International Journal of Engineering Applied Sciences and Technology, 2021
Vol. 6, Issue 6, ISSN No. 2455-2143, Pages 119-123
Published Online October 2021 in IJEAST (http://www.ijeast.com)

MATHEMATICAL CORRELATION OF THERMOPHYSICAL PROPERTIES FOR ACETONITRILE + N, N - DIMETHYLFORMAMIDE FROM 293.15-313.15K BY JOUYBAN ACREE MODEL

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***Abstract*— Density, viscosity and refractive indices were measured for a weak interacting liquid formed by acetonitrile and N, N-dimethylformamide (DMF) at 293.15, 298.15,303.15,308.15,313.15K temperature and 1atm pressure over the whole concentration range (0.2142-0.9567). Jouyban Acree model was used to calculate the physicochemical properties. Results obtained from Jouyban Acree model for various physicochemical properties were compared and tested with experimental values. Standard deviation was calculated from calculated and experimental values at different temperatures for all the three physicochemical properties and used as a criterion for the success of correlation. Mathematical calculation by the Jouyban Acree model deals a fair agreement with experimental results for all the three physico-chemical properties.**

Keywords— **Density, viscosity, refractive index, Jouyban Acree, acetonitrile, DMF**

I. INTRODUCTION

In the Continuation of our previously published work [1], an attempt has been made to corelate the experimental data of density, viscosity and refractive index of weakly interacting liquids at different temperature with Jouyban Acree model [2-6]. Khattab et al [7] correlate the physicochemical properties of water and ethanol system. Awasthi et al [8] corelate the viscosity of binary system at different temperatures.
Different physicochemical properties were calculated by Jouyban Acree [2-6] corelation model

$$\ln PCP_{AB} = X_A.\ln PCP_A + X_B.\ln PCP_B + J_x\left[\frac{X_A.X_B}{T^0}\right] + J_y\left[\frac{X_A.X_B.(X_A - X_B)}{T^0}\right] + J_z\left[\frac{X_A.X_B.(X_A - X_B)^2}{T^0}\right] \quad (1)$$

where J_x, J_y, J_z are coefficients which could be calculated using no -intercept regression of the experimental values. PCP_{AB}, PCP_A and PCP_B are physicochemical properties of binary system, acetonitrile and dimethylformamide respectively.

II. MATERIALS AND METHOD

A. Experimental section

Experimental work [1] has been performed by using AR quality acetonitrile and dimethyl formamide (DMF). Before starting the experiments each of liquid was purified by distillation process. Which was verified by chromatographic technique (Gas). Bicapillary pakynometer Ubbelohde suspended-level viscometer, and Abbe refractometer (Atago-3T) thermostatically controlled were used to determine the experimental density, viscosity and refractive index respectively at different temperatures. Physical properties of pure liquids at different temperatures were compared with the literature values presented in table 1.

B. computational method

computation of these physicochemical properties has been performed by no intercept regression method. Experimental and calculated values of these properties were compared and tested in term of standard deviation which was calculated by the given equation

$$\sigma = \left[\sum_{i=1}^{m}\left(\frac{\Delta\eta}{(k)}\right)^2\right]^{1/2} \quad (2)$$

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$\Delta\eta = (\eta_{exp} - \eta_{cal})$ where η_{exp} and η_{cal} are experimental and theoretical viscosity and k = (number of data point -number of adjustable parameter).

Table-1 Experimental and literature values of pure liquids

T/K	ρx10^{-3}(Kg.m^{-3})		η X 10^{3}(Pa. s)		N	
	Exp	Lit [1]	Exp	Lit[1]	Exp	Lit [1]
			Acetonitrile			
293.15	0.7865	0.7822	0.3699	-	1.3409	1.3441
298.15	0.7811	0.7765	0.3426	0.3410	1.3402	1.3416
303.15	0.7733	0.7713	0.3201	0.3240	1.3392	-
308.15	0.7665	-	0.3408	-	1.3283	-
313.15	0.7605	-	0.3348	-	1.3260	-
			N, N- dimethyl formamide			
293.15	0.9551	0.94873	0.9224	0.9243	1.4285	1.430
298.15	0.9501	0.94387	0.80006	0.802	1.4267	1.428
303.15	0.9419	0.9412	0.7399	-	1.4240	-
308.15	0.9357	-	0.7214	-	1.4221	-
313.15	0.9325	-	0.7204	-	1.4205	-

