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Research Article

Thermodynamic Properties of A Binary system

Optimization of Thermo-Physical Properties For The Binary System Of Acetone–Water At 303.15-318.15 K By Response Surface Quadratic Model

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Abstract: Thermo bodily residences of binary liquid combos are very beneficial in biotechnology, pharmaceutical, chemical and petroleum refining industries for improved favoured products from diverse raw materials. The physical property data on mixed solvents are important for the theoretical and applied areas of research and are frequently used in many chemical and industrial processes such as design of new process and process equipment (fluid flow, mass transfer or heat transfer calculation) and designing of bioreactor/fermenter. The objective of the current paper is to determine the density, viscosity, ultrasonic velocity, refractive index and surface tension of acetone (1) + water (2) at temperatures of 303.15K to 318.15K for the complete composition degrees and atmospheric pressure. These experimental values were used to calculate the respective excess homes in conjunction with a few acoustic properties. The experimental facts and excess residences have been used to calculate the interacting coefficients and well known deviations from different existing models. Also the new model equations have been evolved with the aid of the use of Design Expert application for density, viscosity, ultrasonic velocity, refractive indices and surface tension. Experimental consequences have been analysed on the premise of molecular interactions among element molecules with the assistance of FT-IR spectrum. Acetone-water binary structures of the prevailing observer have positive values of excess molar volumes and deviations in isentropic compressibility over whole composition range and at all temperatures which suggests sturdy interactions among the components of binary mixtures. Thermodynamic observations of acetone and water mixtures were made. Negative viscosity deviation of acetone-water combinations suggests robust dipole-dipole interactions within the device. Fourier remodel infrared spectroscopy also indicates the sturdy interaction made at 3589 cm^{-1} and based on the response surface method outcomes, more interplay takes area at zero. Five and zero six moles of acetone and water combination and the consequences are conformed with reference to the R^2 cost (0.89). Excess molar extent and isentropic compressibility were decided and kinds of interactions have been discussed primarily based on the derived properties.

Key words: Density, viscosity, ultrasonic velocity, refractive indices, intermolecular interactions, FT-IR spectrum.

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1. INTRODUCTION

The thermodynamic, acoustic and transport residences of liquids and liquid mixtures [1,2] were used to take a look at the molecular interactions between the various components of the combinations and also to recognize engineering packages concerning transport methods like warmness, mass switch and fluid flow. In chemical system industries, materials are normally dealt in fluid form, and thus, the thermo-body, chemical and shipping properties of fluids assume significance. Thus, statistics on a number of homes associated with the drinks and liquid combos like density, viscosity, refractive indices, ultrasonic pace and surface tension discover good sized utility in answer idea and molecular dynamics [2,3]. Such consequences are important for interpretation of facts obtained from thermo chemical, electrochemical, biochemical and kinetic studies[3,4]. Thermo physical, acoustic and transport homes are required inside the oil and gas industries to go with the flow warranty and oil recovery[5,6]. In the chemical industries for the layout of separation strategies, in the pharmaceutical and polymer industries for solvent selection and emission control and additionally within the environmental technology for the estimation of the distribution of chemicals in diverse ecosystems and additionally in biotechnology for the foundation of many illnesses records are traced to aggregation of proteins and numerous protein separations[6,7]. Many separation tactics in chemical, biochemical and engineering as well as in petroleum industries depend on section equilibrium information. Depending on the applications and compounds worried, extraordinary forms of data are wished for instance vapour–liquid equilibrium for plenty distillations, liquid–liquid equilibrium for liquid extractions and solid–liquid equilibrium for crystallization and leaching[8]. The reaction floor quadratic model extensively used statistical design technique for the interplay between binary or ternary structures, and the variables screened by using reaction floor quadratic model design have been in addition optimized in a 23 factorial Box–Behnken design methodology[9]. Response floor method (RSM) changed into a notably used statistical approach for additives optimization and for designing experiments, evaluating the consequences of element and relative significance and looking at the choicest elements associated with favoured response. It has the intense capacity to interpret the interactive effects among entered variables are a few appealing functions of RSM[10]. In the present research, we measure the density, viscosity, ultrasonic pace, refractive indices and floor anxiety at temperatures 303.15, 308.15, 313.15 and 318.15K and zero.1 MPa. Thermodynamic residences explains the steadiness of micro emulsions. Interfacial anxiety takes place due floor anxiety; a complicated relationship between 0 interfacial anxiety and thermodynamic stability holds the key for the formation of micro emulsion systems[9]. The intermolecular interactions of the binary system which helps to develop the formation of new micro emulsions in the bioreactor operations[9]. Literature surveys suggest that no reports have been stated in this combination.

2. MATERIALS AND METHODS

Acetone was acquired from Merck (India), Bombay and Sisco Research Laboratories (India) of AR grade with purity higher than 99 percent. The Doubly distilled water was used to keep together the answer. The blended solvent of ACETONE–WATER has been organized using acetone and water in 1:1 (v/v) solution. Eleven sets of answers from 0.0259 to at least one m concentration have been organized and used on the identical day. The viscosity of the answer changed to determine the usage of pre-calibrated Ostwald's viscometer[10] having uncertainity inside the order of ± 0.067%. The viscosity measurements are primarily based on the size of drift time of the answers taken for the research with an uncertainty as much as ±0.01s. The density measurement has been done using a capillary pycknometer[11] with an uncertainity of ±0.06%. Ultrasonic pace of solutions had been measured using an ultrasonic interferometer[12] (Model F-85) with a single frequency of 2 MHz having uncertainity inside the order of ±0.056%. Refractive index has been measured using Abbe's refractometer[13] with an uncertainty of ±0.062%. Surface tension was determined using a drop volume tensiometer and the accuracy of the surface anxiety estimation turned out to be 0.1mNm^{-1}. All the units and apparatus were calibrated with trendy liquids like benzene, 1, four-dioxane, acetophenone, n-hexane and water earlier than taking measurements. The temperature is maintained steady within ±0.10°C with the aid of the thermostatically managed refrigerated water bath tub with circulating water across the mobile. The weighing was finished using the denver stability with an uncertainty of ±0.1 mg. The experimental values of the natural additives were tested with the literature values (Table 1). Fourier Transform Infrared Spectroscopy, also known as FTIR Analysis or FTIR Spectroscopy, is an analytical technique used to identify organic, polymeric, and, in some cases, inorganic materials. The FTIR analysis method uses infrared light to scan test samples and observe chemical properties. The FTIR instrument sends infrared radiation of about 10,000 to 100 cm^{-1} through a sample, with some radiation absorbed and some passed through. The absorbed radiation is converted into rotational and/or vibrational energy by the sample molecules. The resulting signal at the detector presents as a spectrum, typically from 4000 cm^{-1} to 400cm^{-1}, representing a molecular fingerprint of the sample. Each molecule or chemical structure will produce a unique spectral fingerprint, making FTIR analysis a great tool for chemical identification. The FTIR instrument sends infrared radiation of about 10,000 to 100 cm^{-1} through a sample, with some radiation absorbed and some passed through. The absorbed radiation is converted into rotational and/or vibrational energy by the sample molecules. The resulting signal at the detector presents as a spectrum, typically from 4000 cm^{-1} to 400cm^{-1}, representing a molecular fingerprint of the sample. Each molecule or chemical structure will produce a unique spectral fingerprint, making FTIR analysis a great tool for chemical identification.

Table 1. Comparison of experimental density, viscosity, ultrasonic velocity, refractive index and surface tension of pure liquids with literature values at (303.15, 308.15, 313.15 and 318.15) K and 0.1 MPa

Pure Liquids	T,K	ρ, kg m^{-3}		η, m Pa s		u, m s^{-1}		N		σ, mN m^{-1}	
		lit.	exp.	lit.	exp.	lit.	exp.	lit.	exp.	lit.	exp.
Acetone	303.15	779	769.3	0.289	0.4569	-	1153.6	1.353	1.3586	-	25.14
	308.15	773	746.1	0.277	0.4352	-	1131	-	1.3567	-	24.53
	313.15	-	718.6	-	0.4152	-	1099	-	1.3537	-	23.96
	318.15	-	689.1	-	0.3923	-	1047	-	1.3499	-	22.97
Water	303.15	998	999.5	-	0.6550	1483.1	1540.6	1.333	1.3327	-	72.74
	308.15	-	993.9	-	0.6420	-	1520	-	1.3318	-	71.23
	313.15	-	980.2	-	0.6307	-	1505	-	1.3312	-	69.97
	318.15	-	977.2	-	0.6152	-	1499	-	1.3302	-	64.85

T=Temperature (K),ρ=Density (Kg/m^3),η=Viscosity (m Pa.s),u=Ultrasonic velocity (m/s), N=Refractive index, σ=surface Tension (mN.m^{-1}).

