

Heat Capacity of Alkanolamine Aqueous Solutions

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Heat capacities of monoethanolamine, diglycolamine, diethanolamine, di-2-propanolamine, triethanolamine, *N*-methyldiethanolamine, 2-amino-2-methyl-1-propanol, and 2-piperidineethanol aqueous solutions were measured from 30 to 80 °C with a differential scanning calorimeter (DSC). The mole fractions of alkanolamines studied are 0.2, 0.4, 0.6, and 0.8. Heat capacities of *N*-methyldiethanolamine aqueous solutions have been measured to verify the validity of C_p measurements for alkanolamine aqueous solutions. The estimated uncertainty of the measured heat capacities is $\pm 3\%$, including the effect of up to 5% impurities in a substance. An excess molar heat capacity expression using the Redlich–Kister equation for the composition dependence is used to represent the measured C_p of alkanolamine aqueous solutions. For a total of 374 data points, the calculation results for eight alkanolamine solutions give the overall average absolute deviations of 11.9% and 0.29% for the excess molar heat capacity and the heat capacity, respectively. The heat capacities presented in this study are, in general, of sufficient accuracy for most engineering-design calculations.

Introduction

Solutions of alkanolamines are industrially important mixtures used in the natural gas industry, oil refineries, petroleum chemical plants, and synthetic ammonia plants for the removal of acidic components such as CO_2 and H_2S from gas streams. A wide variety of alkanolamines such as monoethanolamine (MEA), diglycolamine (DGA), diethanolamine (DEA), di-2-propanolamine (DIPA), triethanolamine (TEA), *N*-methyldiethanolamine (MDEA), 2-amino-2-methyl-1-propanol (AMP), and 2-piperidineethanol (2-PE) can be used as absorbents for acid gas removal processes (Kohl and Riesenfeld, 1985).

Heat capacity data for alkanolamine solutions are required for the design of the heat-exchanger equipment used in gas-treating processes. The C_p values of MEA, DEA, TEA, and MDEA are available in the literature (Riddick et al., 1986; Lee, 1994; Lide, 1995). Chiu et al. (1999) recently measured the heat capacity of eight alkanolamines (MEA, DGA, DEA, DIPA, TEA, MDEA, AMP, 2-PE) at temperatures ranging from 30 to 80 °C with a differential scanning calorimeter. For the heat capacities of alkanolamine aqueous solutions, little information is available in the literature. Hayden et al. (1983) have studied the heat capacities of 23 wt % and 50 wt % MDEA aqueous solutions at 25, 50, and 75 °C. Presented in graphical form, C_p values of MEA aqueous solutions (15, 30, and 50 wt %) (Union Carbide Chemical Co., 1957), DGA aqueous solutions (50, 60, 70, 80, and 90 wt %) (Texaco Chemical Co., 1969), and DEA aqueous solutions (15, 30, and 50 wt %) (Union Carbide Chemical Co., 1957) have been reported for temperature ranges from 10 to 110 °C (Kohl and Riesenfeld, 1985). At 25 °C, the heat capacities of CO_2 -loaded, aqueous solutions of MEA, DEA, MDEA, aqueous MDEA + MEA, and MDEA + DEA were also studied (Weiland et al., 1997). Except for the C_p data of Hayden et al. (1983), most of the C_p data are presented in a graphical form. It is the purpose of this study to determine experimentally the heat capaci-

ties of alkanolamine aqueous solutions by using a differential scanning calorimeter (DSC). The systems chosen for C_p measurements are MEA, DGA, DEA, DIPA, TEA, MDEA, AMP, and 2-PE aqueous solutions. The temperature range will be from 30 to 80 °C; the concentration range will be 0.2, 0.4, 0.6, and 0.8 mole fractions. An excess molar heat capacity expression, using the Redlich–Kister equation for the concentration dependence, will be applied to represent the measured C_p data.

Experimental Section

Some chemicals are Riedel–de Haën reagent grade with the following purities: MEA, min. 99% (water max. 0.5%); DEA, min. 99% (water max. 0.3%); MDEA, 98.5% (water max. 0.5%); TEA, min. 99% (water max. 0.2%); AMP, min. 95%. Other chemicals are from Aldrich Chemical Co. with the following purities: DGA, min. 98%; DIPA, min. 95%; 2-PE, min. 95%. The estimated uncertainty of the measured heat capacities is $\pm 3\%$, including the effect of impurities in a substance with a purity of 95%. The water is liquid chromatography grade from Alps Chemical Co.

