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Theoretical estimation of heat capacity of binary liquid mixtures at different temperatures by associated and non associated processes

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Abstract

In the present investigation experimental density (ρ), ultrasonic speed (U), thermal expansion coefficient (α) isothermal compressibility (β_T), characteristic pressure (P), characteristic volume (V*) and characteristic temperature (T*) were used to evaluate heat capacity (C_P) of two weakly interacting binary liquid mixtures such as 1-butanol+dodecane and 2-butanol+dodecane over the entire range of concentration and atmospheric pressure from 288.15-318.15K by Prigogine-Flory-Patterson model based on non- associated process. Ramaswamy (RS) as well as model devised by Glinski (GLI) based on association process were also considered for evaluation of aforementioned thermodynamic properties at different temperatures. Deviations of heat capacity were fitted to redlich kister polynomial to estimate the binary coefficient and standard deviation. McAllister Multi body interaction model was used to correlate the experimental findings. Results were discussed in terms of average absolute % deviation for both the liquid mixtures at different temperatures. McAllister four body (Mc_4) was found to be more consistent than McAllister three body (Mc_3) model. Excess heat capacities of binary liquid mixtures were also computed to analyze the intermolecular interactions. Prigogine-Flory-Patterson model deals a fair agreement with experimental findings in comparison to other two models based on associated process.*

Keywords: Heat capacity, Butanol, PFP, Binary mixture, Ultrasonic speed.

Introduction

In recent past internal pressure, excess internal pressure, pseudo-Gruneisen parameter, isobaric heat Capacity, heat capacity ratio, Debye temperature of multi-component liquid mixtures evaluated by various researchers[1,2]. The information obtained from these thermodynamic parameters play a significant role in understanding the behavior of molecular interactions[3-6] present in multi-component liquid mixtures and development of new empirical relations. Some time it is very difficult to determine various thermodynamic properties experimentally then to handle such situation empirical relations become beneficial for researchers. In present investigation, we are applying most widely accepted Flory's statistical theory[7-11] based on non–associated process for estimating heat capacity of two binary liquid mixtures 1-butanol+dodecane and 2-butanol+dodecane in conjugation with Ramaswamy-Anbananthan[3] and model suggested by Glinski[12] based on association process over the entire range of concentration from temperature 288.15-318.15K. From the knowledge of reduced volume ($\widetilde{V}$), thermal expansion coefficient (α), isothermal compressibility (β_T), characteristic pressure (P^*), characteristic volume (V^*) and characteristic temperature (T^*), heat capacity can be theoretically evaluated from statistical approach. Previously, we have analyzed ultrasonic, transport and optical properties by such processes[13-17]. Estimation of heat capacity from these approaches is our first attempt. The entire estimation approach is new and as for as our knowledge is concerned, nobody has attempted entirely different approaches together for the evaluation of heat capacity of weakly interacting liquids at different temperatures. The observed thermodynamic property derived from the measured data were fitted to Redlich kister polynomial[18] to calculate the binary coefficient and standard deviation. McAllister[19] three (Mc_3) and four body (Mc_4) interaction model was used to correlate the experimental findings. Excess heat capacities of binary liquid mixtures were also computed for both the associated and non associated process to understand the extent of molecular interactions between the binary components. The main aim of this work was to evaluate heat capacity of weakly interacting liquid mixtures theoretically by two different approaches at different temperatures and test their accuracy by comparing with literature values[20].

Methodology

Theoretical: Prigogine-Flory-Patterson model: Heat capacity of liquid mixture at constant pressure is defined as,

$$C_{P,Mix} = C_P^E + C_P^{Idel} \quad (1)$$

Where C_P^E is explained by Khanwalkar according to statistical liquid state model of Flory as;

$$C_P^E = \frac{P^*V^*}{T^*}\left[\frac{1}{\left((4/3)\tilde{V}_i^{-1/3}-1\right)} - \sum\left\{\frac{x_i}{(4/3)\tilde{V}_i^{-1/3}-1}\right\}\right] \qquad (2)$$

Ideal heat capacity of mixing can be computed by the given relation:

$$C_P^{Ideal} = \sum_{i=1}^{2} x_i C_{P,i} \qquad (3)$$

Flory evaluated characteristic pressure (P^*), characteristic temperature (T^*) and characteristic volume (V^*) of liquid mixture from reduced equation of state derived from given partition function as;

$$\frac{\tilde{P}\tilde{V}}{\tilde{T}} = \frac{\tilde{V}^{1/3}}{\tilde{V}^{1/3} - 1} - \frac{1}{\tilde{V}\tilde{T}}$$

$$\tilde{P} = \frac{P}{P^*}\ , \tilde{T} = \frac{T}{T^*}\ , = \frac{V}{V^*}$$

Where, $\tilde{P}$, $\tilde{T}$, and $\tilde{V}$ are reduced pressure, reduced temperature and reduced volume respectively.

