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Evaluation of excess surface tension of ternary liquid mixture of hexane, decane, hexadecane using Brock and Bird's relation at 303.16K temperature

S.K. MISHRA* and S.N.TRIPATHI

Chemical Research Laboratories, Post Graduate Department of Chemistry, Government College, Amarpatan, (A.P.S. University) Amarpatan - 485 775 (India).

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ABSTRACT

The present investigation deals with the evaluation of surface tension and excess surface. Tension values in organic liquid mixture of hexane, decane and hexadecane a typical interest from Brock and Bird relation using experimental data.

Key words: Surface Tension, hexane, decane and hexadecane.

INTRODUCTION

Surface tension is diagnostic parameter for describing various properties of liquids mixtures. In the case of liquid mixtures adhesive and cohesive forces change with composition of the mixture and this change is reflected in the form of excess surface tension, defined by the relation:

$$\sigma^{E} = \sigma mix \frac{\Sigma X_i \sigma_i}{i=1}$$

Where σ_{mix} is the surface tension of the mixture and Xi and σ_i are the mole fraction and surface tension of the component in the mixture.

Pioneer attempts [1-5] have been made by several investigations to calculate theoretically the surface tension of liquids and liquids mixtures. Summarized discussions have been given by Defay and Priogogine[7] .H. Hildebrand [6], Guggenheion [8], Onno and Kohno and Gubbins and Haile, Flory's theory[11] recently expanded to enable the calculation of the surface tension of the pure liquids and liquid mixtures and average potential model (APM) theory of Priogogine has been examined by singh et al and both have been compared by Mishra el al [13] over wide range of temperatures and compositions. The increasing importance of surface tension in oil recovery and dam engineering inspired the author towards its theoretical evaluation in mixture following a simple but efficient and correct method due to Brock and Bird [14].

Mathematical expressions for excess surface tension from Brock and Bird's relation
According to Brock and Bird's the surface tension (o-) is given by the equation:

$$\sigma(P_c^{2/3}T_c)^{1/3} = (-0.951 + 0.432)/Z_c.(1-Tr)^{11/9} \quad ...(1)$$

Here Pc,Tc,Vc,Zc and Tr stands for critical pressure, critical temperatures, critical volume, compressibility factor and reduced temperature respectively.

Critical compressibility factor and reduced temperature are given by:

$$Z_c = P_c V_c / RT_c \quad ...(2)$$

$$T_r = T/T_c \quad ...(3)$$

T stand for absolute temperature and R for the gas constant. However it does not work well for associated liquids. This technique has been claimed to give errors of less than 7% for many non aqueous solutions. Eq.(1.01) when extended to mixtures may be written as:

$$\sigma_{mix}/(Pc_m {}^{2}Tc_m)^{1/3} = (-0.951+0.432)/Zc_m.(1-Tr_m)^{11/9} \quad ...(4)$$

Table 1: Surface tension, critical constants and related parameters of pure liquids at 303.16 K

Liquid	Pc Atm Ref. 17	Vc -1 (1.mole^{-1})	Tc Ok Ref.17	Tr. Eq. 1.03	Zc Eq. 1.02	Caled: Dyn cm-1eq.(1.01
Hexane	29.30	0.370	504.70	0.60067	0.26179	17.23
Decane	20.80	0.608	617.60	0.49087	0.24960	22.01
Hexadecane	14.00	0.920	720.60	0.42071	0.21784	22.58

Table 2: Surface tension and excess surface tension values of ternary mixture of Hexane (X1) - Decane (X2) - Hexadecane (X3) at 303.16 K

Mole fract. X2	Mole Frac. X3	Expt1 dyn.cm.ref 16	Clacd 1 dyn.cm. ref16	Calcd dyn. Cm. eq. (1.04)	% ref. 16	%
0.9491	0.0509	23.16	22.94	21.99	0.9	5.0
0.8256	0.1744	23.82	23.59	23.10	0.9	3.0
0.7346	0.2654	24.18	24.05	23.67	0.5	2.1
0.5988	0.4012	24.79	24.70	24.48	0.4	1.2
0.8580	0.0000	22.28	22.09	21.48	0.8	3.5
0.7535	0.1048	22.44	22.71	22.17	-1.2	1.2
0.6457	0.2123	22.74	23.31	22.87	-2.5	-0.57
0.5975	0.2605	23.06	23.57	23.18	-2.2	-0.52
0.4467	0.4113	23.24	24.33	24.15	-4.7	-3.9
0.7329	0.0000	21.68	21.58	20.93	0.5	3.4
0.6353	0.0974	21.84	22.19	21.62	-1.7	1.0
0.4795	0.2534	21.99	23.10	22.62	-5.0	-3.0
0.3902	0.3427	22.16	23.59	23.27	-6.4	-5.0
0.3253	0.4076	22.24	23.81	23.70	-7.0	-6.5
0.4963	0.0000	20.44	20.52	19.86	-0.4	2.8
0.3784	0.1185	20.38	21.35	20.69	-4.7	-1.5
0.3058	0.1911	20.30	21.83	21.21	-7.4	10.4
0.1547	0.3422	20.25	22.75	22.29	-12.3	-10.0
0.0980	0.3989	20.27	23.06	22.68	-13.8	-11.8
0.3998	0.0000	19.98	20.85	19.38	-0.3	3.0
0.2671	0.1237	19.80	20.97	20.22	-5.9	-2.1
0.1895	0.2103	19.66	21.55	20.88	-9.6	-6.2
0.1190	0.2808	19.52	22.00	21.39	-12.7	-10.4
0.0690	0.3300	19.35	22.31	21.74	-15.3	-12.3
Average Deviation %					-4.54	-1.54