The differential scanning calorimeter used for this study consists of a DSC-2010 and a thermal analysis controller from TA Instruments. The DSC operating range is from room temperature to 725 °C. Both the temperatures and the heat flow associated with transitions in materials can be easily and rapidly measured with the system. The DSC operates with a temperature repeatability of ± 0.1 °C. The calorimetric sensitivity is 1 μW (rms). The calorimetric precision is $\pm 1\%$, on the basis of measurements of metal samples. The purge gas is nitrogen with a flow rate of 40 $\text{mL}\cdot\text{min}^{-1}$. By using the sample-encapsulating press, the liquid sample was prepared within a hermetic sample pan. The internal volume of the hermetic pan is approximately 10 mm^3 . The sample weight is in the range 15–20 mg. The accuracy of the C_p measurements is estimated to be $\pm 2\%$ on the basis of the measurement of the C_p of liquid water (Chiu et al., 1999). The apparatus and the experimental

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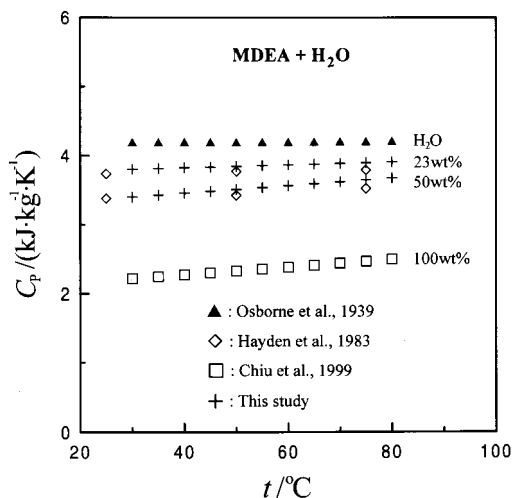


Figure 1. Heat capacity of MDEA (23, 50 wt %) aqueous solutions.

Table 1. Heat Capacities of MDEA + H₂O

temp (°C)	heat capacity, C_p /(kJ·kg ⁻¹ ·K ⁻¹)			
	$x_1 = 0.0432$ (23 wt % MDEA)		$x_1 = 0.1313$ (50 wt % MDEA)	
	Hayden et al., 1983	this study	Hayden et al., 1983	this study
30		3.81		3.40
35		3.82		3.43
40		3.83		3.46
45		3.84		3.49
50	3.773	3.85	3.428	3.51
55		3.86		3.54
60		3.87		3.57
65		3.88		3.60
70		3.89		3.62
75	3.794	3.90	3.527	3.65
80		3.91		3.68
AAD %		2.4%		2.9%

procedure are the same as those described by Chiu et al. (1999).

Results and Discussion

For alkanolamine aqueous solutions, heat capacities of 23 wt % and 50 wt % MDEA aqueous solutions at 25, 50, and 75 °C have been reported in the literature (Hayden et al., 1983) with an uncertainty of $\pm 0.5\%$. To validate the apparatus and the experimental procedure of the heat capacity measurement for alkanolamine aqueous solutions, the C_p values of 23 wt % and 50 wt % MDEA aqueous solutions were measured. The results of C_p measurements for MDEA aqueous solutions are presented in Table 1 and Figure 1. For the C_p values of MDEA aqueous solutions, the difference for the C_p values at 50 and 75 °C between the measurement in this study and that of Hayden et al. (1983) is 2.4% and 2.9% for 23 wt % and 50 wt % MDEA, respectively. Thus, there is good agreement between literature results and the present study for the C_p measurements for alkanolamine aqueous solutions.

The C_p values of eight alkanolamine aqueous solutions were then measured for temperatures ranging from 30 to 80 °C and mole fractions of amine of 0.2, 0.4, 0.6, and 0.8. The results are presented in Tables 2–9. Due to the melting point of DIPA at 45.5 °C, the C_p measurements for DIPA aqueous solution start at 50 °C. At 50 °C, the plots of C_p versus mole fraction of alkanolamine for all alkanolamine aqueous solutions are shown in Figure 2. As

Table 2. Heat Capacities of MEA + H₂O

temp (°C)	heat capacity C_p and excess heat capacity C_p^E / (J·mol ⁻¹ ·K ⁻¹)							
	$x_1 = 0.2$		$x_1 = 0.4$		$x_1 = 0.6$		$x_1 = 0.8$	
	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E
30	93.8	0.127	112.	0.359	131	0.531	149	-0.144
35	94.5	0.558	114	1.02	132	1.04	150	0.208
40	95.2	0.974	115	1.69	134	1.56	152	0.556
45	95.9	1.39	116	2.34	135	2.06	153	0.882
50	96.6	1.79	117	2.97	137	2.57	155	1.23
55	97.4	2.20	119	3.63	138	3.08	156.	1.57
60	98.1	2.58	120	4.26	139	3.57	158	1.92
65	98.8	2.98	121	4.90	141	4.06	159	2.24
70	99.5	3.36	122	5.52	142	4.58	161	2.57
75	100	3.74	124	6.15	144	5.06	162	2.91
80	101	4.10	125	6.77	145	5.54	164	3.23