Ramaswamy - Anbananthan model: Ramaswamy-Anbananthan model is based on the assumption of linearity of acoustic impedance with the mole fraction of components. Ramaswamy-Anbananthan model states that when liquid Liq (1) is added to liquid Liq (2), then molecules associate according to the equilibrium as;

$$Liq_{(1)} + Liq_{(2)} \leftrightarrow Liq_{(12)} \qquad (6)$$

K_{as} can be calculated by the following equation as;

$$K_{as} = \frac{[Liq_{(12)}]}{[Liq_{(1)}]\times[Liq_{(2)}]} \qquad (7)$$

Where: $[Liq_{(1)}]$, $[Liq_{(2)}]$ and $[Liq_{(12)}]$ are concentrations of $Liq_{(1)}$, $Liq_{(2)}$ and $Liq_{(12)}$ respectively.

By applying the condition of linearity with composition, heat capacity can be obtained as;

$$C_{P,(Cal)} = x_{(1)}C_{P,(1)} + x_{(12)}C_{P,(12)} \qquad (8)$$

Table-1: Experimental and Literature values of pure liquids at different temperatures.

Liquid	T/K	α X10^3	β_T x10^{12}	V	ρ_{exp} [21]	ρ_{lit} [21]
		K^{-1}	Pa	cm^3mol^{-1}	$g.cm^{-3}$	$g.cm^{-3}$
Dodecane	288.15	1.3044	116.21	226.40	0.7524	0.7526
	298.15	1.3298	123.13	228.59	0.7452	0.7453
	308.15	1.3564	130.66	230.82	0.7380	0.7380
	318.15	1.3843	138.89	233.12	0.7307	0.7307
1-Butanol	288.15	1.2886	112.04	91.12	0.8135	0.8133
	298.15	1.3111	118.00	91.98	0.8059	0.8057
	308.15	1.3348	124.50	92.88	0.7980	0.7980
	318.15	1.3596	131.59	93.82	0.7901	0.7901
2-Butanol	288.15	1.3091	117.47	91.48	0.8103	-
	298.15	1.3342	124.34	92.40	0.8022	0.8026
	308.15	1.3614	132.10	93.38	0.7038	0.7939
	318.15	1.3911	140.93	94.44	0.7849	0.7849

In case of high solute concentration non-associated components are also present with associated component in liquid mixture. So Equation (8) can be modified as;

$$C_{P,(Cal)} = x_{(1)}C_{P,(1)} + x_{(2)}C_{P,(2)} + x_{(12)}C_{P,(12)} \quad (9)$$

The general idea of Ramaswamy-Anbananthan model can be exploited as;

$$K_{as} = \frac{[Liq_{(12)}]}{\left(C_{Liq_{(1)}} - [Liq_{(12)}]\right)\left(C_{Liq_{(2)}} - [Liq_{(12)}]\right)} \quad (10)$$

In computational analysis, concentration of associated component $Liq_{(12)}$ can be computed for entire range of molar concentration in liquid mixture by considering any hypothetical value of association constant (Kas) and Equation (10) can be modifying into Equation (11) by replacing molar concentration with activity for concentrated solution.

$$K_{as} = \frac{a_{Liq_{(12)}}}{\left(a_{Liq_{(1)}} - a_{Liq_{(12)}}\right)\left(a_{Liq_{(2)}} - a_{Liq_{(12)}}\right)} \quad (11)$$

$a_{Liq_{(1)}}, a_{Liq_{(2)}}$ And $a_{Liq_{(12)}}$are activities of components $Liq_{(1)}$, $Liq_{(2)}$ and associate $Liq_{(12)}$ respectively.

Now assuming any value of heat capacity for hypothetical pure associate $Liq_{(12)}$, theoretical value of heat capacity, $C_{P,(Cal)}$ can be computed by substituting the value of Kas. On changing these adjustable parameters K_{as} and CP, Liq (12), we can get different values of sum of squares of deviations of experimental and theoretical values of heat capacity.

$$S = \sum\left(C_{P,(Exp)} - C_{P,(Cal)}\right)^2 \quad (12)$$

Model of Glinski: On the bases of theoretical results obtained from Ramaswamy model, Glinski proposed an empirical equation assuming the concept of additivity with volume fractions (ϕ) of components of binary liquid mixtures based on Natta-Baccaredda model as;

$$C_{P,Cal} = \frac{C_{P_{Liq(1)}}C_{P_{Liq(2)}}C_{P_{Liq(12)}}}{\phi_{Liq_{(1)}}C_{P_{Liq(2)}}C_{P_{Liq(12)}} + \phi_{Liq_{(2)}}C_{P_{Liq(1)}}C_{P_{Liq(12)}} + \phi_{Liq_{(12)}}C_{P_{Liq(1)}}C_{P_{Liq(2)}}}$$
(13)

$\phi_{Liq_{(1)}}$, $\phi_{Liq_{(2)}}$ and $C_{P_{Liq(1)}}$, $C_{P_{Liq(2)}}$ are volume fractions and heat capacity of pure liquid components 1 and 2 respectively. Computational procedure and determination of association constant, Kas of both these associated processes are almost similar. One of the most interesting features of this method over the earlier one is that density of liquid mixture is not required for computation of various thermodynamic and transport properties.

