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Solvent reclaiming by sulfate precipitation for CO_2 capture

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Solvent reclaiming by sulfate precipitation for CO_2 capture

by

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Dedication

To my loving parents, my sister, and her family

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Last, but definitely not the least, I would like to express my thanks to my parents. Without their support I would not be where I am right now.

Abstract

Solvent reclaiming by sulfate precipitation for CO_2 capture

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The University of Texas at Austin, 2011

Supervisor: Gary. T. Rochelle

Sulfate accumulates in the post-combustion CO_2 capture system and must be removed to re-use amine efficiently. Removal of sulfate from the amine-based post-combustion CO_2 capture system through a solvent reclaiming process may reduce CO_2 capture costs. This work determines the solubility of K_2SO_4 and Na_2SO_4 in 2 to 8 m PZ loaded with CO_2 and develops a thermodynamic and process model for the reclaiming process.

At 40°C the solubility of Na_2SO_4 in 8 m PZ with a CO_2 loading of 0.3 is 0.3 m Na_2SO_4 and that of K_2SO_4 is 0.1 m K_2SO_4.

Sulfate solubility in PZ solutions is represented by the empirical models:

K_2SO_4: $ln(Ksp) = 10.53I^{0.3} - 0.98[PZ]_T - 3440/T - 2.42$

Na_2SO_4: $ln(Ksp) = 2.137I^{0.3} - 0.6505[PZ]_T - 826/T + 265$

where $[PZ]_T$ = 2*(molality of PZ).

A K_2SO_4 and Na_2SO_4 solubility thermodynamic model was developed in the e-NRTL framework in the Fawkes model for $PZ/CO_2/H_2O$ in Aspen Plus®.

The energy cost of the Na process when removing the equivalent of 100 ppm SO_2 from the flue gas, ranging from \$0.1-0.5/ton CO_2, was practically the same as the K process(ranging from \$0.1-0.8/ton CO_2). The K_2SO_4 recovered in the process can be used as fertilizer. However, the KOH will still cost \$0.6/tonne CO_2. If it is not possible to sell the K_2SO_4 as fertilizer because of the impurities that may be present on the K_2SO_4 crystals, the chemical cost of the process would increase to \$2/tonne CO_2. The chemical cost for the Na case is \$0.7/tonne of CO_2.

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Chapter 1: Introduction

1.0 Background and Motivation

The demand for energy is ever increasing and as fossil fuels continue to be burned to meet these increased demands, the atmospheric levels of carbon dioxide (CO_2) have risen which have in turn contributed to global warming. The International Energy Agency (IEA) has pointed out that the carbon emission due to energy production in 2010 was 30.6 gigatonnes, 5% higher than what was recorded in 2008 (IEA, 2011). With this escalation in greenhouse gases, CO_2 capture technology and its viability must be considered seriously.

CO_2 removal from natural gas was first studied by Bottoms in 1930 (Bottoms, 1930). The use of aqueous amines to capture CO_2 in a related process of absorption stripping is shown in Figure 1.1.

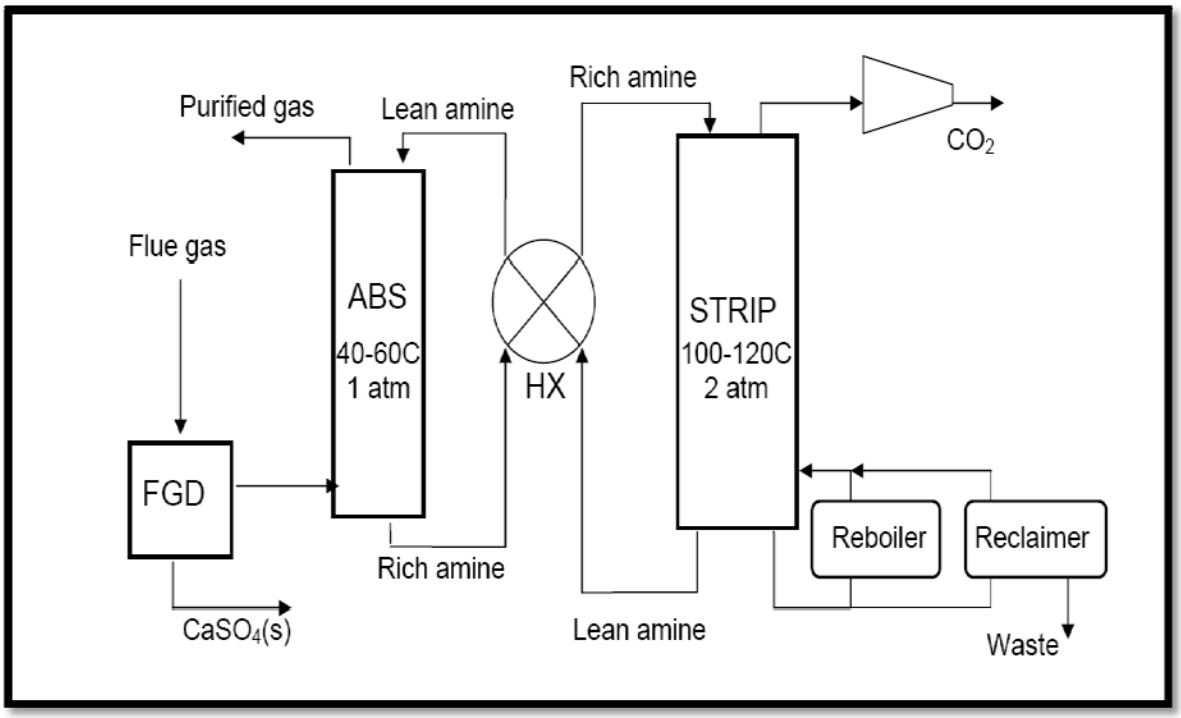

Figure 1.1 Typical amine absorption/stripping process (Xu, 2008)

The process employs flue gas consisting of CO_2, SO_2, O_2, and particulate matter entering the absorber at a temperature between 40-60°C and a pressure of 1 atm. The aqueous amine absorbs the CO_2 which is then sent to the stripper where it is regenerated, compressed, and ready to be used in different industrial and geological applications. Some applications of the CO_2 generated are Enhanced Oil Recovery (EOR) where the CO_2 is used to extract crude oil from wells as well as applications in the beverage industry for soft drinks.

SO_2 (and SO_3) is also absorbed from the flue gas. It oxidizes readily to sulfate and accumulates in the solvent. Because the sulfate in the system hinders the absorption and stripping capacity of the amine, the sulfate in the solvent must be removed.

1.1 SOLVENT RECLAIMING METHODS

Thermal reclaiming, ion exchange, and electrodialysis are solvent reclaiming methods that have either been studied or employed in the gas treating industry.

Thermal reclaiming separates contaminants from the amine based on volatility. In a thermal reclaimer, the amine is evaporated to concentrate the solution. The concentrated solvent is treated with sodium hydroxide to remove heat stable salts. The vaporized amine is returned to the system. The nonvolatile sulfate sludge is removed as a waste stream for disposal.

Ion exchange uses cations immobilized on polymer resin to remove heat stable salts from the amine. In anion exchange, the heat stable salt anion is removed by replacing a hydroxide ion as shown in the following reaction:

$$(R_3NH^+) + (SO_4)^{-2} + (Resin)^+(OH)^- \rightarrow R_3N + (Resin)^+(SO_4)^{-2} + H_2O \qquad 1.1$$

The ion exchange resin is then treated with caustic to regenerate the resin. Cations can be removed by a similar method with a cation exchange resin (Cummings A. L., 2007)

Electrodialysis uses membrane technology for the removal of heat stable salts. In electrodialysis, a potential is created by placing back to back cation and anion exchange resins. The amine solution is neutralized as it passes through the resin pack. However, fouling and replacement of membranes increases costs of the electrodialysis process (Rochelle, CO2 Capture by Aqueous Absorption, Fourth Quarterly Progress Report 2009, 2010).

Sulfate (SO_4^{-2}) is the main contaminant accumulated in the CO_2 capture system and needs to be dealt with exclusively. SO_4^{-2} removal through the addition of potassium hydroxide (KOH) or sodium hydroxide (NaOH) to a slip stream from the stripper as shown in Figure 1.1 is solvent reclaiming by neutralization. This was initially studied by

Xu for monoethanolamine (MEA) of varying concentrations and for MEA/PZ. Xu measured the solubility of K_2SO_4 in CO_2 loaded amine systems using ionic conductivity and correlated it to an empirical model (Xu, 2008).

Aqueous piperazine (PZ) has been investigated as a novel amine solvent for CO_2 removal. The CO_2 absorption rate of aqueous PZ is more than double that of 7 m MEA, the baseline amine used in CO_2 capture. The amine volatility of the PZ solvent at 40 °C and atmospheric pressure ranges from 11 to 21 ppm. Thermal degradation is almost negligible up to a temperature of 150 °C, making it a much better solvent than MEA. Initial system modeling suggests that 8 m PZ will use 10 to 20% less energy than 7 m MEA. The fast mass transfer and low degradation rates suggest that PZ has the potential to be a preferred solvent for CO_2 capture (Freeman et. al, 2009). However, because pure makeup piperazine has a greater cost per pound than makeup MEA, PZ may have an economic disadvantage for use in CO_2 capture if high makeup rates are required.

1.2 SCOPE OF WORK

To effectively use PZ in large scale CO_2 capture, the solvent must be reclaimed and reused to reduce amine replacement costs. SO_x is the main impurity and needs to be removed to avoid reducing amine CO_2 capture capacity. Sulfate in the system can be easily removed using the neutralization methodology employed by Xu in 2008. However, the solubility of sulfate in PZ has not been studied previously.

This thesis focuses on the following two topics:

- A solid solubility experimental method measuring the solubility of K_2SO_4 and Na_2SO_4 in PZ solutions of varying concentrations.
- A process model of sulfate removal in Aspen Plus®.

K_2SO_4 is studied because it has the potential of being used as commercial fertilizer once precipitated in the reclaiming system. However, NaOH has the advantage of being less expensive. Thus, the solubility of Na_2SO_4 in PZ is studied for economic purposes. A process model and economic analysis of the reclaiming method is developed to determine the feasibility of the process using either KOH or NaOH.

Chapter 2: Solubility of sulfate in Piperazine (PZ)

2.0 INTRODUCTION

This chapter focuses on the experimental and analytical methods employed to determine the solubility of Na_2SO_4 and K_2SO_4 in 2-8 m PZ solutions. The solid solubility method is validated with data from Xu (2008). Xu correlated the solubility of the salt in the amine solution with the ionic strength. The solid solubility method used excess salt in a loaded PZ solution and the concentration of the salt in the solution is measured using ion chromatography.

2.1 SOLID SOLUBILITY EXPERIMENTAL METHOD

Loaded solutions were prepared from aqueous piperazine and CO_2. 2, 5, and 8 m amine solutions were prepared gravimetrically using Sigma Aldrich® anhydrous piperazine (PZ) and Distilled de-ionized (DDI) water. The solution was then sparged with CO_2 gravimetrically as shown in Figure 2.1 below.

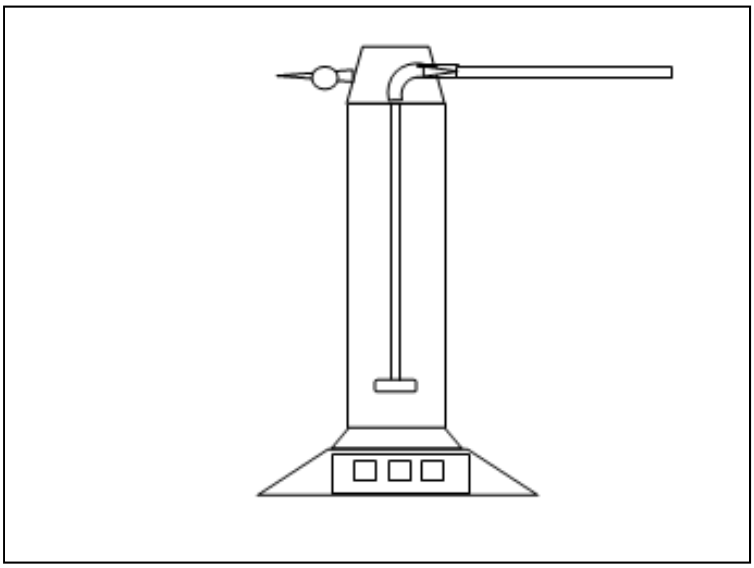

Figure 2.1 Schematic of loading amine with CO_2

For all experiments, CO_2 loading was defined as follows:

$$\text{Loading (A)} = \frac{moles\ of\ CO2}{moles\ of\ equivalent\ amine}$$

For PZ, moles of equivalent amine = 2*(molality of PZ).

Sulfate solid solubility was then measured by analysis of saturated liquid samples from an agitated slurry. 40 g of CO_2 loaded solution was placed in a 100 ml Ace Glass Incorporated® jacketed glass reactor. Excess sodium or potassium sulfate solid was added and the solution was agitated with a magnetic stirrer at 400 rpm. The jacketed reactor was heated by a water bath (Lauda®) as shown in Figure 2.2.

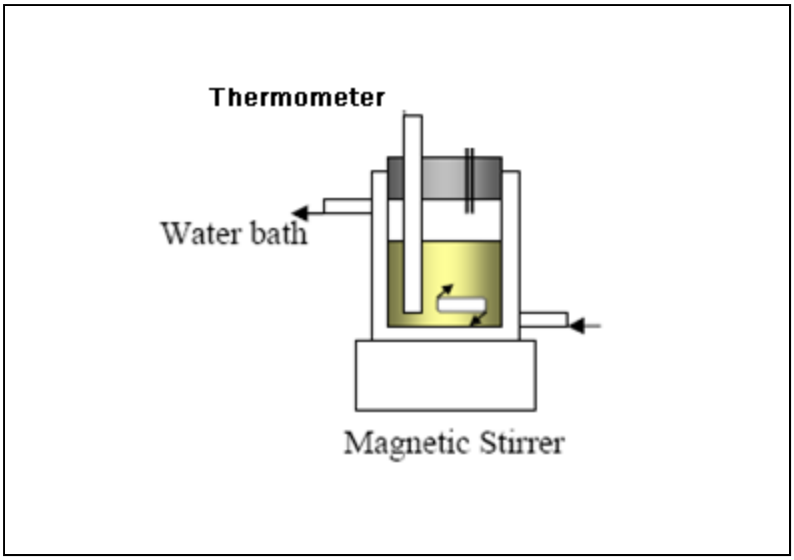

Figure 2.2 Solid solubility experimental apparatus

. The reactor was capped with a rubber stopper. A thermometer was inserted in the solution through the rubber stopper to measure the temperature of the solution. The temperature of the solution was varied between room temperature and 80 °C. Solution was sampled every hour at 10°C intervals using a filtered (0.45 μm PTFE Fisherbrand®)

syringe (Luer lok® tip). The syringe was at room temperature. Thus, the sample was diluted in DDI water immediately to prevent salt crystallization. An initial dilution of 10x was prepared. Further dilutions of 100x and 10000x were prepared for anion and cation chromatography, respectively. Experimental samples were analyzed for Na^+, K^+, SO_4^{-2}, CO_2, and PZ concentrations using cation chromatography, anion chromatography, and TIC as detailed in the next section.

2.2 ANALYTICAL TECHNIQUES

The concentrations of Na^+, K^+ and PZ in the samples were analyzed using a cation chromatograph. CO_2 concentration in solution was determined using a Total Inorganic Carbon (TIC) Analyzer, and the SO_4^{-2} concentration was analyzed using an anion chromatograph.

Cation Chromatography: The cation IC was used to determine the concentration of Na^+, K^+, and PZ in experimental samples. A Dionex ICS-2500 instrument was used as previously described by Sexton (2008) and Freeman (2011) It consisted of:

- A CS17 IonPac column (containing ethylvinylbenzene cross-linked with 55% divinylbenzene resin as a separation medium)
- A 4-mm Cationic Self-Regenerating Suppressor (CSRS) to suppress anions
- Methanesulfonic acid (MSA) in the eluent

The method used for detecting cation concentrations was the 'Jason3Auto.pgm' method and 'Stephanie3Auto.pgm' method (attached in Appendix B). Calibrated samples of Na^+, K^+, and PZ were used to determine the amount of Na^+, K^+, and PZ present in the sampled solution. Na^+, K^+, and PZ peaked on the chromatograph at retention times of 9.3, 12.9, and 33.5 minutes respectively.

Anion Chromatography: The anion IC was used to determine the concentration of SO_4^{-2} in the experimental samples. A Dionex ICS-3000 (as described by Sexton (2008) and Freeman (2011)) instrument was used and consisted of:

- AS15 IonPac column (containing ethylvinylbenzene cross-linked with 55% divinylbenzene resin with quaternary ammonium groups as a separation medium)
- 4-mm Anionic Self-Regenerating Suppressor (ASRS) used to suppress the cations
- Carbonate removal device (CRD) and carbonate removal from eluent generation.

The method used for detecting SO_4^{-2} concentrations was the 'Anions.pgm' (attached in Appendix B). KOH was used in the eluent and its concentration changed over the 35 minute time frame that the electrochemical detector (ECD) detected the concentration of the anions in the sample. SO_4^{-2} in particular peaked on the chromatograph at a retention time of 27.2 minutes.

Total Inorganic Carbon Analyzer: Quantification of CO_2 loading was performed using a total inorganic carbon analyzer. In this method, a sample is acidified with 30 wt % H_3PO_4 to release the CO_2 present in solution (Hilliard, 2008). The CO_2 is carried in the nitrogen carrier gas stream to the detector. PicoLog software was used to record the peaks produced from each sample. A calibration curve was prepared at the end of each analysis using a TIC standard mixture of K_2CO_3 and $KHCO_3$. The TIC method quantifies the total CO_2, CO_3, and HCO_3 present in solution. These species are in equilibrium in the series of reactions shown below:

$$CO_3^{-2} + 2H^+ \leftrightarrow HCO^{-3} + H^+ \leftrightarrow H_2CO_3 \leftrightarrow CO_2 + H_2O \qquad 2.1$$

Acidification of the sample shifts the equilibrium toward CO_2 which bubbles out of solution and is detected in the analyzer (Rochelle et al., 2010). The TIC analysis helps identify whether loss of CO_2 was prevalent at higher temperatures of the experiment.

2.3 EXPERIMENTAL RESULTS

Eight solid solubility experiments were performed. The results are tabulated in Table 2.1 and Table 2.2 below.

Table 2.1 Analytical Results for K_2SO_4 solid solubility experiments

	T (°C)	K^+ (mmol/kgsol)	PZ (mmol/kgsol)	SO_4^{-2} (mmol/kgsol)	CO_2 (mmol/kgsol)
Exp 1	21	74	2151	33	3160
8m PZ	30	111	1869	47	2963
A = 0.3	40	171	2485	68	3731
	50	198	2465	87	3879
	60	191	2301	104	3638
	70	192	2185	122	3520
	80	246	2728	133	3994
Exp 2	21	38	2116	27	3154
8m PZ	30	94	2311	37	4587
A = 0.3	40	134	2565	57	3493
	50	164	3034	85	3810
	60	177	2938	90	3785
	70	108	1384	46	2148
	80	232	3525	115	4423
Exp 3	30	133	2867	57	3904
8m PZ	40	181	2939	81	3929
A = 0.4	50	250	3801	119	4735
	60	233	3121	132	3945
	70	290	3543	137	4410
	80	242	2881	117	3706
Exp 4	23.0	779	1930	356	1172
2m PZ	31.0	854	1889	389	2177
A = 0.4	40.0	943	1856	430	2114
	50.0	1008	1828	467	1126
	60.0	1100	1910	516	1114
	70.0	1122	1785	519	1076
	80.0	1182	1901	560	1016
	70.0	1104	1917	520	1044
	60.0	985	1843	456	1027

Table 2.1 continued

Exp 5	22.5	358	3030	150	2358
5m PZ	32.0	412	3098	175	2319
A = 0.4	40.0	447	3016	194	2297
	50.0	362	2259	165	2268
	60.0	556	3198	256	2211
	68.5	606	3293	279	2307
	80.0	624	2924	256	2200
	69.5	525	3183	238	2310
	60.0	463	3272	208	2270

Table 2.2 Analytical Results for Na_2SO_4 solid solubility experiments

	T (°C)	Na^+ (mmol/kg)	PZ (mmol/kgsol)	SO_4^{-2} (mmol/kgsol)	CO_2 (mmol/kgsol)
Exp 6	25.2	1883	711	1143	1188
2m PZ	30.0	3305	1241	1070	1125
A = 0.4	40.0	3271	1298	1335	1121
	50.0	3102	1152	1096	1120
	59.0	3270	1267	1442	1091
	70.0	2919	1210	1282	1071
	80.0	3189	1289	1162	1087
	70.0	2855	1121	1014	941
	61.0	2957	1138	1292	1031
	50.0	3014	1290	1331	1057
Exp 7	25.0	1339	2229	730	2024
5m PZ	30.0	1002	1646	732	2200
A = 0.4	40.0	940	1439	721	2312
	50.5	1186	1842	664	2215
	61.0	1185	1936	711	2193
	70.0	1211	2254	736	2187
	80.0	1428	2301	771	2200
Exp8	23.5	647	2269	217	1037
8m PZ	30.0	753	3675	284	2178
A = 0.3	40.0	668	3852	354	2292
	50.5	638	2919	277	1715
	60.0	805	3953	299	2296
	80.5	681	3708	313	2182
	70.0	638	3882	331	2194
	60.0	563	3564	301	2079
	50.0	653	4046	337	2311

2.4 PREVIOUS WORK AND EXPERIMENTAL METHOD VALIDITY

The solubility of K_2SO_4 and Na_2SO_4 has been studied in solvents such as H_2O, methanol, ethyl alcohol, and ammonia (Linke, 1965). Xu studied the solubility of K_2SO_4 in MEA, MEA/PZ and at some temperatures of PZ (Xu, 2008). There is no previous study of the solubility of Na_2SO_4 in PZ. Experimental data obtained was compared with the work of Xu (2008) to determine whether the results from the solid solubility method employed were comparable to that of published data.

Table 2.3 Data comparison with Xu (2008)

Experiment	T (°C)	K+ (mmol/kg sol) (Xu, 2008)	K+ (mmol/kg sol)	% Difference
8 m PZ A=0.3	80	261	246	5.7
8 m PZ A=0.3	40	176	171	2.8
8 m PZ A=0.4	80	273	242	11.5
8 m PZ A=0.4	40	159	181	-13.9

Table 2.3 shows the percentage difference between the concentrations of K^+ obtained by Xu (2008) and those by the solid solubility method for 8m PZ at 0.3 loading and 0.4 loading at 40°C and 80°C. The concentrations of K^+ in 8 m PZ with 0.3 CO_2 loading at 80 °C were within 2-5% of the results obtained by Xu. However, the concentration of sulfate in 8 m PZ with 0.4 CO_2 loading at 80 °C was -14 to +11% different from Xu's values. This could be due to experimental error or analytical instrumentation error.

Once the solid solubility data was validated, the results were further analyzed and regressed. This analysis is presented in Chapter 3.

Chapter 3: Solubility of Na_2SO_4 and K_2SO_4 in Piperazine (PZ) – Experimental Methods Analysis

3.0 Comparison with Literature Data

The solubility of Na_2SO_4 and K_2SO_4 in various organic and inorganic solvents has been studied extensively. Caven and Johnston (1927, 1928), Wright (1927), Flottman (1928) and many others studied the solubility of K_2SO_4 in water. Schiff (1861), Barken (1955), Wright (1927), and Gerardin (1865) studied the solubility of K_2SO_4 in aqueous ethyl alcohol. Similarly, the $Na_2SO_4 – H_2O$ system was originally studied by Berkeley in 1904. The $Na_2SO_4 – H_2O – C_2H_5OH$ system was studied by Schreinemakers and deBaat in 1909 (Linke, 1965). While other systems have been studied, the solubility of the salt in H_2O and in aqueous C_2H_5OH systems will be compared here with the solubility of Na_2SO_4 and K_2SO_4 in PZ and K_2SO_4 in MEA from Xu, 2008.

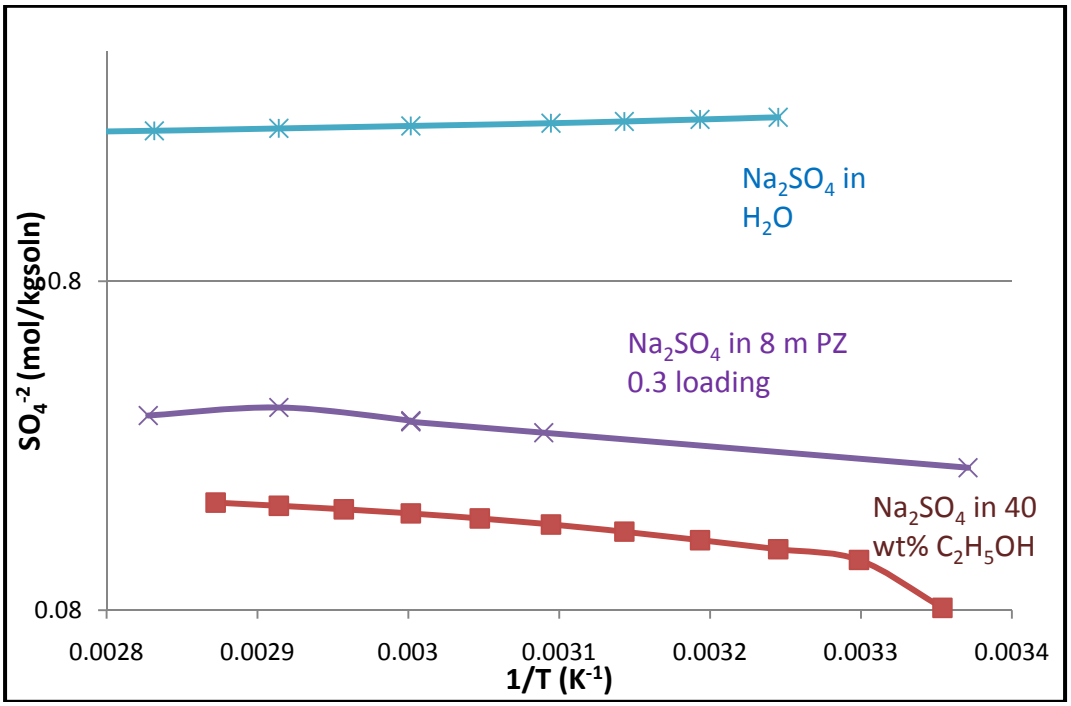

Figure 3.1 Solubility of Na_2SO_4 in H_2O, 8m PZ, and C_2H_5OH (Linke, 1965)

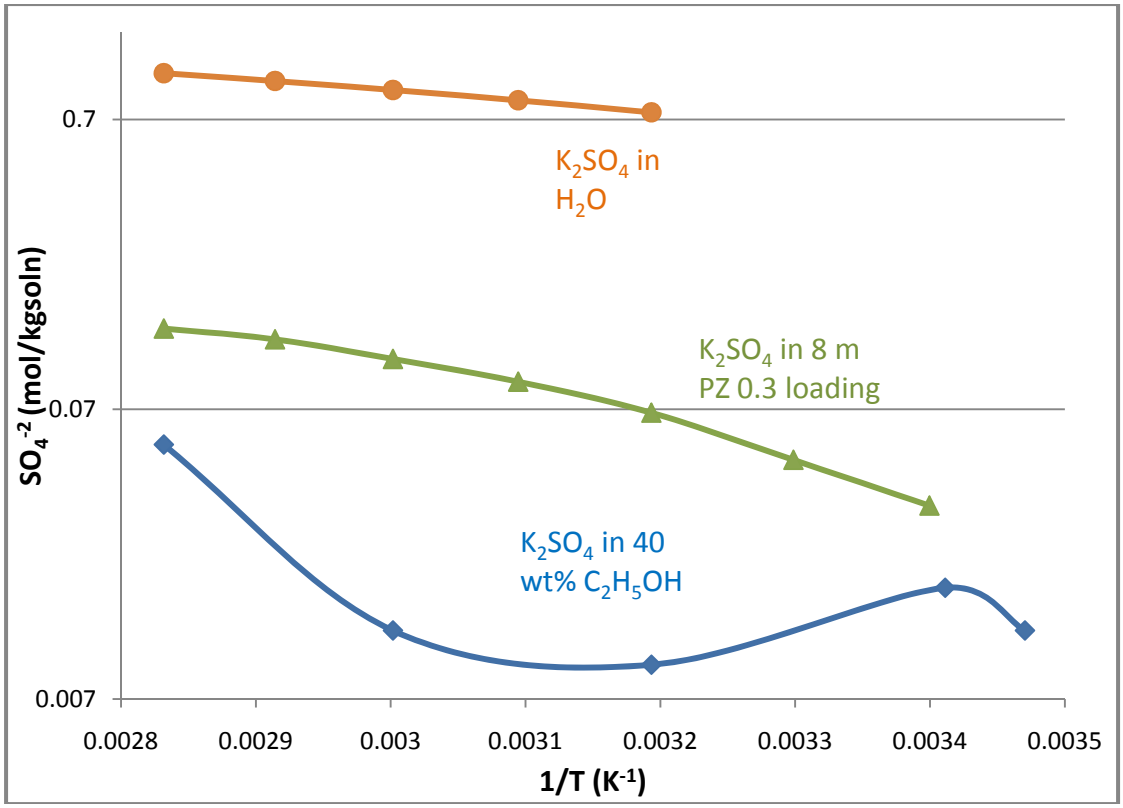

Figure 3.2 Solubility of K_2SO_4 in H_2O, 8 m PZ, and C_2H_5OH (Linke, 1965)

Figure 3.1 and Figure 3.2 show how the solubility of Na_2SO_4 and K_2SO_4 vary in H_2O, 8m PZ, and C_2H_5OH respectively. The solubility of Na_2SO_4 does not seem to be temperature dependent but is more dependent on the organic nature of the solvent. However, the solubility of K_2SO_4 in C_2H_5OH has a more abnormal dependence on temperature. Abnormalities in solubility are normal for salts that exist in various hydrated forms. If the solubility of Na_2SO_4 in H_2O is observed for a wider range of temperature, a sharp increase in the solubility is observed up to 32°C. This is because Na_2SO_4 exists as $Na_2SO_4.10H_2O$ and then in its anhydrous form. Figure 3.3 below shows this change in state of the salt.

