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Validation of Theoretical Approach of Viscosity in Polar-Apolar Liquid Mixtures Containing a Nuclear Extractant at 303.15K

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ABSTRACT

Viscosities (η) of binary liquid mixtures of a nuclear extractant, di-(2-ethyl hexyl) phosphoric acid (DEHPA, $C_{16}H_{35}O_4P$) with three apolar solvents, namely n-pentane (C_5H_{12}), benzene (C_6H_6) and carbon tetrachloride (CCl_4), were experimentally measured at 303.15K and pressure 0.1MPa. Again viscosities of the studied mixtures were computed using several theoretical models such as Grunberg-Nissan, Katti and Chaudhri, Hind , Tamura and Kurata, Heric and Eyring-Margules. The experimentally measured viscosities of the studied mixtures were analysed on the basis of above said theoretical models.

Keywords: Viscosity, DEHPA, Apolar Liquids, Molecular Interaction, TheoriticalModels

I. INTRODUCTION

Viscometric study of liquid mixtures plays an important role in engineering such as mass transfer, heat transfer and fluid flow [1, 2]. In extraction process di-(2-ethyl hexyl) phosphoric acid (DEHPA) is used commercially to recover cobalt, zinc, uranium, plutonium, vanadium and other lanthanide /actinide elements from their respective ores [3 - 5]. The extraction efficacy of an extractant increases with the addition of suitable diluents / modifiers [5, 6]. The viscosity measurements is also helpful to find its application in characterizing aspects of mixture behavior in extraction process. In continuation of our earlier work [7], we are extending our present study on theoretical values of viscosity of the three binary mixtures using Grunberg-Nissan, Katti and Chaudhri, Hind, Tamura and Kurata, Heric and Eyring-Margules.The theoretical viscosity values were correlated with those experimental values. The relative merits of these models for the studied liquid mixtures was verified in terms of standard deviations.

II. METHODS AND MATERIAL

The chemicals used in this present investigation were of analytical reagent (AR) grade and obtained from E-Merck chemicals Ltd India. The procedure of measurement of viscosity is same as reported in earlier works [8, 9] at temperature 303.15K and pressure 0.1MPa. All samples were kept in air tight bottles and adequate precautions were taken to avoid evaporation and contamination. Temperature of all samples was maintained to an accuracy of 0.1K in an electronically controlled thermostatic waterbath.

III. RESULTS AND DISCUSSION

Experimental data on viscosity of the three liquid mixtures over entire molefraction range of DEHPA (X_2) have been reported in our earlier investigations [7], presented in Table-1. These data have been correlated with predicted viscosities by using different theoretical models [10-13]. The viscosity (dynamic, η / kinematic, ν) of liquid mixtures have been correlated with the following theoretical models (Eq. 1 – 6):

Grunberg-Nissan

$$\eta = \exp\left(x_1 \ln \eta_1 + x_2 \ln \eta_2 + x_1 x_2 d_{12}\right) \quad (1)$$

where d_{12} is a parameter proportional to the interchange energy and has been regarded as an indicator for the non-ideal behaviour of binary mixtures.

Katti and Chaudhri

$$\ln \eta V = x_1 \ln \eta_1 V_1 + x_2 \ln \eta_2 V_2 + x_1 x_2 \left(\frac{W_{vis}}{RT}\right) \quad (2)$$

where W_{vis} is an interaction term.

Hind

$$\eta = x_1^2 \eta_1 + x_2^2 \ln \eta_2 + 2 x_1 x_2 \eta_{12} \quad (3)$$

where η_{12} is attributed to unlike pair interactions.

Tamura and Kurata

$$\eta = x_1 \phi_1 \eta_1 + x_2 \phi_2 \eta_2 + 2 (x_1 x_2 \phi_1 \phi_2)^{1/2} C \quad (4)$$

where (x_1 and x_2), (ϕ_1 and ϕ_2) and (η_1 and η_2) are the molefraction, volume fraction and viscosities of pure components respectively and C is an adjustable parameter.