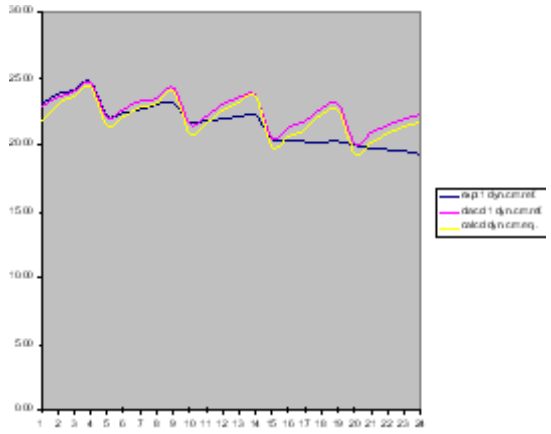

Fig. 1:

Characteristic parameters Pc_m, $Tc_m$and Vc_m for the mixtures are calculated from the critical constants of pure liquids. The simplest procedure is to assume that Pc_m, Tc_m and Vc_m are the mole fraction averages i.e.

$$Pc_m = \frac{\Sigma^3}{I} xi\ P_{ci} \quad etc \qquad ....(5)$$

In case of ternary mixtures

$$Pc_m = X_1 P_{c1} + X_2 P_{c2} + X_3 P_{c3}$$
$$Vc_m = X_1 V_{c1} + X_2 V_{c2} + X_3 V_{c3}$$
$$Tc_m = X_1 T_{c1} + X_2 T_{c2} + X_3 T_{c3} \qquad ...(6)$$

Where X_1, X_2 and X_3 are the mole fractions of the pure components. Tr_m and Zc_m are given by

$$Tr_m = T/Tcm \qquad ...(7)$$

$$Zc_m = (Pc_m X Vc_m)/RTc_m \qquad ...(8)$$

Excess surface tension 0- is calculated by using the expressions:

$$\sigma^E calcd = \sigma mix\ (calcd) - \Sigma^3 X\ 1\ \sigma 1 \qquad ...(9)$$
$$i=1$$

Where i = 1, 3 stands for respective components in the system.

Evaluation of excess surface tension of Hexane, Decane and Hexadecane mixture using Brock's and Bird's relation at 303.16 K.

The present investigation deals with evaluation of surface tension and excess surface tension values in organic liquid mixture of hexane, decane, hexadecane typical interest from Brock and Bird's relation using experimental data of J.D. Pandey and N.Pant [16]. The calculated surface tension óvalues of pure liquids Viz. hexane, decane and hexadecane are enlisted in the last column of the table (1.1) critical constants and related parameters of pure liquids: critical pressure Pc, citical Volume Vc, critical temperature Tc[17], reduced temperature (1.3) and critical Compressibility Zc (1.2) are tabulated in the column first to fifth of the table 1.1. The calculated values for the mixtures of hexane-decane and hexadecane are enlisted in the table 1.2

A perusal of the column fifth of the table 1.2 and plotted graph 1.3 shows that values of surface tension obtained, have the same trend as in the experimental values. The results in not beyond of expectation which confirms the validity of Brock and Bird's relation, which further confirms the assumption on which the relation based. The percentage deviation obtained from Brock and Bird's relation has been given in the column seventh of the table 1.2 the percentage deviation is obtained as positive and negative both. The negative magnitude of deviation are generally obtained when second component i.e. decane as taken with lowest mole fraction. The positive lowest deviation has been obtained when the mole fraction is taken in the least amount.

The average percentage deviation given the column has also same trend as obtained by the previous workers[15-29]. The magnitude of average percentage deviation (-1.54) is less than average percentage deviation (-4.54) obtained which reveals better agreement and confirms the validity of Brock and Bird's relation.

The Brock and Bird's relation is used for the determination of surface tension of ternary mixture and evaluation of excess surface tension

of non polar liquids in précised way without bothering the determining the other parameters as in the other theories. Moreover the method is simpler to operate and only knowledge of critical parameters is needed. Critical constant's values are easily available in literature [17] can be widely used for determination of the surface tension of multicomponent systems.

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