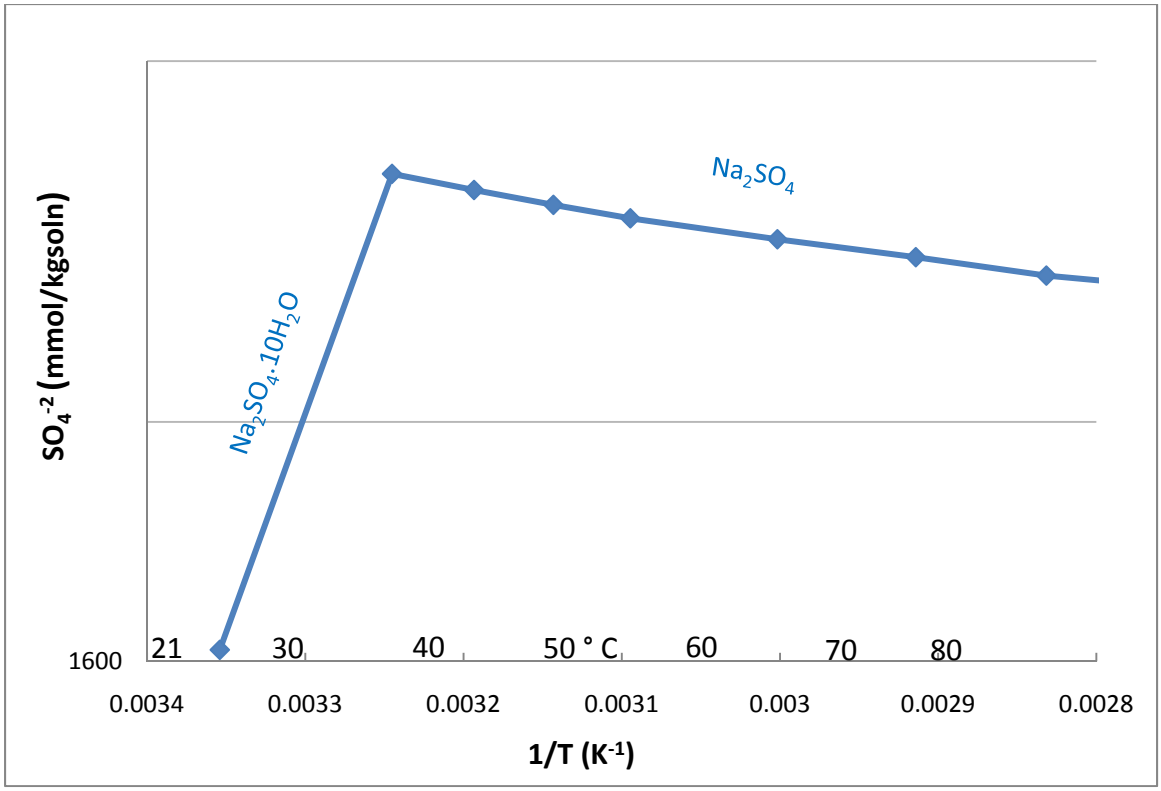

Figure 3.3 Abnormal solubility of Na_2SO_4 in water (Linke, 1965)

The concentrations of Na^+, K^+, and SO_4^{-2} in the sampled solution were measured by cation chromatography and anion chromatography, respectively. Their concentrations were plotted against the inverse of temperature to determine the solubility dependence on temperature, ionic conductivity, CO_2 loading, and the organic nature of solvent used.

The first set of experiments carried out were that of K_2SO_4 in PZ. Figure 3.4 compares the solubility of K^+ in different solvent media; the solubility of K_2SO_4 in water (Linke, 1965), K_2SO_4 solubility in 7 m and 11 m MEA at 0.3 and 0.4 loading was obtained from Xu (2008), and the solubility of K_2SO_4 in PZ is from the solid solubility experimental method.

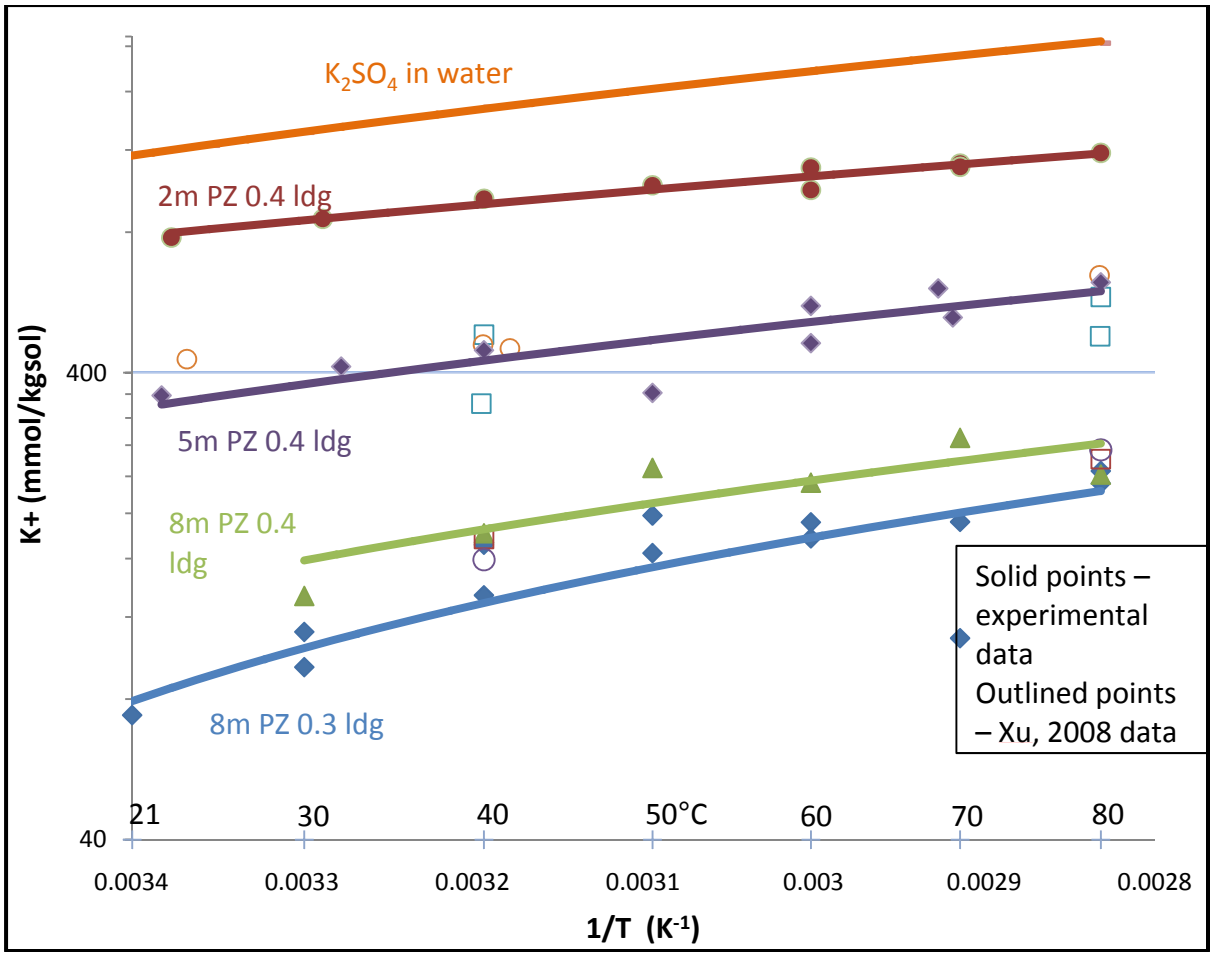

Figure 3.4 Concentration of Potassium in PZ saturated to K_2SO_4

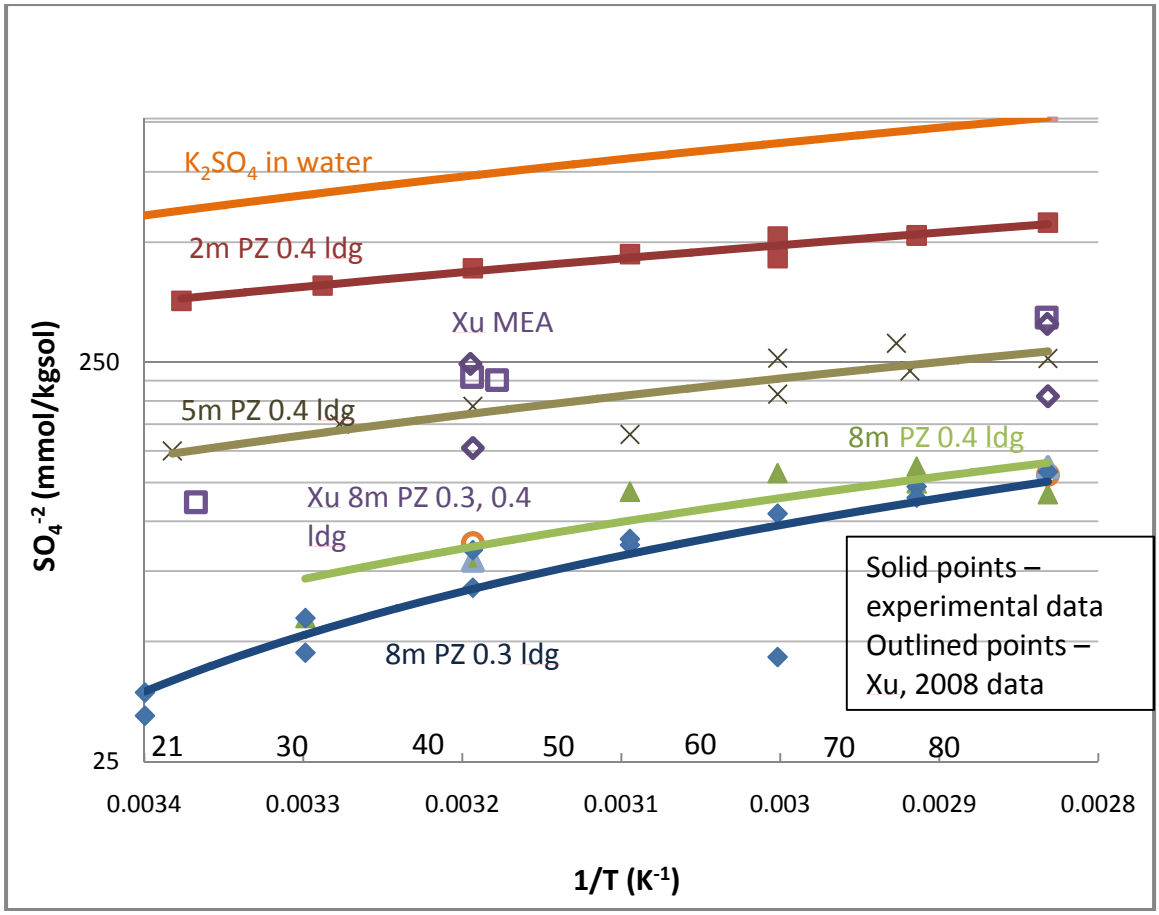

Figure 3.5 Concentration of Sulfate in PZ solutions saturated to K2SO4

Figure 3.4 and Figure 3.5 both show that the solubility of K_2SO_4 in solution increases with increasing loading because of a greater concentration of carbamate and protonated amine in the system. The solubility of the sulfate also increases with the temperature of the solution. The solubility of K_2SO_4, however, is lower in PZ than in MEA. This is because the ring-structured PZ is more organic in nature than MEA. A solvent reclaiming process would ideally require a large difference in solubility at different loadings to create a driving force to precipitate out the sulfate in the system.

The concentration of CO_2 in solution at the various sampling temperatures was also analyzed using the Total Inorganic Carbon analysis method explained in Section 2.2. The raw data obtained were translated into mmol/kgsol and plotted against the inverse of temperature in Figure 3.6 below.

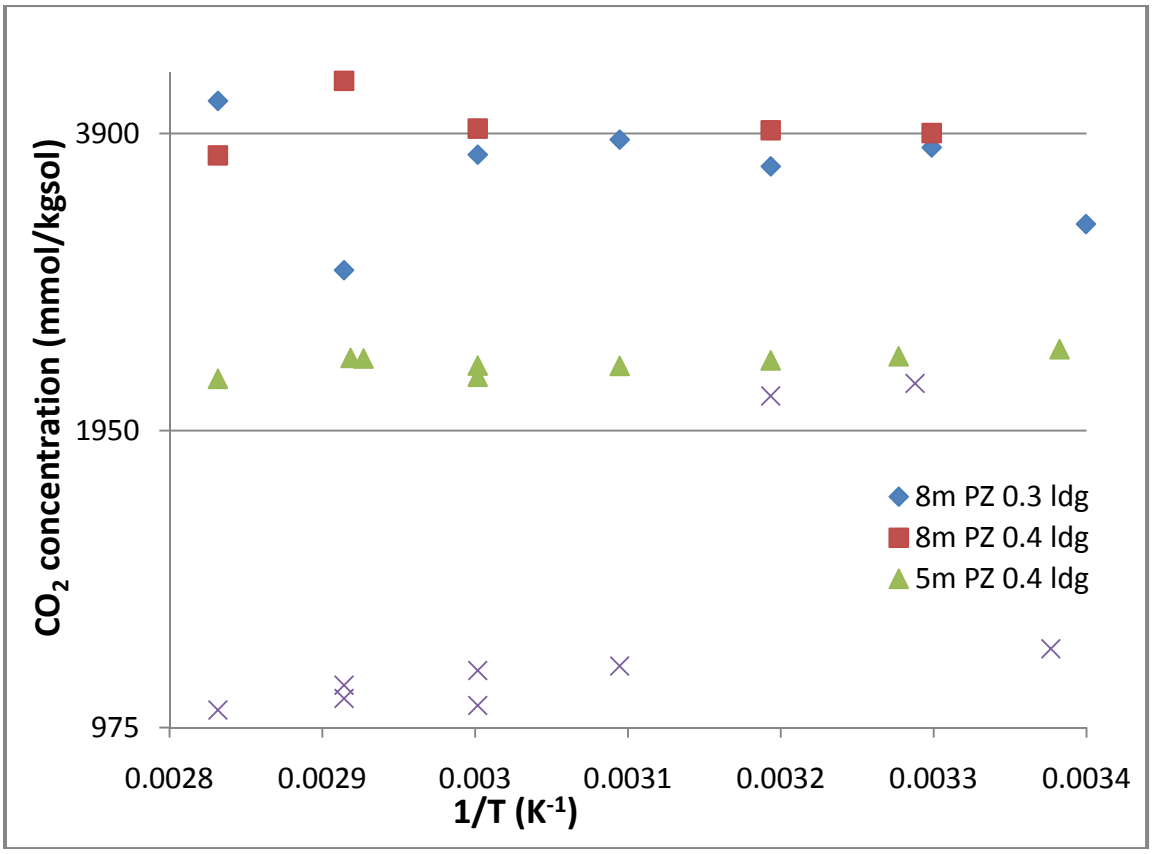

Figure 3.6 Concentration of CO_2 in K_2SO_4 - PZ solution

The reason for analyzing for CO_2 in PZ solutions is to determine if CO_2 was lost during the solid solubility experimental procedure. From Figure 3.6, a general observation can be made that at higher temperatures, some loss of CO_2 in solution does occur in higher piperazine concentrations.

3.1 COMPARISON OF Na_2SO_4 AND K_2SO_4 SOLUBILITY IN CO_2 LOADED PZ SOLUTION

The second set of solid solubility experiments carried out were that of Na_2SO_4 in PZ. The solubility of Na_2SO_4 in PZ is graphed in Figure 3.7.

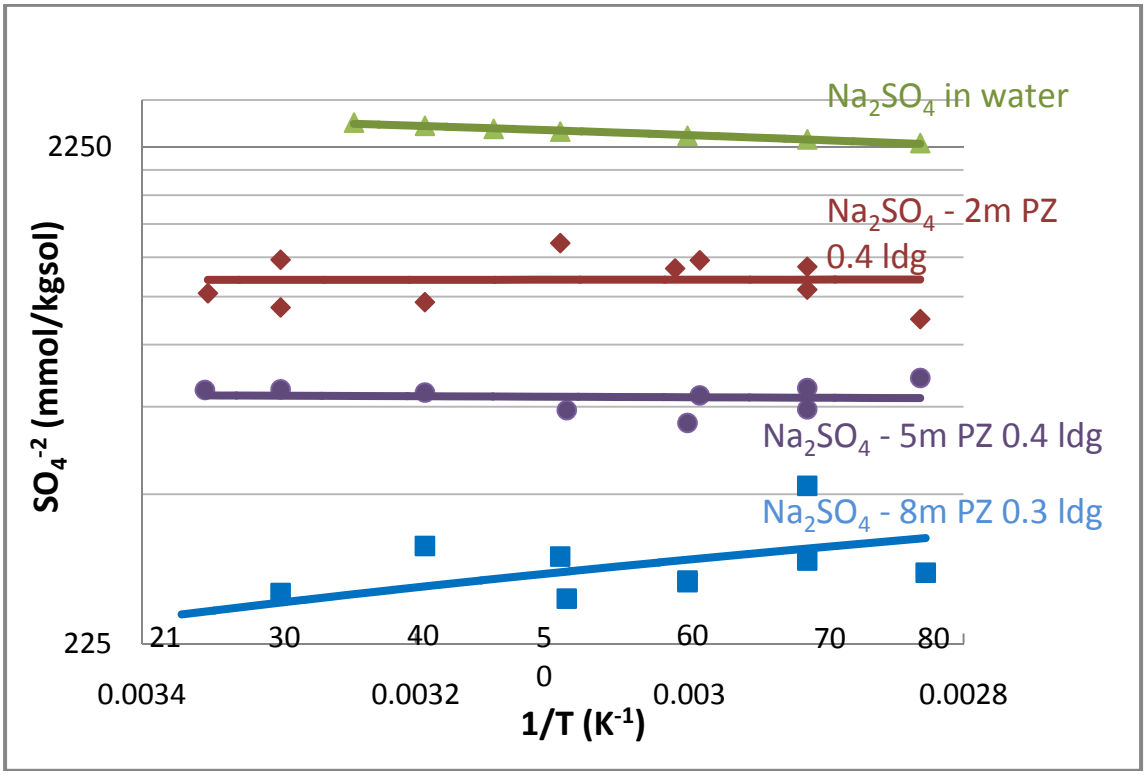

Figure 3.7 Effect of PZ concentration on solubility of Na_2SO_4

Figure 3.7 shows that the solubility of Na_2SO_4 in PZ solution is not as temperature dependent as it is amine concentration dependent. For 2 m and 5 m PZ, there is hardly any change in concentration of SO_4^{-2} as the temperature of the solution is increased from room temperature to 80 °C. For 8 m PZ, there is very little change in concentration of SO_4^{-2} present in solution with temperature increase. However, the concentration of SO_4^{-2} in solution increases from 354 mmol/kgsol for 8 m PZ at 40 °C to

721 mmol/kgsol for 5 m PZ and to 1335 mmol/kgsol for 2 m PZ. As expected, the solubility of Na_2SO_4 is the highest for water.

Figure 3.8 below compares solid solubility data for K_2SO_4 and Na_2SO_4 in 8 m PZ at 0.3 loading obtained from solid solubility experiments and literature data for solubility of the salts in water. The figure also contains data for solubility of K_2SO_4 in MEA obtained from Xu (2008).

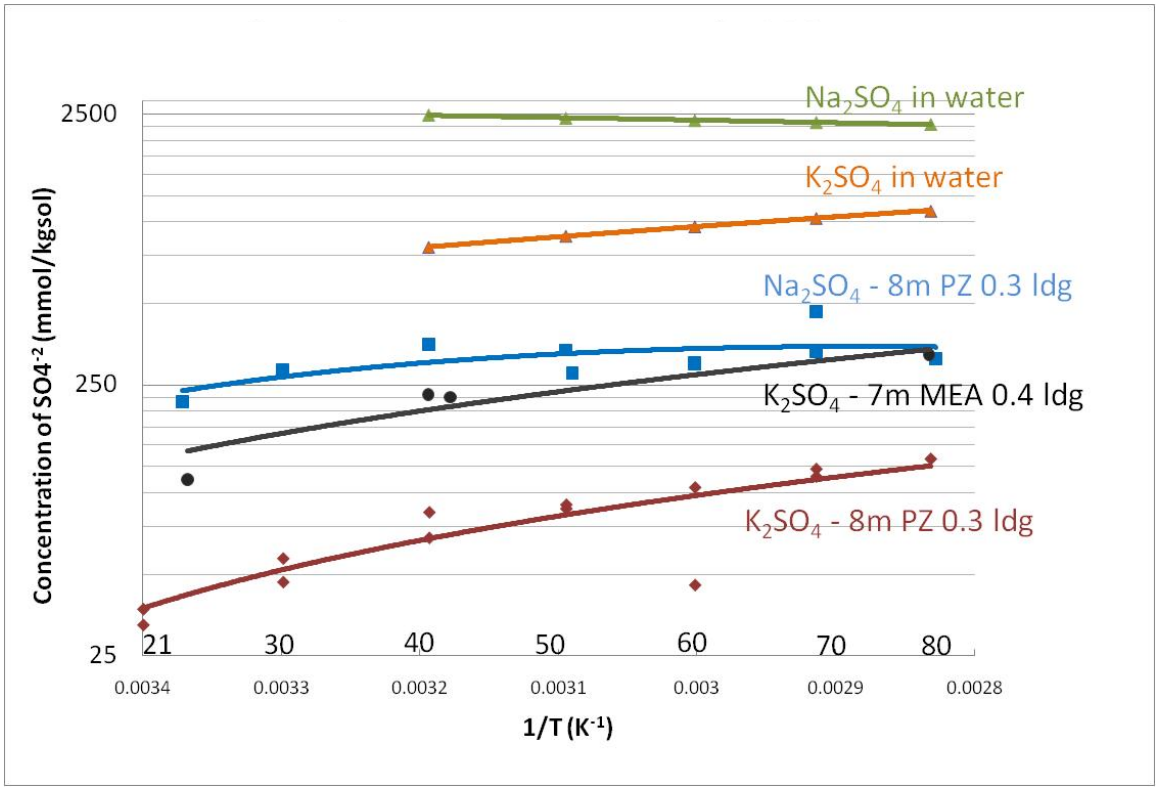

Figure 3.8 Comparison of Na_2SO_4 and K_2SO_4 solubility in 8 m PZ

Figure 3.8 shows that the solubility of Na_2SO_4 in 8 m PZ is ten times greater than K_2SO_4. If SO_4^{-2} is the main impurity in the CO_2 capture system, the amine removed for reclaiming can be concentrated to high PZ concentrations at high temperatures (without

affecting the solubility of SO_4^{-2} in PZ). This way SO_4^{-2} along with the other heat stable salts present can be removed together in a single thermal reclaiming procedure.

3.2 SOLUBILITY PRODUCT (KSP) AND EMPIRICAL MODEL

In the solubility work produced by Xu (2008), an empirical model was developed to predict the solubility of K_2SO_4 for amine aqueous solutions of 3.5 m to 11 m MEA, 4 to 10 m PZ, and 7 m MEA/2 m PZ for temperatures between 25 °C and 80 °C:

$$\ln(Ksp) = 7.82*I^{0.2} - 0.37[amine]_T - 2273.4/T(K) - 1.445 \quad (3.1)$$

where:

I is the ionic strength,

[amine] = $[MEA]^{+2}$·[PZ] with unit of m (molal, mole per kg water) for Xu, 2008

For PZ only, [amine] = 2*(molality of PZ).

Ksp,m for K_2SO_4 = $([K^+],m)^2*([SO_4^{-2}],m)$

Ksp,m for Na_2SO_4 = $([Na^+],m)^2*([SO_4^{-2}],m)$

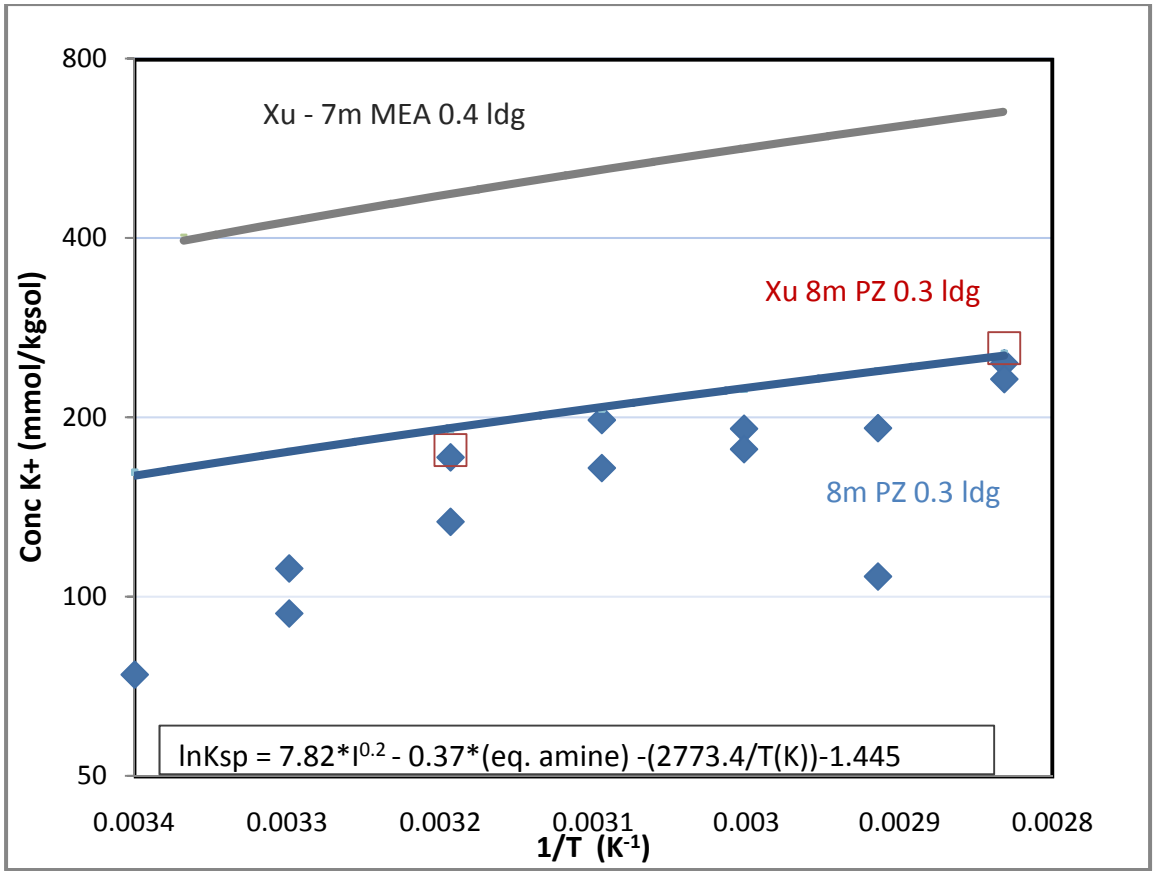

Figure 3.9 K_2SO_4 solubility modeled with Xu, 2008 regression model

Figure 3.9 shows that the equation obtained by Xu, 2008 does not fit well for solubility of K_2SO_4 in PZ. For this reason, the solubility data obtained from the solid solubility method was regressed and a similar equation obtained for both the solubility of Na_2SO_4 and K_2SO_4 in PZ

Regressing the data obtained by the solid solubility experiments carried out for 2 m to 8 m PZ between 25 °C and 80 °C, the empirical model developed for the solubility of K_2SO_4 is given by equation 3.2 shown below:

$$\ln(Ksp) = 10.53*I^{0.3} - 0.98[PZ]_T - 3440/T - 2.42 \qquad 3.2$$

As with all experimental methods, there were errors associated with the solid solubility experimental method as well as the process of analyzing the samples.

Errors are associated with the scale used for gravimetrically preparing the solution and loading the CO_2. At higher temperatures during the course of the experiment, there are errors associated in transferring the sample using a syringe at room temperature to the vial for immediate dilution. This is the main source of error for any changes in PZ and CO_2 concentration over the course of the temperature (due to the evaporation of water and/or CO_2 when the rubber stopper is removed for sampling). Table 3.1 below shows the standard error associated with the coefficient of each parameter in equation 3.2.

Table 3.1 K_2SO_4 regression statistical analysis

	Coefficients	***Standard Error***
Intercept	-2.42	4.86
PZ (eq mol amine)	-0.98	0.046
1/T (1/K)	-3440	668
$\mathbf{I^{0.3}}$	10.5	2.66

The standard error in the regression analysis is an estimate of the standard deviation of the coefficient or the precision with which the coefficient is measured. The experimental data was then fit to the equation and plotted as shown in Figure 3.10.

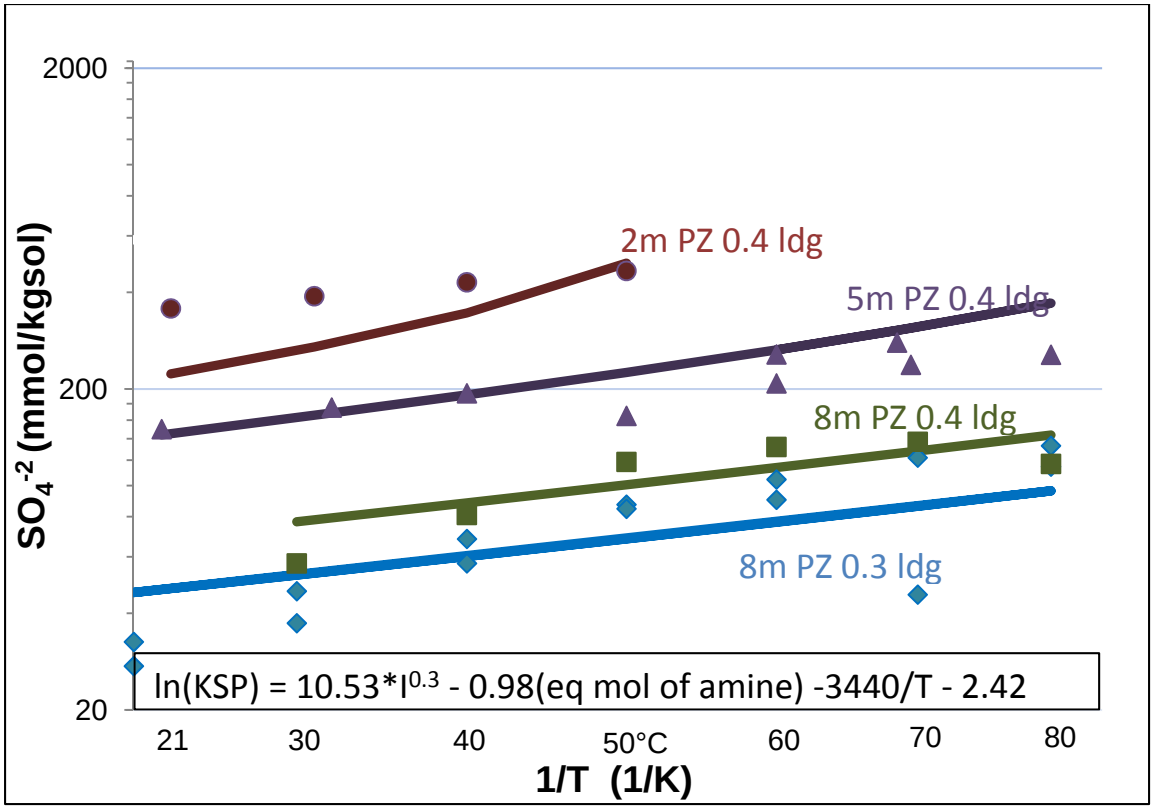

Figure 3.10 K_2SO_4 solubility in 2 m to 8 m PZ solution

Per Figure 3.10, even the empirical model shows that the equivalent amine concentration has a larger effect on the solubility of K_2SO_4 than ionic strength and temperature.

