Naveen Awasthi, 2024, 12:3
ISSN (Online): 2348-4098
ISSN (Print): 2395-4752

International Journal of Science, Engineering and Technology

An Open Access Journal

Estimation of Transport Properties of Polar Solvents from 298.15-318.15K

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Abstract- In this paper, we have computed the viscosity of a solution containing to polar solvents such as benzyl alcohol and 2-propanol from Jouyban Acree (JA) model based on least square regression analysis method and McAllister multi body interaction model based on Eyring's theory absolute reaction rate from 298.15-318.15K. Results obtained from were compared with the literature value. Standard deviation was the criterion of the success of results. Jouyban Acree (JA) model found to be more consistent with experimental findings

Keywords- Jouyban Acree, molecular interactions, transports property, 2- Propenol.

I. INTRODUCTION

Sometimes experimental determination of transport and other thermodynamic properties of liquid mixtures are very difficult. In that case theoretical models play a significant role in the determination of various thermodynamic and transport properties. In recent past transport behavior of pure solvent mixtures of different solvents has become subject of deep interest for researchers in the synthesis of various drugs1 and industrial application such as process simulation, equipment design2 and molecular dynamics.

To fulfill this requirement various researchers3-4 have formulated theoretical models to determine the theoretical viscosity in the absence of experimental results. In the continuation of previously published work 5-6, this paper deals with a comparative study of two correlation models such as McAllister7 and Jouyban Acree model Jouyban8-9at different temperatures to determine the theoretical values of viscosity and compared with the literature values10. The main aim of this investigation is analyze the effect of temperature on the molecular association of aforementioned polar solvent mixture and test the accuracy of these mixing rules.

II. MODELING

Jouyban Acree model8-9 based on no intercept regression method is one of the most useful correlation models.

$$\ln \eta = X_A.\ln \eta_1 + X_B.\ln \eta_2 + J_0\left[\frac{X_A.X_B}{T}\right] + J_1\left[\frac{X_A.X_B.(X_A - X_B)}{T}\right] + J_2\left[\frac{X_A.X_B.(X_A - X_B)^2}{T}\right] \quad (1)$$

Where J0, J1, J2 are numerical coefficient calculated by least square method.

McAllister multi body interaction model based on Eyring's theory of absolute reaction rate According to him a temperature dependent empirical equation relate to kinematic viscosity can be represented as:

$$\partial = \frac{hN}{M} e^{\Delta G^*/RT^{\#}} \quad (2)$$

Where
∂=Kinematic viscosity
h = Planck constant
R = Gas constant
M = Molar mass
N = Avogadro number
T# = Absolute temperature
ΔG* = Movement of molecule between two layers of liquid

McAllister -3-body model

$$\ln \eta = x_1^3 \ln \eta_1 + 3x_1^2 x_2 \ln \eta_{12} + 3x_1 x_2 \ln \eta_{21} + x_2^3 \ln \eta_2 - \ln[x_1 + x_2 M_2/M_1] + 3x_1^2 x_2 \ln[(2 + M_2/M_1)/3] + 3x_1 x_2^2 \ln[(1 + 2M_2/M_1)/3] + x_2^3 \ln[M_2/M_1] \quad (3)$$

McAllister -4-body model

$$\ln \eta = x_1^4 \ln \eta_1 + 4x_1^3 x_2 \ln \eta_{1112} + 6x_1^2 x_2^2 \ln \eta_{1122} + 4x_1 x_2^2 \ln \eta_{222} + x_2^4 \ln \eta_2 - \ln[(x_1 + x_2 M_2/M_1)] + 4x_1^3 x_2 \ln[(3 + M_2/M_1)/4] + 6x_1^2 x_2^2 \ln[(1 + M_2/M_1)/2] + 4x_1 x_2^3 \ln[(1 + 3M_2/M_1)/4] + x_2^4 \ln(M_2/M_1) \quad (4)$$

M1 and M2 are molecular weight of corresponding liquids.

