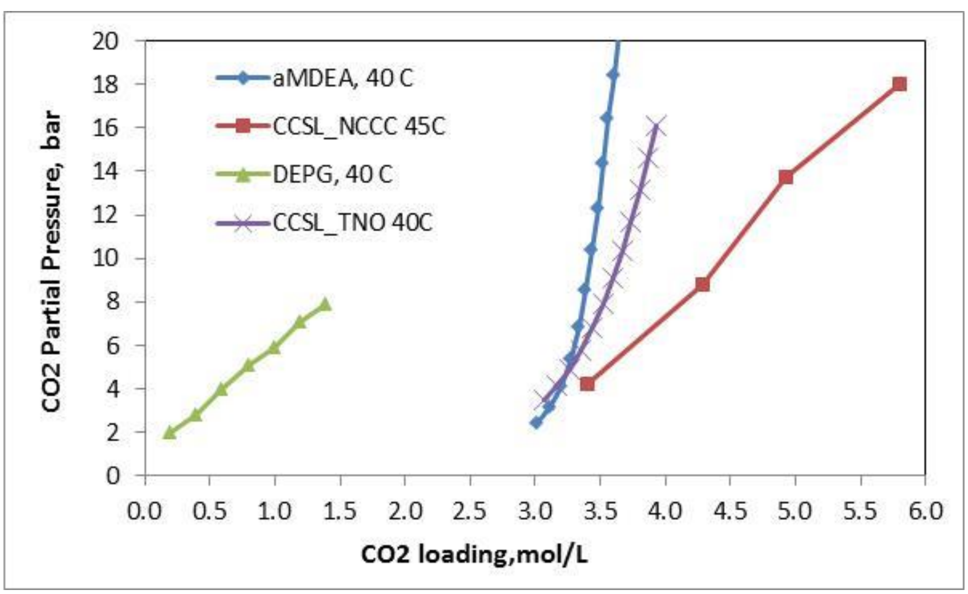

Figure 2: CCSL Solvent comparison with a-MDEA and DEPG (40-45 C)

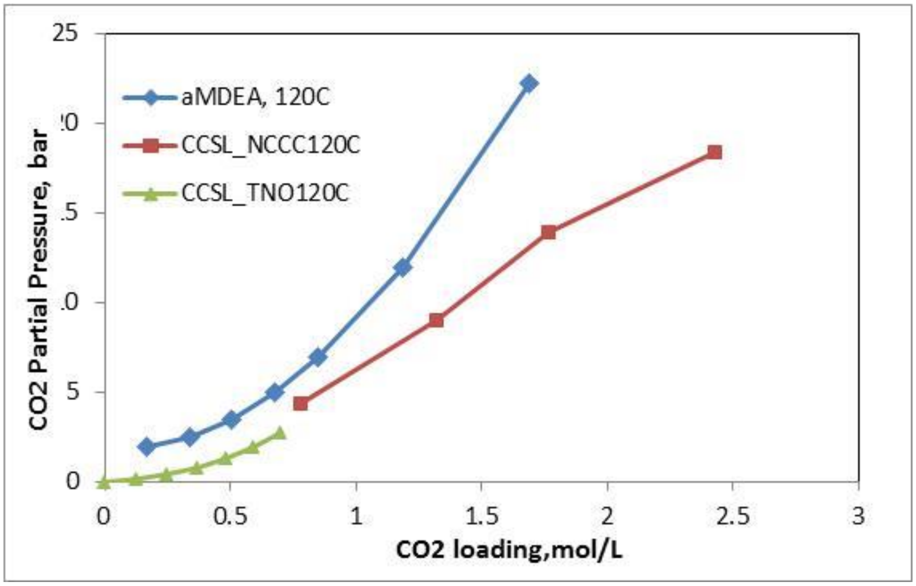

Figure 3: Comparison of VLE data for CCSL solvent and a-MDEA at 120 C

Figure 3 compares the VLE data at 120 C for CCSL solvent at NCCC and a-MDEA (at a lab in India). Data for CCSL solvent, obtained at TNO, is also plotted. It covers the low pressure range. The data for a-MDEA is slightly better than that for CCSL solvent.

4.2 Heat of Reaction

Heat of reaction/absorption is a major contributing factor in the total energy consumption of the CO_2 capture process. CCSL estimated the heat of reaction value from the VLE data. These are:

1. Activated MDEA: 48.9 kJ/mol CO_2
2. CCSL solvent: 39.2 kJ/mol CO_2

It shows that CCSL solvent requires 20% lower energy when compared to activated MDEA.

Table 3: Results with Syngas from Gasification Pilot Plant at NCCC with CCS Solvent

Actual		CO_2	CO_2	Solvent	Corrected	Ideal	Corrected	Ideal	Solvent	Corrected	Ideal	Inlet H_2S
Temp	Press	Conc	PP	Volume	mol CO_2	mol CO_2	mol CO_2/L	mol CO_2/L	Mass	mol CO_2/kg solvent		Ppmv
C	Psig	%	Psig	L					g			
40.4	168	8.7	15.0	4.6	12.7	13.6	2.73	2.93	4895.0	2.6	2.8	1848.7
42.2	169	43.4	73.0	4.4	16.4	18.3	3.73	4.16	4765.0	3.4	3.8	1222.7
46.1	168	21.5	36.0	4.6	15.8	16.3	3.41	3.53	4895.0	3.2	3.3	1457.6
46.6	169	22.2	38.0	4.6	15.8	16.4	3.42	3.54	4950.0	3.2	3.3	1616.4
54.3	164	62.8	103.0	4.4	16.6	18.5	3.78	4.22	4765.0	3.5	3.9	896.6

These data are spread over 5 temperatures with one data at each temperature. Thus, the data cannot be plotted like those in Figures 1 to 3. CCSL was hoping to get H_2S absorption data from these runs. However, the instrumentation at the site, a Gas Chromatograph (GC), had a much longer response time than the reaction of H_2S. **So, it was not possible to measure absorbed H_2S.**

4.3 Conclusions

1. The VLE for CO_2 was measured at four temperatures (Figure 1).
2. Figure 2 shows that, at 40 C and CO_2 partial pressures above 5 bar, CCSL solvent is superior to a-MDEA. The data from TNO, a lab in Europe, shows that CCSL solvent is better than a-MDEA above 2 Bar at 40 C. Since VLE at partial pressure of CO_2 below 2 bar was not measured, the performance of CCSL solvent could not be compared with that of a-MDEA.
3. Figure 3 provides graphs of VLE data for CCSL solvent at 120 C obtained at NCCC and also at TNO. For comparison, VLE data for a-MDEA at 120 C collected at a lab in India is also plotted. This plot shows that a-MDEA VLE is slightly better than that of CCSL solvent. It is recommended that the VLE at 120 C be measured for both a-MDEA and CCSL solvent be measured the same facility.
4. As stated above, the absorption of H_2S in the CCSL solvent could not be measured at NCCC. Therefore, H_2S VLE data could not be reported. It is recommended that an analytical system that is fast and accurate be used for H2S loadings measurement.