A similar equation was developed for the solubility of Na_2SO_4 in PZ as shown by equation 3.3 below:

$$\ln(Ksp) = 2.137*I^{0.3} - 0.6505*[PZ]_T - 826/T + 265 \qquad 3.3$$

The experimental data was then fit to the equation and plotted as shown in Figure 3.11 below.

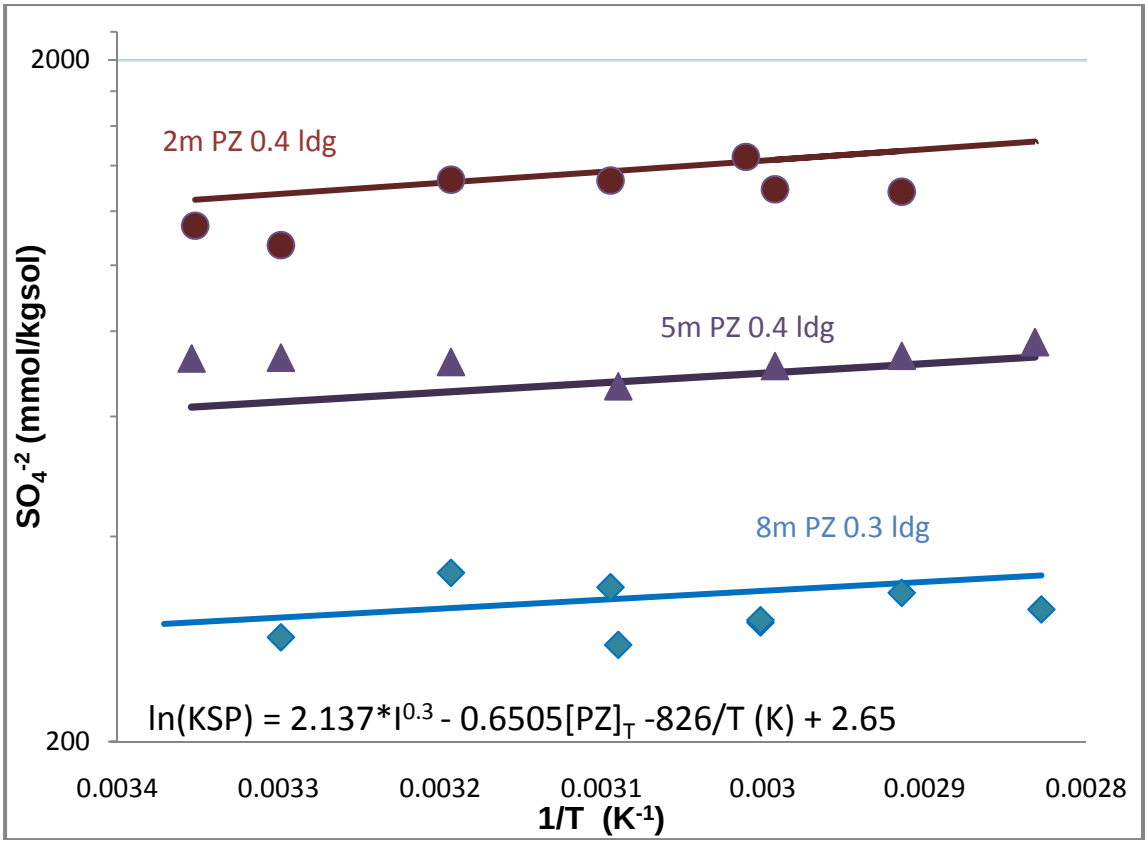

Figure 3.11 Na_2SO_4 solubility in 2 m to 8 m PZ solution

Table 3.2 below shows the standard error associated with the coefficient of each parameter in equation 3.3.

Table 3.2 Na_2SO_4 regression statistical analysis

	Coefficients	***Standard Error***
Intercept	2.65	3.71
PZ (eq mol amine	-0.651	0.059
T (1/K)	-826.0	420.2
$I^{0.3}$	2.14	1.96

One main source of error in the solid solubility experimental method (particularly for solubility in Na_2SO_4 solubility experiments) is the error associated with the analytical equipment used. While the anion and cation IC worked without interruptions when samples were being analyzed, there were instances when the baseline was higher than expected, creating peaks bulkier or higher than anticipated. In the cation IC, a peak for Na was always present (even in Experiments 1 through 3) due to the Na^+ present in either the analytical water used for the equipment or the vials used in the auto sampler. For this reason, when analyzing for Na^+ in the last three experiments, special Na free vials provided by Dionex® were used.

Chapter 4: Regression of interaction parameters in the electrolyte-NRTL model in Aspen Plus®

4.0 ELECTROLYTE-NRTL MODEL IN ASPEN PLUS®

The electrolyte-NRTL model in Aspen Plus® was used to model the sulfate solubility data. For this work in particular, an activity based Aspen Plus® model with regressed thermodynamic data for PZ thermodynamically significant quantities such as Gibbs energy of formation (ΔG_f), heats of formation (ΔH_f), and heat capacities (C_p) were used. This model is primarily used to model MDEA/PZ and PZ CO_2 capture processes for the amine concentration range studied in the solid solubility experiments (Frailie & Marzuka, 2010).

The Aspen Plus® model uses an energy parameter, τ, and a non-randomness factor, α, to calculate the activity coefficient of the ionic species specified in the model. The thermodynamic calculations of the model depend on the ionic forces of the individual ionic species. The forces of the species can be long range forces or short range forces.

Chen et al. (1982) proposed an excess Gibbs energy equation for each of the short and long range interactions. Solubility of K_2SO_4 and Na_2SO_4 in CO_2 loaded PZ can be considered a high electrolyte concentrated solution. Short range interactions dominate regions of high electrolyte concentrations. The excess Gibbs energy (G) for such interactions is calculated below (Hilliard, 2005, Chen, 1982):

$$\frac{G_m^{*E,lc}}{RT} \sum_m Xm \frac{\sum_j X_j G_{jm} \tau_{jm}}{\sum_k X_k G_{km}} + \sum_c X_c \sum_{a'} \left(\frac{X_{a'}}{\sum_{a''} X_{a''}} \right) \frac{\sum_j G_{jc,a'c} \tau_{jc,a'c}}{\sum_k X_k G_{kc,a'c}} + \cdots + \sum_a X_a \sum_{c'} \left(\frac{X_{c'}}{\sum_{c''} X_{c''}} \right) \frac{\sum_j G_{ja,a'c} \tau_{ja,a'c}}{\sum_k X_k G_{ka,a'c}} \quad 4.1$$

Where:

G_{cm} $\frac{\sum_a X_a G_{ca,m}}{\sum_{a'} X_{a'}}$, G_{am} $\frac{\sum_c X_c G_{ca,m}}{\sum_{c'} X_{c'}}$

α_{cm} $\frac{\sum_a X_a \alpha_{ca,m}}{\sum_{a'} X_{a'}}$, α_{am} $\frac{\sum_c X_c \alpha_{ca,m}}{\sum_{c'} X_{c'}}$

$G_{jc,a'c} = \exp(-\alpha_{jc,a'c}\tau_{jc,a'c})$ $G_{jc,c'a} = \exp(-\alpha_{jc,c'a}\tau_{jc,c'a})$

$G_{im} = \exp(-\alpha_{im}\tau_{im})$ $G_{ca,m} = \exp(-\alpha_{ca,m}\tau_{ca,m})$

$\tau_{ma,ca} = \tau_{am} - \tau_{ca,m} + \tau_{m,ca'}$ $\tau_{mc,ac} = \tau_{cm} - \tau_{ca,m} + \tau_{m,ca'}$

$X_j = x_j C_j$ ($C_j = Z_j$ for ions and C_j= unity for molecules);

α is the non randomness parameter;

τ is the binary energy interaction parameter.

The τ parameter has default values in Aspen Plus® for the molecule-electrolyte and electrolyte-water pairs as shown in Table 4.1 below:

Table 4.1 Aspen Plus® default binary interaction parameters

Binary Interaction Pairs	**τ value**
Molecule – Electrolyte	10
Electrolyte – Molecule	-2
Electrolyte – Water	8
Water – Electrolyte	-4

The τ parameters are temperature dependent and are adjusted to fit the experimental data. The τ parameters are fitted using the following equations:

$$\tau_{m,ca} = C_{m,ca} + \frac{D_{m,ca}}{T} + E_{m,ca}\left[\frac{(T_{ref}-T)}{T} + ln\left(\frac{T}{T_{ref}}\right)\right] \quad 4.2$$

$$\tau_{ca,m} = C_{ca,m} + \frac{D_{ca,m}}{T} + E_{ca,m}\left[\frac{(T_{ref}-T)}{T} + ln\left(\frac{T}{T_{ref}}\right)\right] \quad 4.3$$

C, D, and E are given as GMELCC, GMELCD, and GMELCE, respectively in Aspen Plus®. These interaction parameters are then used to calculate the activity coefficients, which in turn are used to calculate the Ksp of the salt in PZ.

The solubility product, Ksp, of a salt is calculated using activity coefficients in the following equation:

$$\text{Ksp} = x_{K^+}^2 * \gamma_{K^+}^2 * x_{SO_4^{-2}} * \gamma_{SO_4^{-2}} \quad 4.4$$

where x is the mole fraction and

γ is the activity coefficient of the ionic species.

The expression for the chemical equilibrium of the dissociation of the salt is given by Hilliard (2005):

$$\ln K = A + \frac{B}{T(K)} + ClnT(K) + D(T(K)) \quad 4.5$$

The values for A, B, and C for K_2SO_4 are input into Aspen Plus® as K-SALT values as follows (Xu, 2008):

Table 4.2: K-salt values for K_2SO_4 (Xu, 2008)

K-SALT/1 (A)	265.7
K-SALT/1 (B)	-14954
K-SALT/1 (C)	-40.7

4.1 NA_2SO_4 - H_2O SYSTEM

For Na_2SO_4, experimental solubility data by Berkeley in 1904 and Richards and Yugve in 1918 between temperatures of 35°C and 200°C (Linke, 1965) are given in the Table 4.3 below.

Table 4.3 Anhydrous Na_2SO_4 solubility in H_2O (Linke, 1965)

Temperature (°C)	Gms of Na_2SO_4/100 gms H_2O
35	49.1
40	48.1
45	47.2
50	46.4
60	45.2
70	44.2
80	43.2
90	42.6
100	42.2
101.9	42.2
110	42
120	41.8
130	41.9
140	42
150	42.2
160	42.5
170	43
180	43.4
190	43.8
200	44.1

Data from Table 4.3 was used to regress the K-SALT values of the Na_2SO_4-H_2O system. Table 4.4 shows the K-SALT values obtained for Na_2SO_4.

Table 4.4: K-salt values for Na_2SO_4

K-SALT/1 (A)	-3457
K-SALT/1 (B)	130527
K-SALT/1 (C)	562.9
K-SALT/1 (D)	-0.649

4.2 EXPERIMENTAL DATA REGRESSION

The following molecules, cations, and anions are assumed to be present in the sulfate reclaiming system:

Molecules: H_2O, PZ, H^+PZCOO^-

Anions: SO_4^{-2}, $PZCOO^-$

Cations: H^+PZ, K^+ /Na^+

While a number of combinations of electrolyte-molecule pairs can be regressed, this work focuses on those including K^+ / Na^+ and SO_4^{-2}. The combinations include:

Table 4.5: Electrolyte-molecule τ parameter pairs to be regressed

Component i	**Component j**
K^+ , SO_4^{-2}	H^+PZCOO^-
H^+PZCOO^-	K^+ , SO_4^{-2}
$PZCOO^-$, K^+	H_2O
H_2O	$PZCOO^-$, K^+
H_2O	H^+PZ, SO_4^{-2}
H^+PZ, SO_4^{-2}	H_2O
K^+ , SO_4^{-2}	PZ
PZ	K^+ , SO_4^{-2}

For Na_2SO_4 solubility, the following τ parameter pairs were varied to fit the experimental data:

Table 4.6 Na_2SO_4 electrolyte-molecule τ parameter pairs to be regressed

Component i	**Component j**
Na^+ , SO_4^{-2}	H^+PZCOO^-
H^+PZCOO^-	Na^+ , SO_4^{-2}
$PZCOO^-$, Na^+	H_2O
H_2O	$PZCOO^-$, Na^+
Na^+ , SO_4^{-2}	PZ
PZ	Na^+ , SO_4^{-2}

Default values from Aspen Plus® were used for the τ parameters of H_2O, K^+, SO_4^{-2} pairs and those of H_2O, Na^+, SO_4^{-2} from Chen et. al (2011) as:

Table 4.7 τ parameters for H_2O, $K^+SO_4^{-2}$ and H_2O, $Na^+SO_4^{-2}$ system (Chen et al., 1982, 2011)

Component i	Component j	τ
H_2O	K^+ , SO_4^{-2}	8
K^+ , SO_4^{-2}	H_2O	-4
H_2O	Na^+ , SO_4^{-2}	8.012
Na^+ , SO_4^{-2}	H_2O	-3.903

4.3 K_2SO_4-PZ-CO_2 -H_2O SYSTEM

After regression of solid solubility experimental data for K_2SO_4 in 2-8 m PZ with CO_2 loadings of 0.3-0.4 mol/mol alkalinity in Aspen Plus®, the following regression output was obtained for the K_2SO_4 system:

Table 4.8 K_2SO_4 τ Parameters regressed in Aspen Plus®

Parameter	Component i	Component j	Value (SI units)	Standard deviation
GMELCC/1	(K+,SO4-2)	PZ	-18.2	194
GMELCC/1	PZ	(K+,SO4-2)	2289.8	330000000
GMELCC/1	(K+,PZCOO-)	H2O	-9.1	207
GMELCC/1	H2O	(K+,PZCOO-)	0.3	1433
GMELCC/1	(K+,SO4-2)	HPZCOO	-0.1	3397
GMELCC/1	HPZCOO	(K+,SO4-2)	57.1	2800000
GMELCC/1	H2O	(PZH+,SO4-2)	11.0	106
GMELCC/1	(PZH+,SO4-2)	H2O	-4.5	68
GMELCD/1	(K+,SO4-2)	PZ	107.4	69700
GMELCD/1	(K+,PZCOO-)	H2O	898.1	74000
GMELCD/1	H2O	(K+,PZCOO-)	-1233.2	503000
GMELCD/1	H2O	(PZH+,SO4-2)	874.1	35200.1
GMELCD/1	(PZH+,SO4-2)	H2O	-136.4	23200
GMELCD/1	PZ	(K+,SO4-2)	233.6	33400000
GMELCD/1	(K+,SO4-2)	HPZCOO	87.4	1370000
GMELCD/1	HPZCOO	(K+,SO4-2)	220.4	45990000

Table 4.8 includes the estimated standard deviation of each parameter from regression of experimental data. Since all of the standard deviations are high, relative to the actual values, some parameters were eliminated after analyzing the correlation matrix of the parameter pairs. The initial correlation matrix is given in Table 4.9 below:

Table 4.9 Correlation Matrix in Aspen Plus®

τ	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	1.00															
2	0.00	1.00														
3	0.07	0.00	1.00													
4	0.76	0.00	-0.22	1.00												
5	-0.41	0.01	-0.10	-0.16	1.00											
6	0.03	0.04	0.06	-0.08	-0.87	1.00										
7	-0.46	0.00	0.00	-0.36	-0.18	0.46	1.00									
8	0.56	0.00	0.03	0.44	0.13	-0.43	-0.99	1.00								
9	-1.00	0.00	-0.07	-0.75	0.40	-0.02	0.47	-0.57	1.00							
10	-0.07	0.00	-1.00	0.22	0.10	-0.06	0.01	-0.03	0.07	1.00						
11	-0.80	0.00	0.12	-0.99	0.21	0.04	0.37	-0.45	0.79	-0.12	1.00					
12	0.53	0.00	0.02	0.40	0.12	-0.43	-0.99	0.99	-0.54	-0.02	-0.41	1.00				
13	-0.63	0.00	-0.04	-0.48	-0.06	0.39	0.97	-0.99	0.63	0.04	0.49	-0.99	1.00			
14	0.00	0.00	0.00	0.00	0.01	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00		
15	0.29	-0.01	0.09	0.08	-0.99	0.94	0.28	-0.24	-0.28	-0.09	-0.13	-0.23	0.18	-0.01	1.00	
16	0.04	-0.70	0.00	0.03	0.07	-0.20	-0.09	0.09	-0.04	0.00	-0.03	0.09	-0.09	-0.70	-0.10	1.00

The correlation coefficient for the parameter pair is a unitless number between 1 and -1. If the number is 1 or -1, then the parameters are said to be correlated and one of the parameters from the pair can then be eliminated. Parameters eliminated were replaced by Aspen Plus® default parameters and/or literature values. Some parameters from literature that were used are given in Table 4.10 below:

Table 4.10 Literature values used to replace independent parameters

Binary Interaction Paramter	τ value
PZ/K^+HCO_3 – GMELCC	7.27 (Hilliard, 2008)
$K^+SO_4^{-2}$/MEA – GMELCC	-1.57 (Xu, 2008)
K^+ HCO_3/PZ – GMELCD	-7.85 (Hilliard, 2008)
$K^+CO_3^{-2}/H_2O$ - GMELCC	-4.24 (Hilliard, 2005)
$K^+CO_3^{-2}/H_2O$ - GMELCD	-96.3 (Hilliard, 2005)
H_2O/K^+CO_3- GMELCD	0.12 (Hilliard, 2005)

After elimination and substitution of parameters, three parameter pairs remained as given in Table 4.11 and the final correlation matrix is given in Table 4.12

Table 4.11 Binary Interaction Parameters regressed for K_2SO_4-PZ-CO_2-H_2O system

Binary Interaction Pairs	Component i	Component j	Value (SI units)	Standard deviation
GMELCC/1	(K+,PZCOO-)	H2O	-4.6	2.7
GMELCC/1	HPZCOO	(K+,SO4-2)	12.0	137.7
GMELCC/1	(PZH+,SO4-2)	H2O	-4.8	0.6

The sum of squares resulting from this regression was 1659.

The residual root mean square was 6.89.

Table 4.12 Final correlation matrix of the K_2SO_4-PZ-CO_2-H_2O system

Parameter	1	2	3
1	1		
2	0.392	1	
3	-0.75	-0.73	1

4.4 VALIDATION OF K_2SO_4-PZ-CO_2 ASPEN PLUS® MODEL

The K_2SO_4-PZ-CO_2 Aspen Plus® model is validated in several different ways. First, a parity plot of the mass fraction of K^+ in 5 m PZ solution between temperatures of 23-80°C is plotted as shown in Figure 4.1.

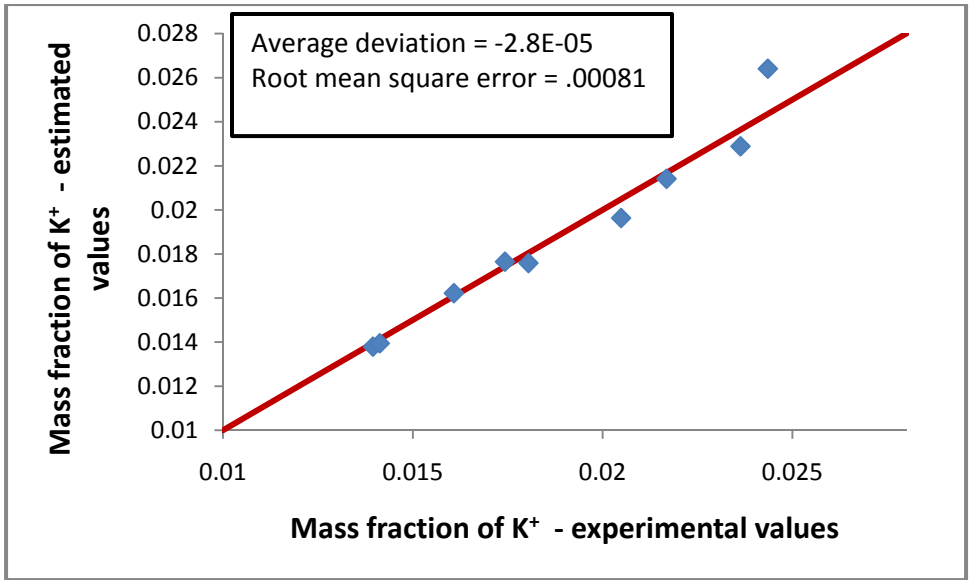

Figure 4.1 Parity plot of Aspen Plus® model adjusted vs. experimental values of K^+ in 5m PZ solution at temperatures between 23 - 80°C

The root mean square of a data set is defined as:

$$\text{Root mean square} = \sum_{i=1}^{k} \left[\frac{(Z_i - ZM_i)2}{K}\right]^{1/2} \quad 4.5$$

Where:

Z is the regressed property value

ZM is the corresponding experimental value from the data set

K is the number of data points.

Table 4.13 below shows the root mean square error of all the other parameters (K^+, PZ, SO_4^{-2}, CO_2) regressed from the solid solubility experiments for 2-8 m PZ for temperatures between 23-80°C.

Table 4.13 Root Mean square error of K_2SO_4-PZ-CO_2 data

		Root Mean Square Error
2m PZ	K^+	0.0026
	PZ	0.0202
	SO_4^{-2}	0.0064
	CO_2	0.0071
5m PZ	K^+	0.0008
	PZ	0.0211
	SO_4^{-2}	0.0003
	CO_2	0.0122
8m PZ	K^+	0.0018
	PZ	0.0015
	SO_4^{-2}	0.2284
	CO_2	0.2154

The K_2SO_4 model was further validated by carrying out a flash calculation for 2-8 m PZ at 0.3 and 0.4 moles of CO_2/mol alkalinity and comparing the SO_4^{-2} concentration with the experimental values. The solution was flashed at 40°C. Figure 4.2 shows Aspen Plus® calculated and measured experimental results.

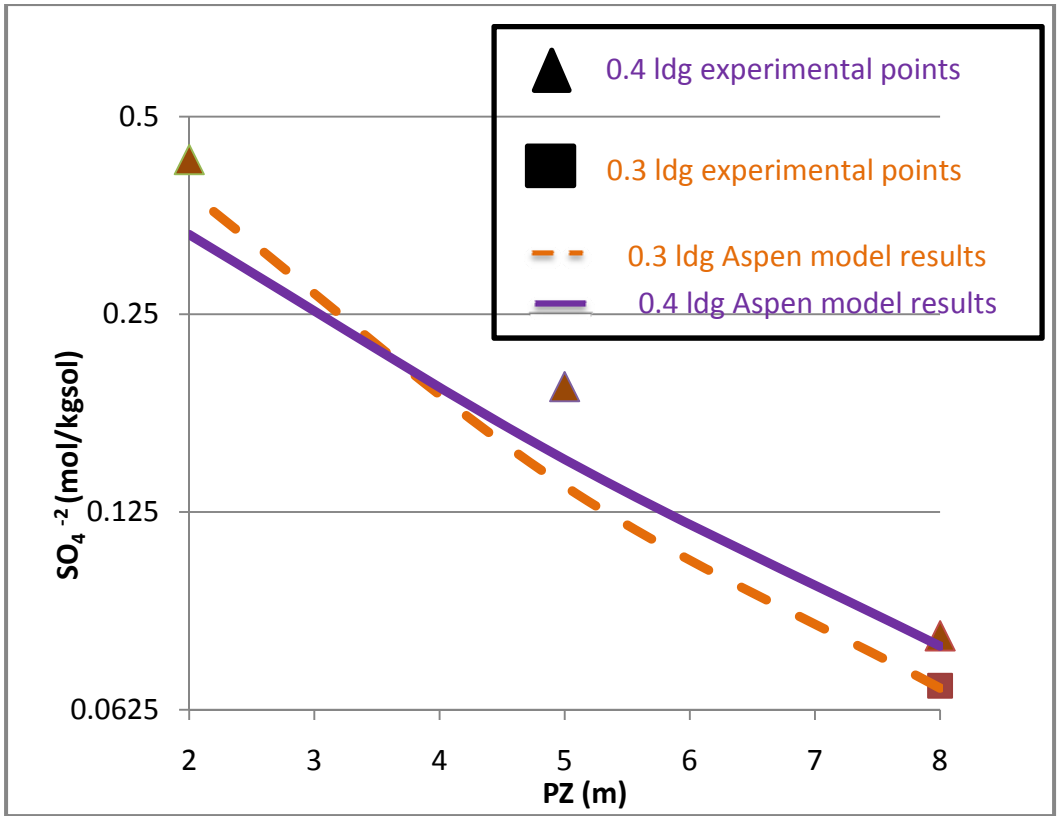

Figure 4.2. Solubility of K_2SO_4, curves predicted by Aspen Plus: points - 40°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus results for 2-8 m PZ at 0.3 loading

In Figure 4.2 above, the lines show Aspen Plus® modeling results and the points show the solid solubility experimental data. From the results it can be deduced that the model predicts SO_4^{-2} solubility well at 8 m PZ and at 2 m PZ but less so at 5 m PZ.

The ratio of the solubility of the experimental data over the solubility of K_2SO_4 in water was plotted against temperature, PZ concentration and CO_2 loading as shown in Figure 4.3, Figure 4.4, and Figure 4.5. The Ksp error varies from -0.09 to 18.5.

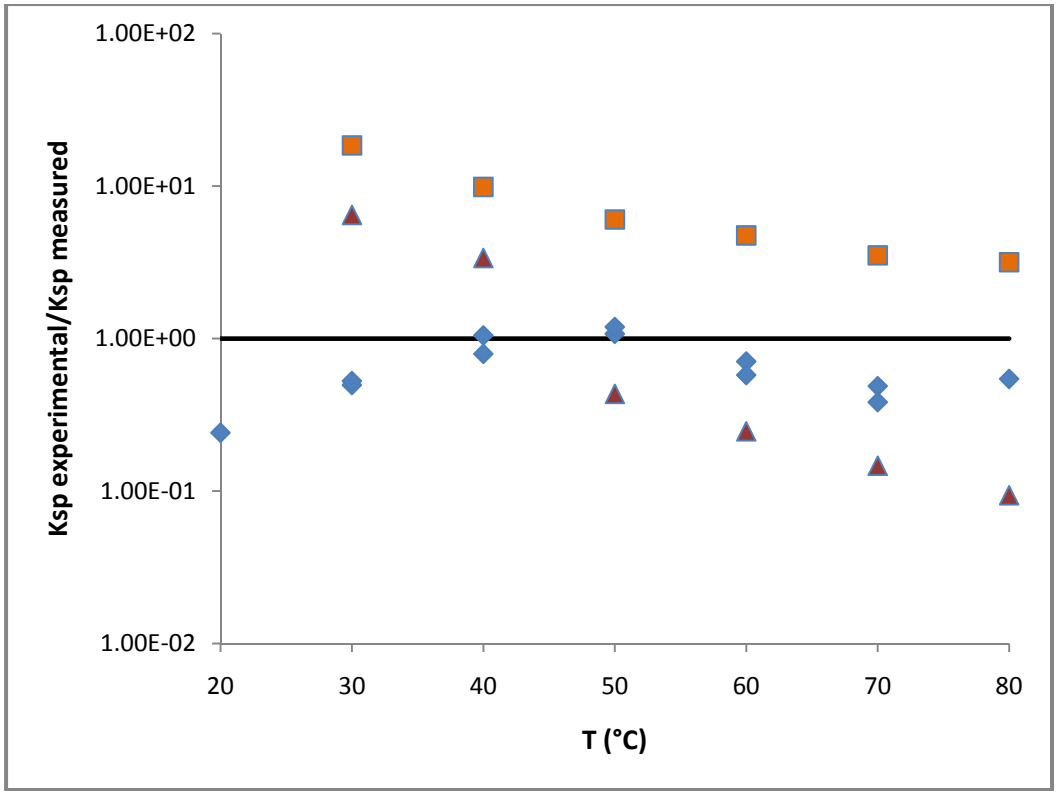

Figure 4.3 Dependence of Ksp error on temperature – K_2SO_4 solubility in 2-8 m PZ; squares – 2 m PZ, triangles – 5 m PZ, diamonds – 8 m PZ

GMELCD parameters, which are the temperature dependent parameters, were eventually eliminated from the regression. Because of the elimination, the slight temperature dependence seen from experimental data in Section 3.2 may not be seen in the Aspen Plus® Model.