III. RESULT AND DISCUSSION

Table1 represents experimental viscosity and computed values of viscosity, by McAllistere-3-body, McAllister-4-body and Jouyban Acree models, their corresponding percentage deviations (%Δ), density of binary solution, reduced volume from 298.15-318.15K. Standard deviations (δ) varies from (0.028-0.018), (0.011-0.024) for McAllister-3 and 4-body whereas (0.008-0.005) for Jouyban Acree model from 298.15-318.15K. A close pursul of table-1 reveals that density of binary solution decreases as mole fraction (x1) increases but it becomes low at higher temperature due to rupture of hydrogen bonds present between the components of solvent mixtures. Viscosity computed from McAllister-3-body and 4-body model gave good result at initial concentrations but as concentration increases both the models show deviations from experimental values whereas Jouyban Acree models deals a fair agreement with experimental findings over the entire range of concentration from 298.15-318.15K. Decreasing order of standard deviations at lower temperature JA <Mc4< Mc3 whereas at higher temperature JA < Mc3 < Mc4.

Table 1: Experimental and theoretical values of viscosity from 298.15-318.15K

X_1	V ~	ρ_{mix}	η_{exp}	η_{Mc3}	η_{Mc4}	η_{JAc}	$\%\Delta_{Mc3}$	$\%\Delta_{Mc4}$	$\%\Delta_{JAc}$
				T=298.15K					
0.05	1.2534	1.0328	5.30	5.14	5.13	5.29	2.94	3.16	0.22
0.1	1.2545	1.0237	5.05	4.95	4.93	5.04	2.00	2.36	0.34
0.15	1.2558	1.0143	4.80	4.76	4.74	4.80	0.77	1.20	0.08
0.2	1.2573	1.0044	4.56	4.58	4.56	4.56	-0.36	0.09	-0.09
0.25	1.2589	0.9942	4.33	4.39	4.37	4.34	-1.41	-0.98	-0.18
0.3	1.2607	0.9836	4.12	4.22	4.20	4.12	-2.44	-2.04	-0.18
0.35	1.2626	0.9726	3.91	4.05	4.03	3.91	-3.46	-3.10	-0.09
0.4	1.2648	0.9612	3.71	3.88	3.87	3.71	-4.57	-4.24	-0.02
0.45	1.2671	0.9494	3.52	3.73	3.72	3.52	-5.85	-5.55	0.00
0.5	1.2696	0.9370	3.34	3.58	3.57	3.34	-7.44	-7.15	-0.14
0.55	1.2724	0.9242	3.17	3.45	3.44	3.17	-8.75	-8.45	0.06
0.6	1.2755	0.9108	3.01	3.32	3.31	3.00	-10.27	-9.93	0.20
0.65	1.2789	0.8969	2.86	3.20	3.19	2.85	-12.02	-11.63	0.22
0.7	1.2826	0.8824	2.72	3.09	3.08	2.71	-13.95	-13.51	0.19
0.75	1.2867	0.8673	2.58	3.00	2.98	2.58	-16.13	-15.63	0.04
0.8	1.2913	0.8515	2.46	2.91	2.90	2.46	-18.24	-17.71	0.05
0.85	1.2963	0.8351	2.35	2.83	2.82	2.35	-20.70	-20.18	-0.12
0.9	1.3017	0.8180	2.25	2.77	2.75	2.25	-22.84	-22.39	0.06
0.95	1.3079	0.8000	2.15	2.71	2.70	2.17	-26.15	-25.85	-1.17
				T=308.15K					