Table 3. Heat Capacities of DGA + H₂O

temp (°C)	heat capacity C_p and excess heat capacity C_p^E / (J·mol ⁻¹ ·K ⁻¹)							
	$x_1 = 0.2$		$x_1 = 0.4$		$x_1 = 0.6$		$x_1 = 0.8$	
	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E
30	114	1.21	150	0.291	186	-0.252	224	0.055
35	115	1.73	151	0.882	188	0.200	226	0.266
40	115	2.25	153	1.45	190	0.621	227	0.439
45	116	2.76	154	2.03	191	1.07	229	0.646
50	117	3.28	155	2.62	193	1.48	231	0.852
55	118	3.79	157	3.19	194	1.92	232	1.06
60	119	4.29	158	3.76	196	2.35	234	1.26
65	120	4.78	159	4.32	197	2.78	236	1.46
70	121	5.27	161	4.86	199	3.19	237	1.63
75	122	5.75	162	5.42	200	3.58	239	1.82
80	123	6.22	163	5.97	202	4.01	241	2.02

Table 4. Heat Capacities of DEA + H₂O

temp (°C)	heat capacity C_p and excess heat capacity C_p^E / (J·mol ⁻¹ ·K ⁻¹)							
	$x_1 = 0.2$		$x_1 = 0.4$		$x_1 = 0.6$		$x_1 = 0.8$	
	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E
30	113	2.02	150	3.11	186	3.36	222	2.60
35	114	2.55	152	3.81	189	3.97	224	2.99
40	115	3.06	154	4.52	191	4.55	227	3.38
45	117	3.54	156	5.23	193	5.15	230	3.77
50	118	4.04	158	5.94	196	5.75	232	4.16
55	119	4.52	160	6.62	198	6.32	235	4.51
60	120	5.01	161	7.31	200	6.92	238	4.90
65	121	5.49	163	8.01	203	7.51	241	5.28
70	122	5.95	165	8.69	205	8.07	243	5.66
75	123	6.42	167	9.36	207	8.66	246	6.05
80	124	6.87	169	10.0	210	9.24	249	6.43

Table 5. Heat Capacities of DIPA + H₂O

temp (°C)	heat capacity C_p and excess heat capacity C_p^E / (J·mol ⁻¹ ·K ⁻¹)							
	$x_1 = 0.2$		$x_1 = 0.4$		$x_1 = 0.6$		$x_1 = 0.8$	
	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E
50	140	5.54	200	6.03	260	7.17	318	6.67
55	141	6.03	202	6.85	263	7.91	322	7.00
60	142	6.49	204	7.63	266	8.62	325	7.28
65	144	6.96	207	8.44	269	9.35	328	7.61
70	145	7.43	209	9.21	272	10.1	332	7.88
75	146	7.88	211	10.0	275	10.8	335	8.25
80	148	8.33	214	10.8	278	11.5	339	8.53

shown in Figure 2, the C_p (in J·mol⁻¹·K⁻¹) of water has the lowest value among C_p values of all pure fluids. The value of C_p increases as the temperature increases and also as the mole fraction of alkanolamine increases. At 50 °C and $x_{\text{amine}} = 0.4$, the values of C_p for alkanolamine aqueous solutions are in the following order: DIPA (200 J·mol⁻¹·K⁻¹),

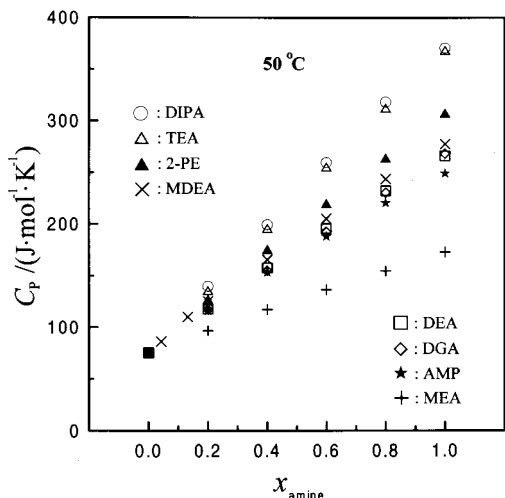


Figure 2. Molar heat capacity of alkanolamine aqueous solutions at 50 °C.