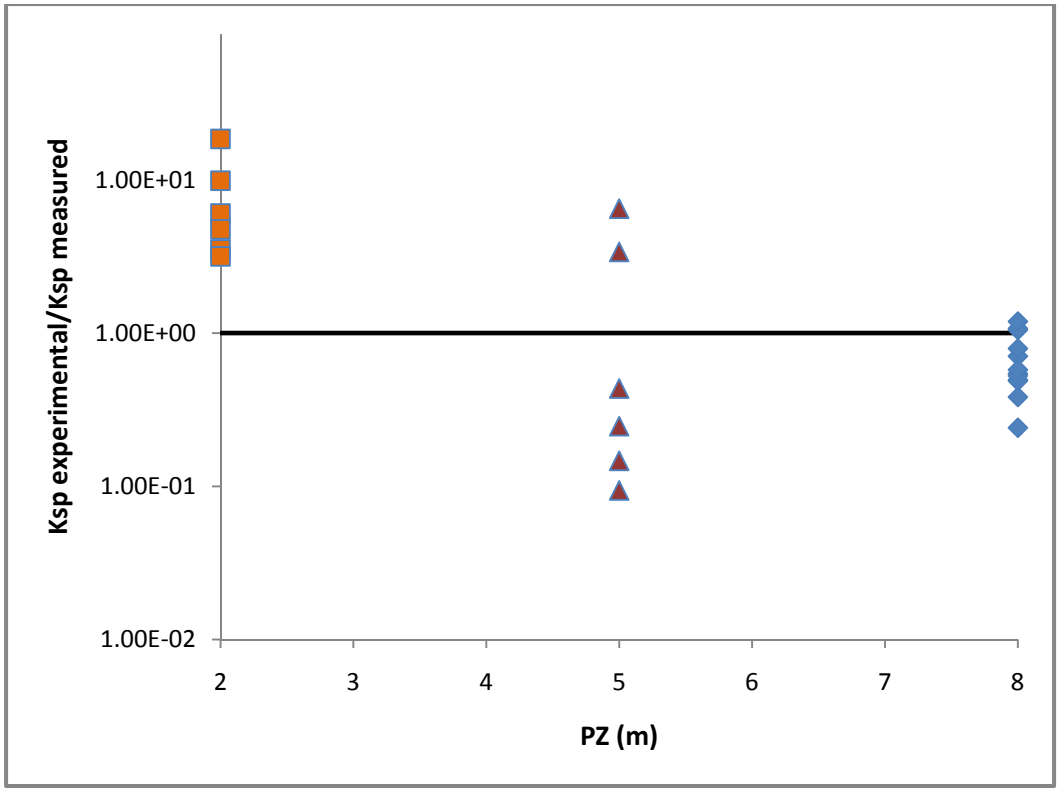

Figure 4.4 Dependence of Ksp error on PZ concentration K_2SO_4 solubility in 2-8 m PZ; squares – 2 m PZ, triangles – 5 m PZ, diamonds – 8 m PZ

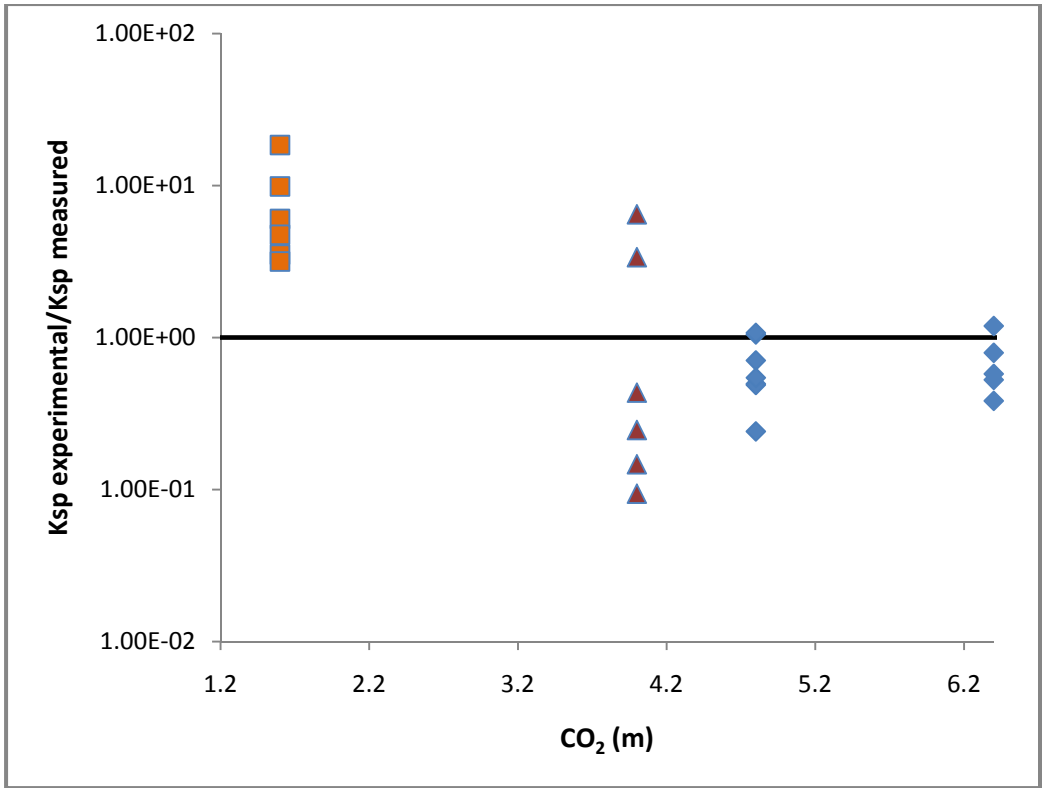

Figure 4.5 Dependence of Ksp error on CO_2 concentration - K_2SO_4 solubility in 2-8 m PZ; squares – 2 m PZ, triangles – 5 m PZ, diamonds – 8 m PZ

The data in Figure 4.4 and Figure 4.5 come close to 1 for the 8 m PZ data set. That may be because there were three experiments carried out for 8 m PZ where as just one experiment for 2 and 5 m PZ. More experimental points could have reduced the error on the 2 and 5 m PZ data.

4.5 Na_2SO_4-PZ-CO_2-H_2O Aspen Plus® Model

Solid solubility experimental data for Na_2SO_4 in 2-8 m PZ with CO_2 loading of 0.3 to 0.4 mol/mol alkalinity were initially fitted to regress the τ parameters shown in Table 4.6. After continuous similar substitution and elimination of parameters as with the K_2SO_4 regression, a sensitivity analysis on the τ parameters was carried out to fit the

experimental data. Default parameters were set for each GMELCC and GMELCD interaction pairs and one pair varied at a time to determine its effect on the model. Table 4.14 shows the variation in parameters. GMELCD pair parameters were set to 0. The corresponding models obtained from the sensitivity analysis are shown in Appendix C. The base case fit of the model is shown in Figure 4.6

Table 4.14 Variation in τ parameters for the Na_2SO_4-PZ-CO_2-H_2O system

Parameter	Component i	Component j	Default value	Change in Value (single change)
GMELCC/1	(NA+,SO4-2)	PZ	-2	-1/ -4
GMELCC/1	PZ	(NA+,SO4-2)	10	7/ 11
GMELCC/1	(NA+,PZCOO-)	H2O	-4	-2/ -6
GMELCC/1	H2O	(NA+,PZCOO-)	8	6/ 10
GMELCC/1	(NA+,SO4-2)	HPZCOO	-2	0/ -4
GMELCC/1	HPZCOO	(NA+,SO4-2)	10	8/ 12
GMELCC/1	(PZH+,SO4-2)	H2O	-4	-2/ -5
GMELCC/1	H2O	(PZH+,SO4-2)	8	5/ 9

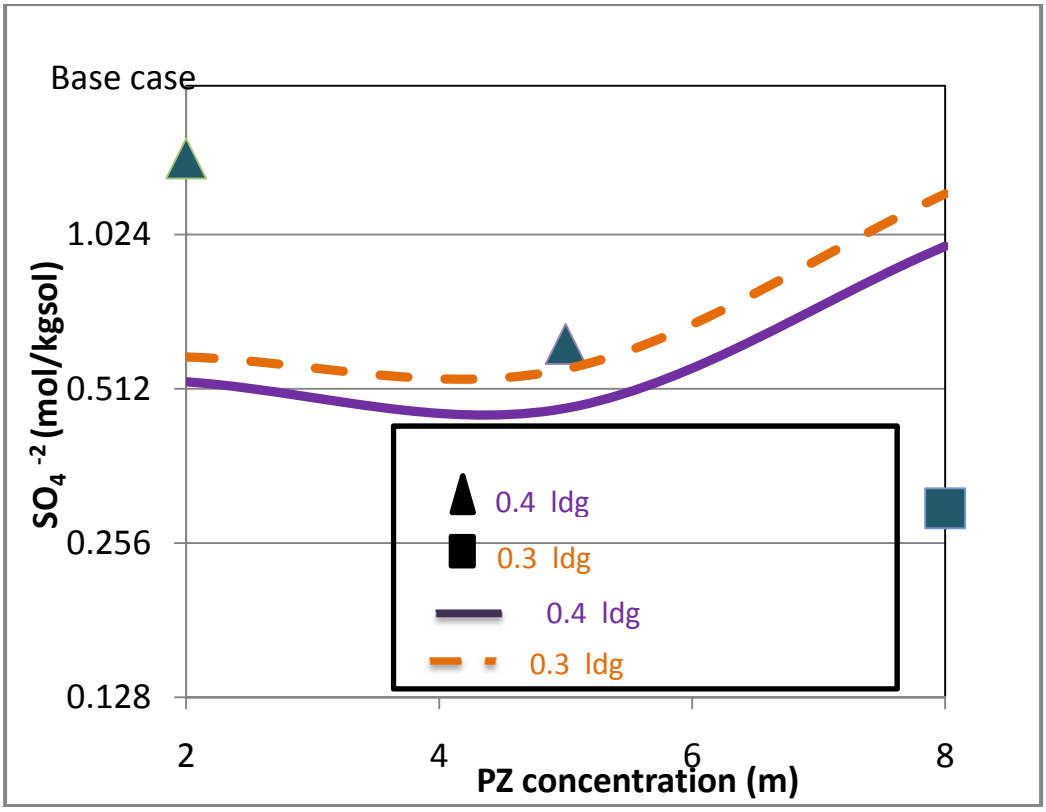

Figure 4.6 Base case fit of the Na_2SO_4-PZ-CO_2-H_2O Aspen Plus® Model. Points – experimental data at 60°C, Curves - Aspen Plus® Model solubility prediction

The PZH^+, SO_4^{-2}/H_2O τ parameter was the only parameter that greatly affected the solubility of Na_2SO_4 in solution when varied from its default value of -4. The τ parameter was varied to determine a fit with the experimental values in 8 m PZ solubility.

Similar to K_2SO_4, the Na_2SO_4 model was further validated by carrying out a flash calculation for 2-8 m PZ at 0.3 and 0.4 moles of CO_2/mol alkalinity and comparing the model SO_4^{-2} concentration with the experimental values. The solution was flashed at 60°C and plotted in Figure 4.7 below.

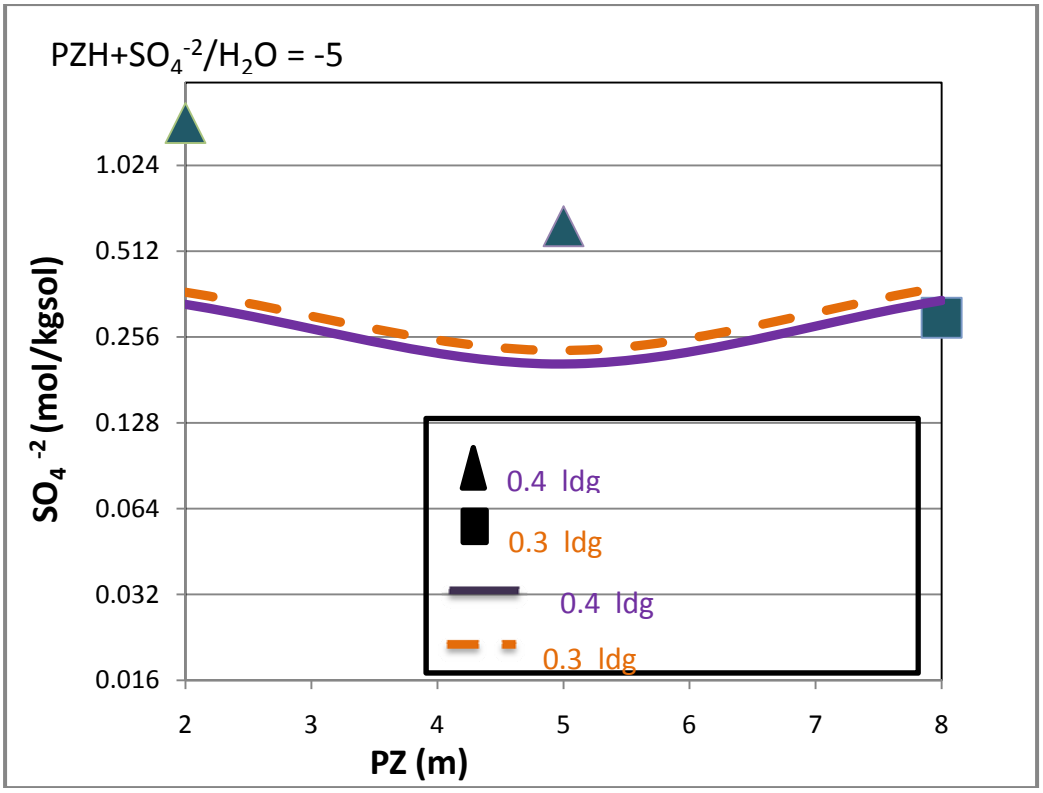

Figure 4.7 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter $PZH+SO_4^{-2}/H_2O$ = -5

The model results work well for 8 m PZ but underpredict the solubility in 2 and 5 m PZ. This could be because there may be two or three combined parameters (including the $PZH^+SO_4^{-2}/H_2O$ parameter**)** that predict the data better than just one parameter alone. Regression of the experimental data in Aspen Plus® did not predict the right combination of the parameters which lead to a sensitivity analysis of the effect of each individual parameter on the solubility of the salt. During the regression analysis, it was noticed that while regressing the τ parameters, the model shifted the Na^+ and SO_4^{-2} experimental mole fraction data in opposite directions skewing the Ksp obtained from experimental data. The trends in the model are, however, similar to those from experimental results in that

the concentration of amine has a greater effect on the solubility of Na_2SO_4 than CO_2 loading of the solution.

The thermodynamic models developed for K_2SO_4 and Na_2SO_4 were used to develop SO_4^{-2} removal by KOH or NaOH reclaiming processes. These models and their results are discussed in Chapter 5.

Chapter 5: Aspen Plus® Reclaiming Process Model

5.0 K_2SO_4 Electrolyte-NRTL Process Simulation in Aspen Plus®

The regression model developed in the e-NRTL framework in Aspen Plus® (as described in Chapter 4) was used to simulate a sulfate reclaiming process. Figure 5.1 shows an Aspen Plus® model using KOH to reclaim sulfate as K_2SO_4. A similar model was developed using NaOH to reclaim Na_2SO_4.

The basis of the model is a CO_2 capture plant that employs 8 m PZ at a lean loading of 0.3 moles CO_2 / mol alkalinity. The flue gas contains 12.38% CO_2 and the CO_2 removal rate is 90%.

A slip stream of the hot lean feed from the stripper at 150°C and 12 atm is flashed though a three-stage flash system. Here CO_2 and H_2O are evaporated and the CO_2 compressed in a two stage compressor. Water is condensed in the pre-cooler and the intercoolers of the compressor. 50% KOH or NaOH is then fed to crystallize the sulfate present in the system. The SO_4^{-2} solids are removed in the separator and the amine is returned to the absorption/stripping process. The reclaiming process has the advantage of removing a significant amount of CO_2 in the process.

There are several areas of the system where the H_2O removed in the process can be re-used. The removal of H_2O concentrates the PZ solution recycled back into the process. The solvent can be diluted back to 8 m PZ using the H_2O removed in the reclaiming process. The H_2O can also be used to wash the crystallized sulfate crystals.

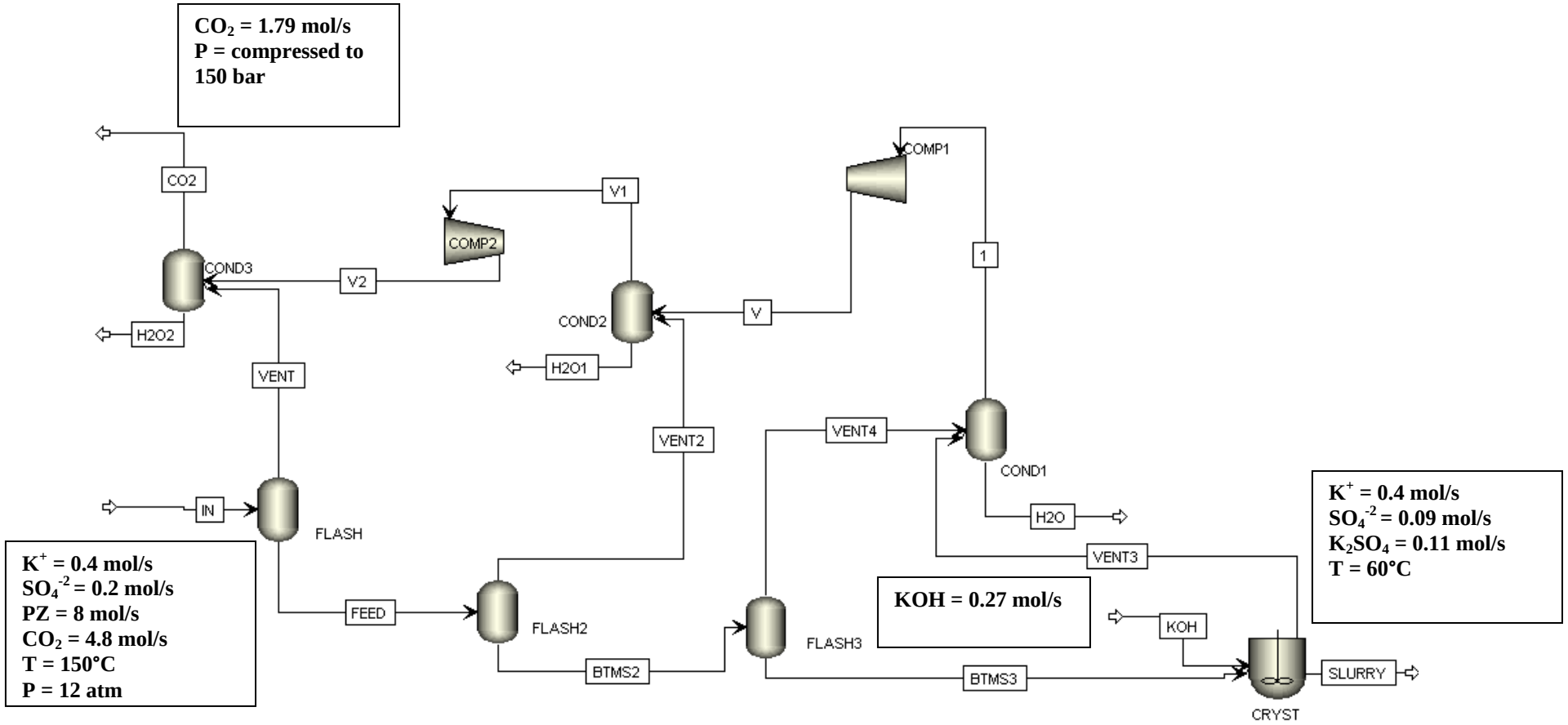

Figure 5.1 Reclaiming by K_2SO_4 crystallization for a CO_2 capture plant using 8 m PZ with a lean loading of 0.3 mol CO_2 / mol alkalinity out of the stripper bottoms– Stoichiometric case (K^+/SO_4^{-2} = 2): 60°C flowrates

Three cases were studied at crystallizer temperatures of 50-100°C:

Stoichiometric case with $K^+/SO_4^{-2} = 2$

Excess sulfate case with $K^+/SO_4^{-2} = 1.3$

Excess K^+ case with $K^+/SO_4^{-2} = 2.5$

The process input for a 8m PZ, 0.3 loaded CO_2 capture process was as follows:

Stream input:

Feed (at 150°C and 5 atm):

55.86 mol/s H_2O

4.8 mol/s CO_2

8 mol/s PZ

For Stoichiometric case: 0.2 mol/s K_2SO_4

Excess sulfate: 0.2 mol/s K_2SO_4 and 0.1 mol/s H_2SO_4

Excess potassium: 0.4 mol/s K_2SO_4 and 0.1 mol/s KOH

The temperature profile between the flash stages was adjusted to be symmetric to minimize the equivalent CO_2 compression work as the temperature of the crystallizer was varied.

The design spec for the simulation was set as follows:

K^+ in steam IN and SLURRY are equal to each other

Flash: T= 117-133.3°C, Q=0

Flash 2: T= 83.4-96.7°C, Q=0

Flash 3: 50-100°C, Q=0

Crystallizer: Q=0

Pressure of streams VENT 2 and V are equal

Pressure of streams VENT and V2 are equal

Pressures in Flash3 = Crystallizer = Cond1

Complete simulation results of all cases and sub-cases are given in Appendix D. A summary of the cases is given in Table 5.1.

Table 5.1 Aspen Plus® modeling results for SO_4^{-2} removal using KOH (Stoich (K^+/SO_4^{-2} = 2), Excess SO_4^{-2} (K^+/SO_4^{-2} = 1.3), and Excess K^+ (K^+/SO_4^{-2} = 2.5))

Case	T (°C)	ΔSO_4^{-2} (mol/kgsolvent)	K_2SO_4 in slurry (mol/s)	CO_2 compressed (mol/s)
Stoich	100	0	0	1.378
Stoich	90	0.010	0.019	1.389
Stoich	70	0.041	0.079	1.352
Stoich	60	0.057	0.110	1.313
Stoich	50	0.072	0.140	1.268
Excess SO_4^{-2}	100	0.043	0.083	1.466
Excess SO_4^{-2}	90	0.058	0.114	1.493
Excess SO_4^{-2}	70	0.090	0.175	1.450
Excess SO_4^{-2}	60	0.106	0.207	1.409
Excess SO_4^{-2}	50	0.122	0.237	1.362
Excess K^+	100	0	0	1.345
Excess K^+	90	0.010	0.020	1.359
Excess K^+	70	0.039	0.076	1.315
Excess K^+	60	0.055	0.107	1.277
Excess K^+	50	0.071	0.138	1.233

In Table 5.1, ΔSO_4^{-2} is the difference in the number of moles of SO_4^{-2} entering the system and that leaving the slurry in moles/kg of process solvent. For the stoichiometric case and the excess K^+ case, no SO_4^{-2} precipitated in the slurry at 100°C. The solubility of K_2SO_4 increases with temperature. Also, there is less driving force and less solvent recirculation in the process system at higher temperatures. Thus, less SO_4^{-2} precipitates at higher temperatures and close to 100°C for the two cases. However, there is some

precipitation in the excess SO_4^{-2} case at 100°C. This is also shown graphically in Figure 5.2

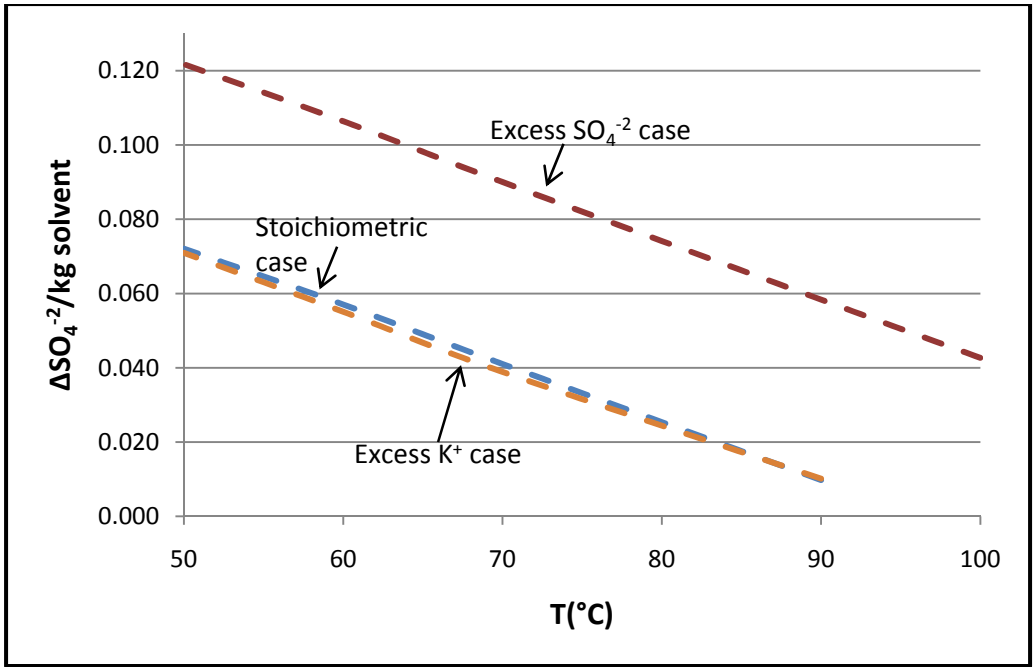

Figure 5.2 Change in ΔSO_4^{-2} with final flash temperature for the three K_2SO_4 cases – stoichiometric ($K^+/SO_4^{-2} = 2$), Excess SO_4^{-2} ($K^+/SO_4^{-2} = 1.3$), and Excess K^+ ($K^+/SO_4^{-2} = 2.5$)

CO_2 is removed in each flash stage of the process system. While the total number of moles for CO_2 compressed remains constant for the different sub-cases within each process case, the amount of CO_2 removed at each flash stage varies, lowering the CO_2 loading. Water vapor is removed in each flash stage as well concentrating the PZ in the solvent. However, the amount removed remains fairly constant at each stage. Figure 5.3 shows how the CO_2 loading and PZ concentration changes at each flash stage for the stoichiometric case at 60°C.

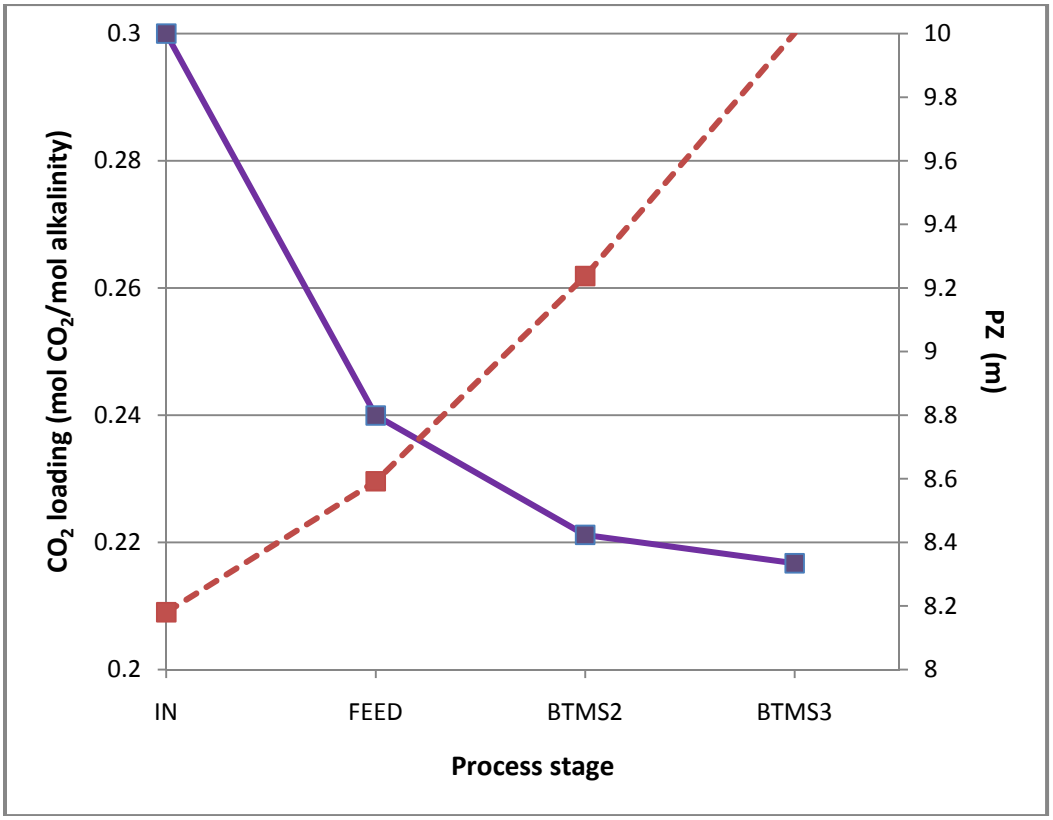

Figure 5.3 Change in CO_2 loading and PZ concentration between flash stages for the stoichiometric case at 60°C for K_2SO_4 stoichiometric case ($K^+/SO_4^{-2} = 2$) – dashed line – PZ concentration, solid line - CO_2 loading

Figure 5.3 shows that the CO_2 loading changes more across the higher temperature flash stage than at the lower temperature flash stages while the PZ concentration changes at the same rate. The partial pressure of CO_2 is higher at higher temperatures and drops a lot faster with temperature than that of water vapor. The heat capacity of a liquid is higher at higher temperatures. Thus, there is more heat available to remove more total vapor at the higher temperature flash stage than the lower temperature flash stages.

5.1 Na_2SO_4 Electrolyte-NRTL Process Simulation in Aspen Plus®

A similar reclaiming process was simulated for the Na_2SO_4 system.

Three cases were also studied at crystallizer temperatures of 50-100°C:

Stoichiometric case with $Na^+/SO_4^{-2} = 2$

Excess sulfate case with $Na^+/SO_4^{-2} = 1.9$

Excess Na^+ case with $Na^+/SO_4^{-2} = 2.04$

The process input for an 8m PZ, 0.3 loaded CO_2 capture process was as follows

Stream input:

Feed (at 150°C and 16 atm):

55.86 mol/s H_2O

4.8 mol/s CO_2

8 mol/s PZ

For Stoichiometric case: 2.3 mol/s Na_2SO_4

Excess sulfate: 2.24 mol/s Na_2SO_4 and 0.07 mol/s H_2SO_4

Excess potassium: 2.3 mol/s Na_2SO_4 and 0.1 mol/s NaOH

The design conditions and specifications of the blocks were kept the same as stated in Section 5.1. A summary of the process result is given in Table 5.2 below.

Table 5.2 Aspen Plus® modeling results for SO_4^{-2} removal using NaOH (Stoich case ($Na^+/SO_4^{-2} = 2$), Excess SO_4^{-2} case ($Na^+/SO_4^{-2} = 1.9$), and Excess Na^+ case ($Na^+/SO_4^{-2} = 2.04$)

Case	T (°C)	ΔSO_4^{-2} (mol/kgsolvent)	Na_2SO_4 in slurry (mol/s)	CO_2 compressed (mol/s)
Stoich	100	0.032	0.0712	1.041
Stoich	70	0.050	0.1118	1.012
Stoich	60	0.044	0.0987	0.990
Stoich	50	0.032	0.0714	0.966
Excess SO_4^{-2}	100	0.038	0.1169	1.084
Excess SO_4^{-2}	70	0.056	0.1576	1.055
Excess SO_4^{-2}	60	0.051	0.1446	1.033
Excess SO_4^{-2}	50	0.038	0.1171	1.009
Excess Na^+	100	0.033	0.0736	1.000
Excess Na^+	70	0.051	0.1136	0.970
Excess Na^+	60	0.045	0.1000	0.948
Excess Na^+	50	0.032	0.0718	0.924

The ΔSO_4^{-2} in the system as a function of temperature behaves differently in the Na^+ case than the K^+ case.