Heric

$$\ln \eta = x_1 \ln \eta_1 + x_2 \ln \eta_2 + x_1 \ln M_1 + x_1 \ln M_2 - \ln (x_1 M_1 + x_2 M_2) + x_1 x_2 \left[\nu_{12} + \nu_{21} (x_1 - x_2)\right] \quad (5)$$

where (ν_{12} and ν_{21})are the adjustable parameters and (M_1 and M_2) are molecular mass of pure components.

Eyring-Margules

$$\ln (\eta V) = x_1 \ln (\eta_1 V_1) + x_2 \ln (\eta_2 V_2) + x_1 x_2 (A_{21} x_1 + A_{12} x_2) \quad (6)$$

where V_1, V_2 and V are the molar volumes of pure components and mixture respectively and A_{21} and A_{12} are adjustable parameters.

TABLE I. Experimental viscosity (η) in polar-apolar liquidmixtures such as DEHPA + n-pentane/ benzene/ CCl_4.

DEHPA + n-pentane		DEHPA + benzene		DEHPA + CCl_4	
x_2	η mPa.s	x_2	η mPa.s	x_2	η mPa.s
0.00	0.6	0.00	0.8	0.00	0.2
0.02	0.7	0.03	1.0	0.07	0.3
0.09	0.8	0.06	1.2	0.12	0.4
0.15	1.0	0.14	1.7	0.20	0.6
0.23	1.6	0.22	2.3	0.28	1.1
0.35	2.6	0.31	3.2	0.34	1.5
0.41	3.3	0.39	3.9	0.42	2.4
0.45	3.8	0.47	5.1	0.46	2.7
0.48	4.1	0.53	6.2	0.48	3.0
0.55	5.4	0.59	7.5	0.56	3.9
0.63	6.7	0.66	9.1	0.68	6.0
0.71	8.5	0.71	10.5	0.71	6.7
0.79	10.5	0.78	12.4	0.79	9.0
0.84	12.1	0.84	14.2	0.84	11.0
0.92	15.1	0.95	16.1	0.92	15.0
1.00	19.3	1.00	19.3	1.00	19.3

TABLE II. Adjustable interaction parameters and standard deviations(σ) in correlating viscosities of the binary mixture.

Theoretical Models		Binary System (taking DEHPA as one component)		
		n-pentane	benzene	carbon tetrachloride
Grunberg-Nissan	d_{12}	1.7693	0.9548	1.5898
	σ	0.0492	0.0390	0.0503

Katti-Chaudhri	W_{vis}/RT	2.3141	1.7773	2.3238
	σ	0.0462	0.0304	0.0594
Hind	η_{12}	-3.9634	-1.4904	1.5688
	σ	0.2096	0.2445	0.1399
Tamura-Kurata	C	-8.2430	-6.6821	-3.3495
	σ	1.3283	1.2005	0.5209
Heric	v_{12}	2.8283	1.9142	1.8799
	v_{21}	1.0179	0.3921	0.7005
	σ	0.0380	0.0291	0.0444
Eyring-Margules	A_{21}	3.0149	3.2374	3.2855
	A_{12}	1.6037	0	1.4205
	σ	0.0464	0.0939	0.0496

The interaction parameters along with the values of standard deviations (σ) using the theoretical models are listed in Table-2. From the average values of standard deviation by considering experimental value of viscosity in the studied binary mixture, the applicability of the theoretical models follows the order:

Heric>Katti and Chaudhri>Grunberg-Nissan >Eyring-Margules>Hind > Tamura and Kurata

The smaller standard deviation for Heric model indicates more suitability than other models, which may predicts viscosity values close to experimental values of the three binary mixtures [10, 13].

IV. CONCLUSION

The variation of viscosity of the three liquid mixtures over entire molefraction range of DEHPA indicates the presence of molecular interaction among unlike molecules. Different theoretical models of viscosity have been correlated with the experimental data of viscosity in all the three mixtures. A good agreement is established between experimental data and theoretical values of viscosities. Out of all the models, Heric has shown smaller standard deviation among all the mixtures and predict viscosity values close to experimental data of the three mixtures.

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