Results and Discussion

Table-1 represents the experimental and literature values of thermal expansion coefficient (α) isothermal compressibility (β_T), density (ρ) ultrasonic speed (U) of pure liquids at different temperatures. Coefficient of redlich kister polynomial Equation (14) and their standard deviations are recorded in Table-2. Standard deviation for 1-butanol+dodecane system varies from 0.6022-2.1307 whereas 2-butanol+dodecane system it varies from 0.2123-0.9905 from 288.15-318.15K.

$$\Delta C_P = X_I(1 - X_1)\sum_{i=0}^{n} A_i(1 - X_1)^i \quad (14)$$

In above equation ΔC_P refers to deviation in heat capacity, X_1 is the mole fraction and A^i is coefficient. The corresponding values of coefficients were evaluated by multiple regression technique based on least square method. The standard deviation (σ) is defined by;

$$\sigma = \left[\left(\sum_{i=1}^{n}\frac{\left(C_{P,(Exp)} - C_{P,(Cal)}\right)^2}{(n-p)}\right)^{1/2}\right] \quad (15)$$

Where n is the number of experimental point and p is the number of adjustable parameters. Results discussed in terms of standard deviations clearly indicate the fair correlation of experimental data for aforementioned liquid mixtures at different temperatures. Since experimental values of α and β_T are not known for considered binary liquid mixtures. So following empirical relations are used for the determination of experimental data. These parameters are already tested by us[21,22] and others[23].

$$\alpha = \frac{75.6\times10^{-3}}{T^{1/9}U^{1/2}\rho^{1/3}}K^{-1} \quad (16)$$

$$\beta_T = \frac{1.17\times10^{-3}}{T^{4/9}\rho^{4/3}U^2}cm^2dyne^{-1} \quad (17)$$

Excess heat capacity is calculated by the following relation;

$$C_P^E = C_{P,Theoetical} - \left(X_1C_{P,1} + X_2C_{P,2}\right) \quad (18)$$

In above equation $C_{P,1}$ and $C_{P,2}$ are heat capacity of pure liquids.

McAllister model is based on the assumption of Eyring's theory of absolute reaction rate. The aforementioned relations are mainly used to correlate the various thermodynamic, transport and acoustical parameter with mole fraction.

McAllister-three- body

$$\ln C_P = x_1^3\ln C_{P,(1)} + 3x_1^2x_2\ln C_{P_{(a)}} + 3x_1{x_2}^2\ln C_{P_{(b)}} + x_2^3\ln C_{P,(2)} - \ln[x_1 + x_2M_2/M_1] + 3x_1^2x_2\ln[(2 + M_2/M_1)/3] + 3x_1x_2^2\ln[(1 + 2\,M_2/M_1)/3] + x_2^3\ln[M_2/M_1] \quad (19)$$

McAllister-four-body

$$\ln C_P = x_1^4\ln C_{P,(1)} + 4x_1^3x_2\ln C_{P_{(a)}} + 6x_1^2x_2^2\ln C_{P_{(b)}} + 4x_1x_2^2\ln C_{P_{(c)}} + x_2^4\ln C_{P,(2)} - \ln[(x_1 + x_2M_2/M_1)] + 4x_1^3x_2\ln[(3 + M_2/M_1)/4] + 6x_1^2x_2^2\ln[(1 + M_2/M_1)/2] + 4x_1x_2^3\ln[(1 + 3M_2/M_1)/4] + x_2^4\ln(M_2/M_1) \quad (20)$$

Table-2: Coefficients and standard deviation (σ) of redlich kister polynomial at different temperatures (ΔC_p J mol^{-1} K^{-1}).

Liquide	T/K	A_0	A_1	A_2	A_3	(σ)
1-Butanol+ Dodecane	288.15	43.6864	-10.0408	45.1026	-56.5478	0.6022
	298.15	54.2751	-12.5112	56.9704	-62.5280	0.6780
	308.15	70.4902	-24.3484	86.9161	-1.4288	0.9685
	318.15	79.9045	-51.5614	61.1528	-18.5052	2.1309
2-Butanol+ Dodecane	288.15	53.3361	15.2145	81.8699	-97.6548	0.8857
	298.15	61.8024	-1.0395	81.3989	-72.6491	0.5467
	308.15	70.8857	-24.1621	66.8007	-24.0098	0.2123
	318.15	81.0506	-50.5939	32.2686	44.6273	0.9905