0.05	1.2615	1.0250	3.91	3.83	3.84	3.91	2.16	1.87	0.08
0.1	1.2627	1.0159	3.73	3.69	3.71	3.73	1.05	0.59	0.03
0.15	1.2641	1.0064	3.56	3.56	3.58	3.56	0.04	-0.51	0.03
0.2	1.2657	0.9965	3.39	3.42	3.44	3.39	-1.03	-1.61	-0.03
0.25	1.2674	0.9863	3.23	3.29	3.31	3.23	-1.98	-2.54	0.04
0.3	1.2693	0.9756	3.08	3.17	3.18	3.07	-2.98	-3.49	0.14
0.35	1.2713	0.9646	2.92	3.05	3.06	2.92	-4.26	-4.72	0.04
0.4	1.2736	0.9531	2.77	2.93	2.94	2.77	-5.63	-6.04	-0.09
0.45	1.2760	0.9412	2.63	2.82	2.83	2.63	-7.02	-7.41	-0.13
0.5	1.2787	0.9288	2.49	2.71	2.72	2.50	-8.81	-9.19	-0.43
0.55	1.2817	0.9159	2.37	2.61	2.62	2.37	-10.08	-10.48	-0.17
0.6	1.2850	0.9025	2.26	2.51	2.52	2.25	-11.46	-11.90	0.09
0.65	1.2885	0.8885	2.15	2.43	2.44	2.14	-13.14	13.64	0.18
0.7	1.2924	0.8740	2.04	2.35	2.36	2.04	-14.87	-15.44	0.33
0.75	1.2967	0.8589	1.95	2.27	2.28	1.94	-16.72	-17.36	0.46
0.8	1.3014	0.8431	1.85	2.20	2.22	1.85	-19.07	-19.75	0.28
0.85	1.3067	0.8266	1.76	2.14	2.16	1.76	-21.73	-22.40	-0.02
0.9	1.3124	0.8094	1.68	2.09	2.10	1.68	-24.81	-25.39	-0.55
0.95	1.3187	0.7915	1.60	2.04	2.05	1.62	-27.63	-28.01	-1.22
				T=318.15K					
0.05	1.2700	1.0171	2.99	2.95	2.96	2.99	1.15	1.00	-0.04
0.1	1.2711	1.0080	2.86	2.86	2.87	2.87	-0.02	-0.26	-0.06
0.15	1.2726	0.9984	2.75	2.77	2.78	2.75	-1.00	-1.29	-0.01
0.2	1.2742	0.9884	2.63	2.68	2.69	2.63	-1.97	-2.26	0.05
0.25	1.2760	0.9781	2.51	2.59	2.59	2.51	-2.94	-3.22	0.11
0.3	1.2780	0.9674	2.40	2.49	2.50	2.40	-3.95	-4.21	0.19
0.35	1.2801	0.9563	2.29	2.40	2.41	2.28	-5.21	-5.45	0.10
0.4	1.2825	0.9448	2.17	2.32	2.32	2.17	-6.61	-6.82	-0.04
0.45	1.2850	0.9328	2.06	2.23	2.23	2.07	-8.28	-8.48	-0.32
0.5	1.2879	0.9203	1.95	2.15	2.15	1.96	-9.91	-10.11	-0.44
0.55	1.2910	0.9074	1.86	2.07	2.07	1.86	-11.25	-11.46	-0.20
0.6	1.2944	0.8939	1.77	1.99	2.00	1.77	-12.57	-12.80	0.18
0.65	1.2981	0.8798	1.68	1.92	1.92	1.67	-14.27	-14.52	0.31
0.7	1.3020	0.8653	1.59	1.85	1.86	1.59	-16.20	-16.50	0.34
0.75	1.3064	0.8502	1.51	1.79	1.79	1.51	-18.42	-18.75	0.22
0.8	1.3114	0.8343	1.43	1.73	1.74	1.43	-20.71	-21.06	0.15
0.85	1.3168	0.8178	1.36	1.68	1.68	1.36	-23.44	-23.78	-0.16
0.9	1.3228	0.8005	1.30	1.63	1.63	1.30	-25.78	-26.08	-0.07
0.95	1.3294	0.7825	1.23	1.59	1.59	1.24	-29.09	-29.29	-1.06

IV. CONCLUSION

It may be concluded that molecular association decreases with increase in temperature due to decrease in density of solution indicating the rupture of hydrogen bonding present between the binary components of polar solvents. McAllister-3-body and 4-body model gave good result at initial concentrations but as concentration increases both the models show deviations from experimental values whereas Jouyban Acree models deals a fair agreement with experimental findings over the entire range of concentration from 298.15-318.15K. Results obtained in terms of their decreasing order of standard deviations at lower and higher temperature were JA <Mc4< Mc3 and JA < Mc3 < Mc4 respectively.

Acknowledgement

Author is very thankful to department of chemistry, Janta College Bakewar Etawah for support and motivation

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