Density (ρ), kinematic viscosity (ν), ultrasonic velocity (u), refractive index (n) and floor tension (σ) were measured at 303.15, 308.15, 313.15 and 318.15 K and atmospheric strain for the entire composition variety of binary mixtures of acetone and water. Dynamic viscosity (η) and the acoustic parameters such as acoustical impedance (Z), isentropic compressibility (βs), intermolecular loose period (L_f), Wada steady (W), relaxation time (τ), molar sound speed (R), extra molar extent (VE) have been calculated by way of using the subsequent equations as given elsewhere[14]

$$\mathbf{\nu = (a \times t) - \left(\frac{b}{t}\right)} \quad \textbf{(1)}$$

Where *a* and *b* are the constants for the viscometer found by calibration method and t is time.

$$\mathbf{u = \left(\frac{\lambda}{2}\right)_{avg} \times 2f} \quad \textbf{(2)}$$

Where λ and *f* are the wavelength and frequency of sound wave respectively.

$$\boldsymbol{\eta = \rho \times \nu} \quad \textbf{(3)}$$

$$\mathbf{Z = \rho u} \quad \textbf{(4)}$$

$$\mathbf{\beta_s = \frac{1}{\rho u^2}} \quad \textbf{(5)}$$

$$\boldsymbol{L_f = K\beta_s^{\frac{1}{2}}} \quad \textbf{(6)}$$

Where *K* is the Jacobson constant[15].

Molar volume (*V*), free volume (V_f), relative association (Ra), isothermal compressibility (βT), thermal expansion coefficient (α) and molar refractivity (R_M) have been calculated from the experimental values with the help of following equations[16]:

$$\mathbf{V = \frac{x_1 \times M_1 + x_2 \times M_2}{\rho}} \quad \textbf{(7)}$$

Where x_1 and x_2 are the mole fraction and M_1 and M_2 are molecular weight of acetone and water, respectively and *M* is the effective molecular mass.

$$\mathbf{M = x_1 \times M_1 + x_2 \times M_2} \quad \textbf{(8)}$$

$$\boldsymbol{W = \left(\frac{M}{\rho}\right) \times \beta_s^{-1/7}} \quad \textbf{(9)}$$

$$\boldsymbol{\tau = \left(\frac{4}{3}\right) \times \eta \times \beta_s} \quad \textbf{(10)}$$

$$\boldsymbol{R = \left(\frac{M}{\rho}\right) \times u^{\frac{1}{3}}} \quad \textbf{(11)}$$

Assuming cubic lattice structure in condensed state of matter free volume of binary mixture has been evaluated by using the relation[17]

$$\mathbf{V_f} = \left[\frac{(\mathbf{M}\times\mathbf{u})}{(\mathbf{K}\times\boldsymbol{\eta})}\right]^{\frac{3}{2}} \quad \textbf{(12)}$$

Where *K* is a constant of proportionality which is not a function of temperature and its value is 4.28×10^9

$$\boldsymbol{Ra} = (\boldsymbol{\rho}/\boldsymbol{\rho_1})\left(\boldsymbol{u_1}/\boldsymbol{u}\right)^{1/3} \quad \textbf{(13)}$$

Where ρ_1 and u_1 are the density and ultrasonic velocity of acetone respectively.

$$\boldsymbol{\beta_T} = \frac{0.00171}{T^{4/9}\times u^2\times\rho^{4/3}} \quad \textbf{(14)}$$

Where *T* is the absolute temperature

$$\boldsymbol{\alpha} = (0.0191 \times \boldsymbol{\beta_T})^{1/4} \quad \textbf{(15)}$$

The molar refractivity (*R*M) of binary system is calculated from Lorentz–Lorentz equation

$$\boldsymbol{R_M} = \left[\frac{n^2-1}{n^2+2}\right]V \quad \textbf{(16)}$$

Excess molar volume (V^E) has been calculated from the density (ρ) of the medium using the following equation

$$V^E = \left(\frac{x_1M_1+x_2M_2}{\rho_m}\right) - \left(\frac{x_1M_1}{\rho_1} + \frac{x_2M_2}{\rho_2}\right) \quad \textbf{(17)}$$

Wherex_1 and $x_2$refer to the mole fraction of components 1 and 2. ρ_1,ρ_2 and ρ_m *are* the density of components 1 and 2 and the density of the mixture, respectively.

Viscosity deviation (Δη) has been determined as follows

$$\Delta\eta = \eta - (\mathrm{x}_1\eta_1 + \mathrm{x}_2\eta_2) \quad \textbf{(18)}$$

Where η, η_1, η_2 are the viscosity of the mixture and the viscosity of pure components 1 and 2, respectively. The uncertainty in the calculation of $\Delta\eta$ from viscosity measurements was estimated to be ±0.0001.

Refractive index deviation (Δn_D) from linear additive value of the mole fraction is obtained by

$$\Delta\mathrm{n_D} = \mathrm{n_D} - (\mathrm{x}_1\mathrm{n_{D1}} + \mathrm{x}_2\mathrm{n_{D2}}) \quad \textbf{(19)}$$

Where n_D, n_{D1}, n_{D2} are the refractive index of the mixture and the refractive index of pure components 1 and 2, respectively.

Ultrasonic velocity deviations (Δu): has been determined as follows

$$\Delta\mathbf{u} = \mathbf{u} - (\mathbf{x_1u_1} + \mathbf{x_2u_2}) \quad \textbf{(20)}$$

Where u, $\mathbf{u_1}$,$\mathbf{u_2}$are the ultrasonic velocity of the mixture and the ultrasonic velocity of pure components 1 and 2, respectively

Surface tension deviations (Δσ): has been determined as follows

$$\Delta\boldsymbol{\sigma} = \boldsymbol{\sigma} - (\boldsymbol{x_1\sigma_1} + \boldsymbol{x_2\sigma_2}) \quad \textbf{(21)}$$

Where $\boldsymbol{\sigma}$, $\boldsymbol{\sigma_1}$, $\boldsymbol{\sigma_2}$ are the ultrasonic velocity of the mixture and the surface tension of pure components 1 and 2, respectively.

Deviation in acoustic impedance (ΔZ) has been determined as follows

$$\Delta\mathrm{Z} = \mathrm{Z} - (\mathrm{x}_1\mathrm{Z}_1 - \mathrm{x}_2\mathrm{Z}_2) \quad \textbf{(22)}$$

Where Z, Z_1 and Z_2 are the acoustic impedance of the mixture and the acoustic impedance of pure components 1 and 2, respectively.

Excess Gibbs free energy of activation of viscous flow (G^{*E}) has been estimated by the available equation[18]

$$G^{*E} = RT[\ln(\eta V) - \{\ln(\eta_1V_1) + \ln(\eta_2V_2)\} \quad (23)$$

Where R, T, η are the molar sound velocity, temperature and viscosity of the mixture and

$$\eta_1, V_1, \eta_2, V_2$$

are the viscosity and molar of pure components 1 and 2 respectively. The experimental values of density, viscosity, refractive index, ultrasonic velocity and surface tension for synthesized acetone-water mixtures are presented in table 2 over the entire temperature range from (303.15 to 318.15)K and 0.1 MPa pressure. The experimental values of viscosity and ultrasonic velocity have been correlated with McAllister model for three body interaction used for binary liquid mixture, model proposed by Krishna-Laddha, Hind, Grunberg–Nissan, and Jouyban–Acree model to derive the binary coefficients and standard deviation (*S*). The corresponding equations for the above models have been given as under:

McAllister Model for viscosity[19],

$$\ln\boldsymbol{\nu} = \boldsymbol{x_1^3}\ln\boldsymbol{\nu_1} + 3\boldsymbol{x_1^2x_2}\ln\boldsymbol{\nu_{12}} + 3\boldsymbol{x_1x_2^2}\ln\boldsymbol{\nu_{21}} + \boldsymbol{x_2^3}\ln\boldsymbol{\nu_2} - \ln\left(\boldsymbol{x_1} + \boldsymbol{x_2}\,\boldsymbol{M_2}/\boldsymbol{M_1}\right) + 3\,\boldsymbol{x_1^2}\,\boldsymbol{x_2}\ln\left((2 + \boldsymbol{M_2}/\boldsymbol{M_1})/3\right) + 3\boldsymbol{x_1x_2^2}\ln((1 + 2\,\boldsymbol{M_2}/\boldsymbol{M_1})/3) + \boldsymbol{x_2^3}\ln(\boldsymbol{M_2}/\boldsymbol{M_1}) \quad \textbf{(24)}$$

In equation 24, ν_1 and ν_2 refer to the kinematic viscosity of pure liquids 1 and 2 having mole fractions x_1 and x_2, respectively. The parameters ν_{12} and ν_{21} represent the interaction parameters obtained by least square method, while M_1 and M_2 are the molecular weight of the components.McAllister Model for ultrasonic velocity[20],

$$\ln\boldsymbol{u} = \boldsymbol{x_1^3}\ln\boldsymbol{u_1} + 3\boldsymbol{x_1^2x_1}\ln\boldsymbol{\nu_{12}} + 3\boldsymbol{x_1x_2^2}\ln\boldsymbol{\nu_{21}} + \boldsymbol{x_2^3}\ln\boldsymbol{u_2} - \ln\left(\boldsymbol{x_1} + \boldsymbol{x_2}\,\boldsymbol{M_2}/\boldsymbol{M_1}\right) + 3\,\boldsymbol{x_1^2}\,\boldsymbol{x_2}\ln\left((2 + \boldsymbol{M_2}/\boldsymbol{M_1})/3\right) + 3\boldsymbol{x_1x_2^2}\ln((1 + 2\,\boldsymbol{M_2}/\boldsymbol{M_1})/3) + \boldsymbol{x_2^3}\ln(\boldsymbol{M_2}/\boldsymbol{M_1}) \quad \textbf{(25)}$$

In equation 25, u_1 and u_2 refer to the kinematic viscosity of pure liquids 1 and 2 having mole fractions x_1 and x_2, respectively. The parameters v_{12} and v_{21} represent the interaction parameters obtained by least square method, while M_1 and M_2 are the molecular weight of the components. The kinematic viscosity was correlated by means of the Krishnan and Laddha model for a two-component mixture[21], which gives

$$\mathbf{lnv_{mix} = x_1 lnv_1 + x_2 lnv_2 - 2.303 x_1 x_2 \left(A + B(x_1 - x_2)\right) - ln(x_1 M_1 + x_2 M_2) + x_1 lnM_1 + x_2 lnM_2} \quad \textbf{(26)}$$

where A and B are interaction parameters. Hind model[22] for binary mixture,

$$\mathbf{\eta = x_1^2 \eta_1 + x_2^2 \eta_2 + 2 x_1 x_2 H_{12}} \quad \textbf{(27)}$$

Where η is the predicted value, η_1 , η_2 are the dynamic viscosity of components 1 and 2, and H_{12} is the Hind interaction constant which is a function of composition and temperature.