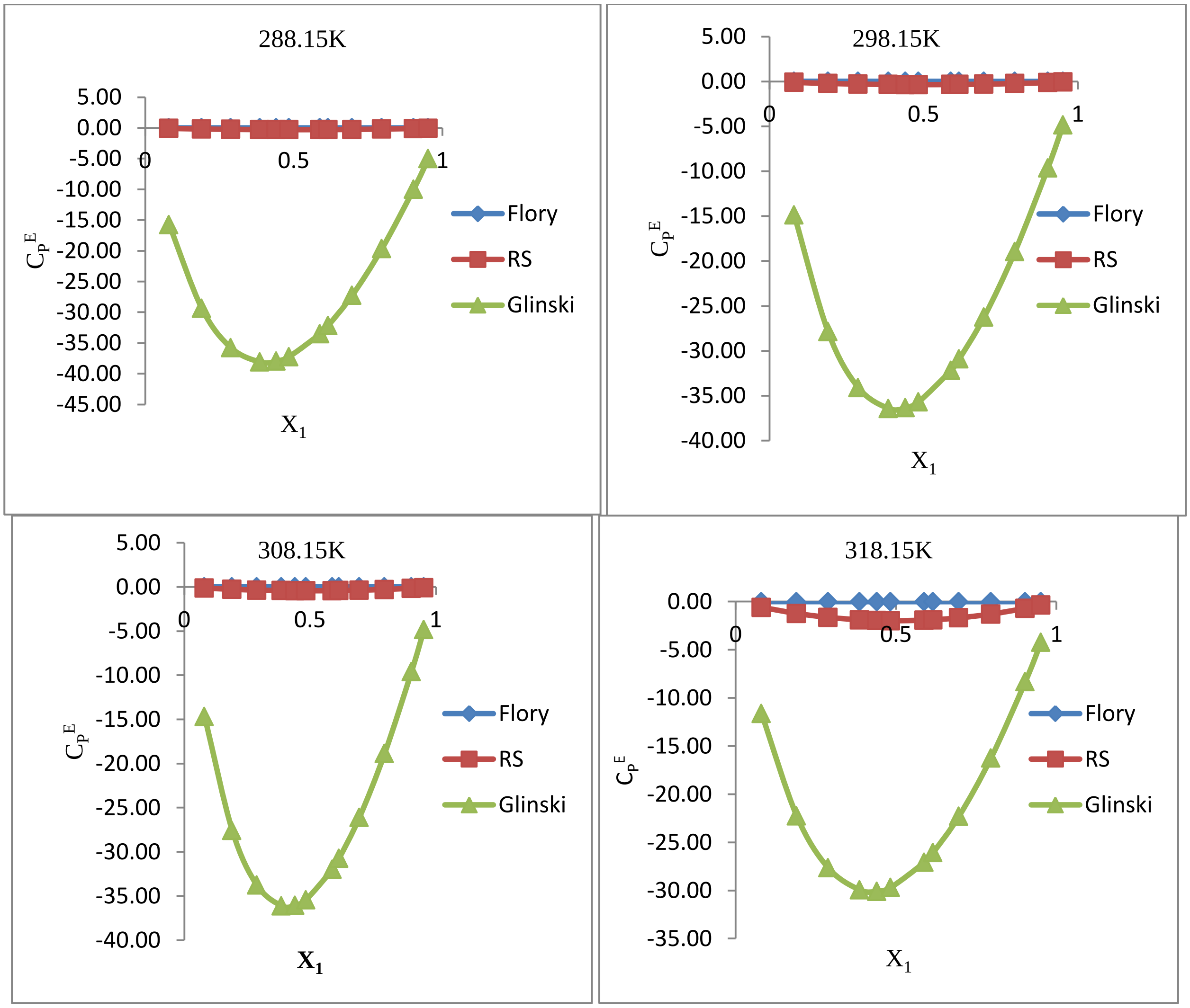

Figure-1: Plot of excess heat capacity of 1-butanol + dodecane with mole fraction X_1 at different temperatures.

In above equations M_1 and M_2 are molecular weight of pure liquids. Standard deviations and Coefficients of McAllister three and four body model were computed from least square method at different temperatures are recorded in Table-3. The values of standard deviations for 1-butanol+dodecane system lie between 3.5883-8.3619 and 1.2131-6.1122 for McAllister three and four body model respectively whereas for 2-butanol+dodecane system the corresponding standard deviations lie between 3.7802-5.5245 and 2.1155-3.2603. This is our first attempt to correlate the experimental data of heat capacity by McAllister multi-body interaction model at different temperatures. A close observation of Table-3 reveals that McAllister-four-body model deals a fair agreement for both the binary liquid mixtures. Absolute percent deviations (AAPD) in heat capacity obtained from non-associated and associated models are recorded in Table-4 whereas experimental density and other binary mixture related data are presented in Table-5. A care full observation of Table-4 and 5 clearly indicate that non-associated process provided fairly good result as compared to associated. Smaller deviation values obtained from Flory model can be explained as model was developed for ϒ-meric spherical non-electrolytic chain.

