

APPENDICES

APPENDIX A Amine Concentration Data Before and After CO₂ Absorption

Table A.1: Amine concentration before and after CO₂ absorption for 1.0 M MAE at 30, 40 and 60 °C

| Temperature (°C) | CO ₂ Partial Pressure (kPa) | Amine Concentration before Test (mol.dm ⁻³) | Amine Concentration after Test (mol.dm ⁻³) | Deviation (%) |
|------------------|--|---|--|---------------|
| 30 | 99.08 | 1 | 1.028 | 2.8 |
| | 49.37 | 1 | 1.031 | 3.1 |
| | 24.69 | 1 | 1.044 | 4.4 |
| | 9.84 | 1 | 1.052 | 5.2 |
| | 4.95 | 1 | 1.038 | 3.8 |
| | 0.98 | 1 | 1.013 | 1.3 |
| 40 | 98.91 | 1 | 1.049 | 4.9 |
| | 49.37 | 1 | 1.007 | 0.7 |
| | 24.64 | 1 | 1.031 | 3.1 |
| 60 | 98.41 | 1 | 1.040 | 4.0 |
| | 49.37 | 1 | 1.063 | 6.3 |
| | 24.64 | 1 | 1.106 | 10.6 |

Table A.2: Amine concentration before and after CO₂ absorption test for 2.0 M MAE at 30, 40 and 60 °C and 4.0 M MAE at 30 °C

| Temperature (°C) | CO ₂ Partial Pressure (kPa) | Amine Concentration before Test (mol.dm ⁻³) | Amine Concentration after Test (mol.dm ⁻³) | Deviation (%) |
|------------------|--|---|--|---------------|
| 30 | 98.75 | 2 | 2.011 | 0.6 |
| | 49.04 | 2 | 1.966 | 1.7 |
| | 24.64 | 2 | 2.052 | 2.6 |
| | 9.87 | 2 | 2.067 | 3.4 |
| | 4.95 | 2 | 2.029 | 1.5 |
| | 0.99 | 2 | 2.059 | 3.0 |
| 40 | 98.58 | 2 | 2.033 | 1.7 |
| | 49.12 | 2 | 2.032 | 1.6 |
| | 24.64 | 2 | 2.004 | 0.2 |
| 60 | 98.58 | 2 | 2.060 | 3.0 |
| | 49.29 | 2 | 2.149 | 7.5 |
| | 24.81 | 2 | 1.809 | 9.6 |
| 30 | 98.41 | 4 | 3.898 | 2.6 |
| | 49.37 | 4 | 3.778 | 5.6 |
| | 24.64 | 4 | 3.930 | 1.8 |
| | 9.89 | 4 | 3.947 | 1.3 |
| | 4.95 | 4 | 3.942 | 1.5 |
| | 0.99 | 4 | 4.071 | 1.8 |

APPENDIX B pH Data and Time to Reach EquilibriumTable B.1: Amine pH data before and after CO₂ absorption and time to reach equilibrium for 1.0 M MAE at 30, 40 and 60 °C

| Temperature (°C) | Amine Concentration (mol.dm ⁻³) | CO ₂ Partial Pressure (kPa) | pH before Test | pH after Test | Time to Reach Equilibrium (min) |
|------------------|---|--|----------------|---------------|---------------------------------|
| 30 | 1 | 99.08 | 11.62 | 7.34 | 32 |
| | 1 | 49.37 | 10.5 | 6.65 | 38 |
| | 1 | 24.69 | 10.51 | 7.87 | 45 |
| | 1 | 9.84 | 11.93 | 8.5 | 70 |
| | 1 | 4.95 | 10.5 | 7.45 | 85 |
| | 1 | 0.98 | 11.38 | 8.87 | 150 |
| 40 | 1 | 98.91 | 10.1 | 6.37 | 25 |
| | 1 | 49.37 | 10.02 | 7.51 | 35 |
| | 1 | 24.64 | 11.41 | 7.83 | 65 |
| 60 | 1 | 98.41 | 10.74 | 7.34 | 20 |
| | 1 | 49.37 | 11.1 | 7.76 | 32 |
| | 1 | 24.64 | 10.73 | 7.76 | 50 |