According to Grunberg Nissan model[23].

$$\mathbf{\ln \eta = x_1 \ln \eta_1 + x_2 \ln \eta_2 + x_1 x_2 G_{12}} \quad \textbf{(28)}$$

Where G_{12} is an interaction constant and is a function of composition and temperature.

Jouyban and Acree model[24] for viscosity of acetone (1) + water (2) mixture

$$\mathbf{\ln \eta_{mix} = x_1 \ln \eta_1 + x_2 \ln \eta_2 + x_1 x_2 \sum A_J (x_1 - x_2)^J / T} \quad \textbf{(29)}$$

Jouyban and Acree model[25] for ultrasonic velocity of acetone (1) + water (2) mixture

$$\mathbf{\ln u_{mix} = x_1 \ln u_1 + x_2 \ln u_2 + x_1 x_2 \sum A_J (x_1 - x_2)^J / T} \quad \textbf{(30)}$$

In equation 29 and 30, where η_{mix} and u_{mix} are the predicted value of viscosity, ultrasonic velocity or at temperature *T*, x_1 and x_2 are the corresponding properties of the components 1 and 2 at pure state, x_1, x_2 are the mole fractions and *Aj* is the model constant.

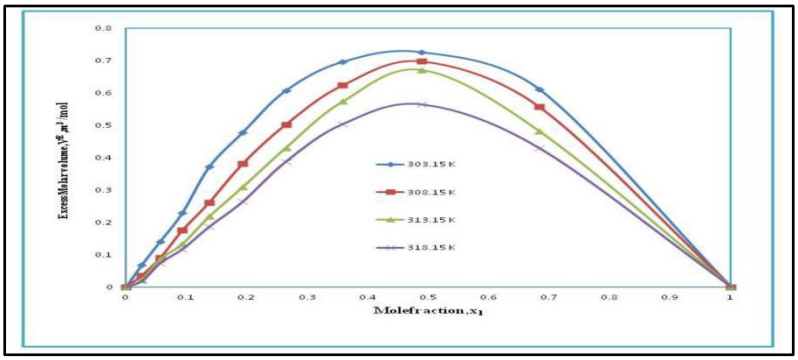


Fig 1. *Variation of excess molar volume with mole fraction for acetone (1) + water (2) at 303.15, 308.15, 313.15 and 318.15 K.*

3. STATISTICAL ANALYSIS

Thermo physical properties of binary liquid mixtures data obtained were analyzed using design expert software (Version 10.2.4).Authors (paired) "t" test was used for analysis of comparison between the binary systems. The data were presented as mean ± standard deviation (SD). Probability values (P) of less than 0.001 was considered statistically significant.

4. RESULTS AND DISCUSSIONS

The variation of excess molar volumes with the mole fraction of acetone (1) + water (2) at diverse temperatures (303 .15, 308.15, 313.15 and 318.15) K are represented in discern 1. The signal of excess molar quantity of a machine relies upon the relative magnitude of enlargement/contraction on mixing of two liquids [23-27]. If the elements inflicting growth dominate the contraction factors, the V^E will become effective. On the other hand, if the contraction elements dominate the expansion factors, then V^E becomes bad. The factors which are liable for expansion in volume are as follows, Loss of dipolar affiliation and geometry of molecular structure, which does not allow becoming of 1 aspect into other factors. The Steric trouble opposes proximity of the constituent molecules[26]. The terrible V^E values get up due to dominance of the following factors Chemical interplay between constituent chemicals and accommodation of molecules of one aspect into the interstitials of the molecules of the opposite component[28-32]. The Geometry of molecular structure that favours becoming of the component molecules with each different. The terrible V^E values inside the combinations underneath observation suggest that interactions between molecules of the mixtures are more potent than interactions between molecules in the pure beverages and that associative force dominate the behaviour of the solution[27-38].In our machine, positive excess molar quantity values are attributed to vulnerable dipole-dipole interactions between like molecules inside the combination. This results are help to design a various unit operations, Bioreactors and downstream processing techniques.

Table 2. Values of density, viscosity, surface tension, ultrasonic velocity and refractive index for the Acetone (1) + water (2) mixture at *T* = (303.15, 308.15,313.15 and 318.15) K and 0.1 MPa

x1	ρ X 10^{-3},kg/m^3	η X 10^3, Pa s	u, m/s	N	σ X 10^3 , N/m
T=303.15 K					
0	0.9995	0.6550	1540.6	1.3327	72.74
0.0259	0.9731	0.6344	1513.1	1.3342	70.09
0.0564	0.9472	0.6154	1481.3	1.3361	66.29
0.0929	0.9214	0.5921	1433.8	1.3385	61.68

0.1374	0.8946	0.5693	1387	1.3415	56.14
0.1928	0.8701	0.5467	1328	1.3448	50.81
0.2638	0.8459	0.5222	1268	1.3484	45.63
0.3579	0.8235	0.5005	1215.9	1.3514	40.52
0.4886	0.8027	0.4823	1179.2	1.3542	35.48
0.6825	0.7839	0.4684	1152	1.3565	31.55
1	0.7693	0.4569	1153.6	1.3586	25.14
		T=308.15 K			
0	0.9939	0.6420	1520	1.3318	71.23
0.0259	0.9668	0.6216	1497.1	1.3329	68.14
0.0564	0.9394	0.5976	1457	1.3349	63.59
0.0929	0.9115	0.5763	1414	1.3369	58.38
0.1374	0.8845	0.5536	1347	1.3393	52.59
0.1928	0.8574	0.5302	1298.1	1.3426	47.76
0.2638	0.8314	0.5046	1234	1.3464	42.86
0.3579	0.8064	0.4822	1188	1.3495	37.71
0.4886	0.7831	0.4647	1152	1.3521	33.45
0.6825	0.7631	0.4457	1128	1.3545	29.23
1	0.7461	0.4352	1131	1.3567	24.53
		T=313.15 K			
0	0.9802	0.6307	1505	1.3312	69.97
0.0259	0.9518	0.6092	1476.4	1.3320	64.48
0.0564	0.9222	0.5815	1434.1	1.3337	58.94
0.0929	0.8941	0.5587	1375.5	1.3353	53.97
0.1374	0.8655	0.5353	1316.2	1.3374	48.68
0.1928	0.8377	0.5110	1264.4	1.3399	44.10
0.2638	0.8102	0.4808	1199.2	1.3431	39.53
0.3579	0.7834	0.4606	1158.2	1.3462	34.63
0.4886	0.7585	0.4393	1120.9	1.3492	30.57
0.6825	0.7378	0.4226	1105	1.3515	27.17
1	0.7186	0.4152	1099	1.3537	23.96
		T=318.15 K			
0	0.9772	0.6152	1499	1.3302	64.85
0.0259	0.9452	0.5845	1435.8	1.3313	59.12
0.0564	0.9124	0.5516	1382.7	1.3324	53.55
0.0929	0.8812	0.5264	1321	1.3338	49.00
0.1374	0.8501	0.4988	1262.4	1.3357	44.42
0.1928	0.8199	0.4735	1216	1.3378	40.52
0.2638	0.7898	0.4501	1153.6	1.34015	36.47
0.3579	0.7612	0.4290	1114.6	1.3427	32.25
0.4886	0.7346	0.4121	1077	1.3448	28.31
0.6825	0.7109	0.3969	1055	1.3472	25.29
1	0.6891	0.3923	1047	1.3499	22.97

X1=Molefraction, T=Temperature (K),ρ=Density (Kg/m^3),η=Viscosity (Pa.s),u=Ultrasonic velocity (m/s), N=Refractive index, σ=surface Tension (mN.m^{-1}).