Molecule and the considered binary liquid Mixtures have weakly interacting properties. A close observation of Table-5 reveals that for a particular temperature as the mole fraction of butanol in binary mixture increases the heat capacity of mixtures decreases but increases with increase in temperature. Positive deviation in heat capacity for both the systems as shown in Figure-1 and 2 are result of molecular association and show weak interactions. On other hand, negative values of excess heat capacity results of strong molecular interaction for both the system at different temperatures. The magnitude and actual sign of excess function depends on the relative strength of these two opposing effects. For positive values of excess function association of molecules are more dominant than packing effect. Conversely, for negative values the dipolar-dipolar and packing effect are more dominant[23]. Percentage deviation obtained from all the models follow the same trend increases up to a maximum limit than decreases.

Results obtained from associative Glinski model was not quite satisfactory in comparison to Ramaswamy model while non-associated Flory deals a fair agreement with experimental finding for all the temperatures. Conclusively it is suggested that although Glinski model work appreciably for various thermodynamic and transport properties but still modification is required.

Table-3: Coefficients and standard deviation (σ) of McAllister multi-body model at different temperatures (Cp / J.mol^{-1}.K^{-1}).

Liquide	T/K	Three body			Four body			
		a	b	(σ)	a	b	c	(σ)
1-Butanol+ Dodecane	288.15	142.2009	242.5594	3.5883	249.8250	289.3095	350.1219	1.2131
	298.15	146.4311	248.6587	4.5028	259.5925	295.5207	360.2972	1.5322
	308.15	152.2695	247.5848	8.3619	266.2728	302.9485	357.1238	6.1122
	318.15	153.5335	266.2014	6.8918	298.1303	292.6504	413.8756	4.3090
2-Butanol+ Dodecane	288.15	149.9408	243.9567	6.2392	268.9836	293.0424	355.4981	3.2603
	298.15	154.3796	252.2814	6.2937	282.8456	297.9627	371.1140	2.1155
	308.15	159.5387	261.2722	5.5245	297.1228	304.6775	386.7465	2.1155
	318.15	166.0183	270.5425	3.7802	312.8629	313.2684	402.2215	2.8795