III. RESULT AND DISCUS SION

Table1 represents the experimental and literature vales of acetonitrile and dimethyl formamide at different temperatures. Table 2-4 represents the variation of standard deviation (σ) and respective parameters (J_x, Jy, Jz) calculated from 293.15 to313.15 for density, viscosity and refractive index respectively. R^2 values calculated for observational physicochemical properties are presented in table 5. table 6 represents the Experimental and calculated values of different physicochemical properties from temperature 293.15 to 313.15K.

Table-2 variation of (σ) for density

T/K	J_x	J_y	J_z	(σ)
293.15	66.05	27.41	-22.26	0.006
298.15	72.47	30.82	-21.36	0.007
303.15	82.57	39.25	-5.35	0.008
308.15	80.58	35.93	36.38	0.009
313.15	80.65	37.68	58.75	0.008

A close observation of table 2 reveals that standard deviation for density calculated from equation (2) lies in the range $0.006 < \sigma < 0.009$. the minimum value of σ was found to be 0.006 at 293.15K. values of (J_x, Jy, Jz) increases with increase in temperature. R^2 values for density presented in table5 decreases with increase in temperature in following order $0.9997 > R^2 > 0.9993$. which confirm the good applicability of model at low temperature. While in case of viscosity (table 3) the value of σ decreases with increase in temperature and lies in the range $1.142 > \sigma > 0.015$ the minimum value for σ (0.015) was observed at 313.15K. R^2 values calculated for viscosity increases with increase in temperature from (-7.2050 to 0.99965). results obtained from σ and R^2 for viscosity confirm that for this system Acree model holds good at 313. 15K.similarly σ value for refractive index presented in table 4 decreases with increase in temperature.

Table-3 variation of(σ) for viscosity

T/K	J_x	J_y	J_z	(σ)
293.15	-992.23	-1075.54	1593.16	1.142
298.15	-998.95	-1231.32	1852.94	0.077
303.15	-1053.43	-1360.09	2160.27	0.079
308.15	-1136.99	-1402.36	1954.61	0.077
313.15	743.6625	341.3274	-219.60	0.015

Its value lies in the range $0.005 > \sigma > 0.003$.the minimum value of σ for refractive index was found to be at 298.15K. values of (J_x, Jy, Jz) also increases with increase in temperature for both these properties. R^2 values calculated for refractive index (table5) confirm the success of the model at all temperatures.

Table-4 variation of (σ) for refractive index

T/K	J_x	J_y	J_z	(σ)
293.15	18.479	3.794	-15.955	0.005
298.15	21.688	8.250	-8.262	0.003
303.15	24.878	11.012	-2.418	0.004
308.15	27.352	16.964	27.876	0.005
313.15	24.887	10.750	19.167	0.004

Comparative study of experimental and calculated values of corresponding physicochemical properties from Jouyban Acree model from 293.15 to313.15K presented in table 6 reveals that experimental and calculated values of all the three physicochemical properties decreases as mole fraction of acetonitrile increases for all the temperatures. Calculated values of density and refractive index are very close to experimental values at 293.15K while for viscosity calculated value shows huge deviation from experimental values.

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Table-5 R^2 values

T/K	$R^2(\rho)$	$R^2(\eta)$	$R^2(n)$
293.15	0.99997	-7.02050	0.99999
298.15	0.99996	0.96001	1.00000
303.15	0.99993	0.95490	0.99999
308.15	0.99993	0.95211	0.99999
313.15	0.99993	0.99965	1.00000

Deviation for density increases while for viscosity and refractive index deviation decreases with increase in temperature. On the basis of above discussion, it is observed that for acetonitrile and dimethyl formamide system model gave excellent result for density at low temperature while for viscosity and refractive index better results are obtained at high temperature.