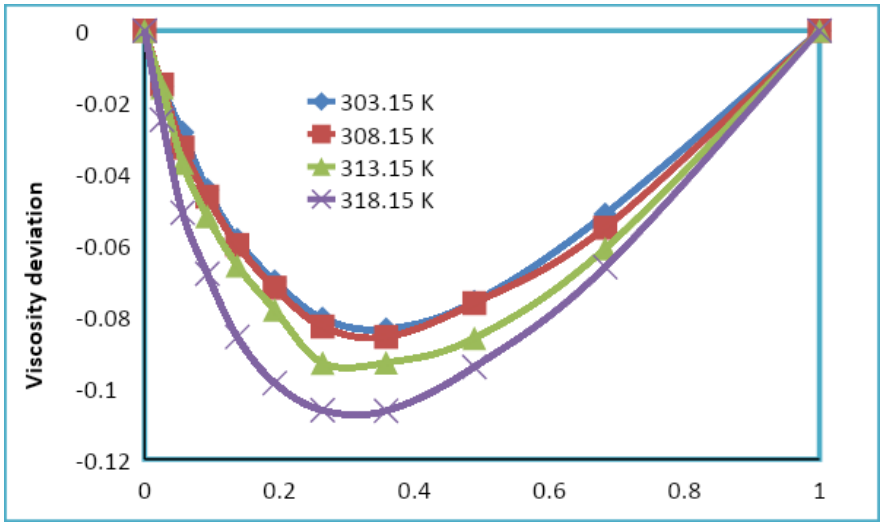


Fig 2. Variation of viscosity deviation (Δη) with mole fraction for acetone (1) + water (2) at 303.15, 308.15, 313.15 and 318.15 K.

It is seen from Fig. 2 that for the whole of composition , viscosity deviation is negative indicating complicated formation because of rate switching between the components. Acetone is electron accepting institution and water is electron donating institution which may additionally cause the opportunity of formation of complicated.

Table 3. Acoustical parameters *Z*, βs, *Lf*, *V*, *W*, τ, *R*, *Vf*, Ra, βT, and α of the Acetone (1) + water (2) mixtures at *T* = (303.15, 308.15, 313.15 and 318.15) K and 0.1 MPa

X	Z X 10^{-6} Kg/m^2 s	β_s X10^{10}, Pa-1	L_f X 10^{11}, m	W X 10^3	τ X 10^{10}, s	V X 10^5, m3/mol	R X 10^3 m^3/mol $(m/s)^{1/3}$	V_f X 10^{12}	Ra	B_T X 10^{15}	α X 10^{-4}	R_m X 10^6 m^3/mol
T=303.15 K												
0	1.53	4.21	4.26	0.39	3.681	1.80	0.20	0.98	1.22	5.68	1.02	3.70
0.0259	1.47	4.48	4.39	0.42	3.7961	1.95	0.22	1.09	1.20	6.11	1.03	4.03
0.0564	1.40	4.81	4.55	0.45	3.9472	2.13	0.24	1.21	1.17	6.60	1.05	4.43
0.0929	1.32	5.27	4.76	0.49	4.1675	2.35	0.26	1.36	1.15	7.31	1.08	4.92
0.1374	1.24	5.81	5.00	0.54	4.4106	2.62	0.29	1.54	1.13	8.13	1.11	5.52
0.1928	1.15	6.51	5.29	0.60	4.75	2.95	0.32	1.76	1.11	9.20	1.15	6.27
0.2638	1.07	7.35	5.62	0.68	5.119	3.37	0.36	2.06	1.09	10.48	1.18	7.23
0.3579	1.00	8.21	5.94	0.77	5.481	3.92	0.41	2.48	1.07	11.82	1.22	8.47
0.4886	0.94	8.95	6.21	0.91	5.7609	4.67	0.49	3.14	1.04	13.00	1.25	10.17
0.6825	0.90	9.61	6.43	1.12	6.0029	5.77	0.60	4.19	1.02	14.06	1.28	12.64
1	0.88	9.76	6.48	1.46	5.9489	7.53	0.79	6.33	1	14.37	1.28	16.58
T=308.15 K												
0	1.51	4.35	4.37	0.39	3.72	1.8	0.20	0.99	1.20	5.84	1.02	3.71
0.0259	1.44	4.61	4.49	0.42	3.82	1.96	0.22	1.10	1.18	6.25	1.04	4.04
0.0564	1.36	5.01	4.68	0.45	3.99	2.15	0.24	1.23	1.15	6.85	1.06	4.45
0.0929	1.28	5.48	4.90	0.50	4.21	2.38	0.26	1.38	1.13	7.57	1.09	4.95
0.1374	1.19	6.23	5.22	0.54	4.59	2.65	0.29	1.54	1.11	8.69	1.13	5.55
0.1928	1.11	6.92	5.50	0.61	4.89	2.99	0.32	1.78	1.09	9.75	1.16	6.33
0.2638	1.02	7.89	5.88	0.68	5.31	3.43	0.36	2.08	1.08	11.25	1.21	7.32
0.3579	0.95	8.78	6.20	0.78	5.64	4.00	0.42	2.53	1.06	12.64	1.24	8.61
0.4886	0.90	9.62	6.49	0.93	5.96	4.79	0.50	3.20	1.04	13.97	1.27	10.37
0.6825	0.86	10.29	6.72	1.14	6.12	5.93	0.61	4.38	1.02	15.09	1.30	12.92
1	0.84	10.47	6.77	1.49	6.08	7.77	0.80	6.60	1	15.47	1.31	17.01
T=313.15 K												
0	1.47	4.50	4.48	0.39	3.78	1.83	0.21	1.00	1.22	6.02	1.03	3.75
0.0259	1.40	4.81	4.63	0.42	3.91	1.99	0.22	1.11	1.20	6.51	1.05	4.10
0.0564	1.32	5.27	4.85	0.46	4.08	2.19	0.24	1.26	1.17	7.20	1.08	4.52
0.0929	1.22	5.91	5.13	0.50	4.40	2.42	0.27	1.39	1.15	8.15	1.11	5.02
0.1374	1.13	6.66	5.45	0.55	4.76	2.71	0.29	1.56	1.13	9.30	1.15	5.65
0.1928	1.05	7.46	5.77	0.61	5.08	3.06	0.33	1.81	1.11	10.53	1.19	6.43

0.2638	0.97	8.58	6.19	0.69	5.50	3.52	0.37	2.14	1.09	12.24	1.23	7.44
0.3579	0.90	9.51	6.51	0.80	5.84	4.12	0.43	2.61	1.07	13.72	1.27	8.79
0.4886	0.85	10.49	6.84	0.94	6.14	4.94	0.51	3.34	1.04	15.29	1.30	10.62
0.6825	0.81	11.10	7.04	1.16	6.25	6.13	0.63	4.60	1.02	16.33	1.32	13.26
1	0.78	11.52	7.17	1.52	6.37	8.07	0.83	6.79	1	17.10	1.34	17.53
T=318.15 K												
0	1.46	4.55	4.54	0.39	3.73	1.84	0.21	1.03	1.25	6.05	1.0372	3.76
0.0259	1.35	5.13	4.82	0.42	3.99	2.01	0.22	1.14	1.23	6.90	1.0716	4.12
0.0564	1.26	5.73	5.10	0.46	4.21	2.21	0.24	1.29	1.20	7.80	1.1049	4.55
0.0929	1.16	6.50	5.43	0.50	4.56	2.46	0.27	1.43	1.18	8.95	1.1436	5.08
0.1374	1.07	7.38	5.79	0.55	4.90	2.76	0.29	1.63	1.15	10.28	1.1839	5.72
0.1928	0.99	8.24	6.12	0.62	5.20	3.13	0.33	1.91	1.13	11.63	1.221	6.53
0.2638	0.91	9.51	6.57	0.70	5.70	3.61	0.37	2.23	1.10	13.58	1.2692	7.58
0.3579	0.84	10.57	6.93	0.81	6.04	4.24	0.44	2.74	1.08	15.29	1.3072	8.96
0.4886	0.79	11.73	7.30	0.96	6.44	5.11	0.52	3.47	1.05	17.17	1.3457	10.85
0.6825	0.75	12.63	7.57	0.11	6.68	6.37	0.64	4.71	1.02	18.69	1.3747	13.61
1	0.72	13.23	7.75	0.15	6.92	8.41	0.85	6.87	1	19.78	1.3943	18.10

X=Molefraction,Z=Acoustical Impedance,β_s=Isentropic compressibility,L_f=Intermolecular loose period,W=wada Steady,T=Relaxation time,V=Kinematic Viscosity, R=molar sound speed, R_m=Molar refractivity,β_T=Isotheral compressibility,α=Thermal Expansion coefficient,R_a=Relative association.