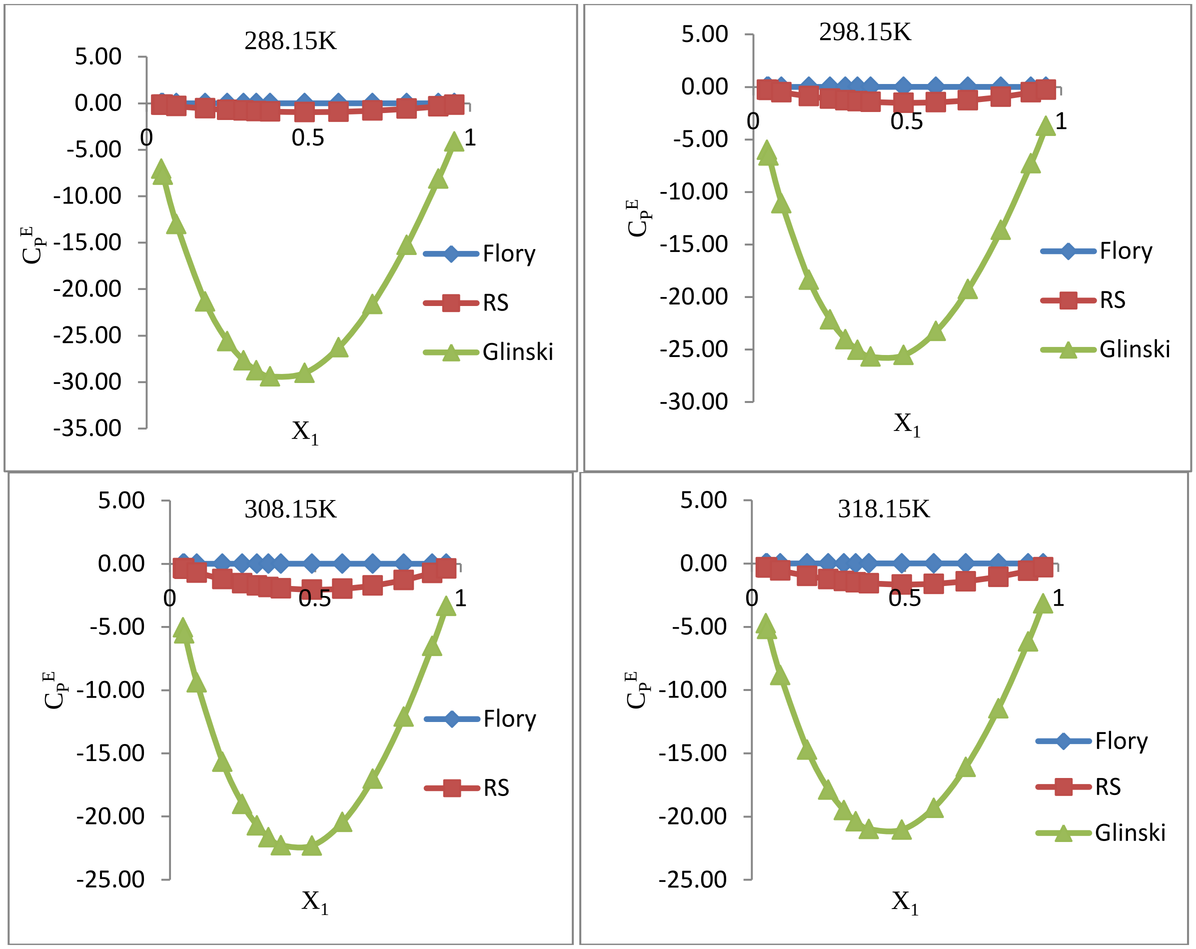

Figure-2: Plot of excess heat capacity of 2-butanol + dodecane with mole fraction X_1 at different temperatures.

Table-4: Average absolute % deviation of binary liquid mixtures at different temperatures.

T/K		AAPD					
	K_{as}	C_pab	C_p^{Flory}	C_p^{RS}	C_p^{Gli}	$C_p^{Mc\text{-}3}$	$C_p^{Mc\text{-}4}$
1-Butanol+ Dodecane							
288.15	0.006	345.67	3.20	3.27	12.84	1.11	0.27
298.15	0.007	350.54	3.89	3.99	12.87	1.37	0.36
308.15	0.009	365.87	5.23	5.34	13.88	2.59	1.81
318.15	0.040	370.78	5.17	5.65	12.18	1.84	1.11
2-Butanol+ Dodecane							
288.15	0.02	365.78	3.79	3.99	10.08	1.81	0.87
298.15	0.03	365.76	4.14	4.45	9.48	1.79	0.54
308.15	0.04	375.67	4.34	4.75	8.85	1.54	0.05
318.15	0.03	376.34	4.37	4.69	8.51	0.97	0.73

Table-5: Experimental density, reduced volume, experimental and theoretical heat capacity obtained from various liquid state models and their corresponding % deviations at different temperatures.

X_1	ρ_{mix}	$\tilde{V}$	Cp^{Exp}	Cp^{flory}	Cp^{RS}	$Cp^{Glinski}$	$\%\Delta^{Flory}$	$\%\Delta^{RS}$	$\%\Delta^{Glinski}$
1-Butanol+ Dodecane: T=288.15K									
0.08048	753.82	1.0008	364.22	355.20	355.12	339.46	2.48	2.50	6.80
0.19017	756.5	1.0015	344.32	333.15	332.97	303.80	3.24	3.30	11.77
0.28812	759.47	1.0019	325.39	313.46	313.22	277.69	3.67	3.74	14.66
0.38654	762.98	1.0023	305.76	293.67	293.40	255.57	3.95	4.04	16.41
0.44097	765.23	1.0024	294.85	282.73	282.45	244.77	4.11	4.21	16.98
0.4835	767.14	1.0025	286.04	274.18	273.89	236.94	4.15	4.25	17.16
0.58849	772.65	1.0026	263.8	253.07	252.80	219.57	4.07	4.17	16.76
0.61515	774.27	1.0026	257.68	247.71	247.45	215.56	3.87	3.97	16.35
0.69605	779.63	1.0026	240.13	231.45	231.21	204.21	3.61	3.71	14.96
0.79594	787.76	1.0025	217.56	211.37	211.19	191.71	2.85	2.93	11.88
0.90295	799.12	1.0019	192.97	189.85	189.77	179.90	1.62	1.66	6.77
0.95231	805.7	1.0013	181.36	179.93	179.89	174.92	0.79	0.81	3.55
1-Butanol+ Dodecane: T=298.15K									
0.08048	746.51	1.0106	370.79	359.94	359.81	345.03	2.93	2.96	6.95
0.19017	749.12	1.0114	351.89	338.09	337.85	310.18	3.92	3.99	11.85
0.28812	752.04	1.0118	333.33	318.58	318.27	284.46	4.42	4.52	14.66
0.38654	755.51	1.0122	313.86	298.98	298.62	262.53	4.74	4.85	16.36
0.44097	757.73	1.0124	303.08	288.14	287.77	251.77	4.93	5.05	16.93
0.4835	759.62	1.0125	294.28	279.67	279.30	243.95	4.97	5.09	17.10
0.58849	765.09	1.0126	272.13	258.76	258.40	226.55	4.91	5.05	16.75
0.61515	766.72	1.0125	265.84	253.45	253.09	222.51	4.66	4.79	16.30
0.69605	772.04	1.0125	248.35	237.33	237.02	211.08	4.44	4.56	15.01
0.79594	780.2	1.0122	225.46	217.44	217.19	198.46	3.56	3.67	11.98
0.90295	791.57	1.0114	200.34	196.12	195.99	186.48	2.11	2.17	6.92
0.95231	798.15	1.0108	188.36	186.29	186.21	181.42	1.10	1.14	3.68
1-Butanol+ Dodecane: T=308.15K									
0.08048	739.13	1.0012	376.59	364.79	364.66	350.10	3.13	3.17	7.03
0.19017	741.67	1.0020	359.80	342.80	342.53	315.23	4.72	4.80	12.39
0.28812	744.51	1.0025	341.79	323.17	322.81	289.40	5.45	5.55	15.33
0.38654	747.93	1.0029	322.51	303.44	303.02	267.32	5.91	6.04	17.11
0.44097	750.12	1.0031	311.79	292.53	292.10	256.47	6.18	6.32	17.74
0.4835	752.00	1.0032	303.09	284.01	283.57	248.57	6.30	6.44	17.99
0.58849	757.40	1.0033	281.00	262.96	262.53	230.98	6.42	6.57	17.80
0.61515	759.03	1.0032	274.56	257.62	257.20	226.89	6.17	6.32	17.36
0.69605	764.36	1.0031	257.05	241.40	241.03	215.31	6.09	6.23	16.24
0.79594	772.50	1.0028	233.92	221.38	221.09	202.50	5.36	5.48	13.43
0.90295	783.88	1.0019	208.32	199.93	199.77	190.34	4.03	4.10	8.63
0.95231	790.48	1.0012	195.95	190.03	189.95	185.19	3.02	3.06	5.49

