Scholarly Research Journal for Interdisciplinary Studies,
Online ISSN 2278-8808, SJIF 2016 = 6.177, www.srjis.com
UGC Approved Sr. No.49366, NOV-DEC 2017, VOL- 4/37

PREDICTION OF SURFACE TENSION FOR BINARY LIQUID MIXTURES FROM ASSOCIATED AND NON-ASSOCIATED PROCESSES AT VARIOUS TEMPERATURES

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Abstract

Prediction of surface tension is of outstanding importance in many scientific and technological areas such as liquid-liquid extraction, gas absorption, distillation, condensation, environmental sciences, material sciences, process simulation, molecular dynamics etc and play a significant role in several industries such as paints, detergents, agrochemicals and petroleum. As a fundamental parameter, surface tension is the single most accessible experimental parameter that describes the thermodynamic state and contains at least implicit information on the internal structure of a liquid interface. Apart from this theoretical interest, a detailed understanding of the behavior of a vapor-liquid interface, such as enrichment of one component in a liquid surface is important for modeling a distillation process. These non-associated and associated models were compared and tested for different systems showing that the associated processes yield fair agreement between theory and experiment as compared to non-associated processes.

Keywords: *Surface Tension, Prigogine-Flory-Patterson, McAllister, Sanchez, Eberhart, GoldSack*

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Introduction

Prediction of surface tension is of out standing importance in many scientific and technological areas such as liquid-liquid extraction, gas absorption, distillation, condensation, environmental sciences, material sciences, process simulation, molecular dynamics etc and play a significant role in several industries such as paints, detergents, agrochemicals and petroleum. As a fundamental parameter, surface tension is the single most accessible experimental parameter that describes the thermodynamic state and contains at least implicit information on the internal structure of a liquid interface. Apart from this theoretical interest, a detailed understanding of the behavior of a vapor-liquid interface, such as enrichment of one component in a liquid surface is important for modeling a distillation process.

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Densities and surface tensions were measured for the binary liquid mixtures formed by formamide, N-methylacetamide, di-methylformamide and di-methylacetamide with acetonitrile at 293.15, 298.15, 303.15 and 313.15 K and atmospheric pressure over the whole concentration range. Prigogine-Flory-Patterson model (PFP), Ramaswamy and Anbananthan (RS), model devised by Glinski, Sanchez equation, Goldsack relation and Eberhart models were utilized to predict the associational behavior of weakly interacting liquids. The measured properties were fitted to Redlich-Kister polynomial relation to estimate the binary coefficients and standard errors. Furthermore, McAllister multi body interaction model was also used to correlate the binary properties. These non-associated and associated models were compared and tested for different systems showing that the associated processes yield fair agreement between theory and experiment as compared to non-associated processes.

Experimental

High purity and AR grade samples used in this experiment were obtained from Merck Co. Inc., Germany and purified by distillation in which the middle fraction was collected. Differential capillary rise method was used for all the reported results. Data were taken from 293.15 K up to 313.15 K in temperature intervals of 5 K. The reported uncertainty ($\pm 4.5.10^{-4}$ $N.m^{-1}$) is the highest uncertainty found from all the data points. The uncertainty in the density measurement was within ± 6.4 $kg.m^{-3}$. The densities of the pure components and their mixtures were measured with the bi-capillary pyknometer. The liquid mixtures were prepared by mass in an air tight stopped bottle using an electronic balance model SHIMADZUAX-200 accurate to within ±0.1 mg. The average uncertainty in the composition of the mixtures was estimated to be less than ±0.0001. All molar quantities were based on the IUPAC relative atomic mass table.

Results and Discussion

The values of standard deviation obtained from Redlish-Kister polynomial lie between 0.11 - 0.97 and the largest value corresponds to acetonitrile + DMA mixture at 313.15 K. It is observed that McAllister four body model is correlated the mixture surface tension to a significantly higher degree of accuracy for all the systems than the three body model. Generally McAllister model is adequate in correlating the systems having small deviations. With the increase of mole fraction, the values of surface tension obtained from all the models decrease at all temperatures except at few places. The overall average estimated error for all the systems under investigation at all temperatures obtained from various equations (5, 19, 10, 22, 25 & 29) are (3.24, 6.94, 9.80, 5.83, 6.47 & 6.54), (6.12, 11.73, 5.72,

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7.19, 8.78 & 11.77), (8.52, 9.60, 8.01, 7.70, 9.50 & 14.60) and (11.10, 20.15, 10.22, 9.01, 11.38 & 14.50) respectively.

Conclusively, associated process give more reliable results as compared to non-associated processes and helpful in deducing the internal structure of associates through the fitted values of surface tension in a hypothetical pure associate and observed dependence of concentration on composition of a mixture.

Comparison of absolute average deviation values obtained from various liquid state models

acetonitrile+formamide

Temperature	Kas	σ_{ab}/ mN.m^{-1}	σ_{rs}/ mN.m^{-1} RS	σ_{ab}/ mN.m^{-1} PFP	σ/ mN.m^{-1} Gelinski	σ/ mN.m^{-1} Sanchez	σ/ mN.m^{-1} Goldsack	σ/ mN.m^{-1} Eberhart
293.15	0.00013	57.80	4.98	3.88	6.48	5.24	4.46	11.13
298.15	0.00010	57.90	2.40	4.05	9.80	8.11	7.17	4.87
303.15	0.00012	57.20	2.62	3.60	10.15	8.52	7.44	2.90
313.15	0.00011	56.80	2.96	16.24	12.82	9.57	6.84	7.29

acetonitrile+NMA

293.15	0.00014	33.90	7.90	9.60	7.33	6.66	8.25	11.71
298.15	0.00015	33.10	8.26	18.54	7.72	7.10	8.68	11.47
303.15	0.00016	32.80	1.10	10.76	1.10	8.97	10.53	13.26
313.15	0.00018	32.20	7.24	8.02	6.73	6.04	7.67	10.65

acetonitrile+DMF

293.15	0.00012	36.30	8.55	10.19	7.97	7.63	9.37	14.26
298.15	0.00012	35.90	8.53	9.20	8.01	7.69	9.53	14.40
303.15	0.00012	35.50	8.68	9.36	8.19	7.91	9.73	16.19
313.15	0.00013	35.30	8.32	9.66	7.87	7.58	9.38	13.55

acetonitrile+DMA

293.15	0.00013	32.90	10.02	19.28	9.18	7.65	10.26	13.27
298.15	0.00014	32.10	10.81	19.14	9.93	8.52	11.10	13.96
303.15	0.00014	31.80	12.69	20.80	11.80	10.45	12.99	16.36
313.15	0.00014	31.20	10.89	21.41	9.98	9.45	11.18	14.44

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Acknowledgement

Author is thankful to Department of Chemistry, DBS.College, for their help and cooperation

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