Table 4. Δη, V^E, Δσ, Δ*u*, Δ*n*, Δ*Z*, $\Delta\beta_s$, and ΔL_f of the acetone (1) + water (2) mixtures at *T* = (303.15, 308.15,313.15 and 318.15) K and 0.1 MPa

X	Δη m.Pa s	V^E m^3 /mol	Δσ m N/m	Δu m/ s	Δn	ΔZ X 10-4 Kg/m^2 s	$\Delta\beta s X 10^{11}$ Pa^{-1}	$\Delta L_f X 10^{12}$ m
0	0	0	0	0	0	0	0	0
0.0259	-0.01	0.06	-1.41	-17.52	0.0008	-5.05	1.36	0.72
0.0564	-0.02	0.14	-3.76	-37.50	0.0019	-9.99	2.86	1.65
0.0929	-0.04	0.22	-6.63	-70.88	0.0034	-15.81	5.53	2.94
0.1374	-0.05	0.37	-10.05	-100.52	0.0052	-20.94	8.36	4.35
0.1928	-0.07	0.47	-12.74	-138.06	0.0071	-25.86	12.37	6.02
0.2638	-0.08	0.60	-14.54	-170.60	0.0088	-29.52	16.73	7.74
0.3579	-0.08	0.69	-15.18	-186.23	0.0094	-30.51	20.10	8.85
0.4886	-0.075	0.72	-13.99	-172.34	0.0088	-27.45	20.33	8.65
0.6825	-0.05	0.61	-8.70	-124.55	0.0062	-19.15	15.55	6.35
1	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0
0.0259	-0.015	0.0357	-1.8810	-12.8371	0.0005	-4.6083	1.00	0.67
0.0564	-0.0327	0.0901	-5.0007	-41.0792	0.0017	-10.4439	3.13	1.84
0.0929	-0.0464	0.1752	-8.5140	-69.8755	0.0028	-15.993	5.68	3.16
0.1374	-0.06	0.2614	-12.2220	-119.5632	0.0042	-22.7688	10.35	5.29
0.1928	-0.0719	0.3816	-14.4607	-146.7987	0.0061	-26.9059	13.84	6.75
0.2638	-0.0828	0.5021	-16.0450	-183.3871	0.0081	-30.8849	19.27	8.84
0.3579	-0.0857	0.6235	-16.7979	-192.6881	0.0088	-31.3958	22.39	9.77
0.4886	-0.0763	0.6972	-14.9527	-177.8810	0.0082	-28.2657	22.65	9.52
0.6825	-0.0552	0.5570	-10.1214	-126.4995	0.0057	-19.4747	16.52	7.05
1	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0
0.0259	-0.0159	0.0225	-4.2938	-18.0421	0.0002	-5.2183	1.39	0.90
0.0564	-0.0371	0.0857	-8.4286	-47.9322	0.0013	-11.3965	3.75	2.18
0.0929	-0.0519	0.1329	-11.7186	-91.7643	0.0020	-18.1682	7.59	4.10
0.1374	-0.0658	0.2175	-14.9604	-133.0073	0.0032	-24.1851	12.08	6.10
0.1928	-0.0782	0.3089	-16.9890	-162.2729	0.0044	-28.381	16.20	7.71
0.2638	-0.0930	0.4296	-18.3029	-198.6673	0.0060	-32.2765	22.33	10.00
0.3579	-0.0930	0.5728	-18.8723	-201.4238	0.0070	-32.2492	25.04	10.80
0.4886	-0.0861	0.6703	-16.9189	-185.7051	0.0070	-29.006	25.79	10.50
0.6825	-0.0610	0.4819	-11.3908	-122.8967	0.0049	-19.2091	18.22	7.24
1	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0
0.0259	-0.0250	0.0179	-4.6410	-51.4863	0.0006	-8.8459	3.56	1.97

0.0564	-0.0510	0.0737	-8.9373	-90.7873	0.0011	-16.132	6.92	3.69
0.0929	-0.0681	0.1164	-11.9521	-136.0250	0.0018	-23.1727	11.46	5.92
0.1374	-0.0858	0.1859	-14.6677	-174.4294	0.0028	-29.9487	16.41	7.99
0.1928	-0.0987	0.2636	-16.2508	-195.8493	0.0038	-32.45	20.30	9.51
0.2638	-0.1063	0.3869	-17.3253	-226.0820	0.0047	-35.7559	26.81	11.80
0.3579	-0.1064	0.5031	-17.6088	-222.5437	0.0055	-35.0829	29.27	12.30
0.4886	-0.0942	0.5636	-16.0744	-201.1393	0.0050	-31.0448	29.59	11.80
0.6825	-0.0662	0.4290	-10.9711	-135.5007	0.0036	-20.7481	21.84	8.39
1	0	0	0	0	0	0	0	0

X = Molefraction, $\Delta\eta$ = Viscosity deviation, V^E = Excess molar volume, $\Delta\sigma$ = Surface tension deviation, Δu = Ultrasonic velocity deviation, Δn = Refractive index deviation , Δz = Acoustical Impedance deviation, $\Delta\beta_s$ = Isentropic compressibility deviation , ΔL_f = Intermolecular loose period deviation.

Table 5. Interaction parameters and standard deviations of the McAllister, Krishna-Laddha, and Hind model for acetone (1) + water (2) mixtures at *T* = (303.15, 308.15,313.15 and 318.15) K and 0.1 MPa

T,K	McAllister			Krishna-Laddha			Hind	
	v_{12}	v_{21}	S	B	C	S	H_{12}	S
For viscosity								
303.15	0.543958	0.857292	0.02441	0.3925	0.0019	0.5178	0.0003	0.1341
308.15	0.533605	0.842507	0.02448	0.3977	0.0276	0.3887	0.0003	0.1262
313.15	0.520832	0.817451	0.02744	0.4029	0.0359	0.5920	0.0003	0.1141
318.15	0.532722	0.735512	0.02564	0.4156	0.0549	0.7854	0.0002	0.0977
Ultrasonic Velocity								
303.15	1044.29	1611.22	0.9875	0.8256	0.4741	0.1681	1524.23	0.6614
308.15	1026.72	1549.79	0.9889	0.8074	0.4739	0.1574	1512.45	0.6204
313.15	1029.73	1461.47	1.0235	0.7998	0.4724	0.1404	1502.31	0.6012
318.15	1036.78	1313.51	1.0965	0.7986	0.4705	0.1354	1497.21	0.6009

v12=Kinematic viscosity of 1 to 2, v21=Kinematic viscosity of 2 to 1, S=constant, B and C=Krishnan Ladha coefficients, H12=Hind Interaction constant.

Table 6. Interaction parameters and standard deviations of Jouyban-Acree and Gruenberg–Nissan models for the viscosity of the acetone (1) + water (2) mixtures at (303.15, 308.15, 313.15 and 318.15) K and 0.1 MPa

T,K	Jouyban-Acree						Gruenberg and Nissan Viscosity	
	Viscosity			ultrasonic velocity				
	A1	A2	S	A1	A2	S	G_{12}	S
303.15	-108.42	299.78	0.0478	-8.925	107.616	0.0265	-0.6877	0.0127
308.15	-86.95	155.64	0.0452	-8.146	102.356	0.0264	-0.7289	0.0129
313.15	-59.78	287.63	0.0497	-8.023	99.444	0.0263	-0.8274	0.0133
318.15	-28.63	369.74	0.0512	-7.898	89.656	0.0262	-1.1181	0.0230

A1 and A2 = Jouyban Acree coefficients , S= constant , G12 = Gruenberg & Nissan viscosity coefficient

Table 7. Interaction parameters and standard deviations of Katti and Chaudari, Heric and Brewer, Frenkel and Tamura and Kurata model for the viscosity of the acetone (1) + water (2) mixtures at (303.15, 308.15, 313.15 and 318.15) K and 0.1 MPa

T,K	Katti and Chaudari model for Viscosity		Heric and Brewer model for viscosity		Frenkel model for viscosity		Tamura and Kurata model for viscosity	
	W_{vis} /RT	S	Δ_{12}	S	F_{12}	S	T_{12}	S
303.15	0.3529	0.0073	0.3529	0.0073	0.3889	0.0125	0.6055	0.0038
308.15	0.3356	0.006	0.0947	0.0016	0.3682	0.0127	0.5802	0.0032
313.15	0.272	0.0057	-0.0038	0.0027	0.3395	0.013	0.5447	0.0039
318.15	0.0535	0.005	-0.2945	0.0132	0.2847	0.022	0.4741	0.0036

T = Temperature , W_{is}/RT= Katti and Chaudari model coefficient ,S = Constant , Δ12 = Heric and Brewer model coefficient , F12 = Frenke model coefficient , T12 = Tamura and Kurata model coefficient.

Table 8. APE and Chi square of U_{NOM}, U_{IMP}, U_{VDV} , U_{JM} , U_{FLT} and U_R model for the ultrasonic velocity of the acetone (1) + water (2) mixtures at (303.15, 308.15, 313.15 and 318.15) K and 0.1 MPa

Acetone + Water	U_{NOM}	U_{IMP}	U_{VDV}	U_{JM}	U_{FLT}	U_R
	ms^{-1}	ms^{-1}	ms^{-1}	ms^{-1}	ms^{-1}	ms^{-1}
303.15 K						
APE	0	-8.2516	-0.9026	0.0736	0	9.6379

Chi square	0	129.63	3.2469	7.188	0	204.408
308.15 K						
APE	0	-8.9171	-1.4248	-0.0077	0	9.8969
Chi square	0	146.97	6.3432	8.0954	0	209.346
313.15 K						
APE	0	-9.9227	-2.2562	0.0294	0	10.118
Chi square	0	171.94	12.056	6.9806	0	212.777
318.15 K						
APE	0	-12.612	-4.5078	-0.2527	0	10.107
Chi square	0	243.21	34.683	3.1409	0	211.065

U_{NOM} , U_{IMP} , U_{VDV} , U_{JM} , U_{FLT} , U_R = APE and Chi square

The derived properties from experimental values calculated with the use of Equations (4)–(16) have been given in Table 3. Standard deviation (*S*) is calculated by using the equation[33-35],

$$S(Y) = \left(\frac{\sum_{i=0}^{n}(A_{exp}-A_{cal})^2}{N-n}\right)^{1/2} \quad \textbf{(31)}$$

Where *A* is the thermo physical property or derived property or deviation in property, *N* is the number of data points and *n* is the number of coefficients.The coefficients and standard deviation for McAlister, Krishna-Laddha, Hind, Jouyban–Acree, and Grunberg–Nissan have been given in Tables 5, 6 and Katti and Chaudari, Heric and Brewer, Frenkel and Tamura and Kurata model have been given in Table 7. APE and Chi square of U_{NOM}, U_{IMP}, U_{VDV} , U_{JM} , U_{FLT} and U_R model for the ultrasonic velocity values are reported in Table 8.