1-Butanol+ Dodecane: T=318.15K									
0.08048	731.65	1.0018	382.63	370.66	370.07	359.04	3.13	3.28	6.16
0.19017	734.12	1.0032	376.77	349.33	348.10	327.09	7.28	7.61	13.18
0.28812	736.86	1.0043	350.48	330.28	328.65	302.65	5.76	6.23	13.65
0.38654	740.20	1.0054	331.46	311.15	309.26	281.21	6.13	6.70	15.16
0.44097	742.36	1.0060	320.93	300.56	298.60	270.49	6.35	6.96	15.72
0.4835	744.23	1.0064	312.27	292.29	290.31	262.61	6.40	7.03	15.90
0.58849	749.54	1.0075	290.20	271.88	269.95	244.81	6.31	6.98	15.64
0.61515	751.18	1.0076	283.62	266.70	264.81	240.63	5.97	6.63	15.16
0.69605	756.46	1.0084	266.23	250.97	249.28	228.68	5.73	6.37	14.11
0.79594	764.59	1.0093	242.97	231.54	230.25	215.30	4.70	5.23	11.39
0.90295	775.98	1.0100	216.75	210.74	210.04	202.43	2.77	3.10	6.61
0.95231	782.60	1.0101	204.16	201.14	200.78	196.93	1.48	1.66	3.54
2-Butanol+ Dodecane: T=288.15K									
0.04602	752.79	1.0009	371.2	362.89	362.73	355.83	2.24	2.28	4.14
0.0507	752.85	1.0010	370.87	362.03	361.85	354.32	2.38	2.43	4.46
0.09287	753.61	1.0014	365.51	354.26	353.93	341.23	3.08	3.17	6.64
0.18128	755.47	1.0022	351.44	337.95	337.39	316.59	3.84	4.00	9.92
0.24985	757.15	1.0027	339.54	325.31	324.60	299.69	4.19	4.40	11.74
0.30044	758.57	1.0031	330.4	315.98	315.18	288.29	4.36	4.61	12.75
0.33974	759.79	1.0033	323.35	308.73	307.88	279.98	4.52	4.78	13.41
0.38271	761.21	1.0036	315.22	300.81	299.91	271.40	4.57	4.86	13.90
0.48939	765.43	1.0040	295.51	281.13	280.18	252.11	4.86	5.19	14.69
0.59429	770.68	1.0042	276.16	261.79	260.87	235.51	5.20	5.54	14.72
0.69831	777.27	1.0039	255.61	242.60	241.80	220.97	5.09	5.40	13.55
0.80469	785.96	1.0033	233.26	222.98	222.39	207.74	4.41	4.66	10.94
0.90245	796.36	1.0021	210.78	204.95	204.62	196.83	2.76	2.92	6.62
0.95177	802.84	1.0012	198.92	195.86	195.68	191.72	1.54	1.63	3.62
2-Butanol+ Dodecane: T=298.15K									
0.04602	745.46	1.0011	375.87	367.72	367.45	361.73	2.17	2.24	3.76
0.0507	745.51	1.0012	375.91	366.88	366.59	360.34	2.40	2.48	4.14
0.09287	746.19	1.0017	371.99	359.35	358.83	348.24	3.40	3.54	6.38
0.18128	747.97	1.0025	359.44	343.55	342.65	325.17	4.42	4.67	9.53
0.24985	749.59	1.0031	348.04	331.30	330.16	309.13	4.81	5.14	11.18
0.30044	750.94	1.0035	339.21	322.26	320.98	298.19	5.00	5.37	12.09
0.33974	752.15	1.0038	332.29	315.23	313.87	290.17	5.13	5.54	12.67
0.38271	753.51	1.0041	324.42	307.55	306.12	281.85	5.20	5.64	13.12
0.48939	757.62	1.0046	304.59	288.49	286.97	262.94	5.29	5.78	13.67
0.59429	762.72	1.0048	285.33	269.74	268.28	246.47	5.46	5.98	13.62
0.69831	769.2	1.0046	265.16	251.15	249.87	231.89	5.28	5.77	12.55
0.80469	777.8	1.0039	243.52	232.14	231.18	218.50	4.67	5.07	10.27
0.90245	788.21	1.0025	221.25	214.67	214.13	207.37	2.98	3.22	6.27