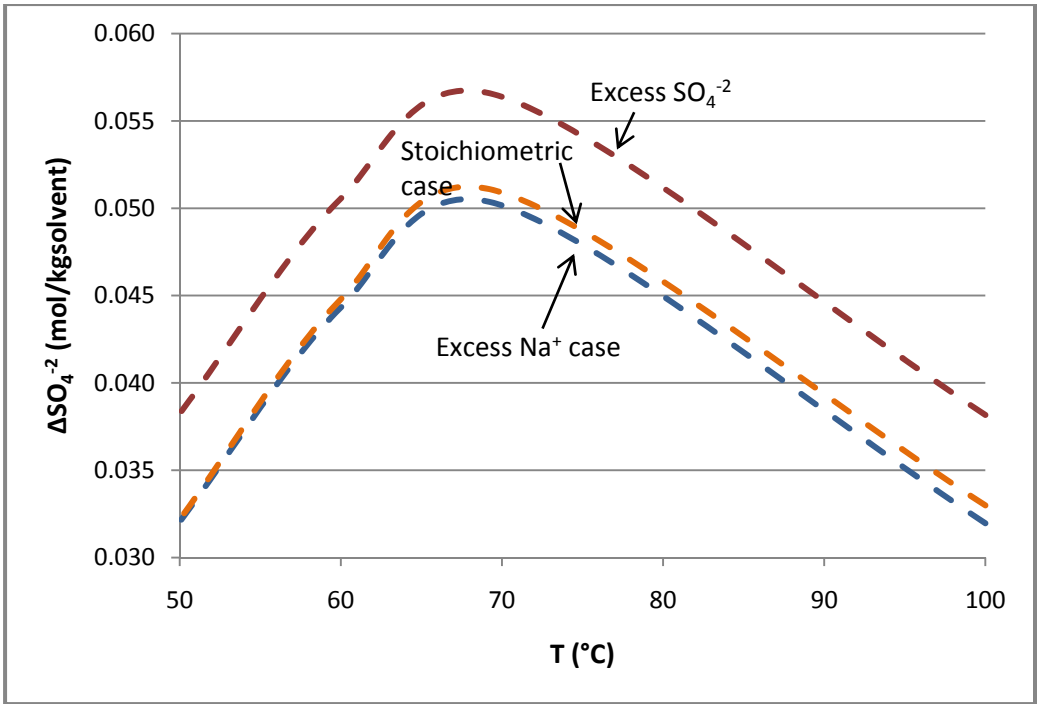

Figure 5.4 Change in ΔSO_4^{-2} with final flash temperature for the three Na_2SO_4 cases – stoichiometric case ($Na^+/SO_4^{-2} = 2$), Excess SO_4^{-2} case ($Na^+/SO_4^{-2} = 1.9$), and Excess Na^+ case ($Na^+/SO_4^{-2} = 2.04$)

The ΔSO_4^{-2} reaches a maximum at approximately 70°C and then decreases again. A reason for this may be that because the solvent is saturated with Na_2SO_4, which remains fairly constant with temperature. It may be that the NaOH reacts more readily with the PZ species that contribute to the ionic strength of the solvent (PZH^+ and/or $PZCOO^-$) than the SO_4^{-2}.

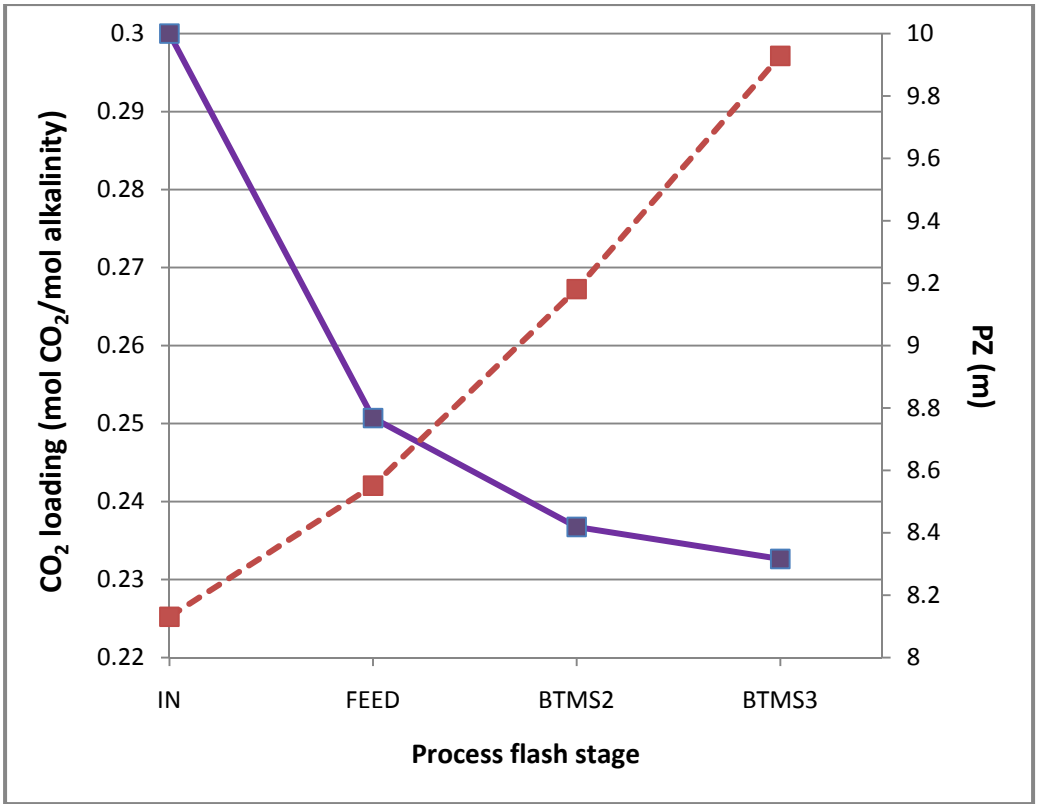

Figure 5.5 Change in CO_2 loading and PZ concentration between flash stages for Na_2SO_4 Excess SO_4^{-2} case (Na^+/SO_4^{-2} = 1.9) at 70°C - dashed line – PZ concentration, solid line CO_2 loading

5.3 Energy and Chemical Cost Estimation For K_2SO_4 System

The equivalent work that is lost in the reclaiming process per mole of sulfate comprises of the equivalent work lost in the main process, the work from the compressor, and the work benefitted from the CO_2 compressed during the reclaiming process. The equivalent work lost in the process is given by equation 5.1:

$$W_{eq1} = m * 0.75 * \int_{Tref}^{T} \frac{T-Tref}{T} * C_p * dT \qquad 5.1$$

Where m is the feed rate in kg/s

C_p is = average heat capacity of the feed 3.54 kJ/kgK (Xu, 2008)

The equivalent work that is saved results from CO_2 produced here rather than in the main process is given by

$$W_{eq2} = (\frac{moles}{s} of\ CO2\ produced * 35 \frac{kJ}{mol} CO2) \quad 5.2$$

Van Wagener (Van Wagener, 2011) regressed a compressor correlation to calculate the work from the compressor:

$$W_{comp} = 4.572 * \ln(\frac{150}{Pin}) - 4.096 \quad 5.3$$

where P_{in} in the compressor feed vapor coming from the highest pressure stage in bar (Van Wagener, 2011).

Using a typical electricity cost of \$65/MWh and the ratio of CO_2 to SO_2 in the flue gas, the cost of sulfate removal in \$/ton of CO_2 can be calculated.

The equivalent work and energy costs are summarized in Table 5.3 below for the K_2SO_4 case and shown graphically in Figure 5.6.

Table 5.3 Work and cost summary for sulfate reclaiming by KOH (stoichiometric ($K^+/SO_4^{-2} = 2$), Excess SO_4^{-2} ($K^+/SO_4^{-2} = 1.3$), and Excess K^+ ($K^+/SO_4^{-2} = 2.5$))

Case	T (°C)	W_{comp} (MJ/mol K_2SO_4 in slurry)	W_{eq1} (MJ/mol K_2SO_4 in slurry)	W_{eq2} (MJ/mol K_2SO_4 in slurry)	W_{eq}MJ/mol K_2SO_4 in slurry	Energy cost ($/ton$CO_2$)
Stoich	100	0	0	0	0	0
Stoich	90	1.55	3.29	2.57	2.26	0.833
Stoich	70	0.43	0.92	0.60	0.75	0.277
Stoich	60	0.32	0.70	0.42	0.60	0.223
Stoich	50	0.27	0.57	0.32	0.52	0.191
Excess SO_4^{-2}	100	0.34	0.65	0.62	0.37	0.135
Excess SO_4^{-2}	90	0.28	0.54	0.46	0.36	0.132
Excess SO_4^{-2}	70	0.21	0.42	0.29	0.34	0.124
Excess SO_4^{-2}	60	0.18	0.37	0.24	0.32	0.118
Excess SO_4^{-2}	50	0.17	0.34	0.20	0.31	0.113
Excess K^+	100	0	0	0	0	0
Excess K^+	90	1.45	3.16	2.41	2.20	0.810
Excess K^+	70	0.44	0.97	0.61	0.80	0.294
Excess K^+	60	0.32	0.72	0.42	0.63	0.231
Excess K^+	50	0.26	0.58	0.31	0.53	0.194

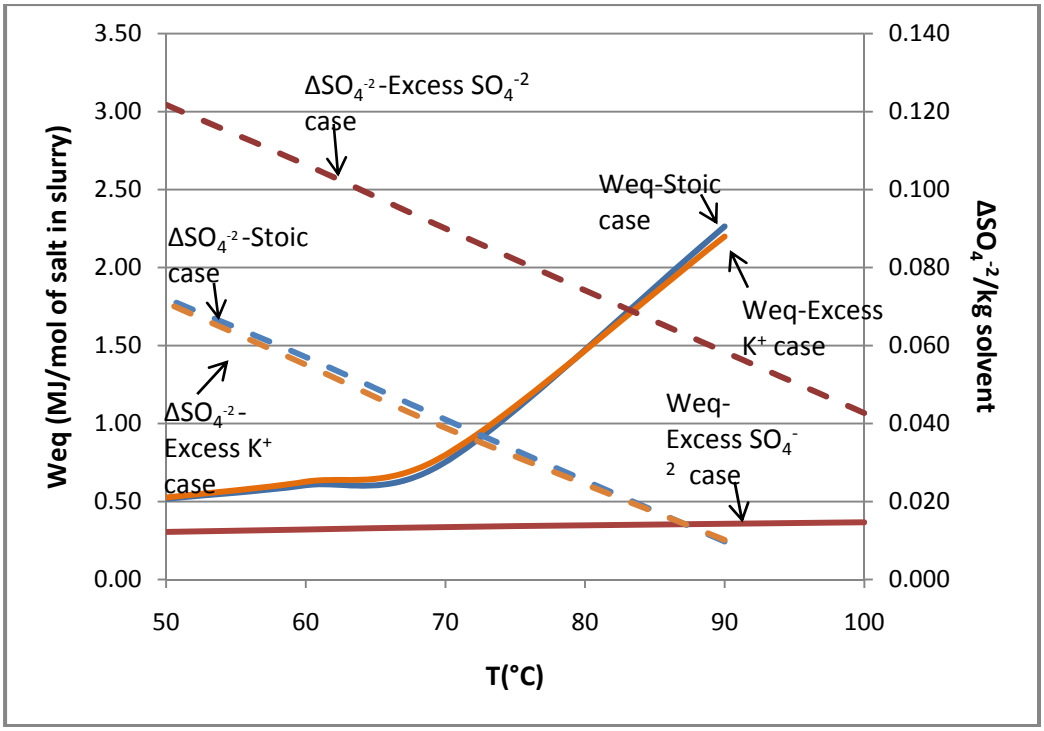

Figure 5.6 Change in equivalent work and ΔSO_4^{-2} with temperature for the three K_2SO_4 cases – stoichiometric ($K^+/SO_4^{-2} = 2$), Excess SO_4^{-2} ($K^+/SO_4^{-2} = 1.3$), and Excess K^+ ($K^+/SO_4^{-2} = 2.5$)

Adding sulfate increases the capacity and lowers the equivalent work of the process. The stoichiometric case and excess K^+ case show a minimum work requirement between 65-70°C. This could be an optimized temperature to run the reclaimer for the two conditions.

The energy cost of the system is given by:

$$\text{Energy cost} = \frac{\text{Weq kJ}}{\text{mol SO2}} \frac{\text{1e-04 mol SO2}}{\text{12.4\%mol CO2*90\%}} \frac{\text{mol CO2}}{\text{44.01g}} \frac{\text{1e6g}}{\text{tonne}} \frac{\text{MWhr}}{\text{3.6e6 kJ}} \frac{\text{\$65}}{\text{MWhr}} \qquad 5.4$$

The energy cost in \$/ton CO_2 is directly proportional to the increase in temperature of the last flash stage. However, this is still a small number compared to a typical CO_2 capture cost of \$50/tonne.

Two chemical costs based on different assumptions were calculated. The first assumption is that the K_2SO_4 precipitated can be sold as fertilizer. For this, a price of \$200/ton of K_2SO_4 fertilizer was use (ICIS, 2011). The second assumption is that the K_2SO_4 is removed and treated in a waste water treatment facility. For this case, a price of \$0 was used. A cost of \$40/100 lb of KOH was used (ICIS, 2011). This is equivalent to:

$$\frac{\$40}{100\text{lb KOH}}\frac{56\text{ g}}{\text{gmol}}\frac{1\text{ lb}}{454\text{ g}}=\frac{\$0.049}{\text{gmol }K^{+}}=\frac{\$0.098}{\text{gmol }SO_4^{-2}} \qquad 5.5$$

The chemical cost in \$/ton of CO_2 was calculated using the following equation:

$$\text{Chemical cost}=\frac{\$}{\text{mol SO2}}\frac{\text{1e-04 mol SO2}}{12.38\%\text{mol CO2}*90\%}\frac{\text{mol CO2}}{44.01\text{g}}\frac{\text{1e6g}}{\text{tonne}} \qquad 5.6$$

The chemical cost if the K_2SO_4 is recovered in the process is used as fertilizer is \$0.6/tonne CO_2. However, if this is not possible because of the impurities that may be present on the K_2SO_4 crystals, the chemical cost would increase to \$2 / tonne CO_2

5.4 Energy and Chemical Cost Estimation For Na_2SO_4 System

The equivalent work and energy costs for the Na_2SO_4 system are summarized in the Table 5.4 below and shown graphically in Figure 5.6

Table 5.4 Work and cost summary for the sulfate reclaiming by NaOH (Stoich (Na^+/SO_4^{-2} = 2), Excess SO_4^{-2} (Na^+/SO_4^{-2} = 1.9), and Excess Na^+ (Na^+/SO_4^{-2} = 2.04)

Case	T (°C)	W_{comp} (MJ/moles Na_2SO_4 in slurry)	W_{eq1} (MJ/moles Na_2SO_4 in slurry)	W_{eq2} (MJ/mol Na_2SO_4 in slurry)	W_{eq}MJ/mol Na_2SO_4 in slurry	Energy cost ($/tonCO2)
Stoich	100	0.3	0.9	0.5	0.6	0.236
Stoich	70	0.2	0.8	0.3	0.7	0.246
Stoich	60	0.3	0.9	0.4	0.8	0.305
Stoich	50	0.4	1.3	0.5	1.2	0.449
Excess SO_4^{-2}	100	0.2	0.5	0.3	0.4	0.147
Excess SO_4^{-2}	70	0.2	0.5	0.2	0.5	0.176
Excess SO_4^{-2}	60	0.2	0.6	0.2	0.6	0.209
Excess SO_4^{-2}	50	0.3	0.8	0.3	0.7	0.275
Excess Na^+	100	0.3	0.9	0.5	0.6	0.239
Excess Na^+	70	0.2	0.7	0.3	0.7	0.247
Excess Na^+	60	0.3	0.9	0.3	0.8	0.305
Excess Na^+	50	0.4	1.3	0.5	1.2	0.450

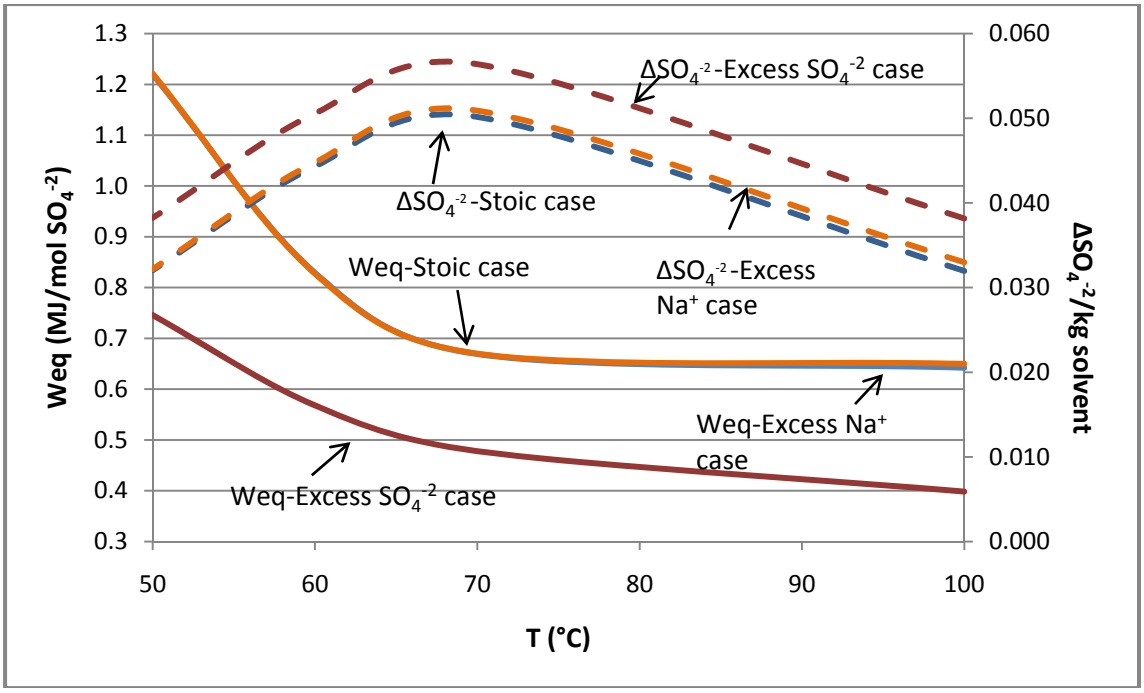

Figure 5.7 Change in equivalent work and ΔSO_4^{-2} with temperature for the three Na_2SO_4 cases – stoichiometric ($Na^+/SO_4^{-2} = 2$), Excess SO_4^{-2} ($Na^+/SO_4^{-2} = 1.9$), and Excess Na^+ ($Na^+/SO_4^{-2} = 2.04$)

Similar to K^+, adding sulfate increases the capacity and lowers the equivalent work of the Na_2SO_4 precipitation process. All cases show a minimum work requirement between 65-70°C. This could be an optimized temperature to run the reclaimer for if SO_4^{-2} is to be removed using NaOH.

The energy cost of the Na process, ranging from \$0.1-0.5/ton CO_2 is the same order of magnitude as the K^+ case (ranging from \$0.1-0.8/ton CO_2).

The price of 50 wt% NaOH is \$450/short ton of NaOH (ICIS, 2011). The solids from the crystallizer are most likely to be treated in wastewater treating. For this reason, the cost for Na_2SO_4 is \$0. The chemical cost in \$/tonne of CO_2 calculated by Equation 5.5 is \$0.7 / tonne of CO_2. This is less than compared to the chemical cost for the K^+ case if the K_2SO_4 crystals cannot be sold as fertilizer. This is one of the reasons why it

may be cheaper to use NaOH to remove sulfate in the reclaiming process rather than KOH. Another reason why removal process may be cheaper for the Na case is that the process requires less equivalent work compared to the K case because less solvent is required in the process reducing the size of the equipment and the capital cost of the project.

SO_4^{-2} crystals removed from the crystallizer are impure. Impurities such as nitrosamines and PZ may be attached to the crystals that would need to be washed off. For 100 ppm removal of K_2SO_4 and 20 wt% of 8 m PZ of impurity attached to the SO_4^{-2} crystals, the cost of PZ loss can be estimated as follows:

$$\frac{\$3}{\text{lb PZ}}\frac{(0.2)*(0.4)\text{lb PZ}\ (1e\text{-}4)\text{mol SO2}}{(0.8\ \text{solids})(12.38\%\ \text{gmol CO2})*(90\%\ \text{removal})}\frac{174\ \text{lb solids}}{\text{lbmol solids}}\frac{1\text{gmolCO2}}{44.01\ \text{g}}\frac{1e6\ \text{g}}{\text{ton CO2}} = \frac{\$2.3}{\text{tonne CO2}} \quad 5.7$$

In the above equation, the cost of PZ is assumed to be \$3/lb of PZ. If 50 wt% of 8 m PZ of impurities are attached to the SO_4^{-2} crystals, a PZ loss of \$9.4/tonne CO_2 is estimated. Both these costs of loss of PZ are high. If such a small amount of PZ lost is expensive, it will be far more expensive to replace amine solvent if it is not reclaimed and reused. The solids from the crystals should be washed and sent back to the process to reduce PZ replacement costs.

Chapter 6: Recommendations and conclusions

Sulfate accumulates in the post-combustion CO_2 capture system and must be removed to re-use amine efficiently. Removal of sulfate from the amine-based post-combustion CO_2 capture system through a solvent reclaiming process may reduce CO_2 capture costs. Solvent reclaiming by solids precipitation requires the knowledge of the solubility of sulfate in PZ solution. Solid solubility experiments determined the solubility of K_2SO_4 and Na_2SO_4 in 2-8 m CO_2 loaded PZ solutions. Data regression gave an empirical equation to determine the solubility of sulfate over a range of PZ concentrations. Aspen Plus® process simulations determined the amount of sulfate that can be removed from a process using 8m PZ with a lean loading of 0.3 mol CO_2/mol alkalinity. The results from the simulation determined the energy cost and economics of the reclaiming process.

6.0 EXPERIMENTAL RESULTS

At 40°C the solubility of Na_2SO_4 in 8 m PZ with a CO_2 loading of 0.3 is 0.3 m Na_2SO_4 and that of K_2SO_4 is 0.1 m K_2SO_4.

The solubility of both K_2SO_4 and Na_2SO_4 in aqueous PZ increased with CO_2 loading and decreased with increasing PZ. At higher CO_2 loading, the solvent is more ionic since it contains greater concentrations of carbamate and protonated amines. As a result, salt crystals are more soluble in the solution. In addition, sulfate solubility decreased as the organic nature and concentration of the solvent increased. There was minimal effect of temperature on the solubility of K_2SO_4 and almost no effect of temperature on the solubility of Na_2SO_4 in PZ.

Sulfate solubility in PZ solutions is represented by the empirical models:

K_2SO_4: $ln(Ksp) = 10.53I^{0.3} - 0.98[PZ]_T - 3440/T - 2.42$

Na_2SO_4: $ln(Ksp) = 2.137I^{0.3} - 0.6505[PZ]_T - 826/T + 265$

Where Ksp is the solubility product of a salt

I is the ionic strength

and $[PZ]_T$ = 2*(molality of PZ)

The experiments were carried out at loadings of 0.3 and 0.4 moles of CO_2/mol of alkalinity and at concentrations of 2-8 m PZ. The sulfate containing PZ solution is flashed in the reclaiming process resulting in a higher PZ concentration at lower loadings. It is recommended that more experiments be carried out at leaner loadings and at higher PZ concentrations for sulfate solubility analysis closer to the proposed reclaiming process.

6.1 PROCESS SIMULATION RESULTS

A K_2SO_4 and Na_2SO_4 solubility thermodynamic model was developed in the e-NRTL framework in PZ Fawkes Aspen Plus® model. Reclaiming processes for removal of SO_4^{-2} with KOH and NaOH were simulated using the thermodynamic model developed. The K_2SO_4 thermodynamic model developed in Aspen Plus seemed to fit the experimental data obtained from the solid solubility experiments. However, the Na_2SO_4 regression in Aspen Plus® did not fit the experimental data as well as K case did. The trends obtained from the model were similar to those obtained in experimental work.

The energy cost of the Na process, ranging from \$0.1-0.5/ton CO_2 is in the same order of magnitude as the K^+ case (ranging from \$0.1-0.8/ton CO_2).

The K_2SO_4 recovered in the process can be used as fertilizer. However, the KOH will still cost \$0.6/tonne CO_2. If it is not possible to sell the K_2SO_4 as fertilizer because of the impurities that may be present on the K_2SO_4 crystals, the chemical cost would increase to \$2/tonne CO_2.

The chemical cost in \$/tonne of CO_2 for the Na case is \$0.7/tonne of CO_2. This is less than compared to the chemical cost for the K case if the crystals cannot be sold as fertilizer and one of the reasons why it may be cheaper to use NaOH to remove sulfate in the reclaiming process rather than KOH.

For 100 ppm removal of SO_4^{-2} and 20 wt% of 8 m PZ of impurity attached to the SO_4^{-2} crystals, the cost of PZ loss is \$2.3/tonne CO_2. If 50 wt% of 8 m PZ of impurities are attached to the SO_4^{-2} crystals, a PZ loss of \$9.4/tonne CO_2.SO_4^{-2} crystals removed from the crystallizer are impure. Impurities such as nitrosamines and PZ may be attached to the crystals that would need to be washed off.

Removing SO_4^{-2} exclusively in a neutralization process than with the other heat stable salts in a thermal reclaiming process prevents the thermal reclaiming heat exchanger to be exposed to SO_4^{-2} solids. The crystallizer employed in the process is also at ambient pressures which reduces the cost of the SO_4^{-2} removal process proposed.

In conclusion, removing SO_4^{-2} by neutralization with either KOH or NaOH is a straight forward method that can be employed in the post combustion CO_2 capture system. It has the advantage of removing more CO_2 and re-using a relatively clean solvent back to the absorber, reducing the cost of replacing expensive solvents used for CO_2 capture.

Appendix A

Table A.0 Experimental Apparatus

Equipment	Supplier
100 ml Jacketed Beaker Reactor	Chemglass®
Rubber Stopper	Fisherbrand®
Thermometer	Fisherbrand®
Stir bar	Fisherbrand®
Tubing	Tygon® - 3603
Heater and water bath	Lauda® Ecoline E-100
Nonsterile; PTFE; Pore size: 0.45µm; Diameter: 25mm filter	Fisherbrand®
3mL; 0.10mL graduation luer lok syringes	BD Medical®
6 dram, 22.2 ml clear glass vials	Fisherbrand®
10ml, 2ml Pipettes	Eppendorf® Research
250 ml CO_2 loader and frit	Wilmad® labglass
500 ml Bottles	Wheaton®
Cation Chromatograph	Dionex ICS-2100
Anion Chromatograph	Dionex ICS-3000
Total Inorganic Carbon Analyzer	Horiba PIR 2000, PICOlog

Table A.1 Chemicals Used

Chemical	Supplier
Piperazine	Sigma-Aldrich®
Anhydrous Sodium Sulfate	Fisher Scientific®
Potassium Sulfate	Fisher Scientific®
Carbon Dioxide	Matheson® Co.

Appendix B

B.0 CHROMELEON CATION CHROMATOGRAPHY PROGRAM

B.0.1 Jason3 Auto.pgm

```
;Sampler.AcquireExclusiveAccess
          ;Sampler_DiverterValve.Position_1
          Pressure.LowerLimit =          200 [psi]
          Pressure.UpperLimit =          3000 [psi]
          %A.Equate =                    "%A"
          CR_TC =                        On
          ;Flush                         Volume = 100
          ;Wait                          FlushState
          ;NeedleHeight =                0 [mm]
          ;CutSegmentVolume =            0 [µl]
          ;SyringeSpeed =                -1
          ;TrayTemperature =             Off
          ;CycleTime =                   0 [min]
          ;Flush                         Volume = 100
          ;Wait                          FlushState
          ;NeedleHeight =                2 [mm]
          ;CutSegmentVolume =            0 [µl]
          ;SyringeSpeed =                3
          ;TrayTemperature =             10
          ;CycleTime =                   0 [min]
          WaitForTemperature =           False
          Data_Collection_Rate =         5.0 [Hz]
          CellTemperature.Nominal =      30.0 [°C]
          ColumnTemperature.Nominal =    30.0 [°C]
          Suppressor_Type =              CSRS_4mm
          ; Pump_ECD.H2SO4 =            0.0
          ; Pump_ECD.MSA =              38.5
          ; Pump_ECD.Other eluent =     0.0
          ; Pump_ECD.Recommended Current =             136
          Suppressor_Current =           136 [mA]
          ECD_Total.Step =               0.20 [s]
          ECD_Total.Average =            Off
          Wait                           SampleReady
          ;Wait                          SampleReady
          Flow =                         1.20 [ml/min]

 0.000    Concentration =                5.50 [mM]
          Autozero
```

```
          ;Load
          ;Wait                              CycleTimeState
          ;Wait                              StartRun
          Inject
          ;Wait                              InjectState
          ECD_1.AcqOn
          ECD_Total.AcqOn
          ;Sampler.ReleaseExclusiveAccess
          Concentration =                    5.50 [mM]
          Pump_ECD_Relay_2.Closed            Duration=10.00

 0.100    Pump_ECD_Relay_1.State             Closed

 1.000    Pump_ECD_Relay_1.State             Open

 2.300    Pump_InjectValve.InjectPosition    Duration=60.00

10.000    Concentration =                    5.50 [mM]

10.001    Concentration =                    11.00 [mM]

15.000    Concentration =                    11.00 [mM]

20.000    Concentration =                    38.50 [mM]

28.000    ECD_1.AcqOff
          ECD_Total.AcqOff
          Concentration =                    38.50 [mM]
          End
```

B.0.2 Stephanie3 Auto.pgm

```
Pressure.LowerLimit =                        200 [psi]
          Pressure.UpperLimit =              3000 [psi]
          %A.Equate =                        "%A"
          CR_TC =                            On
          DeliverSpeed =                     4.0 [ml/min]
          DelayVolume =                      125 [µl]
          FlushFactor =                      10
          Sampler.LoadPosition
          DeliverSample                      Volume=1666
          EndSamplePrep
          Data_Collection_Rate =             5.0 [Hz]
          CellTemperature.Nominal =          30.0 [°C]
```

```
          ColumnTemperature.Nominal =     30.0 [°C]
          Suppressor_Type =               CSRS_4mm
          ; Pump_ECD.H2SO4 =              0.0
          ; Pump_ECD.MSA =                38.5
          ; Pump_ECD.Other eluent =       0.0
          ; Pump_ECD.Recommended Current =              57
          Suppressor_Current =            77 [mA]
          Channel_Pressure.Average =      On
          Flow =                          0.50 [ml/min]

 0.000    Autozero
          Concentration =                 5.50 [mM]
          Curve =                         5
          Wait                            CycleTimeState
          Inject
          ECD_1.AcqOn
          Channel_Pressure.AcqOn
          Concentration =                 5.50 [mM]
          Curve =                         5

 0.500    BeginOverlap

16.400    Concentration =                 5.50 [mM]
          Curve =                         5

16.501    Concentration =                 11.00 [mM]
          Curve =                         5

26.400    Concentration =                 11.00 [mM]
          Curve =                         5

36.400    Concentration =                 38.50 [mM]
          Curve =                         5

47.400    Concentration =                 38.50 [mM]
          Curve =                         5

47.500    Concentration =                 5.50 [mM]
          Curve =                         5

50.000    ECD_1.AcqOff
          Concentration =                 5.50 [mM]
          Curve =                         5
          Channel_Pressure.AcqOff
```

```
End
```