Table B.2: Amine pH data before and after CO₂ absorption and time to reach equilibrium for 2.0 M MAE at 30, 40 and 60 °C and 4.0 M at 30 °C

| Temperature (°C) | Amine Concentration (mol.dm ⁻³) | CO ₂ Partial Pressure (kPa) | pH before Test | pH after Test | Time to Reach Equilibrium (min) |
|------------------|---|--|----------------|---------------|---------------------------------|
| 30 | 2 | 98.75 | 11.89 | 7.49 | 35 |
| | 2 | 49.04 | 11.48 | 7.86 | 45 |
| | 2 | 24.64 | 11.66 | 7.98 | 75 |
| | 2 | 9.87 | 12.28 | 8.68 | 80 |
| | 2 | 4.95 | 12.25 | 8.88 | 100 |
| | 2 | 0.99 | 11.56 | 8.18 | 170 |
| 40 | 2 | 98.58 | 11.76 | 7.51 | 30 |
| | 2 | 49.12 | 10.22 | 7.86 | 40 |
| | 2 | 24.64 | 11.8 | 8.2 | 65 |
| 60 | 2 | 98.58 | 10.51 | 7.68 | 25 |
| | 2 | 49.29 | 11.36 | 7.86 | 35 |
| | 2 | 24.81 | 10.82 | 7.79 | 55 |
| 30 | 4 | 98.41 | 12.36 | 8.25 | 60 |
| | 4 | 49.37 | 12.09 | 8.47 | 72 |
| | 4 | 24.64 | 11.97 | 8.67 | 85 |
| | 4 | 9.89 | 12.17 | 8.94 | 92 |
| | 4 | 4.95 | 12.5 | 9.03 | 150 |
| | 4 | 0.99 | 12.3 | 9.18 | 200 |

APPENDIX C Non-Linear Regression Program Results for Estimating the Parameters for K_2 Correlation

NLREG version 6.5
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Non-Linear Regression to fit experimental $\ln K_2$, T, M, and P to Model

Number of observations = 17

Maximum allowed number of iterations = 500

Convergence tolerance factor = 1.000000E-010

Stopped due to: Relative function convergence.

Number of iterations performed = 5

Final sum of squared deviations = 2.6814277E+001

Final sum of deviations = -3.3801547E-009

Standard error of estimate = 1.49483

Average deviation = 0.973436

Maximum deviation for any observation = 2.67345

Proportion of variance explained (R^2) = 0.5284 (52.84%)

Adjusted coefficient of multiple determination (R_a^2) = 0.3712 (37.12%)

Durbin-Watson test for autocorrelation = 2.204

Analysis completed 24-Apr-2010 01:44. Runtime = 0.05 seconds.

---- Descriptive Statistics for Variables ----

| Variable | Minimum value | Maximum value | Mean value | Standard dev. |
|-----------|---------------|---------------|------------|---------------|
| $\ln K_2$ | -3.905 | 3.1041 | -1.357082 | 1.885126 |
| P | 303 | 333 | 312.4118 | 12.48529 |
| M | 0.9841 | 98.913 | 30.93721 | 34.6903 |
| T | 0.9605 | 4.0416 | 1.708041 | 0.9986274 |

---- Calculated Parameter Values ----

| Parameter | Initial guess | Final estimate | Standard error | t | Prob(t) |
|-----------|---------------|----------------|----------------|-------|---------|
| a | 1 | 1.30081964 | 11.46776 | 0.11 | 0.91156 |
| b | 1 | -4.23040899 | 1.32262 | -3.20 | 0.00765 |
| c | 1 | 0.002474157 | 0.037044 | 0.07 | 0.94785 |
| d | 1 | -0.0334237468 | 0.050418 | -0.66 | 0.51990 |
| e | 1 | 0.00035097811 | 0.0004516 | 0.78 | 0.45207 |