0.95177	794.74	1.0014	209.36	205.85	205.57	202.13	1.68	1.81	3.45
2-Butanol+ Dodecane: T=308.15K									
0.04602	738.06	1.0013	380.02	372.94	372.58	367.90	1.86	1.96	3.19
0.0507	738.11	1.0014	380.01	372.13	371.73	366.62	2.07	2.18	3.52
0.09287	738.72	1.0020	377.88	364.82	364.13	355.43	3.46	3.64	5.94
0.18128	740.36	1.0029	367.12	349.49	348.27	333.82	4.80	5.13	9.07
0.24985	741.9	1.0036	356.53	337.60	336.06	318.59	5.31	5.74	10.64
0.30044	743.22	1.0040	348.12	328.83	327.10	308.10	5.54	6.04	11.50
0.33974	744.36	1.0043	341.43	322.01	320.17	300.37	5.69	6.23	12.03
0.38271	745.69	1.0046	333.69	314.56	312.62	292.28	5.73	6.31	12.41
0.48939	749.62	1.0052	313.86	296.06	294.01	273.76	5.67	6.32	12.78
0.59429	754.56	1.0055	294.46	277.87	275.89	257.43	5.63	6.31	12.58
0.69831	760.88	1.0053	274.5	259.83	258.10	242.81	5.34	5.97	11.54
0.80469	769.39	1.0045	253.41	241.38	240.09	229.27	4.75	5.26	9.53
0.90245	779.73	1.0029	231.68	224.43	223.71	217.92	3.13	3.44	5.94
0.95177	786.27	1.0016	219.79	215.88	215.50	212.55	1.78	1.95	3.29
2-Butanol+ Dodecane: T=318.15K									
0.04602	730.61	1.0015	383.08	378.56	378.26	373.83	1.18	1.26	2.42
0.0507	730.64	1.0016	383.28	377.77	377.44	372.60	1.44	1.52	2.79
0.09287	731.15	1.0023	382.79	370.66	370.10	361.85	3.17	3.32	5.47
0.18128	732.63	1.0034	374.26	355.76	354.77	341.03	4.94	5.21	8.88
0.24985	734.07	1.0042	364.7	344.20	342.95	326.31	5.62	5.96	10.53
0.30044	735.32	1.0046	356.68	335.68	334.27	316.16	5.89	6.28	11.36
0.33974	736.4	1.0049	350.35	329.05	327.56	308.66	6.08	6.51	11.90
0.38271	737.68	1.0053	342.58	321.81	320.23	300.81	6.06	6.52	12.19
0.48939	741.45	1.0059	323.17	303.83	302.16	282.78	5.98	6.50	12.50
0.59429	746.23	1.0062	303.75	286.15	284.54	266.83	5.80	6.33	12.15
0.69831	752.33	1.0061	284	268.61	267.21	252.52	5.42	5.91	11.09
0.80469	760.64	1.0052	263.01	250.68	249.63	239.21	4.69	5.09	9.05
0.90245	770.88	1.0033	241.63	234.20	233.61	228.03	3.08	3.32	5.63
0.95177	777.38	1.0019	230.03	225.88	225.58	222.73	1.80	1.94	3.17

Conclusion

Finally, it is concluded that the theoretical results computed from Flory's statistical liquid state model deal a fair agreement with experimental findings for all the temperatures in comparison to Ramaswamy and Glinski model. The decreasing order of average absolute percentage deviation is as follows Glinski > Ramaswamy > Flory. The magnitude and actual sign of excess function depends on the relative strength of these two opposing effects. For positive values of excess function association of molecules are more dominant than packing effect. Conversely, for negative values the dipolar-dipolar and packing effect are more dominant. McAllister four body provides excellent results in comparison to three body model for all the temperatures.

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