B.1 CHROMELEON ANION CHROMATOGRAPHY PROGRAM

B1.1 Anions.pgm

```
Sampler.AcquireExclusiveAccess
          Sampler_DiverterValve.Position_2
          Column_TC.AcquireExclusiveAccess
          Compartment_TC.AcquireExclusiveAccess
          Pressure.LowerLimit =              200 [psi]
          Pressure.UpperLimit =              3000 [psi]
          MaximumFlowRamp =                  6.00 [ml/min²]
          %A.Equate =                        "%A"
          CR_TC =                            On
          Flush                              Volume = 250
          Wait                               FlushState
          NeedleHeight =                     2 [mm]
          CutSegmentVolume =                 10 [µl]
          SyringeSpeed =                     4
          CycleTime =                        0 [min]
          WaitForTemperature =               False
          Data_Collection_Rate =             5.0 [Hz]
          Temperature_Compensation =         1.7 [%/°C]
          CellHeater.Mode                    = On
          CellHeater.TemperatureSet =        35.00 [°C]
          Column_TC.Mode =                   On
          Column_TC.TemperatureSet =         30.00 [°C]
          Compartment_TC.Mode =              On
          Compartment_TC.TemperatureSet =    30.00 [°C]
          Suppressor2.Type =                 ASRS_4mm
          Suppressor2.CurrentSet =           179 [mA]
          Flow =                             1.600 [ml/min]
          Pump_2.Curve =                     5
          Wait                               SampleReady
          ;Wait  Column_TC.TemperatureState
          ;Wait Compartment_TC.TemperatureState
          ;Wait  Column_TC.TemperatureState
          ;Wait Compartment_TC.TemperatureState
          ; Suppressor1.Carbonate =          0.0
          ; Suppressor1.Bicarbonate =        0.0
          ; Suppressor1.Hydroxide =          45.0
          ; Suppressor1.Tetraborate =        0.0
          ; Suppressor1.Other eluent =       0.0
          ; Suppressor1.Recommended Current =              179

-6.100    Concentration =                    45.00 [mM]
          EGC_1.Curve =                      5
```

```
-6.000     Concentration =                    2.00 [mM]
           EGC_1.Curve =                      5

 0.000     CDet1.Autozero
           Load
           Wait                               CycleTimeState
           Inject
           Wait                               InjectState
           Pump_2_Pressure.AcqOn
           CD_1.AcqOn
           CD_1_Total.AcqOn
           Sampler.ReleaseExclusiveAccess
           Compartment_TC.ReleaseExclusiveAccess
           Column_TC.ReleaseExclusiveAccess

10.000     ;ompartment_TC.ReleaseExclusiveAccess
           ;column_TC.ReleaseExclusiveAccess

17.000     Concentration =                    2.00 [mM]
           EGC_1.Curve =                      5

25.000     Concentration =                    45.00 [mM]
           EGC_1.Curve =                      5

35.000     Concentration =                    45.00 [mM]
           Pump_2_Pressure.AcqOff
           CD_1.AcqOff
           CD_1_Total.AcqOff
           EGC_1.Curve =                      5
           End
```

Appendix C

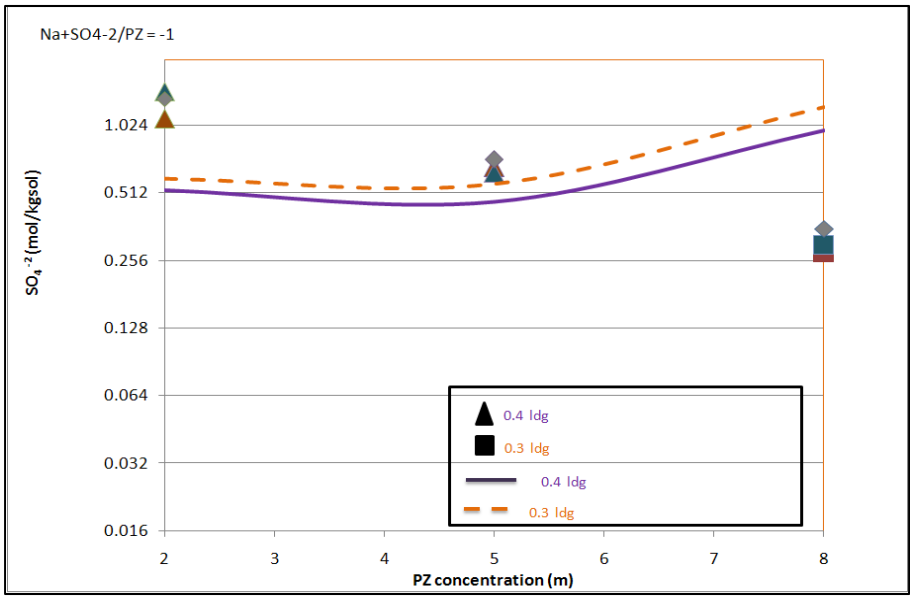

Figure C.1 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter $Na+SO_4^{-2}/PZ = -1$

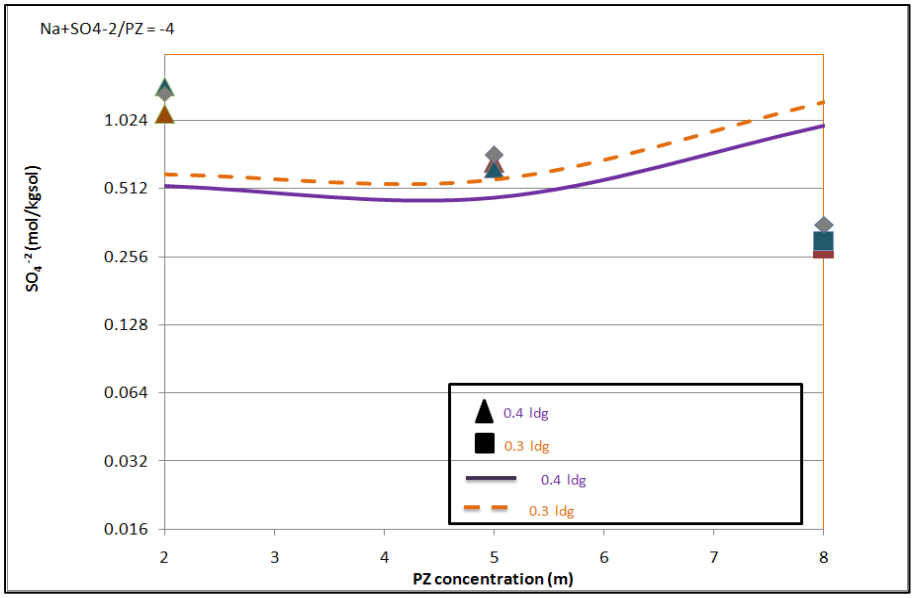

Figure C.2 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter $Na+SO_4^{-2}/PZ = -4$

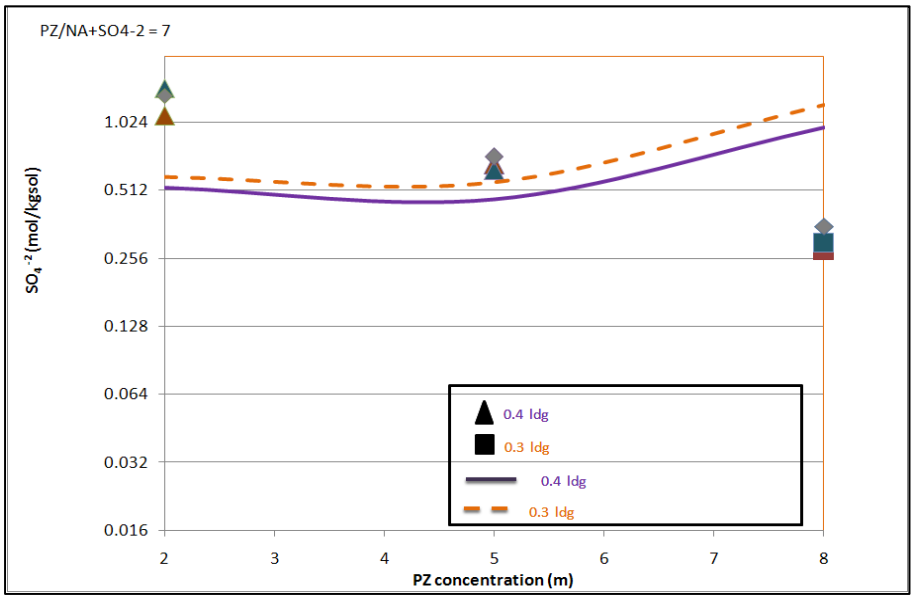

Figure C.3 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter PZ/ $Na+SO_4^{-2} = 7$

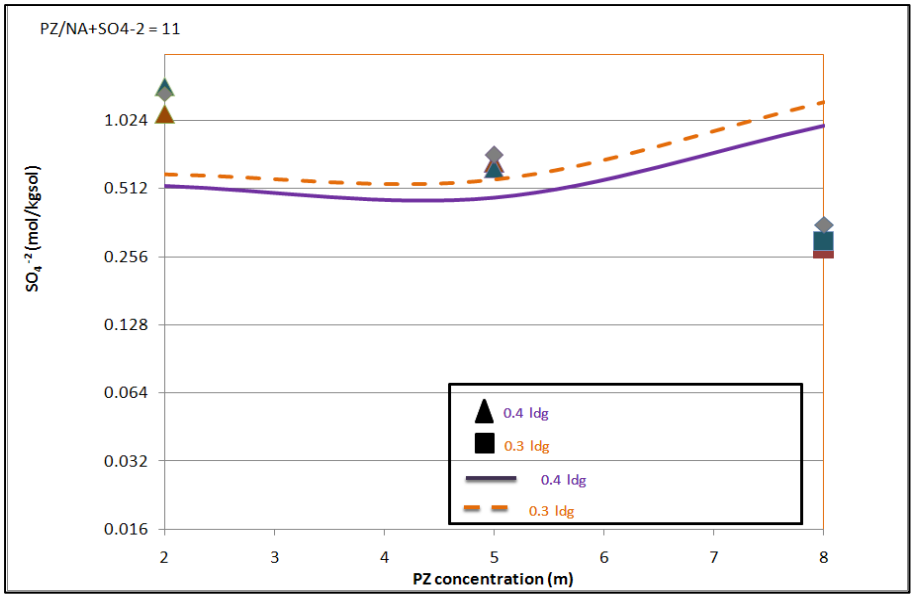

Figure C.4 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter PZ/ $Na+SO_4^{-2}$ = 11

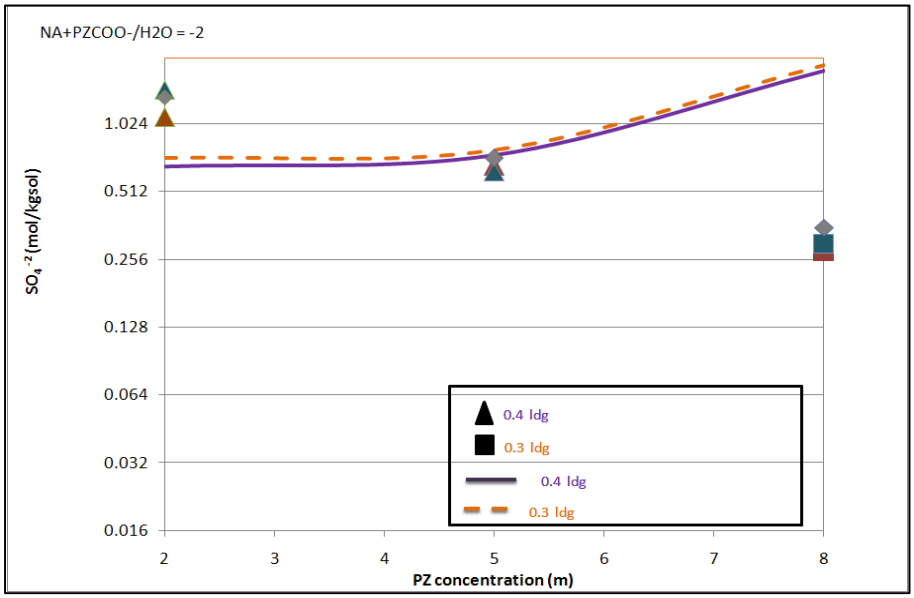

Figure C.5 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter Na+PZCOO-/H2O = -2

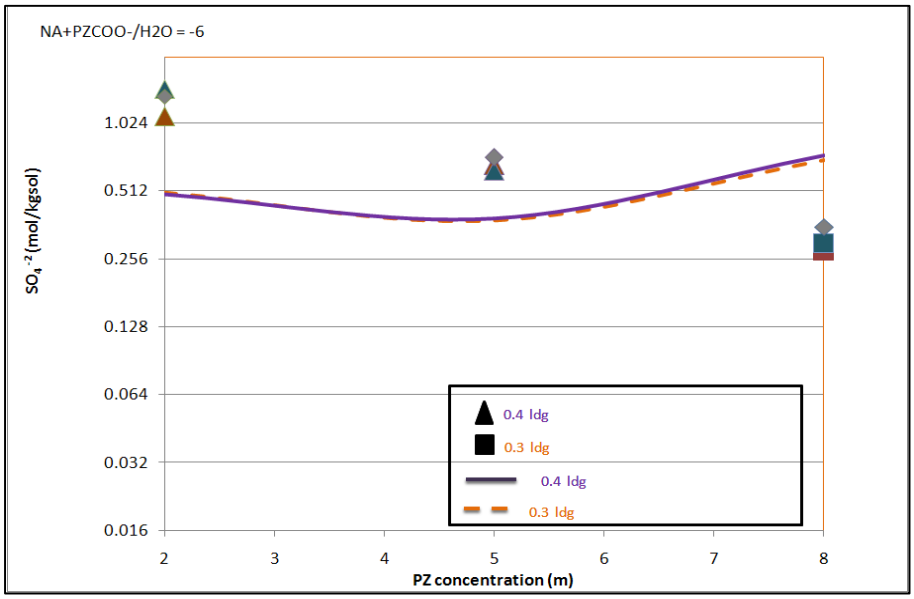

Figure C.6 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter Na+PZCOO-/H2O = -6

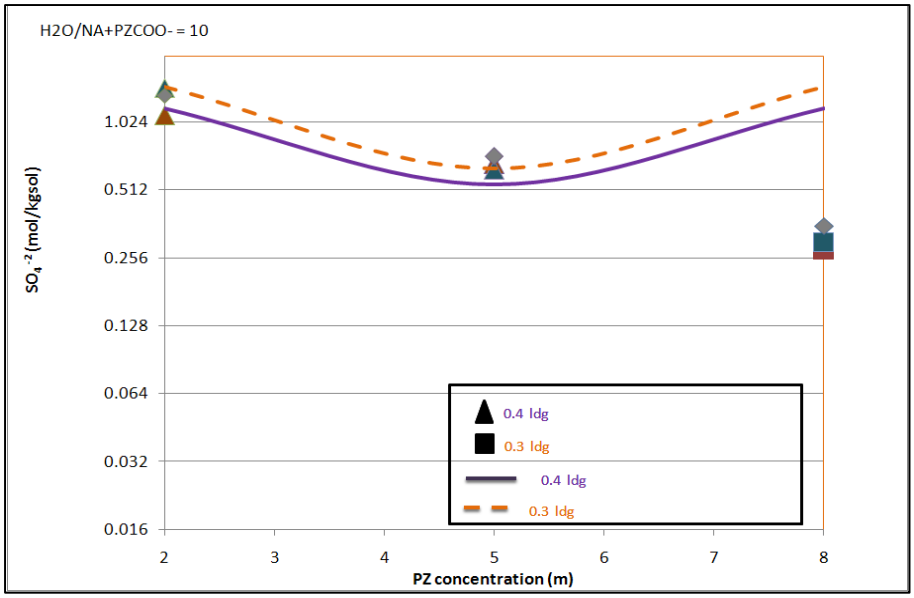

Figure C.7 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter H2O /Na+PZCOO- = 10

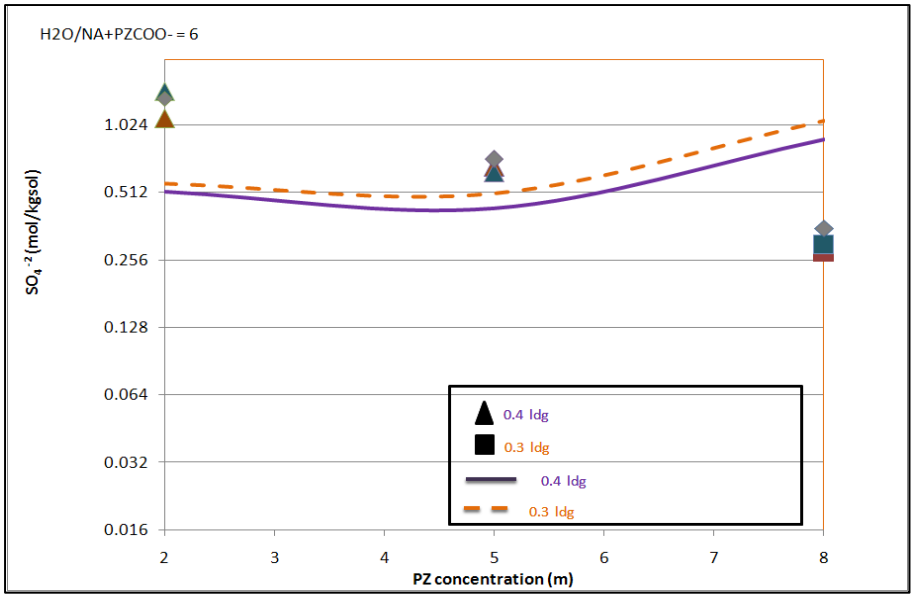

Figure C.8 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter H2O /Na+PZCOO- = 6

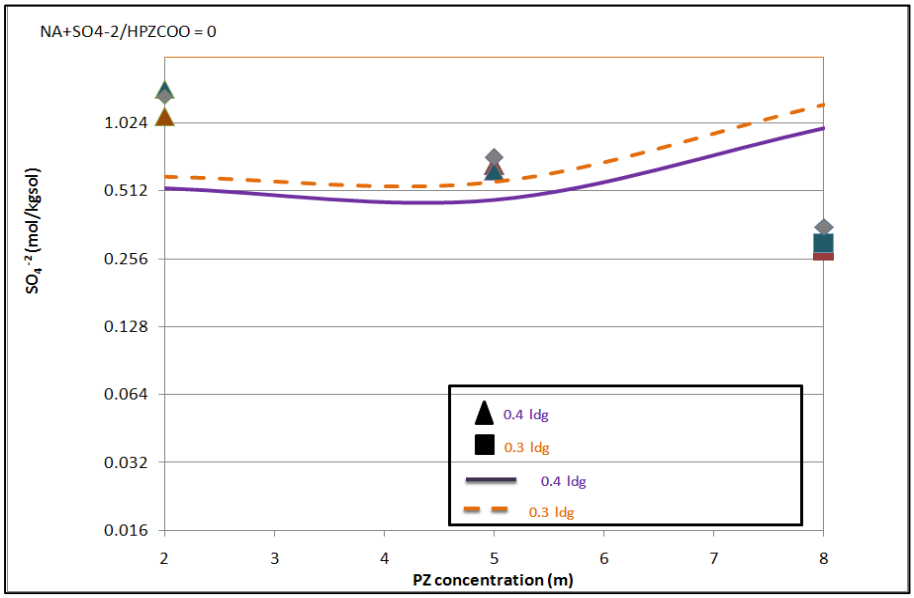

Figure C.9 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter Na+SO4-2/HPZCOO = 0

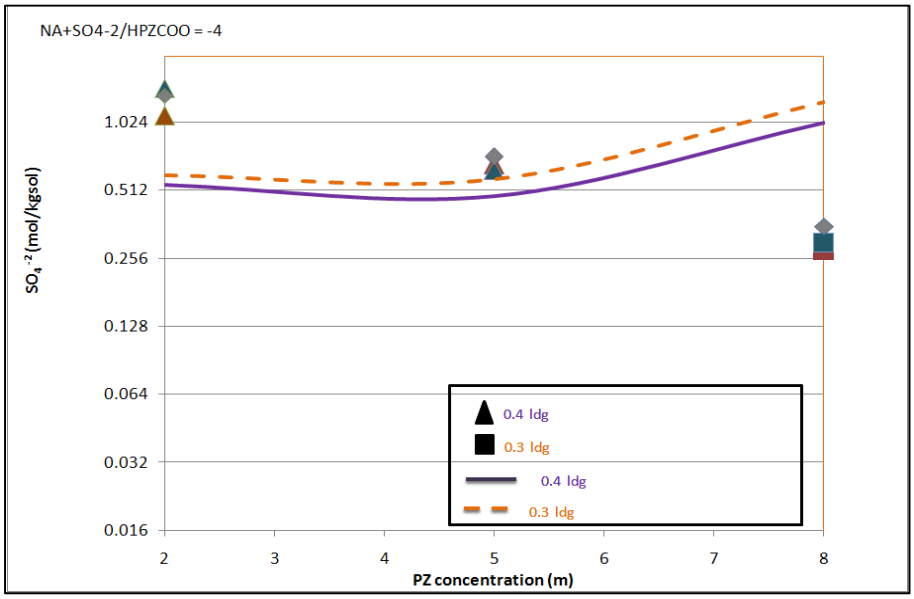

Figure C.10 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter Na+SO4-2/HPZCOO = -4

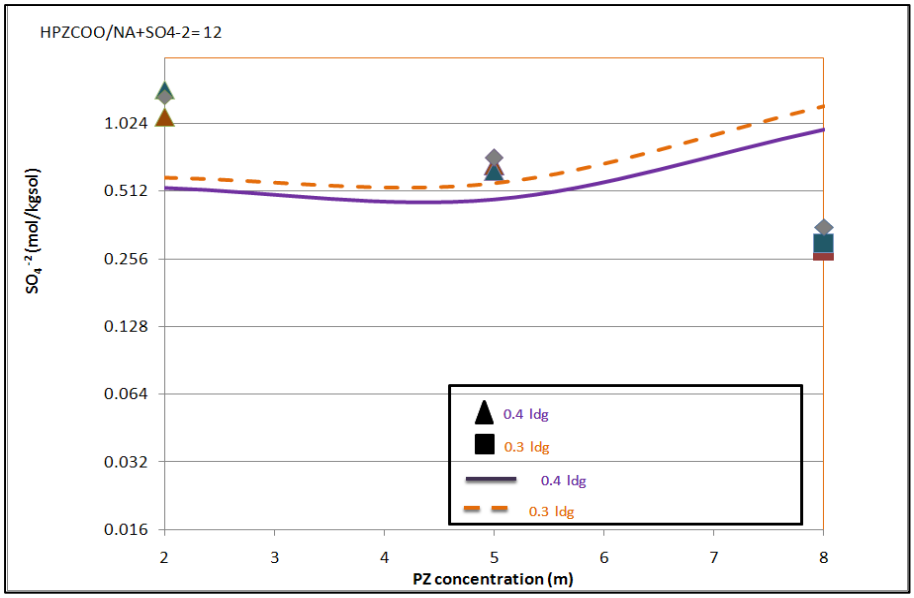

Figure C.11 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter HPZCOO / Na+SO4-2 = 12

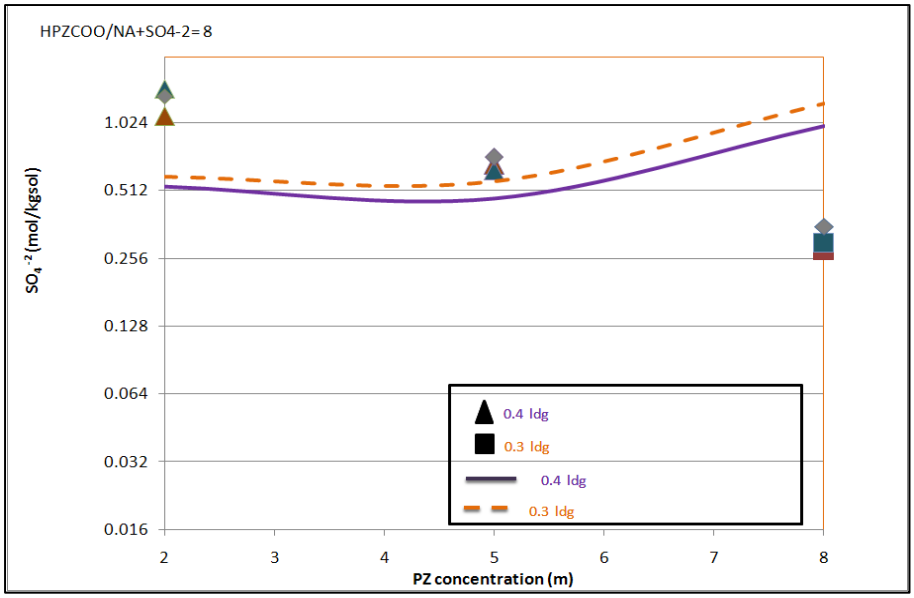

Figure C.12 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter HPZCOO / Na+SO4-2 = 8

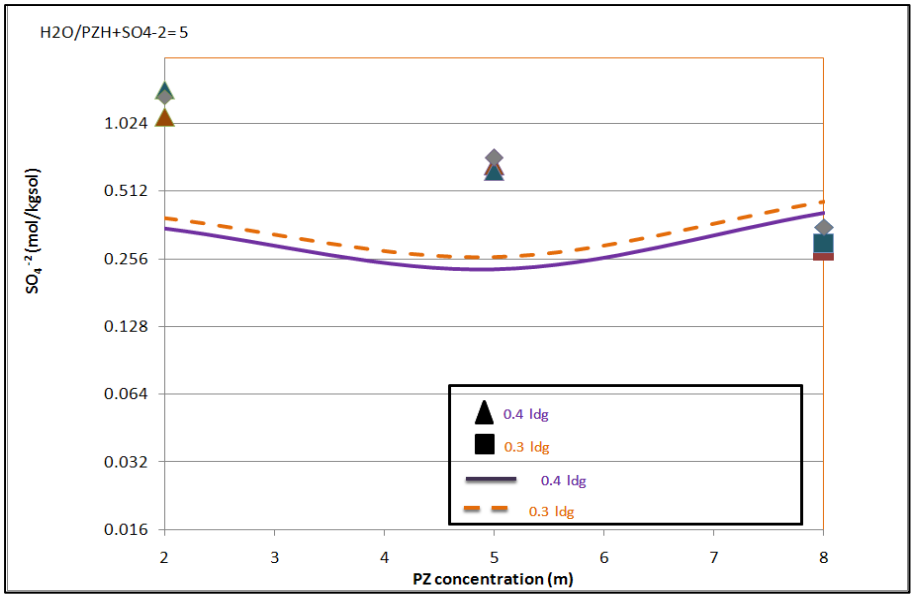

Figure C.13 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter H2O/PZH+SO4-2 = 5

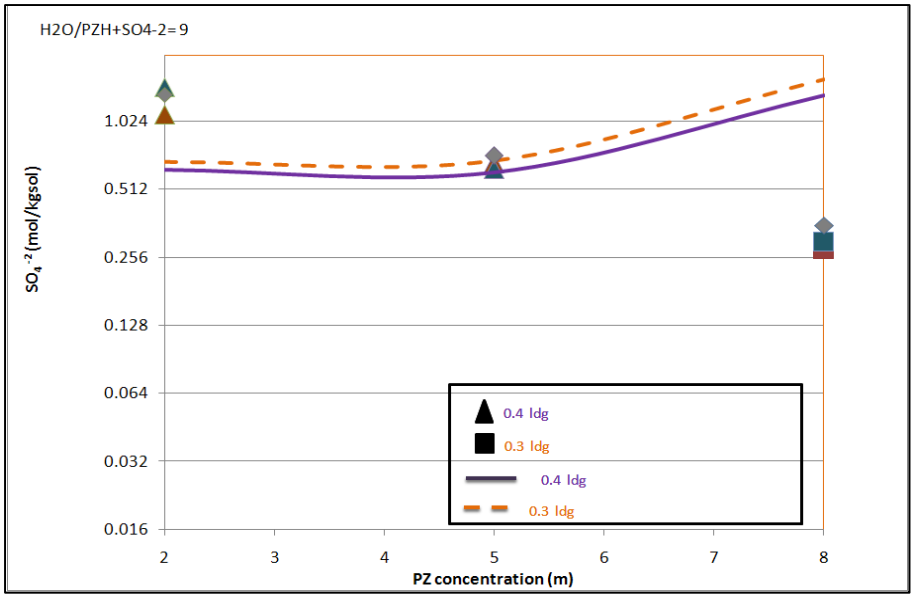

Figure C.14 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter H2O/PZH+SO4-2 = 9

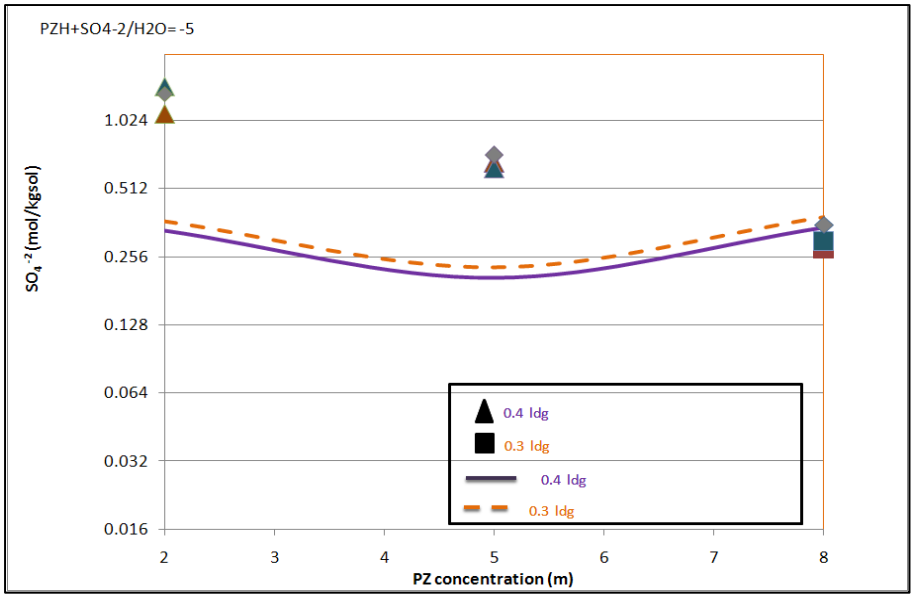

Figure C.15 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter PZH+SO4-2 /H2O = -5