Table 6. Heat Capacities of TEA + H₂O

temp (°C)	heat capacity C_p and excess heat capacity C_p^E ($J \cdot mol^{-1} \cdot K^{-1}$)							
	$x_1 = 0.2$		$x_1 = 0.4$		$x_1 = 0.6$		$x_1 = 0.8$	
	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E
30	133	-0.082	191	0.573	250	1.83	306	0.864
35	134	0.388	192	1.30	251	2.47	308	1.26
40	134	0.830	194	2.01	253	3.10	309	1.70
45	135	1.25	195	2.69	254	3.69	311	2.04
50	136	1.68	196	3.40	256	4.31	312	2.48
55	136	2.11	197	4.10	257	4.93	314	2.87
60	137	2.52	199	4.80	259	5.55	315	3.26
65	138	2.94	200	5.49	260	6.17	317	3.69
70	139	3.34	201	6.18	261	6.82	318	4.07
75	139	3.73	202	6.84	263	7.39	320	4.41
80	140	4.13	204	7.52	264	8.00	321	4.84

K^{-1}) > TEA (196 $J \cdot mol^{-1} \cdot K^{-1}$) > 2-PE (176 $J \cdot mol^{-1} \cdot K^{-1}$) > MDEA (166 $J \cdot mol^{-1} \cdot K^{-1}$) > DEA (158 $J \cdot mol^{-1} \cdot K^{-1}$) > DGA (155 $J \cdot mol^{-1} \cdot K^{-1}$) > AMP (154 $J \cdot mol^{-1} \cdot K^{-1}$) > MEA (117 $J \cdot mol^{-1} \cdot K^{-1}$). The order of C_p for alkanolamine aqueous solutions generally follows the order of C_p for pure alkanolamines. The heat capacities of the pure fluids including water and alkanolamines are available in the literature (Chiu et al., 1999). The molar C_p values (in $J \cdot mol^{-1} \cdot K^{-1}$) for pure alkanolamines are listed in the Appendix for reference.

In Figure 3, heat capacities are shown for three alkanolamine aqueous solutions, MEA + H₂O, DEA + H₂O, and MDEA + H₂O. At 25 °C, heat capacities of MEA + H₂O, DEA + H₂O, and MDEA + H₂O for concentrations up to 60 mass % have been reported in the literature (Weiland

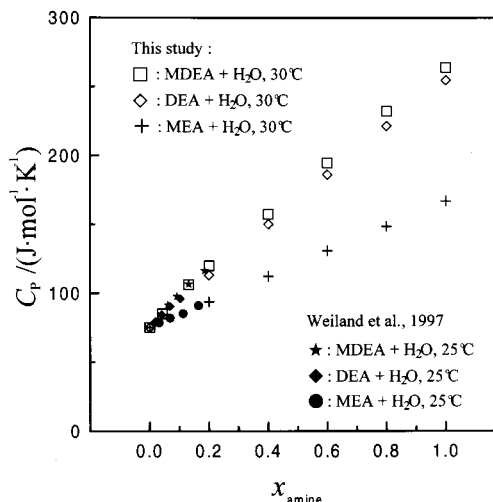


Figure 3. Heat capacity of three alkanolamine aqueous solutions.

et al., 1997). As shown in Figure 3, the C_p data measured in this study for MEA + H₂O, DEA + H₂O, and MDEA + H₂O at 30 °C are in good agreement with the data of Weiland et al. (1997) at 25 °C.

An excess molar heat capacity expression, using the Redlich–Kister equation for the concentration dependence, is applied to represent the measured C_p data of alkanolamine aqueous solutions. The excess molar heat capacity C_p^E for a binary mixture is defined as (Lide and Kehiaian, 1994)

$$C_p^E = C_p - (x_1 C_{p,1} - x_2 C_{p,2}) \quad (1)$$

where $C_{p,i}$ is the molar heat capacity of the pure component i . The C_p^E can be calculated from the measured C_p and $C_{p,i}$. The calculated C_p^E values from eq 1 for eight alkanolamine aqueous solutions are also presented in Tables 2–9. In Table 7, the values of C_p^E for 23 wt % ($x_{MDEA} = 0.0432$) and 50 wt % ($x_{MDEA} = 0.1313$) MDEA aqueous solutions are also presented. The value of C_p^E increases as the temperature increases. In Figure 4, plots of C_p^E for alkanolamine aqueous solutions versus mole fraction of alkanolamine at 80 °C are shown. At 80 °C and $x_{amine} = 0.4$, the values of C_p^E for alkanolamine aqueous solutions are in the following order: MDEA (13.6 $J \cdot mol^{-1} \cdot K^{-1}$) > AMP (12.9 $J \cdot mol^{-1} \cdot K^{-1}$) > 2-PE (11.2 $J \cdot mol^{-1} \cdot K^{-1}$) > DIPA (10.8 $J \cdot mol^{-1} \cdot K^{-1}$) > DEA (10.0 $J \cdot mol^{-1} \cdot K^{-1}$) > TEA (7.52 $J \cdot mol^{-1} \cdot K^{-1}$) > MEA (6.77 $J \cdot mol^{-1} \cdot K^{-1}$) > DGA (5.97 $J \cdot mol^{-1} \cdot K^{-1}$). In general, the value of C_p^E indicates the degrees of nonideality of the binary mixtures. The smaller the value of C_p^E is, the closer the system approaches an