Table 9.ANOVA table for density

Source	Sum of squares	df	Mean square	F-Value	P-Value Prob>F	Remarks
Model	0.13	5	0.025	1225.1	< 0.0001	significant
A-T	4.85E-03	1	4.85E-03	234.86	< 0.0001	
B-X	0.098	1	0.098	4736.64	< 0.0001	
AB	8.38E-04	1	8.38E-04	40.58	0.0004	
A^2	4.59E-04	1	4.59E-04	22.22	0.0022	
B^2	0.022	1	0.022	1045.77	< 0.0001	
Residual	1.45E-04	7	2.07E-05			
Lack of Fit	1.45E-04	3	4.82E-05			
Pure Error	0	4	0			
Cor Total	0.13	12				

df=Degrees of freedom,F-Value=F-Test value,P-Value=P test value

From the ANOVA Table 9, The Model F-value of 1225.10 implies the model is significant. There is only a 0.01% chance that an F-value, this large could occur due to noise. Values of "Prob > F" less than 0.0500 indicates model terms are significant. In this case A, B, AB, A^2, B^2 are significant model terms. Values greater than 0.1000 indicate the model terms are not significant. If there are many insignificant model terms (not counting those required to support hierarchy), model reduction may improve your model. The "Pred R-Squared" of 0.9886 is in reasonable agreement with the "Adj R-Squared" of 0.9980; i.e. the difference is less than 0.2. "Adeq Precision" measures the signal to noise ratio. A ratio greater than 4 is desirable. Your ratio of 101.134 indicates an adequate signal. This model can be used to navigate the design space. From the response surface graph as shown in Fig. 3, it has been seen that with increase in temperature, density decreases and with increase in mole fraction, density decreases in a concave upward manner. From the R^2 values it has been seen that the predicted values of density is a linear function of actual one having intercept 0 and of slope 1.

Final equation in terms of coded factors:

$$\textbf{Density} = +0.78 - 0.028 * A - 0.13 * B - 0.014 * AB - 0.013 * A^2 + 0.088 * B^2 \quad (32)$$

The final equation in terms of actual factors is,

$$\textbf{Density} = -20.53971 + 0.14053 * T + 0.58999 * X - 3.86000E - 003 * T * X - 2.29180E - 004 * T^2 + 0.35373 * X^2 \quad (33)$$

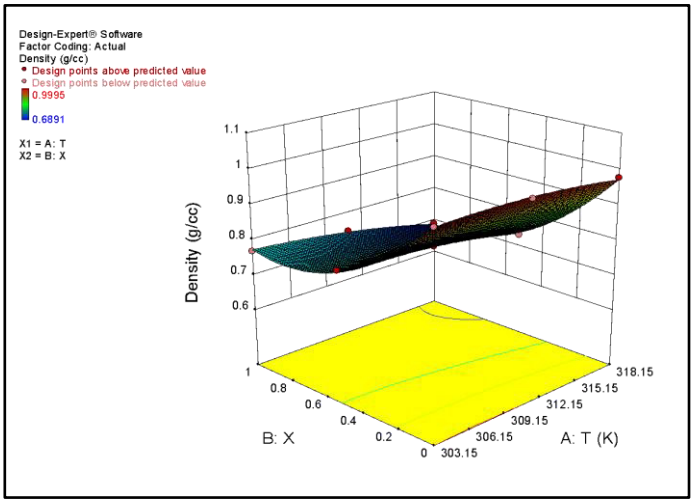


Fig 3. Combined effect of mole fraction and temperature on density.

Table 10.ANOVA table for viscosity

Source	Sum of squares	df	Mean square	F-Value	P-Value Prob>F	Remarks
Model	0.082	5	0.016	187.07	< 0.0001	significant
A-T	2.48E-03	1	2.48E-03	28.21	0.0011	
B-X	0.066	1	0.066	747.33	< 0.0001	
AB	1.53E-04	1	1.53E-04	1.74	0.2284	
A^2	3.04E-07	1	3.04E-07	3.46E-03	0.9547	
B^2	0.012	1	0.012	134.59	< 0.0001	
Residual	6.15E-04	7	8.79E-05			
Lack of Fit	6.15E-04	3	2.05E-04			
Pure Error	0	4	0			
Cor Total	0.083	12				

df=Degrees of freedom,F-Value=F-Test value,P-Value=P test value

From the ANOVA table 10, The Model F-value of 187.07 implies the model is significant. There is only a 0.01% chance that an F-value this large could occur due to noise. Values of "Prob > F" less than 0.0500 indicate model terms are significant. In this case A, B, B^2 are significant model terms. Values greater than 0.1000 indicate the model terms are not significant. If there are many insignificant model terms (not counting those required to support hierarchy), model reduction may improve your model. The "Pred R-Squared" of 0.9330 is in reasonable agreement with the "Adj R-Squared" of 0.9873; i.e. the difference is less than 0.2."Adeq Precision" measures the signal to noise ratio. A ratio greater than 4 is desirable. Your ratio of 39.239 indicates an adequate signal. This model can be used to navigate the design space. The response surface graph has been given in Fig.4 in which the values of viscosity decrease slightly in a concave upward with increase in temperature and increases major portion of compositions.

Final Equation in terms of coded factors

$$\mathbf{Viscosity} = +0.47 - 0.020 * A - 0.10 * B - 6.187E - 003 * AB + 3.319E - 004 * A^2 + 0.065 * B^2 \quad (34)$$

Final equation in terms of actual factors

$$\mathbf{Viscosity} = +1.79244 - 5.55180E - 003 * T + 0.041482 * X * T - 1.65000E - 003 * X + 5.90038E - 006 * T^2 + 0.26181 * X^2 \quad (35)$$

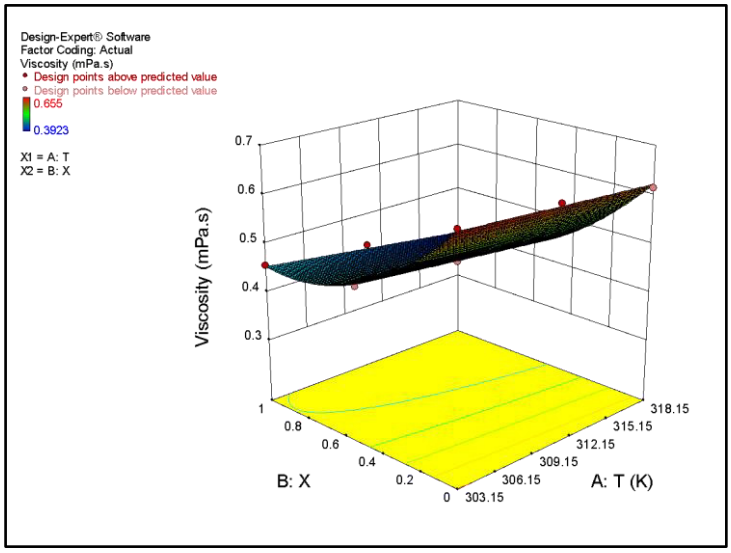


Fig 4. Combined effect of mole fraction and temperature on viscosity.

Table 11.ANOVA table for ultrasonic velocity

Source	Sum of squares	df	Mean square	F-Value	P-Value Prob>F	Remarks
Model	3.57E+05	5	71465.17	803.75	< 0.0001	significant
A-T	10467.89	1	10467.89	117.73	< 0.0001	
B-X	2.51E+05	1	2.51E+05	2826.64	< 0.0001	
AB	1056.2	1	1056.2	11.88	0.0107	
A^2	1083.94	1	1083.94	12.19	0.0101	
B^2	87078.69	1	87078.69	979.35	< 0.0001	
Residual	622.41	7	88.92			
Lack of Fit	622.41	3	207.47			
Pure Error	0	4	0			
Cor Total	3.58E+05	12				

df=Degrees of freedom,F-Value=F-Test value,P-Value=P test value

From the ANOVA table 11,The Model F-value of 803.75 implies the model is significant. There is only a 0.01% chance that an F-value this large could occur due to noise. Values of "Prob > F" less than 0.0500 indicate model terms are significant. In this case A, B, AB, A^2, B^2 are significant model terms. Values greater than 0.1000 indicate the model terms are not significant. If there are many insignificant model terms (not counting those required to support hierarchy), model reduction may improve your model. The "Pred R-Squared" of 0.9828 is in reasonable agreement with the "Adj R-Squared" of 0.9970; i.e. the difference is less than 0.2. "Adeq Precision" measures the signal to noise ratio. A ratio greater than 4 is desirable. Your ratio of 76.938 indicates an adequate signal. This model can be used to navigate the design space.