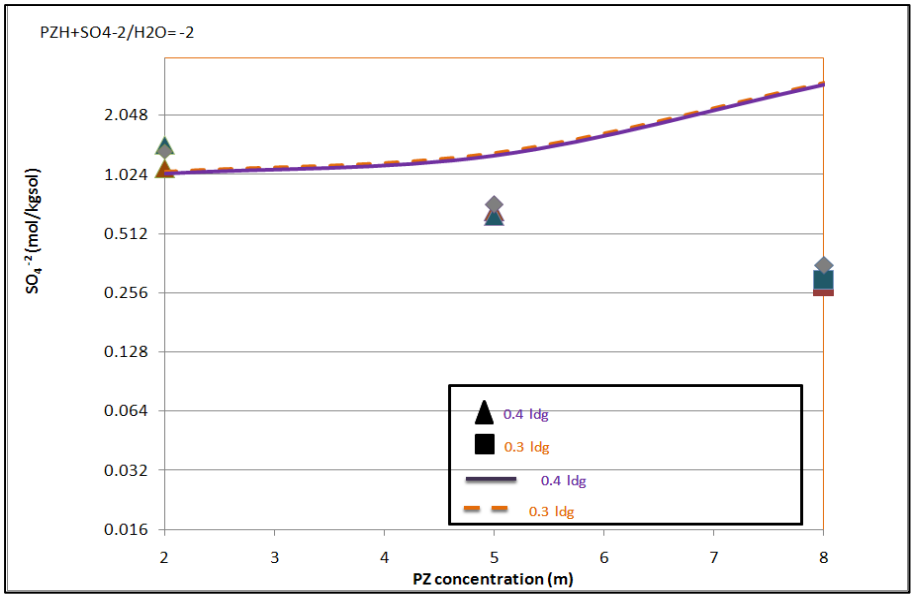

Figure C.16 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameter PZH+SO4-2 /H2O = -2

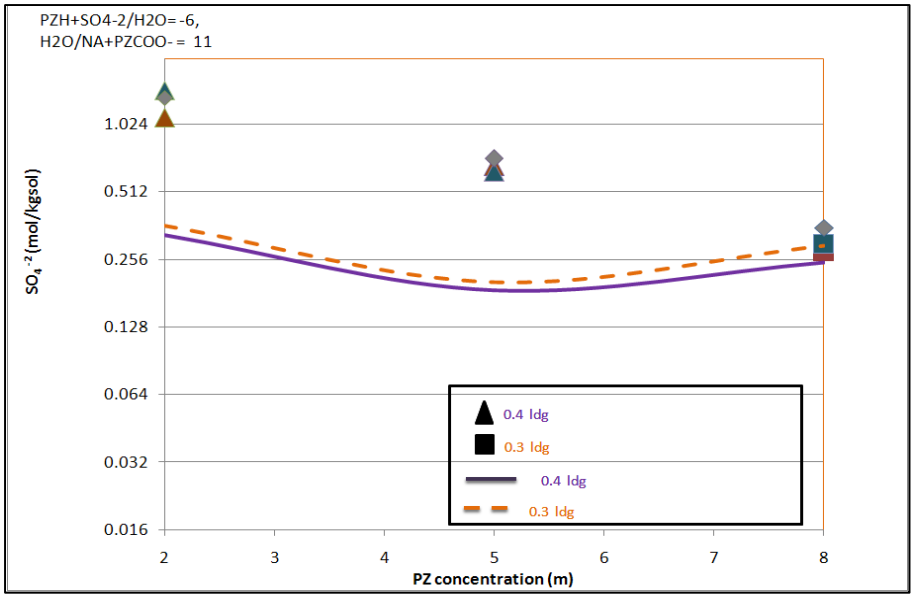

Figure C.17 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameters PZH+SO4-2 /H2O = -6, H2O/Na+PZCOO- = 11

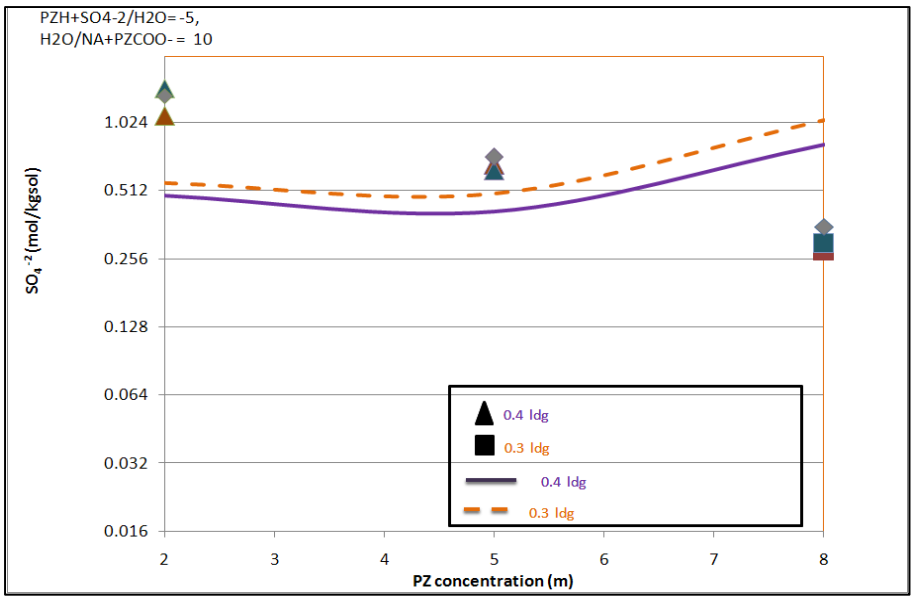

Figure C.18 Solubility of Na_2SO_4 in PZ, curve predicted by Aspen Plus®: points - 60°C experimental data, solid line – Aspen Plus results for 2-8 m PZ at 0.4 loading, dashed lines - Aspen Plus® results for 2-8 m PZ at 0.3 loading for parameters PZH+SO4-2 /H2O = -5, H2O/Na+PZCOO- = 10

Appendix D

SIMULATION RESULTS

Table D.1 Stream summary for SO_4^{-2} reclaiming by KOH (stoichiometric case ($K^+/SO_4^{-2} = 2$) –50°C

		1	BTMS 2	BTMS 3	CO2	FEED	H2O	H2O1	H2O2	IN	KOH	SLURRY	V	V1	V2	VENT	VENT 2	VENT 3	VENT 4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYST	COMP1	COND2	COMP2	FLASH	FLASH2	CRYST	FLASH3
To		COMP1	FLASH3	CRYST		FLASH2				FLASH	CRYST		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.74	0.84	0.83	0.25	0.85	1.00	1.00	0.99	0.85	0.61	0.83	0.74	0.26	0.26	0.79	0.94	0.99	0.99
CO2		0.26	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.26	0.74	0.74	0.21	0.06	0.01	0.01
HCO3-		0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO3--		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K+		0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.20	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZ		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.02	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZH+		0.00	0.05	0.05	0.00	0.05	0.00	0.00	0.00	0.05	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00

HPZCOO		0.00	0.02	0.02	0.00	0.02	0.00	0.00	0.00	0.02	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO4-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4-02		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
KOH		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flow	MOL/HR	633	201125	185164	6053	217297	15518	16073	12589	231096	5138	189444	633	1470	1470	17234	16957	596	15577
Mass Flow	KG/HR	16	6229	5942	228	6563	282	295	234	6970	113	6044	16	55	55	407	334	11	287
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	1
Temperature	C	40	83	50	40	117	40	40	40	150	40	50	238	40	271	117	83	50	50
Pressure	KPA	10	47	10	30	190	10	28	30	1216	101	10	47	28	190	190	47	10	10
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.2 Stream summary for SO_4^{-2} reclaiming by KOH (stoichiometric case ($K^+/SO_4^{-2} = 2$) – 60°C

		1	BTMS2	BTMS3	CO2	FEED	H2O	H2O1	H2O2	IN	KOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYST	COMP1	COND2	COMP2	FLASH	FLASH2	CRYST	FLASH3
To		COMP1	FLASH3	CRYST		FLASH2				FLASH	CRYST		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			

Phase:		Vapor	All	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.45	0.84	0.84	0.25	0.85	1	0.99	0.99	0.85	0.61	0.83	0.45	0.26	0.26	0.77	0.92	0.98	0.98
CO2		0.55	0	0	0.75	0	0	0	0	0	0	0	0.55	0.74	0.74	0.22	0.07	0.02	0.02
HCO3-		0	0	0	0	0.01	0	0	0	0.02	0	0	0	0	0	0	0	0	0
CO3--		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H+		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH-		0	0	0	0	0	0	0	0	0	0.2	0	0	0	0	0	0	0	0
K+		0	0.01	0	0	0.01	0	0	0	0.01	0.2	0.01	0	0	0	0	0	0	0
PZ		0	0.04	0.04	0	0.03	0	0	0	0.02	0	0.04	0	0	0	0	0	0	0
PZCOO-2		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PZCOO-		0	0.04	0.04	0	0.03	0	0	0	0.03	0	0.04	0	0	0	0	0	0	0
PZH+		0	0.05	0.05	0	0.05	0	0	0	0.05	0	0.05	0	0	0	0	0	0	0
HPZCOO		0	0.02	0.02	0	0.02	0	0	0	0.02	0	0.02	0	0	0	0	0	0	0
K2SO4		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SO4-2		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
K2SO4-02		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
KOH		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2SO4		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow	MOL/HR	450.17	204735.6	190243.2	6266.71	218932.9	14145.85	13870	10979.63	231096.3	4066.91	193715.6	450.17	1763.85	1763.85	155400.05	152301.04	398.2	142244.23
Mass Flow	KG/HR	14.52	6289.1	6024.11	235.77	6595.38	257.87	255.28	204.37	6970	89.23	6105.94	14.52	65.53	65.53	374.62	306.29	7.4	264.99
Volume Flow	CUM/SEC	0.02	0	0	0.15	0	0	0	0	0		0	0.01	0.05	0.01	0.07	0.21	0.02	0.67
Temperature	C	40	90	60	40	120	40	40	40	150	40	60.11	196.34	40	288.78	120	90	60.11	60
Pressure	KPA	16.35	61.64	16.35	30	214.56	16.35	28	30	1215.9	101.33	16.35	61.64	28	214.56	214.56	61.64	16.35	16.35
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1

Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.3 Stream summary for SO_4^{-2} reclaiming by KOH (stoichiometric case ($K^+/SO_4^{-2} = 2$) – 70°C

		1	BTMS2	BTMS3	CO2	FEED	H2O	H2O1	H2O2	IN	KOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4	
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYST	COMP1	COND2	COMP2	FLASH	FLASH2	CRYST	FLASH3	
To		COMP1	FLASH3	CRYST		FLASH2				FLASH	CRYST		COND2	COMP2	COND3	COND3	COND2	COND1	COND1	
Substream: MIXED																				
Phase:		Vapor	Liquid	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor	
Component Mole Fraction																				
H2O		0.29	0.84	0.84	0.25	0.85	1	0.99	0.99	0.85	0.61	0.84	0.29	0.26	0.26	0.75	0.91	0.97	0.97	
CO2		0.71	0	0	0.75	0	0	0	0	0	0	0	0.71	0.74	0.74	0.25	0.09	0.03	0.03	
HCO3-		0	0	0	0	0.01	0	0	0	0.02	0	0	0	0	0	0	0	0	0	
CO3--		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
H+		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
OH-		0	0	0	0	0	0	0	0	0	0.2	0	0	0	0	0	0	0	0	
K+		0	0.01	0.01	0	0.01	0	0	0	0.01	0.2	0.01	0	0	0	0	0	0	0	
PZ		0	0.04	0.04	0	0.03	0	0	0	0.02	0	0.04	0	0	0	0	0	0	0	
PZCOO-2		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	

PZCOO-		0	0.03	0.04	0	0.03	0	0	0	0.03	0	0.04	0	0	0	0	0	0	0	
PZH+		0	0.05	0.05	0	0.05	0	0	0	0.05	0	0.05	0	0	0	0	0	0	0	
HPZCOO		0	0.02	0.02	0	0.02	0	0	0	0.02	0	0.02	0	0	0	0	0	0	0	
K2SO4		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
SO4-2		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
K2SO4-02		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
KOH		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
H2SO4		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Mole Flow	MOL/HR	490.64	208331	195409	6453	220526	12582	11780	9424	231096	2925	197961	491	2072	2072	13857	13407	232	12871	
Mass Flow	KG/HR	17.96	6352	6108	243	6628	230	217	176	6970	64	6168	18	77	77	342	277	4	244	
Volume Flow	CUM/SEC	0.01	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0	
Temperature	C	40	97	70	40	123	40	40	40	150	40	70	167	40	307	123	97	70	70	
Pressure	KPA	25.93	81	26	30	243	26	28	30	1216	101	26	81	28	243	243	81	26	26	
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1	
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0	
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	

Table D.4 Stream summary for SO_4^{-2} reclaiming by KOH (stoichiometric case ($K^+/SO_4^{-2} = 2$) –90°C

		1	BTMS2	BTMS3	CO2	FEED	H2O	H2O1	H2O2	IN	KOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYST	COMP1	COND2	COMP2	FLASH	FLASH2	CRYST	FLASH3
To		COMP1	FLASH3	CRYST		FLASH2				FLASH	CRYST		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			

Phase:		Vapor	Liquid	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.12	0.85	0.84	0.25	0.85	0.99	0.99	0.99	0.85	0.61	0.84	0.12	0.26	0.26	0.70	0.85	0.93	0.93
CO2		0.88	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.88	0.74	0.74	0.30	0.14	0.06	0.07
HCO3-		0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO3--		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K+		0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.01	0.20	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZ		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.02	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-		0.00	0.03	0.03	0.00	0.03	0.00	0.00	0.00	0.03	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZH+		0.00	0.05	0.05	0.00	0.05	0.00	0.00	0.00	0.05	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HPZCOO		0.00	0.02	0.02	0.00	0.02	0.00	0.00	0.00	0.02	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO4-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4-02		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
KOH		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flow	MOL/HR	700	215260	205870	6628	224012	9230	8095	6085	231096	699	206507	700	2759	2759	9991	10194	27	9937
Mass Flow	KG/HR	29	6485	6287	249	6709	170	150	114	6970	15	6302	29	103	103	261	224	1	198
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0
Temperature	C	40	110	90	40	130	40	40	40	150	40	90	126	40	353	130	110	90	90
Pressure	KPA	61	138	61	30	327	61	28	30	1216	101	61	138	28	327	327	138	61	61
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.5 Stream summary for SO_4^{-2} reclaiming by KOH (stoichiometric case ($K^+/SO_4^{-2} = 2$) –100°C

		1	BTMS2	BTMS3	CO2	FEED	H2O	H2O1	H2O2	IN	KOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYST	COMP1	COND2	COMP2	FLASH	FLASH2	CRYST	FLASH3
To		COMP1	FLASH3	CRYST		FLASH2				FLASH	CRYST		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	Liquid	Liquid	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.08	0.85	0.85	0.25	0.85	0.99	0.99	0.99	0.85	0.61	0.85	0.08	0.26	0.26	0.66	0.82	0.90	0.90
CO2		0.92	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.92	0.74	0.74	0.34	0.18	0.09	0.09
HCO3-		0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO3--		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K+		0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.01	0.20	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZ		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.02	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-		0.00	0.03	0.03	0.00	0.03	0.00	0.00	0.00	0.03	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZH+		0.00	0.05	0.04	0.00	0.05	0.00	0.00	0.00	0.05	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HPZCOO		0.00	0.02	0.02	0.00	0.02	0.00	0.00	0.00	0.02	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO4-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4-02		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
KOH		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flow	MOL/HR	821	218591	210974	6573	225519	7554	6183	4664	231096	1	210969	821	3013	3013	8253	8410	6	8401
Mass Flow	KG/HR	34	6554	6380	247	6747	140	115	87	6970	0	6380	34	112	112	223	193	0	174
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0
Temperature	C	40	117	100	40	133	40	40	40	150	40	100	110	40	378	133	117	100	100
Pressure	KPA	92	181	92	30	381	92	28	30	1216	101	92	181	28	381	381	181	92	92
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0

Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.6 Stream summary for SO_4^{-2} reclaiming by KOH (excess SO_4^{-2} case (K^+/SO_4^{-2} = 1.3) –50°C

		1	BTM S2	BTM S3	CO2	FEED	H2O	H2O 1	H2O 2	IN	KOH	SLURRY	V	V1	V2	VENT	VENT 2	VENT 3	VENT 4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYST	COMP1	COND2	COMP2	FLASH	FLASH2	CRYST	FLASH3
To		COMP1	FLASH3	CRYST		FLASH2				FLASH	CRYST		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	All	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.74	0.84	0.84	0.25	0.85	1.00	1.00	0.99	0.85	0.61	0.83	0.74	0.26	0.26	0.77	0.94	0.99	0.99
CO2		0.26	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.26	0.74	0.74	0.22	0.06	0.01	0.01
HCO3-		0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO3--		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K+		0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.20	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZ		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.02	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZH+		0.00	0.05	0.05	0.00	0.05	0.00	0.00	0.00	0.05	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HPZCOO		0.00	0.02	0.02	0.00	0.02	0.00	0.00	0.00	0.02	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO4-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4-02		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
KOH		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flow	MOL/HR	714	201749	186065	6500	218150	15903	15997	11956	231473	8723	192902	714	1593	1593	16923	16921	1185	15455
Mass Flow	KG/HR	18	6263	5978	245	6598	289	293	222	7005	191	6147	18	59	59	408	335	22	285

Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	1
Temperature	C	40	83	50	40	117	40	40	40	150	40	50	239	40	274	117	83	50	50
Pressure	KPA	10	47	10	30	194	10	28	30	1216	101	10	47	28	194	194	47	10	10
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.7 Stream summary for SO_4^{-2} reclaiming by KOH (excess SO_4^{-2} case (K^+/SO_4^{-2} = 1.3) –60°C

		1	BTM S2	BTM S3	CO2	FEED	H2O	H2O 1	H2O 2	IN	KOH	SLURRY	V	V1	V2	VENT	VENT 2	VENT 3	VENT 4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYST	COMP1	COND2	COMP2	FLASH	FLASH2	CRYST	FLASH3
To		COMP1	FLASH3	CRYST		FLASH2				FLASH	CRYST		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	All	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.45	0.84	0.84	0.25	0.85	1.00	0.99	0.99	0.85	0.61	0.84	0.45	0.26	0.26	0.75	0.92	0.98	0.98
CO2		0.55	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.55	0.74	0.74	0.24	0.08	0.02	0.02
HCO3-		0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO3--		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K+		0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.20	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZ		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.02	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-		0.00	0.03	0.04	0.00	0.03	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZH+		0.00	0.05	0.05	0.00	0.05	0.00	0.00	0.00	0.05	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HPZCOO		0.00	0.02	0.02	0.00	0.02	0.00	0.00	0.00	0.02	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO4-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4-02		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
KOH		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

H2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flow	MOL/HR	500	205327	191080	6724	219816	14470	13748	10359	231473	7623	197242	500	1905	1905	15233	15199	873	14124
Mass Flow	KG/HR	16	6323	6059	253	6630	264	253	193	7005	167	6210	16	71	71	375	308	16	264
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	1
Temperature	C	40	90	60	40	120	40	40	40	150	40	60	197	40	292	120	90	60	60
Pressure	KPA	16	62	16	30	219	16	28	30	1216	101	16	62	28	219	219	62	16	16
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.8 Stream summary for SO_4^{-2} reclaiming by KOH (excess SO_4^{-2} case (K^+/SO_4^{-2} = 1.3) – 70°C

		1	BTMS2	BTMS3	CO2	FEED	H2O	H2O1	H2O2	IN	KOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYST	COMP1	COND2	COMP2	FLASH	FLASH2	CRYST	FLASH3
To		COMP1	FLASH3	CRYST		FLASH2				FLASH	CRYST		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.28	0.85	0.84	0.25	0.85	1.00	0.99	0.99	0.85	0.61	0.84	0.28	0.26	0.26	0.73	0.90	0.97	0.97
CO2		0.72	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.72	0.74	0.74	0.27	0.10	0.03	0.03
HCO3-		0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO3--		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K+		0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.20	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZ		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.02	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-		0.00	0.03	0.04	0.00	0.03	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZH+		0.00	0.05	0.05	0.00	0.05	0.00	0.00	0.00	0.05	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00

PZH+2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HPZCOO		0.00	0.02	0.02	0.00	0.02	0.00	0.00	0.00	0.02	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO4-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4-02		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
KOH		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flow	MOL/HR	539	209006	196216	6919	221418	12817	11593	8822	231473	6452	201598	539	2234	2234	13556	13332	589	12798
Mass Flow	KG/HR	20	6386	6143	260	6663	234	214	165	7005	142	6274	20	83	83	342	277	11	243
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0
Temperature	C	40	97	70	40	123	40	40	40	150	40	70	168	40	311	123	97	70	70
Pressure	KPA	26	82	26	30	249	26	28	30	1216	101	26	82	28	249	249	82	26	26
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.8 Stream summary for SO_4^{-2} reclaiming by KOH (excess SO_4^{-2} case (K^+/SO_4^{-2} = 1.3) –90°C

		1	BTMS2	BTMS3	CO2	FEED	H2O	H2O1	H2O2	IN	KOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYST	COMP1	COND2	COMP2	FLASH	FLASH2	CRYST	FLASH3
To		COMP1	FLASH3	CRYST		FLASH2				FLASH	CRYST		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.12	0.85	0.85	0.25	0.85	0.99	0.99	0.99	0.85	0.61	0.85	0.12	0.26	0.26	0.67	0.84	0.93	0.93
CO2		0.88	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.88	0.74	0.74	0.33	0.15	0.06	0.07
HCO3-		0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO3--		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

K+		0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.20	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZ		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.02	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-		0.00	0.03	0.03	0.00	0.03	0.00	0.00	0.00	0.03	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZH+		0.00	0.05	0.04	0.00	0.05	0.00	0.00	0.00	0.05	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HPZCOO		0.00	0.02	0.02	0.00	0.02	0.00	0.00	0.00	0.02	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO4-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4-02		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
KOH		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flow	MOL/HR	754	21606	20635	7120	22481	9294	7838	5579	23147	4185	21049	754	2957	2957	9777	10081	169	9911
Mass Flow	KG/HR	31	6518	6319	268	6743	171	146	104	7005	92	6408	31	110	110	262	225	3	199
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0
Temperature	C	40	110	90	40	130	40	40	40	150	40	90	127	40	360	130	110	90	90
Pressure	KPA	61	140	61	30	340	61	28	30	1216	101	61	140	28	340	340	140	61	61
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.9 Stream summary for SO_4^{-2} reclaiming by KOH (excess SO_4^{-2} case ($K^+/SO_4^{-2} = 1.3$) –100°C

		1	BTMS2	BTMS3	CO2	FEED	H2O	H2O1	H2O2	IN	KOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYST	COMP1	COND2	COMP2	FLASH	FLASH2	CRYST	FLASH3
To		COMP1	FLASH3	CRYST		FLASH2				FLASH	CRYST		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.08	0.85	0.85	0.25	0.85	0.99	0.99	0.99	0.85	0.61	0.85	0.08	0.26	0.26	0.63	0.80	0.90	0.89
CO2		0.92	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.92	0.74	0.74	0.36	0.20	0.09	0.10

HCO3-		0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO3--		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K+		0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.01	0.20	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZ		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.02	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-		0.00	0.03	0.03	0.00	0.03	0.00	0.00	0.00	0.03	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZH+		0.00	0.05	0.04	0.00	0.05	0.00	0.00	0.00	0.05	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HPZCOO		0.00	0.02	0.02	0.00	0.02	0.00	0.00	0.00	0.02	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO4-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4-02		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
KOH		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flow	MOL/HR	884	219496	211726	6994	226253	7456	5869	4250	231473	3062	214514	884	3246	3246	8026	8264	37	8335
Mass Flow	KG/HR	37	6590	6416	263	6783	138	110	80	7005	67	6482	37	121	121	222	193	1	174
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0
Temperature	C	40	117	100	40	133	40	40	40	150	40	100	111	40	384	133	117	100	100
Pressure	KPA	92	184	92	30	396	92	28	30	1216	101	92	184	28	396	396	184	92	92
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.10 Stream summary for SO_4^{-2} reclaiming by KOH (excess K^+ case ($K^+/SO_4^{-2} = 2.5$) –50°C

		1	BTMS2	BTMS3	CO2	FEED	H2O	H2O1	H2O2	IN	KOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYST	COMP1	COND2	COMP2	FLASH	FLASH2	CRYST	FLASH3
To		COMP1	FLASH3	CRYST		FLASH2				FLASH	CRYST		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor

Component Mole Fraction																			
H2O		0.74	0.84	0.83	0.25	0.85	1.00	1.00	0.99	0.85	0.61	0.83	0.74	0.26	0.26	0.80	0.94	0.99	0.99
CO2		0.26	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.26	0.74	0.74	0.20	0.05	0.01	0.01
HCO3-		0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO3--		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K+		0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.01	0.20	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZ		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.02	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZH+		0.00	0.05	0.05	0.00	0.05	0.00	0.00	0.00	0.05	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HPZCOO		0.00	0.02	0.02	0.00	0.02	0.00	0.00	0.00	0.02	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO4-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4-02		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
KOH		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flow	MOL/HR	601	201537	185375	5883	217839	15524	16151	12793	231809	5074	189868	601	1412	1412	17330	17010	482	15664
Mass Flow	KG/HR	15	6249	5961	221	6583	282	296	238	6990	111	6063	15	52	52	407	334	9	288
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	1
Temperature	C	40	83	50	40	117	40	40	40	150	40	50	238	40	269	117	83	50	50
Pressure	KPA	10	47	10	30	188	10	28	30	1216	101	10	47	28	188	188	47	10	10
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.11 Stream summary for SO_4^{-2} reclaiming by KOH (excess K^+ case (K^+/SO_4^{-2} = 2.5) –60°C

		1	BTMS2	BTMS3	CO2	FEED	H2O	H2O1	H2O2	IN	KOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYST	COMP1	COND2	COMP2	FLASH	FLASH2	CRYST	FLASH3

To		COMP1	FLASH3	CRYST		FLASH2				FLASH	CRYST		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.45	0.84	0.84	0.25	0.85	1.00	0.99	0.99	0.85	0.61	0.83	0.45	0.26	0.26	0.78	0.93	0.98	0.98
CO2		0.55	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.55	0.74	0.74	0.22	0.07	0.02	0.02
HCO3-		0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO3--		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K+		0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.01	0.20	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZ		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.02	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZH+		0.00	0.05	0.05	0.00	0.05	0.00	0.00	0.00	0.05	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HPZCOO		0.00	0.02	0.02	0.00	0.02	0.00	0.00	0.00	0.02	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO4-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4-02		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
KOH		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flow	MOL/HR	429	205193	190519	6092	219487	14149	13948	11170	231809	3938	194104	429	1694	1694	15629	15262	306	14299
Mass Flow	KG/HR	14	6310	6044	229	6616	258	257	208	6990	86	6124	14	63	63	374	306	6	266
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	1
Temperature	C	40	90	60	40	120	40	40	40	150	40	60	196	40	287	120	90	60	60
Pressure	KPA	16	61	16	30	212	16	28	30	1216	101	16	61	28	212	212	61	16	16
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.12 Stream summary for SO_4^{-2} reclaiming by KOH (excess K^+ case (K^+/SO_4^{-2} = 2.5) – 70°C

		1	BTMS2	BTMS3	CO2	FEED	H2O	H2O1	H2O2	IN	KOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYST	COMP1	COND2	COMP2	FLASH	FLASH2	CRYST	FLASH3
To		COMP1	FLASH3	CRYST		FLASH2				FLASH	CRYST		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	Liquid	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.29	0.84	0.84	0.25	0.85	1.00	0.99	0.99	0.85	0.61	0.84	0.29	0.26	0.26	0.76	0.91	0.97	0.97
CO2		0.71	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.71	0.74	0.74	0.24	0.09	0.03	0.03
HCO3-		0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO3--		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K+		0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.01	0.20	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZ		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.02	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-		0.00	0.03	0.04	0.00	0.03	0.00	0.00	0.00	0.03	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZH+		0.00	0.05	0.05	0.00	0.05	0.00	0.00	0.00	0.05	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HPZCOO		0.00	0.02	0.02	0.00	0.02	0.00	0.00	0.00	0.02	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO4-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4-02		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
KOH		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flow	MOL/HR	469	208791	195710	6276	221093	12594	11902	9600	231809	2780	198299	469	1992	1992	13938	13474	169	12925
Mass Flow	KG/HR	17	6372	6128	236	6649	230	220	179	6990	61	6186	17	74	74	341	277	3	244
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0
Temperature	C	40	97	70	40	123	40	40	40	150	40	70	167	40	305	123	97	70	70
Pressure	KPA	26	81	26	30	240	26	28	30	1216	101	26	81	28	240	240	81	26	26
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0

Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.13 Stream summary for SO_4^{-2} reclaiming by KOH (excess K^+ case (K^+/SO_4^{-2} = 2.5) – 90°C

		1	BTM S2	BTM S3	CO2	FEED	H2O	H2O 1	H2O 2	IN	KOH	SLURRY	V	V1	V2	VENT	VENT 2	VENT 3	VENT 4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYST	COMP1	COND2	COMP2	FLASH	FLASH2	CRYST	FLASH3
To		COMP1	FLASH3	CRYST		FLASH2				FLASH	CRYST		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	Liquid	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.12	0.85	0.84	0.25	0.85	0.99	0.99	0.99	0.85	0.61	0.84	0.12	0.26	0.26	0.70	0.86	0.93	0.93
CO2		0.88	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.88	0.74	0.74	0.30	0.14	0.06	0.06
HCO3-		0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO3--		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K+		0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.01	0.20	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZ		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.02	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-		0.00	0.03	0.03	0.00	0.03	0.00	0.00	0.00	0.03	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZH+		0.00	0.05	0.05	0.00	0.05	0.00	0.00	0.00	0.05	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZH+2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HPZCOO		0.00	0.02	0.02	0.00	0.02	0.00	0.00	0.00	0.02	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO4-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4-02		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
KOH		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flow	MOL/HR	671	215779	206310	6485	224627	9270	8213	6200	231809	727	207012	671	2665	2665	10059	10250	20	9956

Mass Flow	KG/HR	27	6505	6307	244	6729	171	153	116	6990	16	6322	27	99	99	261	224	0	198
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0
Temperature	C	40	110	90	40	130	40	40	40	150	40	90	126	40	351	130	110	90	90
Pressure	KPA	61	137	61	30	323	61	28	30	1216	101	61	137	28	323	323	137	61	61
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.14 Stream summary for SO_4^{-2} reclaiming by KOH (excess K^+ case (K^+/SO_4^{-2} = 2.5) – 100°C