Table 7. Heat Capacities of MDEA + H₂O

temp (°C)	heat capacity C_p and excess heat capacity C_p^E ($J \cdot mol^{-1} \cdot K^{-1}$)											
	$x_1 = 0.0432$		$x_1 = 0.1313$		$x_1 = 0.2$		$x_1 = 0.4$		$x_1 = 0.6$		$x_1 = 0.8$	
	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E
30	85.2	1.76	107	6.41	120	7.04	158	6.71	195	6.32	232	5.85
35	85.4	1.86	107	6.84	121	7.60	160	7.41	198	6.88	235	6.03
40	85.6	1.94	108	7.26	123	8.18	162	8.13	200	7.45	238	6.26
45	85.9	2.01	109	7.67	124	8.72	164	8.82	203	8.01	241	6.44
50	86.1	2.08	110	8.08	125	9.25	166	9.50	205	8.53	244	6.62
55	86.3	2.14	111	8.48	126	9.79	168	10.2	208	9.12	247	6.84
60	86.6	2.19	112	8.87	128	10.3	170	10.9	210	9.64	250	7.02
65	86.8	2.24	113	9.25	129	10.9	172	11.6	213	10.2	253	7.20
70	87.1	2.28	113	9.63	130	11.4	174	12.3	216	10.8	255	7.41
75	87.3	2.31	114	10.0	131	11.9	176	12.9	218	11.3	258	7.58
80	87.5	2.34	115	10.4	132	12.4	178	13.6	221	11.9	261	7.80

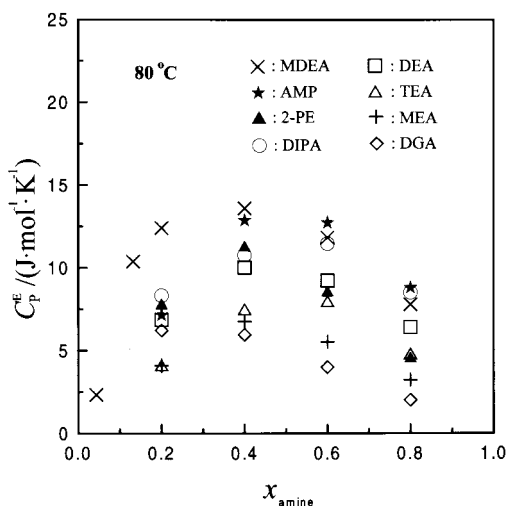


Figure 4. Excess molar heat capacity of alkanolamine aqueous solutions at 80 °C.

Table 8. Heat Capacities of AMP + H₂O

temp (°C)	heat capacity C_p and excess heat capacity C_p^E ($\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$)							
	$x_1 = 0.2$		$x_1 = 0.4$		$x_1 = 0.6$		$x_1 = 0.8$	
	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E
30	113	4.96	147	5.76	179	5.61	211	4.29
35	114	5.22	148	6.50	181	6.35	213	4.77
40	115	5.44	150	7.22	184	7.07	216	5.22
45	115	5.68	152	7.94	186	7.78	218	5.67
50	116	5.91	154	8.65	188	8.49	221	6.11
55	117	6.13	155	9.36	191	9.20	223	6.56
60	118	6.34	157	10.1	193	9.93	226	7.03
65	118	6.55	159	10.8	195	10.6	228	7.47
70	119	6.76	161	11.5	197	11.3	231	7.91
75	120	6.95	162	12.2	200	12.0	233	8.35
80	121	7.15	164	12.9	202	12.7	236	8.82

Table 9. Heat Capacities of 2-PE + H₂O

temp (°C)	heat capacity C_p and excess heat capacity C_p^E ($\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$)							
	$x_1 = 0.2$		$x_1 = 0.4$		$x_1 = 0.6$		$x_1 = 0.8$	
	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E	C_p	C_p^E
30	123	3.84	167	4.83	209	3.31	252	2.20
35	124	4.25	169	5.50	212	3.84	255	2.48
40	125	4.66	171	6.12	215	4.36	258	2.67
45	126	5.06	174	6.79	217	4.88	261	2.91
50	127	5.47	176	7.45	220	5.43	264	3.14
55	128	5.84	178	8.08	223	5.94	267	3.37
60	130	6.24	180	8.71	226	6.45	271	3.60
65	131	6.62	182	9.36	228	7.00	274	3.83
70	132	6.99	184	9.98	231	7.47	277	4.06
75	133	7.35	186	10.6	234	8.00	280	4.28
80	134	7.73	189	11.2	237	8.50	283	4.50

ideal solution. As far as the degree of nonideality of the solution is concerned, the ratio of C_p^E to C_p may also be a suitable replacement factor for the absolute value of C_p^E . At 80 °C and $x_{\text{amine}} = 0.4$, the values of the ratio of C_p^E to C_p for eight alkanolamine aqueous solutions are in the following order: AMP (7.87%) > MDEA (7.64%) > 2-PE (5.93%) > DEA (5.92%) > MEA (5.42%) > DIPA (5.05%) > TEA (3.69%) > DGA (3.66%). This order exhibits the degree of nonideality of the binary mixtures of water and alkanolamines. Among eight alkanolamine aqueous solutions, AMP + H₂O shows the strongest nonideality behavior while DGA + H₂O shows the weakest nonideality behavior.