Final Equation in Terms of Coded Factors:

$$\mathbf{Ultrasonic\ Velocity} = +1150.87 - 41.77 * A - 204.67 * B - 16.25 * AB - 19.81 * A^2 + 177.56 * B^2 \quad \textbf{(36)}$$

Final Equation in Terms of Actual Factors:

$$Ultrasonic\ velocity = -31397.36958 + 215.41271 * T + 226.53160 * X - 4.33322 * T * X - 0.35219 * T^2 + 710.25056 * X^2 \quad \textbf{(37)}$$

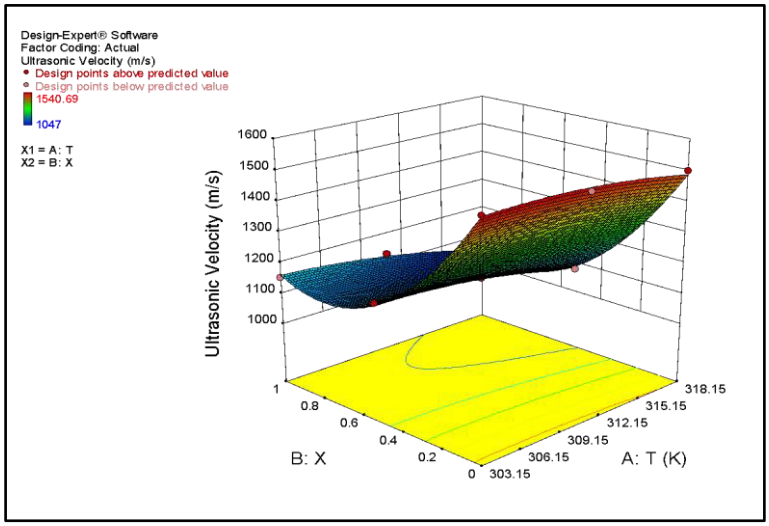


Fig 5. Combined effect of mole fraction and temperature on ultrasonic velocity.

Table 12. Standard deviation, mean and R^2 values for density and viscosity in the predicted model

Density				Viscosity			
Std.dev.	4.55E-03	R-Squared	0.9989	Std.dev.	9.38E-03	R-Squared	0.9926
Mean	0.82	Adj.R-squared	0.998	Mean	0.5	Adj. R-squared	0.9873
C.V., %	0.56	Pred. R-squared	0.9886	C.V., %	1.88	Pred. R-squared	0.933
PRESS	1.45E-03	Adeq. Precision	101.134	PRESS	5.55E-03	Adeq. Precision	39.239

Std.Dev.=Standard deviation , R-Squared=R2 ,C.V.=Variant coefficient

Table13. Standard deviation, mean and R^2 values for ultrasonic velocity in the predicted model

Ultrasonic Velocity			
Std.dev.	9.43	R-Squared	0.9983
Mean	1223.68	Adj. R-squared	0.997
C.V., %	0.77	Pred. R-squared	0.9828
PRESS	6168.77	Adeq. Precision	76.938

Std.Dev.=Standard deviation , R-Squared=R2 ,C.V.=Variant coefficient

Table 14.ANOVA table for refractive index

Source	Sum of squares	Df	Mean square	F-Value	P-Value Prob>F	Remarks
Model	1.13E-03	5	2.26E-04	216.99	< 0.0001	significant
A-T	7.09E-05	1	7.09E-05	68.14	< 0.0001	
B-X	8.27E-04	1	8.27E-04	794.81	< 0.0001	
AB	9.39E-06	1	9.39E-06	9.02	0.0198	
A^2	1.15E-05	1	1.15E-05	11.07	0.0126	
B^2	1.47E-04	1	1.47E-04	140.9	< 0.0001	
Residual	7.29E-06	7	1.04E-06			
Lack of Fit	7.29E-06	3	2.43E-06			
Pure Error	0	4	0			
Cor Total	1.14E-03	12				

df=Degrees of freedom,F-Value=F-Test value,P-Value=P test value

The Model F-value of 216.99 implies the model is significant. There is only a 0.01% chance that an F-value this large could occur due to noise. Values of "Prob > F" less than 0.0500 indicate model terms are significant. In this case A, B, AB, A^2, B^2 are significant model terms. Values greater than 0.1000 indicate the model terms are not significant. If there are many insignificant model terms (not counting those required to support hierarchy), model reduction may improve your model. The "Pred R-Squared" of 0.9379 is in reasonable agreement with the "Adj R-Squared" of 0.9890; i.e. the difference is less than 0.2."Adeq Precision" measures the signal to noise ratio. A ratio greater than 4 is desirable. Your ratio of 43.804 indicates an adequate signal. This model can be used to navigate the design space.

Final Equation in Terms of Coded factors

$$\text{Refractive index} = +1.35 - 3.438E - 003 * A + 0.012 * B - 1.532E - 003 * AB - 2.043E - 003 * A^2 - 7.288E - 003 * B^2 \quad (38)$$

The equation in terms of coded factors can be used to make predictions about the response for given levels of each factor. By default, the high levels of the factors are coded as +1 and the low levels of the factors are coded as -1. The coded equation is useful for identifying the relative impact of the factors by comparing the factor coefficients.

Final Equation in Terms of Actual Factors:

$$\text{Refractive index} = -2.09240 + 0.022307 * T + 0.17959 * X - 4.08667E - 004 * T * X - 3.63126E - 005 * T^2 - 0.029150 * X^2 \quad (39)$$

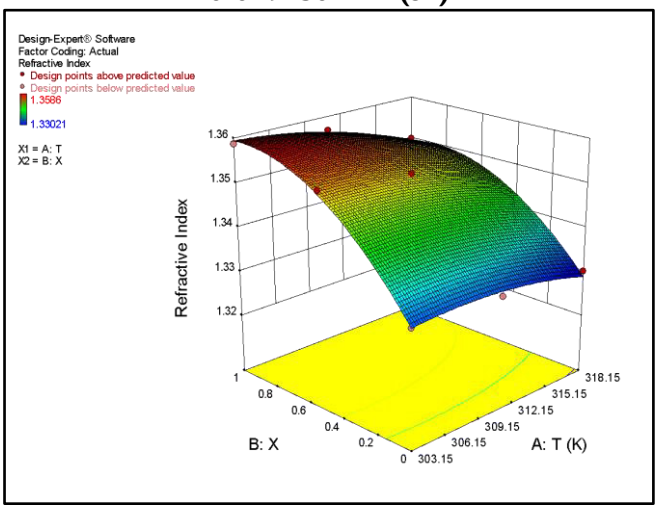


Fig. 6. Combined effect of mole fraction and temperature on Refractive index.

Table 15.ANOVA table for surface tension

Source	Sum of squares	df	Mean square	F-Value	P-Value Prob>F	Remarks
Model	3778.79	5	755.76	1877.16	< 0.0001	significant
A-T	49.48	1	49.48	122.91	< 0.0001	
B-X	3090.9	1	3090.9	7677.24	< 0.0001	
AB	8.18	1	8.18	20.32	0.0028	
A^2	6.3	1	6.3	15.66	0.0055	
B^2	578.46	1	578.46	1436.8	< 0.0001	
Residual	2.82	7	0.4			
Lack of Fit	2.82	3	0.94			
Pure Error	0	4	0			
Cor Total	3781.61	12				

df=Degrees of freedom,F-Value=F-Test value,P-Value=P test value

Table16. Standard deviation, mean and R^2 values for refractive index and surface tension in the predicted model

Refractive index				Surface Tension			
Std.dev.	1.02E-03	R-Squared	0.9936	Std.dev.	0.63	R-Squared	0.9993
Mean	1.35	Adj. R-squared	0.989	Mean	39.43	Adj. R-squared	0.9987
C.V., %	0.076	Pred. R-squared	0.9379	C.V., %	1.61	Pred. R-squared	0.9924
PRESS	7.06E-05	Adeq.Precision	43.804	PRESS	28.67	Adeq.Precision	118.63

Std.Dev.=Standard deviation , R-Squared=R2 ,C.V.=Variant coefficient

The Model F-value of 1877.16 implies the model is significant. There is only a 0.01% chance that an F-value this large could occur due to noise. Values of "Prob > F" less than 0.0500 indicate model terms are significant. In this case A, B, AB, A^2, B^2 are significant model terms. Values greater than 0.1000 indicate the model terms are not significant. If there are many insignificant model terms (not counting those required to support hierarchy), model reduction may improve your model. The "Pred R-Squared" of 0.9924 is in reasonable agreement with the "Adj R-Squared" of 0.9987; i.e. the difference is less than 0.2."Adeq Precision" measures the signal to noise ratio. A ratio greater than 4 is desirable. Your ratio of 118.630 indicates an adequate signal. This model can be used to navigate the design space.