		1	BTM S2	BTM S3	CO2	FEED	H2O	H2O 1	H2O 2	IN	KOH	SLURRY	V	V1	V2	VENT	VENT 2	VENT 3	VENT 4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYST	COMP1	COND2	COMP2	FLASH	FLASH2	CRYST	FLASH3
To		COMP1	FLASH3	CRYST		FLASH2				FLASH	CRYST		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	Liquid	Liquid	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.08	0.85	0.84	0.25	0.85	0.99	0.99	0.99	0.85	0.61	0.84	0.08	0.26	0.26	0.67	0.82	0.90	0.91
CO2		0.92	0.00	0.00	0.75	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.92	0.74	0.74	0.33	0.17	0.09	0.09
HCO3-		0.00	0.01	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO3--		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H+		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K+		0.00	0.01	0.01	0.00	0.01	0.00	0.00	0.00	0.01	0.20	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZ		0.00	0.04	0.04	0.00	0.03	0.00	0.00	0.00	0.02	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZCOO-		0.00	0.03	0.03	0.00	0.03	0.00	0.00	0.00	0.03	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PZH+		0.00	0.05	0.04	0.00	0.05	0.00	0.00	0.00	0.05	0.00	0.04	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HPZCOO		0.00	0.02	0.02	0.00	0.02	0.00	0.00	0.00	0.02	0.00	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO4-2		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
K2SO4-02		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

KOH		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2SO4		0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mole Flow	MOL/HR	795	219160	211499	6415	226161	7600	6276	4758	231809	1	211495	795	2932	2932	8272	8451	6	8422
Mass Flow	KG/HR	33	6576	6402	241	6768	141	117	89	6990	0	6401	33	109	109	222	193	0	174
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0
Temperature	C	40	117	100	40	133	40	40	40	150	40	100	110	40	375	133	117	100	100
Pressure	KPA	91	180	91	30	376	91	28	30	1216	101	91	180	28	376	376	180	91	91
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.15 Stream summary for SO_4^{-2} reclaiming by NaOH (stoichiometric case (Na^{+}/SO_4^{-2} = 2) – 50°C

		1	BTMS2	BTMS3	CO2	FEED	H20	H2O1	H2O2	IN	NAOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYSTL	COMP1	COND2	COMP2	FLASH	FLASH2	CRYSTL	FLASH3
To		COMP1	FLASH3	CRYSTL		FLASH2				FLASH	CRYSTL		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.86	0.76	0.74	0.25	0.77	1	0.99	0.99	0.77	0.32	0.74	0.86	0.26	0.26	0.84	0.96	0.99	0.99
CO2		0.14	0	0	0.75	0	0	0	0	0	0	0	0.14	0.74	0.74	0.15	0.04	0.01	0.01
HCO3-		0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0
CO3--		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H+		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH-		0	0	0	0	0	0	0	0	0	0.34	0	0	0	0	0	0	0	0
PZ		0	0.01	0.01	0	0.01	0	0	0	0	0	0.02	0	0	0	0	0	0	0
PZCOO-2		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PZCOO-		0	0.05	0.06	0	0.05	0	0	0	0.04	0	0.06	0	0	0	0	0	0	0
PZH+		0	0.06	0.06	0	0.05	0	0	0	0.05	0	0.06	0	0	0	0	0	0	0
HPZCOO		0	0.01	0.01	0	0.01	0	0	0	0.01	0	0	0	0	0	0	0	0	0

SO4-2		0	0.04	0.04	0	0.03	0	0	0	0.03	0	0.04	0	0	0	0	0	0	0
NA2SO-01		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NA+		0	0.07	0.08	0	0.07	0	0	0	0.07	0.34	0.08	0	0	0	0	0	0	0
NA2SO-02		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2SO4		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NAOH		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow	MOL/HR	825	21982	20037	4611	23725	16147	18144	15059	25369	1517	20417	825	972	972	18774	18351	406	16593
Mass Flow	KG/HR	18	7251	6947	173	7603	294	334	280	8021	29	6969	18	36	36	417	352	7	305
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	1
Temperature	C	40	83	50	40	117	40	40	40	150	40	50	248	40	248	117	83	50	50
Pressure	KPA	9	41	9	30	161	9	28	30	1621	101	9	41	28	161	161	41	9	9
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.16 Stream summary for SO_4^{-2} reclaiming by NaOH (stoichiometric case (Na^+/SO_4^{-2} = 2) – 60°C

		1	BTMS2	BTMS3	CO2	FEED	H20	H2O1	H2O2	IN	NAOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYSTL	COMP1	COND2	COMP2	FLASH	FLASH2	CRYSTL	FLASH3
To		COMP1	FLASH3	CRYSTL		FLASH2				FLASH	CRYSTL		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.52	0.76	0.74	0.25	0.77	1	0.99	0.99	0.77	0.32	0.74	0.52	0.26	0.26	0.83	0.95	0.99	0.99
CO2		0.48	0	0	0.75	0	0	0	0	0	0	0	0.48	0.74	0.74	0.17	0.04	0.01	0.01
HCO3-		0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0
CO3--		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H+		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH-		0	0	0	0	0	0	0	0	0	0.34	0	0	0	0	0	0	0	0
PZ		0	0.01	0.01	0	0.01	0	0	0	0	0	0.02	0	0	0	0	0	0	0

PZCOO-2		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PZCOO-		0	0.05	0.05	0	0.05	0	0	0	0.04	0	0.06	0	0	0	0	0	0	0
PZH+		0	0.06	0.06	0	0.05	0	0	0	0.05	0	0.06	0	0	0	0	0	0	0
HPZCOO		0	0.01	0.01	0	0.01	0	0	0	0.01	0	0.01	0	0	0	0	0	0	0
SO4-2		0	0.04	0.04	0	0.03	0	0	0	0.03	0	0.04	0	0	0	0	0	0	0
NA2SO-01		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NA+		0	0.07	0.08	0	0.07	0	0	0	0.07	0.34	0.08	0	0	0	0	0	0	0
NA2SO-02		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2SO4		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NAOH		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow	MOL/HR	323	223117	207923	4724	239489	15412	15672	13308	253769	2098	209493	323	1123	1123	16979	16533	522	15249
Mass Flow	KG/HR	10	7316	7034	178	7637	282	289	248	8021	41	7065	10	42	42	384	321	10	282
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	1
Temperature	C	40	90	60	40	120	40	40	40	150	40	60	200	40	265	120	90	60	60
Pressure	KPA	14	54	14	30	182	14	28	30	1621	101	14	54	28	182	182	54	14	14
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.17 Stream summary for SO_4^{-2} reclaiming by NaOH (stoichiometric case (Na^+/SO_4^{-2} = 2) – 70°C

		1	BTMS2	BTMS3	CO2	FEED	H20	H2O1	H2O2	IN	NAOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYSTL	COMP1	COND2	COMP2	FLASH	FLASH2	CRYSTL	FLASH3
To		COMP1	FLASH3	CRYSTL		FLASH2				FLASH	CRYSTL		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.33	0.76	0.75	0.25	0.77	1	0.99	0.99	0.77	0.32	0.75	0.33	0.26	0.26	0.81	0.94	0.98	0.98
CO2		0.67	0	0	0.75	0	0	0	0	0	0	0	0.67	0.74	0.74	0.18	0.05	0.01	0.02
HCO3-		0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0

CO3--		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H+		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH-		0	0	0	0	0	0	0	0	0	0.34	0	0	0	0	0	0	0	0
PZ		0	0.01	0.02	0	0.01	0	0	0	0	0	0.02	0	0	0	0	0	0	0
PZCOO-2		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PZCOO-		0	0.05	0.05	0	0.05	0	0	0	0.04	0	0.05	0	0	0	0	0	0	0
PZH+		0	0.06	0.06	0	0.05	0	0	0	0.05	0	0.06	0	0	0	0	0	0	0
HPZCOO		0	0.01	0.01	0	0.01	0	0	0	0.01	0	0.01	0	0	0	0	0	0	0
SO4-2		0	0.04	0.04	0	0.03	0	0	0	0.03	0	0.04	0	0	0	0	0	0	0
NA2SO-01		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NA+		0	0.07	0.07	0	0.07	0	0	0	0.07	0.34	0.08	0	0	0	0	0	0	0
NA2SO-02		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2SO4		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NAOH		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow	MOL/HR	311	226976	213036	4830	241240	14073	13564	11576	253769	2375	214830	311	1287	1287	15181	14600	536	13890
Mass Flow	KG/HR	11	7383	7124	182	7671	258	251	216	8021	46	7160	11	48	48	350	288	10	259
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0
Temperature	C	40	97	70	40	123	40	40	40	150	40	70	168	40	282	123	97	70	70
Pressure	KPA	23	70	23	30	204	23	28	30	1621	101	23	70	28	204	204	70	23	23
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.18 Stream summary for SO_4^{-2} reclaiming by NaOH (stoichiometric case ($Na^+/SO_4^{-2} = 2$) – 100°C

		1	BTMS2	BTMS3	CO2	FEED	H20	H2O1	H2O2	IN	NAOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYSTL	COMP1	COND2	COMP2	FLASH	FLASH2	CRYSTL	FLASH3
To		COMP1	FLASH3	CRYSTL		FLASH2				FLASH	CRYSTL		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	Liquid	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole																			

Fraction																			
H2O		0.09	0.77	0.77	0.25	0.78	0.99	0.99	0.99	0.77	0.32	0.76	0.09	0.26	0.26	0.73	0.89	0.95	0.95
CO2		0.91	0	0	0.75	0	0	0	0	0	0	0	0.91	0.74	0.74	0.27	0.11	0.04	0.05
HCO3-		0	0	0	0	0.01	0	0	0	0.01	0	0	0	0	0	0	0	0	0
CO3--		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H+		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH-		0	0	0	0	0	0	0	0	0	0.34	0	0	0	0	0	0	0	0
PZ		0	0.01	0.02	0	0.01	0	0	0	0	0	0.02	0	0	0	0	0.01	0.01	0
PZCOO-2		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PZCOO-		0	0.05	0.05	0	0.04	0	0	0	0.04	0	0.05	0	0	0	0	0	0	0
PZH+		0	0.05	0.05	0	0.05	0	0	0	0.05	0	0.05	0	0	0	0	0	0	0
HPZCOO		0	0.01	0.01	0	0.01	0	0	0	0.01	0	0.01	0	0	0	0	0	0	0
SO4-2		0	0.03	0.04	0	0.03	0	0	0	0.03	0	0.03	0	0	0	0	0	0	0
NA2SO-01		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NA+		0	0.07	0.07	0	0.07	0	0	0	0.07	0.34	0.07	0	0	0	0	0	0	0
NA2SO-02		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2SO4		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NAOH		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow	MOL/HR	465	238726	229496	4967	247058	8921	7876	5882	253769	1513	230762	465	1863	1863	9021	9322	172	9260
Mass Flow	KG/HR	19	7596	7414	187	7793	166	147	110	8021	29	7440	19	69	69	228	197	3	182
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0
Temperature	C	40	117	100	40	133	40	40	40	150	40	100	107	40	348	133	117	100	100
Pressure	KPA	79	152	79	30	316	79	28	30	1621	101	79	152	28	316	316	152	79	79
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.19 Stream summary for SO_4^{-2} reclaiming by NaOH (excess SO_4^{-2} case (Na^+/SO_4^{-2} = 1.9) – 50°C

		1	BTMS2	BTMS3	CO2	FEED	H20	H2O1	H2O2	IN	NAOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYSTL	COMP1	COND2	COMP2	FLASH	FLASH2	CRYSTL	FLASH3
To		COM	FLAS	CRYS		FLAS				FLAS	CRYS		CON	COM	CON	CON	CON	CON	CON

		P1	H3	TL		H2				H	TL		D2	P2	D3	D3	D2	D1	D1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	All	Liquid	Liquid	Liquid	All	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.86	0.76	0.74	0.25	0.77	1	0.99	0.99	0.77	0.32	0.74	0.86	0.26	0.26	0.84	0.96	0.99	0.99
CO2		0.14	0	0	0.75	0	0	0	0	0	0	0	0.14	0.74	0.74	0.16	0.04	0.01	0.01
HCO3-		0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0
CO3--		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H+		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH-		0	0	0	0	0	0	0	0	0	0.34	0	0	0	0	0	0	0	0
PZ		0	0.01	0.01	0	0.01	0	0	0	0	0	0.02	0	0	0	0	0	0	0
PZCOO-2		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PZCOO-		0	0.05	0.06	0	0.05	0	0	0	0.04	0	0.06	0	0	0	0	0	0	0
PZH+		0	0.06	0.06	0	0.06	0	0	0	0.06	0	0.06	0	0	0	0	0	0	0
HPZCOO		0	0.01	0.01	0	0.01	0	0	0	0.02	0	0	0	0	0	0	0	0	0
SO4-2		0	0.04	0.04	0	0.04	0	0	0	0.03	0	0.04	0	0	0	0	0	0	0
NA2SO-01		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NA+		0	0.07	0.08	0	0.07	0	0	0	0.06	0.34	0.08	0	0	0	0	0	0	0
NA2SO-02		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2SO4		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NAOH		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow	MOL/HR	866	219495	203154	4815	237886	16174	18127	14814	253733	1814	204512	866	1017	1017	18686	18336	487	16581
Mass Flow	KG/HR	19	7267	6963	181	7620	295	333	275	8038	35	6989	19	38	38	419	352	9	305
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	1
Temperature	C	40	83	50	40	117	40	40	40	150	40	50	248	40	249	117	83	50	50
Pressure	KPA	9	41	9	30	163	9	28	30	1621	101	9	41	28	163	163	41	9	9
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.20 Stream summary for SO_4^{-2} reclaiming by NaOH (excess SO_4^{-2} case (Na^+/SO_4^{-2} = 1.9) – 60°C

		1	BTMS2	BTMS3	CO2	FEED	H20	H2O1	H2O2	IN	NAOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYSTL	COMP1	COND2	COMP2	FLASH	FLASH2	CRYSTL	FLASH3
To		COMP1	FLASH3	CRYSTL		FLASH2				FLASH	CRYSTL		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	All	Liquid	Liquid	Liquid	All	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.52	0.76	0.75	0.25	0.77	1	0.99	0.99	0.77	0.32	0.74	0.52	0.26	0.26	0.82	0.95	0.99	0.99
CO2		0.48	0	0	0.75	0	0	0	0	0	0	0	0.48	0.74	0.74	0.17	0.05	0.01	0.01
HCO3-		0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0
CO3--		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H+		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH-		0	0	0	0	0	0	0	0	0	0.34	0	0	0	0	0	0	0	0
PZ		0	0.01	0.01	0	0.01	0	0	0	0	0	0.02	0	0	0	0	0	0	0
PZCOO-2		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PZCOO-		0	0.05	0.05	0	0.05	0	0	0	0.04	0	0.05	0	0	0	0	0	0	0
PZH+		0	0.06	0.06	0	0.05	0	0	0	0.06	0	0.06	0	0	0	0	0	0	0
HPZCOO		0	0.01	0.01	0	0.01	0	0	0	0.02	0	0.01	0	0	0	0	0	0	0
SO4-2		0	0.04	0.04	0	0.03	0	0	0	0.03	0	0.04	0	0	0	0	0	0	0
NA2SO-01		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NA+		0	0.07	0.07	0	0.07	0	0	0	0.06	0.34	0.08	0	0	0	0	0	0	0
NA2SO-02		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2SO4		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NAOH		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow	MOL/HR	339	223227	208044	4929	239733	15464	15633	13062	253733	2399	209828	339	1173	1173	16885	16526	598	15241
Mass Flow	KG/HR	10	7332	7050	185	7653	283	288	243	8038	46	7085	10	44	44	385	322	11	282
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	1
Temperature	C	40	90	60	40	120	40	40	40	150	40	60	200	40	266	120	90	60	60
Pressure	KPA	14	54	14	30	183	14	28	30	1621	101	14	54	28	183	183	54	14	14
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0

Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.21 Stream summary for SO_4^{-2} reclaiming by NaOH (excess SO_4^{-2} case (Na^+/SO_4^{-2} = 1.9) – 70°C

		1	BTM S2	BTM S3	CO2	FEED	H20	H2O 1	H2O 2	IN	NAOH	SLURRY	V	V1	V2	VENT	VENT 2	VENT 3	VENT 4
From		CON D1	FLASH2	FLASH3	CON D3	FLASH	CON D1	CON D2	CON D3			CRYSTL	COMP1	CON D2	COMP2	FLASH	FLASH2	CRYSTL	FLASH3
To		COMP1	FLASH3	CRYSTL		FLASH2				FLASH	CRYSTL		CON D2	COMP2	CON D3	CON D3	CON D2	CON D1	CON D1
Phase:		Vapor	All	All	Vapor	All	Liquid	Liquid	Liquid	All	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.33	0.76	0.75	0.25	0.77	1	0.99	0.99	0.77	0.32	0.75	0.33	0.26	0.26	0.81	0.94	0.98	0.98
CO2		0.67	0	0	0.75	0	0	0	0	0	0	0	0.67	0.74	0.74	0.19	0.06	0.01	0.02
HCO3-		0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0
CO3--		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H+		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH-		0	0	0	0	0	0	0	0	0	0.34	0	0	0	0	0	0	0	0
PZ		0	0.01	0.02	0	0.01	0	0	0	0	0	0.02	0	0	0	0	0	0	0
PZCOO-2		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PZCOO-		0	0.05	0.05	0	0.05	0	0	0	0.04	0	0.05	0	0	0	0	0	0	0
PZH+		0	0.06	0.06	0	0.05	0	0	0	0.06	0	0.06	0	0	0	0	0	0	0
HPZCOO		0	0.01	0.01	0	0.01	0	0	0	0.02	0	0.01	0	0	0	0	0	0	0
SO4-2		0	0.04	0.04	0	0.03	0	0	0	0.03	0	0.04	0	0	0	0	0	0	0
NA2SO-01		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NA+		0	0.07	0.07	0	0.07	0	0	0	0.06	0.34	0.08	0	0	0	0	0	0	0
NA2SO-02		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2SO4		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NAOH		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow	MOL/HR	326	227083	213158	5036	241565	14118	13523	11331	253733	2675	215172	326	1345	1345	15083	14600	604	13880
Mass Flow	KG/HR	12	7399	7140	189	7688	259	250	211	8038	52	7180	12	50	50	351	289	11	259
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0
Temperature	C	40	97	70	40	123	40	40	40	150	40	70	168	40	283	123	97	70	70

Pressure	KPA	23	71	23	30	206	23	28	30	1621	101	23	71	28	206	206	71	23	23
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.22 Stream summary for SO_4^{-2} reclaiming by NaOH (excess SO_4^{-2} case (Na^+/SO_4^{-2} = 1.9) – 100°C

		1	BTM S2	BTM S3	CO2	FEED	H20	H2O 1	H2O 2	IN	NAOH	SLURRY	V	V1	V2	VENT	VENT 2	VENT 3	VENT 4
From		COND 1	FLASH 2	FLASH 3	COND 3	FLASH	COND 1	COND 2	COND 3			CRYSTL	COMP 1	COND 2	COMP 2	FLASH	FLASH 2	CRYSTL	FLASH 3
To		COMP 1	FLASH 3	CRYSTL		FLASH 2				FLASH	CRYSTL		COND 2	COMP 2	COND 3	COND 3	COND 2	COND 1	COND 1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	Liquid	Liquid	Liquid	Liquid	All	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.09	0.77	0.77	0.25	0.78	0.99	0.99	0.99	0.77	0.32	0.77	0.09	0.26	0.26	0.72	0.88	0.95	0.94
CO2		0.91	0	0	0.75	0	0	0	0	0	0	0	0.91	0.74	0.74	0.28	0.11	0.04	0.05
HCO3-		0	0	0	0	0.01	0	0	0	0.01	0	0	0	0	0	0	0	0	0
CO3--		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H+		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH-		0	0	0	0	0	0	0	0	0	0.34	0	0	0	0	0	0	0	0
PZ		0	0.01	0.02	0	0.01	0	0	0	0	0	0.02	0	0	0	0	0.01	0.01	0
PZCOO-2		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PZCOO-		0	0.05	0.05	0	0.04	0	0	0	0.04	0	0.05	0	0	0	0	0	0	0
PZH+		0	0.05	0.05	0	0.05	0	0	0	0.06	0	0.05	0	0	0	0	0	0	0
HPZCOO		0	0.01	0.01	0	0.01	0	0	0	0.02	0	0.01	0	0	0	0	0	0	0
SO4-2		0	0.03	0.04	0	0.03	0	0	0	0.03	0	0.03	0	0	0	0	0	0	0
NA2SO-01		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NA+		0	0.07	0.07	0	0.07	0	0	0	0.06	0.34	0.07	0	0	0	0	0	0	0
NA2SO-02		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2SO4		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NAOH		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow	MOL/HR	484	238843	229598	5171	247421	8927	7826	5670	253733	1811	231117	484	1942	1942	8933	9330	204	9252

Mass Flow	KG/HR	20	7612	7429	195	7810	166	146	106	8038	35	7461	20	72	72	228	198	4	182
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0
Temperature	C	40	117	100	40	133	40	40	40	150	40	100	107	40	351	133	117	100	100
Pressure	KPA	79	153	79	30	322	79	28	30	1621	101	79	153	28	322	322	153	79	79
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.23 Stream summary for SO_4^{-2} reclaiming by NaOH (excess Na^+ case (Na^+/SO_4^{-2} = 2.04) – 50°C

		1	BTM S2	BTM S3	CO2	FEED	H20	H2O 1	H2O 2	IN	NAOH	SLURRY	V	V1	V2	VENT	VENT 2	VENT 3	VENT 4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYSTL	COMP1	COND2	COMP2	FLASH	FLASH2	CRYSTL	FLASH3
To		COMP1	FLASH3	CRYSTL		FLASH2				FLASH	CRYSTL		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.87	0.75	0.74	0.25	0.77	1	0.99	0.99	0.77	0.32	0.74	0.87	0.26	0.26	0.85	0.96	0.99	0.99
CO2		0.13	0	0	0.75	0	0	0	0	0	0	0	0.13	0.74	0.74	0.14	0.03	0.01	0.01
HCO3-		0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0
CO3--		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H+		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH-		0	0	0	0	0	0	0	0	0	0.34	0	0	0	0	0	0	0	0
PZ		0	0.01	0.01	0	0.01	0	0	0	0	0	0.02	0	0	0	0	0	0	0
PZCOO-2		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PZCOO-		0	0.05	0.06	0	0.05	0	0	0	0.04	0	0.06	0	0	0	0	0	0	0
PZH+		0	0.06	0.06	0	0.05	0	0	0	0.05	0	0.06	0	0	0	0	0	0	0
HPZCOO		0	0.01	0.01	0	0.01	0	0	0	0.01	0	0	0	0	0	0	0	0	0
SO4-2		0	0.04	0.04	0	0.03	0	0	0	0.03	0	0.04	0	0	0	0	0	0	0
NA2SO-01		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NA+		0	0.07	0.08	0	0.07	0	0	0	0.07	0.34	0.08	0	0	0	0	0	0	0
NA2SO-02		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

H2SO4		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NAOH		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow	MOL/HR	782	219733	203349	4412	238188	16234	18216	15353	254479	1526	204501	782	929	929	18915	18423	407	16637
Mass Flow	KG/HR	17	7265	6960	166	7618	296	335	286	8035	30	6982	17	35	35	417	353	7	305
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	1
Temperature	C	40	83	50	40	117	40	40	40	150	40	50	248	40	247	117	83	50	50
Pressure	KPA	9	41	9	30	160	9	28	30	1621	101	9	41	28	160	160	41	9	9
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.24 Stream summary for SO_4^{-2} reclaiming by NaOH (excess Na^+ case (Na^+/SO_4^{-2} = 2.04) – 60°C

		1	BTMS2	BTMS3	CO2	FEED	H20	H2O1	H2O2	IN	NAOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYSTL	COMP1	COND2	COMP2	FLASH	FLASH2	CRYSTL	FLASH3
To		COMP1	FLASH3	CRYSTL		FLASH2				FLASH	CRYSTL		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.52	0.76	0.74	0.25	0.77	1	0.99	0.99	0.77	0.32	0.74	0.52	0.26	0.26	0.84	0.95	0.99	0.99
CO2		0.48	0	0	0.75	0	0	0	0	0	0	0	0.48	0.74	0.74	0.16	0.04	0.01	0.01
HCO3-		0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0
CO3--		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H+		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH-		0	0	0	0	0	0	0	0	0	0.34	0	0	0	0	0	0	0	0
PZ		0	0.01	0.02	0	0.01	0	0	0	0	0	0.02	0	0	0	0	0	0	0
PZCOO-2		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PZCOO-		0	0.05	0.06	0	0.05	0	0	0	0.04	0	0.06	0	0	0	0	0	0	0
PZH+		0	0.06	0.06	0	0.05	0	0	0	0.05	0	0.06	0	0	0	0	0	0	0
HPZCOO		0	0.01	0.01	0	0.01	0	0	0	0.01	0	0	0	0	0	0	0	0	0

SO4-2		0	0.04	0.04	0	0.03	0	0	0	0.03	0	0.04	0	0	0	0	0	0	0
NA2SO-01		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NA+		0	0.07	0.08	0	0.07	0	0	0	0.07	0.34	0.08	0	0	0	0	0	0	0
NA2SO-02		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2SO4		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NAOH		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow	MOL/HR	307	22377	20839	4523	23961	15477	15773	13593	25479	2124	20983	307	1075	1075	17113	16603	528	15292
Mass Flow	KG/HR	9	7330	7047	170	7652	283	291	253	8035	41	7079	9	40	40	383	322	10	283
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	1
Temperature	C	40	90	60	40	120	40	40	40	150	40	60	200	40	263	120	90	60	60
Pressure	KPA	14	54	14	30	180	14	28	30	1621	101	14	54	28	180	180	54	14	14
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.25 Stream summary for SO_4^{-2} reclaiming by NaOH (excess Na^+ case (Na^+/SO_4^{-2} = 2.04) – 70°C

		1	BTMS2	BTMS3	CO2	FEED	H20	H2O1	H2O2	IN	NAOH	SLURRY	V	V1	V2	VENT	VENT2	VENT3	VENT4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYSTL	COMP1	COND2	COMP2	FLASH	FLASH2	CRYSTL	FLASH3
To		COMP1	FLASH3	CRYSTL		FLASH2				FLASH	CRYSTL		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	All	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.33	0.76	0.75	0.25	0.77	1	0.99	0.99	0.77	0.32	0.75	0.33	0.26	0.26	0.82	0.94	0.98	0.98
CO2		0.67	0	0	0.75	0	0	0	0	0	0	0	0.67	0.74	0.74	0.17	0.05	0.01	0.02
HCO3-		0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0
CO3--		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H+		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH-		0	0	0	0	0	0	0	0	0	0.34	0	0	0	0	0	0	0	0
PZ		0	0.01	0.02	0	0.01	0	0	0	0	0	0.02	0	0	0	0	0	0	0

PZCOO-2		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PZCOO-		0	0.05	0.05	0	0.05	0	0	0	0.04	0	0.05	0	0	0	0	0	0	0
PZH+		0	0.05	0.06	0	0.05	0	0	0	0.05	0	0.05	0	0	0	0	0	0	0
HPZCOO		0	0.01	0.01	0	0.01	0	0	0	0.01	0	0	0	0	0	0	0	0	0
SO4-2		0	0.04	0.04	0	0.03	0	0	0	0.03	0	0.04	0	0	0	0	0	0	0
NA2SO-01		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NA+		0	0.07	0.08	0	0.07	0	0	0	0.07	0.34	0.08	0	0	0	0	0	0	0
NA2SO-02		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2SO4		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NAOH		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow	MOL/HR	297	227348	213358	4628	241722	14139	13668	11849	254479	2414	215183	297	1235	1235	15308	14667	546	13932
Mass Flow	KG/HR	11	7397	7137	174	7686	260	253	221	8035	47	7174	11	46	46	349	289	10	260
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0
Temperature	C	40	97	70	40	123	40	40	40	150	40	70	168	40	280	123	97	70	70
Pressure	KPA	23	70	23	30	202	23	28	30	1621	101	23	70	28	202	202	70	23	23
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table D.26 Stream summary for SO_4^{-2} reclaiming by NaOH (excess Na^+ case (Na^+/SO_4^{-2} = 2.04) – 100°C

		1	BTM S2	BTM S3	CO2	FEED	H20	H2O 1	H2O 2	IN	NAOH	SLURRY	V	V1	V2	VENT	VENT 2	VENT 3	VENT 4
From		COND1	FLASH2	FLASH3	COND3	FLASH	COND1	COND2	COND3			CRYSTL	COMP1	COND2	COMP2	FLASH	FLASH2	CRYSTL	FLASH3
To		COMP1	FLASH3	CRYSTL		FLASH2				FLASH	CRYSTL		COND2	COMP2	COND3	COND3	COND2	COND1	COND1
Substream: MIXED																			
Phase:		Vapor	Liquid	All	Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	All	All	Vapor	All	Vapor	Vapor	Vapor	Vapor
Component Mole Fraction																			
H2O		0.09	0.77	0.76	0.25	0.78	0.99	0.99	0.99	0.77	0.32	0.76	0.09	0.26	0.26	0.74	0.89	0.95	0.95

CO2		0.91	0	0	0.75	0	0	0	0	0	0	0	0.91	0.74	0.74	0.25	0.1	0.04	0.05
HCO3-		0	0	0	0	0	0	0	0	0.01	0	0	0	0	0	0	0	0	0
CO3--		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H+		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
OH-		0	0	0	0	0	0	0	0	0	0.34	0	0	0	0	0	0	0	0
PZ		0	0.01	0.02	0	0.01	0	0	0	0	0	0.02	0	0	0	0	0.01	0.01	0
PZCOO-2		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PZCOO-		0	0.05	0.05	0	0.05	0	0	0	0.04	0	0.05	0	0	0	0	0	0	0
PZH+		0	0.05	0.05	0	0.05	0	0	0	0.05	0	0.05	0	0	0	0	0	0	0
HPZCOO		0	0.01	0.01	0	0.01	0	0	0	0.01	0	0.01	0	0	0	0	0	0	0
SO4-2		0	0.03	0.04	0	0.03	0	0	0	0.03	0	0.03	0	0	0	0	0	0	0
NA2SO-01		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NA+		0	0.07	0.07	0	0.07	0	0	0	0.07	0.34	0.07	0	0	0	0	0	0	0
NA2SO-02		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2SO4		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NAOH		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow	MOL/HR	448	23916	22985	4769	24757	8988	7989	6102	25447	1564	23116	448	1793	1793	9115	9382	182	9302
Mass Flow	KG/HR	19	7611	7428	179	7808	167	149	114	8035	30	7455	19	67	67	227	198	4	182
Volume Flow	CUM/SEC	0	0	0	0	0	0	0	0	0		0	0	0	0	0	0	0	0
Temperature	C	40	117	100	40	133	40	40	40	150	40	100	107	40	345	133	117	100	100
Pressure	KPA	79	151	79	30	311	79	28	30	1621	101	79	151	28	311	311	151	79	79
Vapor Fraction		1	0	0	1	0	0	0	0	0	0	0	1	1	1	1	1	1	1
Liquid Fraction		0	1	1	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
Solid Fraction		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

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