A Redlich–Kister equation was applied to represent the compositional dependence of the excess molar heat capacity

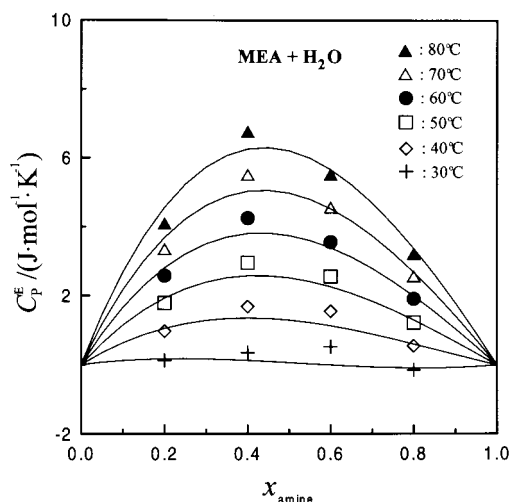


Figure 5. Excess molar heat capacity of MEA + H₂O: points, exptl data; lines, calculated using eq 2.

as follows,

$$C_p^E(\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}) = x_1 x_2 \sum_{i=1}^n A_i (x_1 - x_2)^{i-1} \quad (2)$$

The temperature dependence of A_i is assumed to follow the equation

$$A_i = a_{i,0} + a_{i,1}(T/K) \quad (3)$$

The parameters $a_{i,0}$ and $a_{i,1}$ are determined from the C_p^E calculated with eq 1. The determined parameters $a_{i,0}$ and $a_{i,1}$ and the average absolute percentage deviation (AAD %) for each aqueous solution are presented in Table 10. The values of C_p^E are then calculated with eqs 2 and 3. By adding the ideal solution of heat capacity, as in eq 1, to the C_p^E , the value of C_p is then calculated. Since the alkanolamine aqueous solutions are not strongly nonideal solutions, a two-term Redlich–Kister equation is used in the calculation. For the eight alkanolamine aqueous solutions, the overall average absolute percentage deviation (overall AAD %) is 11.9% for C_p^E . Since some values of C_p^E are quite small, the corresponding AAD % for C_p^E calculation may appear to be rather large while this deviation does not contribute to a large AAD % for the calculation of the C_p . For a total of 374 data points, the overall AAD % for C_p calculations for eight alkanolamine solutions is 0.29%, which is a quite satisfactory result.

On the basis of eq 2 and the parameters in Table 10, the calculation of C_p for the MEA + H₂O, DEA + H₂O, and MDEA + H₂O mixtures at 25 °C is performed and compared with the literature values (Weiland et al., 1997). The results are presented in Table 11. The AAD % values are 0.84%, 2.07%, and 2.25% for MEA + H₂O, DEA + H₂O, and MDEA + H₂O, respectively. The results of the calculations with eq 2 for MEA + H₂O, DEA + H₂O, and MDEA + H₂O are quite satisfactory.

For MEA + H₂O, the AAD % for C_p^E is 17.6; however, the AAD % for C_p is only 0.2%, as shown in Table 10 and Figure 5. Due to the quite small values of C_p^E at 30 °C, the AAD % for C_p^E at this temperature is 60%. However, the calculated C_p^E at 30 °C looks reasonable, as shown in Figure 5.

For DGA + H₂O, the AAD % values are 27.1 and 0.3 for C_p^E and C_p , respectively. As shown in Figure 6, the large values of AAD % (78%) come from quite small C_p^E values