Final Equation in terms of coded factors:

$$\sigma = +33.45 - 2.87 \times A - 22.70 \times B + 1.43 \times AB - 1.51 \times A^2 + 14.47 \times B^2 \quad \textbf{(40)}$$

Final Equation in Terms of actual factors:

$$\sigma = -2343.03907 + 16.11295 \times \mathrm{T} - 221.74379 \times \mathrm{x} + 0.38133 \times \mathrm{T} \times \mathrm{x} - 0.026857 \times \mathrm{T}^2 + 57.88874 \times \mathrm{x}^2 \quad \textbf{(41)}$$

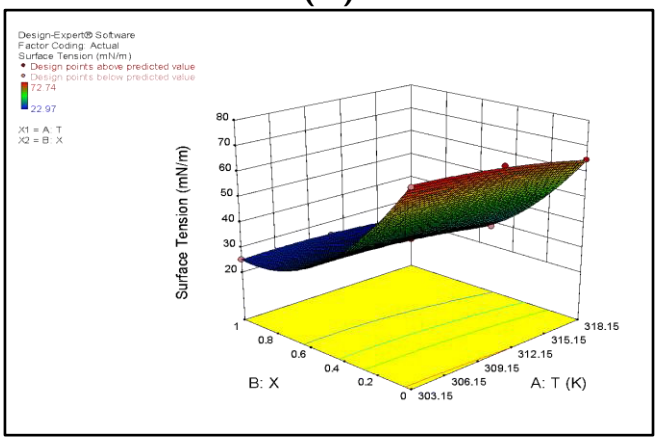
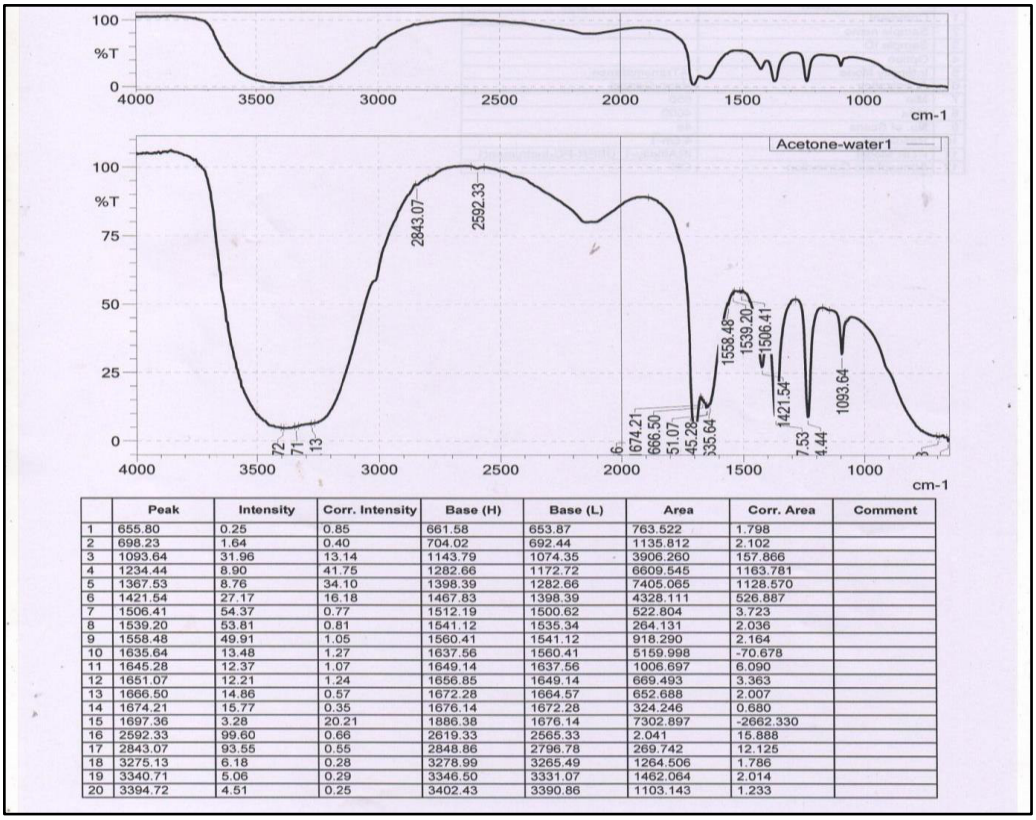


Fig. 7. Combined effect of mole fraction and temperature on Surface Tension.

From equation 32-41, in terms of actual factors can be used to make predictions about the response for given levels of each factor. Here, the levels should be specified in the original units for each factor. This equation should not be used to determine the relative impact of each factor because the coefficients are scaled to accommodate the units of each factor and the intercept is not at the center of the design space.

FT-IR Analysis:

The molecular interactions among Acetone-water mixture also are defined through FT-IR spectroscopy. FT-IR spectroscopy has been used extensively to examine intra and intermolecular hydrogen bonding interactions between acetone-water combination molecules [36-41]. Generally, intermolecular hydrogen bonds supply upward push to a wide band, because the bands bobbing up from intermolecular hydrogen bonds are sharp bands. The carbonyl stretching absorption is one of the strongest IR absorptions, and may be very useful in structure dedication as one could determine each the range of carbonyl businesses (assuming peaks do not now overlap) but also an estimation of which types. The function absorption peaks found for the acetone-water combination as follows: 3394 cm^{-1} (N–H, St), 2843 cm^{-1} (C–H, St), 2592 cm^{-1} (C–H, St in acetone), 1674 cm^{-1} (C = O, St), 1558 cm-1 (C = O, St in carboxylic ion) and 1367 cm-1 (C–O, St).



	Peak	Intensity	Corr. Intensity	Base (H)	Base (L)	Area	Corr. Area	Comment
1	655.80	0.25	0.85	661.58	653.87	763.522	1.798	
2	698.23	1.64	0.40	704.02	692.44	1135.812	2.102	
3	1093.64	31.96	13.14	1143.79	1074.35	3906.260	157.866	
4	1234.44	8.90	41.75	1282.66	1172.72	6609.545	1163.781	
5	1367.53	8.76	34.10	1398.39	1282.66	7405.065	1128.570	
6	1421.54	27.17	16.18	1467.83	1398.39	4328.111	526.887	
7	1506.41	54.37	0.77	1512.19	1500.62	522.804	3.723	
8	1539.20	53.81	0.81	1541.12	1535.34	264.131	2.036	
9	1558.48	49.91	1.05	1560.41	1541.12	918.290	2.164	
10	1635.64	13.48	1.27	1637.56	1560.41	5159.998	-70.678	
11	1645.28	12.37	1.07	1649.14	1637.56	1006.697	6.090	
12	1651.07	12.21	1.24	1656.85	1649.14	669.493	3.363	
13	1666.50	14.86	0.57	1672.28	1664.57	652.688	2.007	
14	1674.21	15.77	0.35	1676.14	1672.28	324.246	0.680	
15	1697.36	3.28	20.21	1886.38	1676.14	7302.897	-2662.330	
16	2592.33	99.60	0.66	2619.33	2565.33	2.041	15.888	
17	2843.07	93.55	0.55	2848.86	2796.78	269.742	12.125	
18	3275.13	6.18	0.28	3278.99	3265.49	1264.506	1.786	
19	3340.71	5.06	0.29	3346.50	3331.07	1462.064	2.014	
20	3394.72	4.51	0.25	3402.43	3390.86	1103.143	1.233	

Fig.8. Normalized FT-IR spectrum of [ACETONE][WATER] over the range (1000 to 4000) cm^{-1}.

5. CONCLUSION

The system Acetone and water has been studied with the aid of measuring density, viscosity, ultrasonic velocity, floor anxiety and refractive index at four one-of-a-kind temperatures of 303.15, 308.15, 313.15 and 318.15 K. These experimental facts and the derived properties were analyzed in phrases of particular interplay because of electron donor-acceptor complex among the issue molecules. The important reality is that the brand new equations evolved for viscosity and ultrasonic pace have been discovered to be in shape nicely compared to the prevailing equations. Finally, FT-IR spectroscopy changed into acetone-water device and corresponding absorption peaks have been observed. The physical property data on mixed solvents (Acetone-water) are important for the theoretical and applied areas of research and are frequently used in many chemical and industrial processes such as design of new process and process equipment (fluid flow, mass transfer or heat transfer calculation) and designing of bioreactor/fermenter.

6. AUTHORS CONTRIBUTION

Golamari Siva Reddy, Nadeem Siddiqui, Jannu Sai Teja, Pamireddy Gari Venkateswar Reddy, conceived of the presented idea, developed the theory and performed the computations. G Siva Reddy verified the analytical methods. G Siva Reddy encouraged Rayapalli Tharun Kumar, Nelluri Krishna Chaitanya, Jamullamudi Vineethanand , Mallu Maheswara Reddy, N Konda Reddy, Varakala Nikhil Reddy,Divyansh Dhakate ,Venkata Ramana Avula to investigate design expert software for medium component analysis and supervised the findings of this work. All authors discussed the results and contributed to the final manuscript. All the authors read and approved the final version of the manuscript.

7. CONFLICT OF INTEREST

Conflict of interest declared none

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