Table-6 Experimental and theoretical results

	$\rho x10^{-3}(Kg.m^{-3})$		η X 10^3(Pa. s)		n	
X_1	EXP	Cal	EXP	Cal	EXP	Cal
			T=293.15K			
0.2142	0.9391	0.9391	0.9752	2.5730	1.4189	1.4218
0.3802	0.9297	0.9296	0.2975	1.9157	1.4128	1.4154
0.5126	0.9158	0.9152	0.2482	1.3155	1.4047	1.4047
0.6206	0.8957	0.8966	0.2314	1.0153	1.3936	1.3920
0.7104	0.8748	0.8761	0.2319	0.8580	1.3823	1.3792
0.7863	0.8569	0.8556	0.2437	0.7527	1.3727	1.3678
0.8513	0.8354	0.8359	0.2642	0.6591	1.3615	1.3582
0.9075	0.8253	0.8178	0.2923	0.5633	1.3559	1.3506
0.9567	0.7902	0.8013	0.3276	0.4650	1.3385	1.3449
			T=298.15K			
0.2142	0.9342	0.9360	0.9531	0.7953	1.4182	1.4191
0.3802	0.9272	0.9276	0.2712	0.3615	1.4143	1.4145
0.5126	0.9215	0.9137	0.2249	0.2188	1.4112	1.4073
0.6206	0.8901	0.8953	0.2096	0.1850	1.3951	1.3978
0.7104	0.8721	0.8746	0.2109	0.1929	1.3859	1.3872
0.7863	0.8504	0.8536	0.2230	0.2214	1.3749	1.3765
0.8513	0.8344	0.8332	0.2436	0.2597	1.3668	1.3662
0.9075	0.8248	0.8143	0.2718	0.2982	1.3620	1.3567
0.9567	0.7899	0.7969	0.3073	0.3280	1.3448	1.3480
			T=303.15K			
0.2142	0.9304	0.9327	0.9512	0.7850	1.4181	1.4193
0.3802	0.9255	0.9248	0.2472	0.3366	1.4157	1.4152
0.5126	0.9192	0.9120	0.2036	0.1967	1.4125	1.4088
0.6206	0.8892	0.8949	0.1900	0.1659	1.3973	1.4002
0.7104	0.8706	0.8751	0.1925	0.1755	1.3880	1.3904

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0.7863	0.8584	0.8541	0.2056	0.2053	1.3819	1.3799
0.8513	0.8261	0.8329	0.2273	0.2446	1.3659	1.3693
0.9075	0.8259	0.8121	0.2570	0.2828	1.3659	1.3589
0.9567	0.7853	0.7922	0.2948	0.3103	1.3460	1.3488
			T=308.15K			
0.2142	0.9280	0.9325	0.8853	0.7250	1.4184	1.4221
0.3802	0.9234	0.9179	0.2342	0.3203	1.4163	1.4123
0.5126	0.9065	0.9025	0.1947	0.1901	1.4079	1.4045
0.6206	0.8801	0.8865	0.1831	0.1600	1.3947	1.3980
0.7104	0.8647	0.8694	0.1864	0.1684	1.3871	1.3909
0.7863	0.8561	0.8508	0.1999	0.1970	1.3830	1.3822
0.8513	0.8248	0.8308	0.2219	0.2368	1.3675	1.3714
0.9075	0.8234	0.8098	0.2516	0.2796	1.3669	1.3586
0.9567	0.7805	0.7882	0.2891	0.3167	1.3459	1.3441
			T=313.15K			
0.2142	0.9255	0.9310	0.8024	0.7899	1.4158	1.4186
0.3802	0.9199	0.9130	0.8529	0.8775	1.4119	1.4084
0.5126	0.9002	0.8965	0.9007	0.8863	1.4010	1.3991
0.6206	0.8751	0.8813	0.8237	0.8253	1.3876	1.3907
0.7104	0.8615	0.8655	0.7250	0.7298	1.3801	1.3822
0.7863	0.8502	0.8479	0.6442	0.6280	1.3738	1.3729
0.8513	0.8227	0.8283	0.5312	0.5344	1.3595	1.3625
0.9075	0.8207	0.8069	0.4500	0.4545	1.3582	1.3512
0.9567	0.7798	0.7841	0.3809	0.3884	1.3379	1.3389

IV. CONCLUSION

It is concluded from the above discussion that the calculated results obtained from Jouyban Acree model are very compatible with experimental results. Model gave an excellent result for density at low temperature while in case viscosity and refractive index excellent results are obtained at high temperature. Correlation results confirm the success of experiment.

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