Table 10. Parameters of Heat Capacity for Alkanolamine Aqueous Solutions

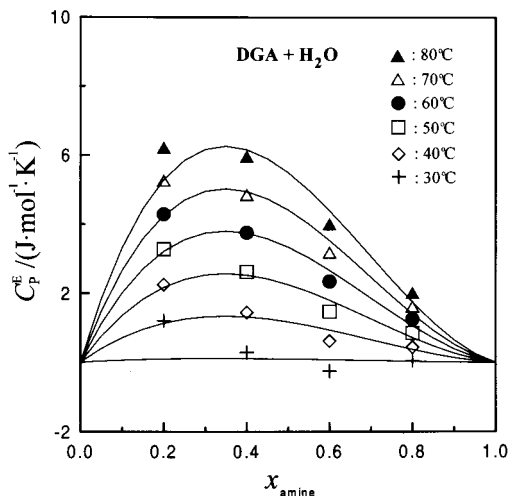
system	parameters				no. of data points	AAD % ^a	
	$a_{1,0}$	$a_{1,1}$	$a_{2,0}$	$a_{2,1}$		C_p^E	C_p
MEA + H ₂ O	-148.90	0.492 08	28.033	-0.096 90	44	17.6	0.20
DGA + H ₂ O	-130.65	0.432 43	109.506	-0.362 25	44	27.1	0.30
DEA + H ₂ O	-150.04	0.541 04	38.682	-0.118 61	44	2.6	0.07
DIPA + H ₂ O	-163.91	0.603 44	48.049	-0.130 99	44	10.8	0.39
TEA + H ₂ O	-160.54	0.540 48	24.096	-0.058 60	44	11.3	0.15
MDEA + H ₂ O	-105.74	0.458 71	11.466	-0.074 49	66	15.1	0.66
AMP + H ₂ O	-130.67	0.516 78	-67.729	0.213 43	44	4.3	0.19
2-PE + H ₂ O	-116.29	0.441 94	52.784	-0.202 38	44	4.8	0.15
overall AAD % ^b					374	11.9	0.29

^a AAD %: average absolute percentage deviation. ^b Overall AAD %: overall average absolute percentage deviation.

Table 11. Comparison of the Calculated Heat Capacity and the Literature Heat Capacity for Alkanolamine Aqueous Solutions at 25 °C

system	mole fraction x_1	$C_p/(J \cdot mol^{-1} \cdot K^{-1})$		AAD % ^a
		data of Weiland et al., 1997	calcd using eq 2	
MEA + H ₂ O	0.0317	78.69	77.99	0.84%
	0.0687	82.00	81.29	
	0.1122	85.29	85.17	
DEA + H ₂ O	0.1643	91.16	89.81	2.07%
	0.0187	79.47	78.62	
	0.0411	84.52	82.75	
MDEA + H ₂ O	0.0684	90.56	87.79	2.25%
	0.1025	96.07	94.08	
	0.0608	91.51	88.76	
	0.0915	97.76	95.46	
	0.1313	106.61	104.0	
	0.1848	116.5	115.2	

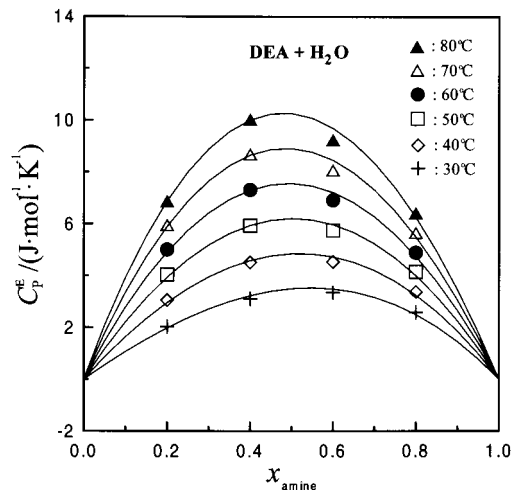
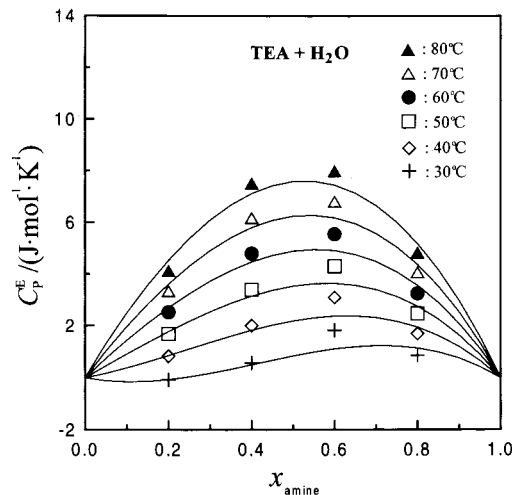
^a AAD %: average absolute percentage deviation.

**Figure 6.** Excess molar heat capacity of DGA + H₂O: points, exptl data; lines, calculated using eq 2.

at the temperature 30 °C. Among eight alkanolamine aqueous solutions, the 27.1% for the C_p^E calculation for DGA + H₂O is the largest deviation.

As shown in Figure 7, the results for C_p calculations for DEA + H₂O are quite satisfactory. For DEA + H₂O, the AAD % for the C_p^E calculation is 2.6 and that for the C_p calculation is only 0.07%, as presented in Table 10. Both results for the C_p^E and the C_p calculations are quite satisfactory for DEA + H₂O.