---- Analysis of Variance ----

| Source | DF | Sum of Squares | Mean Square | F value | Prob(F) |
|------------|----|----------------|-------------|---------|---------|
| Regression | 4 | 30.04493 | 7.511233 | 3.36 | 0.04587 |
| Error | 12 | 26.81428 | 2.234523 | | |
| Total | 16 | 56.85921 | | | |

---- 90.000% Confidence Intervals ----

| Parameter | Lower limit | Best estimate | Upper limit |
|-----------|--------------|---------------|---------------|
| a | -19.1376722 | 1.30081964 | 21.7393115 |
| b | -6.58765765 | -4.23040899 | -1.87316033 |
| c | -0.063548557 | 0.00247415668 | 0.0684968704 |
| d | -0.123281526 | -0.0334237468 | 0.0564340326 |
| e | -0.000453831 | 0.0003509781 | 0.00115578725 |

APPENDIX D Equilibrium Constant Data for Hydrolysis of Carbamate

Table D.1: Equilibrium constant data for hydrolysis of carbamate for 1.0 M MAE at 30, 40 and 60 °C

| Temperature (°C) | Amine Concentration (mol.dm ⁻³) | CO ₂ Partial Pressure (kPa) | Equilibrium Constant (K_2) |
|------------------|---|--|--------------------------------|
| 30 | 1 | 99.08 | 2.73 |
| | 1 | 49.37 | 3.18 |
| | 1 | 24.69 | 3.37 |
| | 1 | 9.84 | 3.49 |
| | 1 | 4.95 | 3.52 |
| | 1 | 0.98 | 3.55 |
| 40 | 1 | 98.91 | 16.27 |
| | 1 | 49.37 | 18.31 |
| | 1 | 24.64 | 19.42 |
| 60 | 1 | 98.41 | 92.17 |
| | 1 | 49.37 | 103.58 |
| | 1 | 24.64 | 109.59 |

Table D.2: Equilibrium constant data for hydrolysis of carbamate ion for 2.0 M MAE at 30, 40 and 60 °C and 4.0 M at 30 °C

| Temperature (°C) | Amine Concentration (mol.dm ⁻³) | CO ₂ Partial Pressure (kPa) | Equilibrium Constant (K_2) |
|------------------|---|--|--------------------------------|
| 30 | 2 | 98.75 | 2.44 |
| | 2 | 49.04 | 2.66 |
| | 2 | 24.64 | 2.91 |
| | 2 | 9.87 | 2.93 |
| | 2 | 4.95 | 2.96 |
| | 2 | 0.99 | 2.98 |
| 40 | 2 | 98.58 | 14.08 |
| | 2 | 49.12 | 15.85 |
| | 2 | 24.64 | 16.80 |
| 60 | 2 | 98.58 | 79.76 |
| | 2 | 49.29 | 89.65 |
| | 2 | 24.81 | 95.03 |
| 30 | 4 | 98.41 | 105.07 |
| | 4 | 49.37 | 117.69 |
| | 4 | 24.64 | 120.89 |
| | 4 | 9.89 | 125.21 |
| | 4 | 4.95 | 130.81 |
| | 4 | 0.99 | 138.05 |

APPENDIX E List of Publications

Haider, H., Yusoff, R., Aroua, M. K. (2009), Solubility of carbon dioxide in 2(methylamino) ethanol, Techpos2009, 14-15th December 2009, Kuala Lumpur, Malaysia.

Haider, H., Yusoff, R., Aroua, M. K. (2011), Equilibrium solubility of carbon dioxide in 2(methylamino) ethanol. Accepted for publication, Fluid Phase Equilibria.