For TEA + H₂O, the AAD % for the C_p^E calculation is 11.3 and that for the C_p calculation is only 0.15%, as shown in Table 10 and Figure 8. Similar to the case of MEA + H₂O, large deviations for C_p^E calculations come from the

**Figure 7.** Excess molar heat capacity of DEA + H₂O: points, exptl data; lines, calculated using eq 2.**Figure 8.** Excess molar heat capacity of TEA + H₂O: points, exptl data; lines, calculated using eq 2.

lowest temperature, 30 °C. As shown in Figure 8, both results for the C_p^E and the C_p calculations are reasonable and are also satisfactory.

For AMP + H₂O, the AAD % for the C_p^E calculation is 4.3 and that for the C_p calculation is only 0.19%, as shown in Table 10 and Figure 9. As shown in Figure 9, both results for the C_p^E and the C_p calculations are quite good.

Conclusions

The heat capacities of MEA, DGA, DEA, DIPA, TEA, MDEA, AMP, and 2-PE aqueous solutions were measured

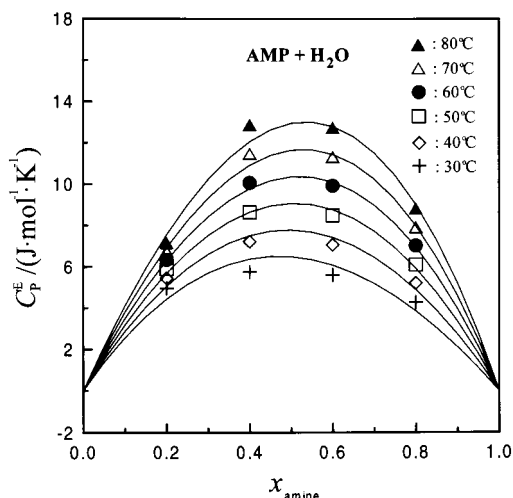


Figure 9. Excess molar heat capacity of AMP + H₂O: points, exptl data; lines, calculated using eq 2.

Table 12. Heat Capacities of Pure Alkanolamines

temp (°C)	heat capacity C_p (J·mol ⁻¹ ·K ⁻¹) (given in Chiu et al., 1999)								
	H ₂ O ^a	MEA	DGA	DEA	DIPA	TEA	MDEA	AMP	2-PE
30	75.253	167	261	255		363	264	239	293
35	75.248	169	263	258		364	268	242	297
40	75.255	170	265	261		366	271	244	300
45	75.271	172	267	264		367	274	247	304
50	75.293	173	268	266	371	369	278	249	308
55	75.323	175	270	269	375	370	281	252	311
60	75.359	176	272	272	378	371	284	255	315
65	75.403	178	274	275	382	373	288	257	319
70	75.453	179	276	278	386	374	291	260	322
75	75.511	180	278	281	390	376	295	262	326
80	75.575	182	280	284	394	377	298	265	330

^a Data of Osborne et al., 1939.

from 30 to 80 °C with a differential scanning calorimeter (DSC). The mole fractions of alkanolamines studied are 0.2, 0.4, 0.6, and 0.8. The heat capacities of MDEA aqueous solutions have been measured to verify the validity of the C_p measurement for alkanolamine aqueous solutions. An excess molar heat capacity expression using the Redlich–Kister equation for the composition dependence is used to represent the measured C_p of alkanolamine aqueous solutions. For a total of 374 data points, the calculation results for eight alkanolamine solutions are 11.9% and 0.29% for the excess molar heat capacity and the heat capacity, respectively. The heat capacities presented in this study are, in general, of sufficient accuracy for most engineering-design calculations.

Appendix

Heat Capacities of Pure Alkanolamines. The heat capacities of pure alkanolamines have been measured for

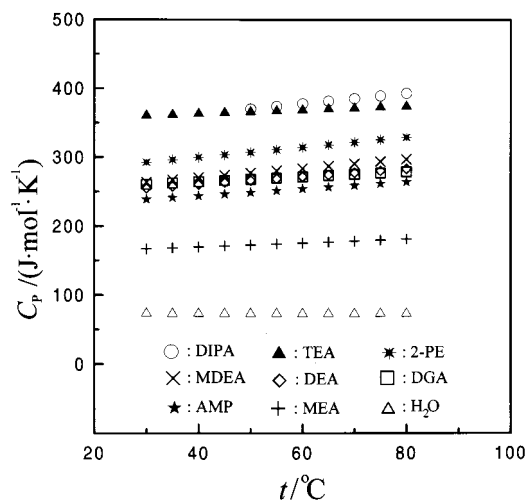


Figure 10. Molar heat capacity of pure alkanolamines.

temperatures from 30 to 80 °C (Chiu et al., 1999). The heat capacities of water were reported by Osborne et al. (1939). The C_p data of pure fluids including water, MEA, DGA, DEA, DIPA, TEA, MDEA, AMP, and 2-PE expressed in molar units are summarized in Table 12 and Figure 10.

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