

PREDICTION OF THERMODYNAMICS AND TRANSPORT PROPERTIES OF BINARY LIQUID MIXTURE USING PROCESS SIMULATION

Submitted in partial fulfillment of the requirements for the award of

Bachelor of Technology degree in
Chemical Engineering
by

ANFAS ROSHAN P (38190001)

KARTHIK RAJA S (38190006)



**DEPARTMENT OF CHEMICAL ENGINEERING
SCHOOL OF BIO AND CHEMICAL ENGINEERING**

SATHYABAMA

**INSTITUTE OF SCIENCE AND TECHNOLOGY
(DEEMED TO BE UNIVERSITY)**

Accredited with grade “A” by NAAC

JEPPIAAR NAGAR, RAJIV GANDHI SALAI, CHENNAI – 600119

MAY 2022



SATHYABAMA
INSTITUTE OF SCIENCE AND TECHNOLOGY
(DEEMED TO BE UNIVERSITY)
Accredited with "A" grade by NAAC
Jeppiaar Nagar, Rajiv Gandhi Salai, Chennai - 600 119
www.sathyabama.ac.in



DEPARTMENT OF CHEMICAL ENGINEERING

BONAFIDE CERTIFICATE

This is to certify that this Project Report is the bonafide work of **ANFAS ROSHAN P (38190001)** and **KARTHIK RAJA S (38190006)** who carried out the project entitled **"PREDICTION OF THERMODYNAMICS AND TRANSPORT PROPERTIES OF BINARY LIQUID MIXTURE USING PROCESS SIMULATION"** under my supervision from September 2021 to April 2022.

Chenkar
Internal Guide

Dr. D.VENKATESAN M.Tech., Ph.D.,

[Signature]
Head of the Department

Dr.S.SATHISH, M.E., Ph.D.,

DEPARTMENT
CHEMICAL ENGINEERING
SATHYABAMA
INSTITUTE OF SCIENCE AND TECHNOLOGY
(DEEMED TO BE UNIVERSITY)
Jeppiaar Nagar, Rajiv Gandhi Salai,
Chennai - 600 119

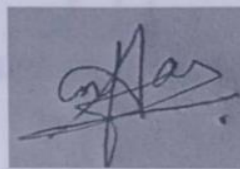
Submitted for Viva voce Examination held on 04-05-22

Internal Examiner

External Examiner

DECLARATION

I ANFAS ROSHAN P (38190001) hereby declare that the Project Report entitled "PREDICTION OF THERMODYNAMICS AND TRANSPORT PROPERTIES OF BINARY LIQUID MIXTURE USING SIMULATION" done by us under the guidance of Dr. D. VENKATESAN, M.Tech., Ph. D., at Sathyabama Institute of Science and Technology is submitted in partial fulfillment of the requirements for the award of Bachelor of Technology degree in Chemical Engineering.



DATE: 19.04.22

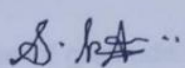
SIGNATURE OF THE CANDIDATE

PLACE: CHENNAI

DECLARATION

I KARTHIK RAJA S (38190006) hereby declare that the Project Report entitled "PREDICTION OF THERMODYNAMICS AND TRANSPORT PROPERTIES OF BINARY LIQUID MIXTURE USING SIMULATION" done by me under the guidance of Dr. D. VENKATESAN, M.E., Ph. D., at Sathyabama Institute of Science and Technology is submitted in partial fulfillment of the requirements for the award of Bachelor of Technology degree in Chemical Engineering.

DATE: 19.04.22


SIGNATURE OF THE CANDIDATE

PLACE: CHENNAI

ACKNOWLEDGEMENT

We are pleased to acknowledge our sincere thanks to the Board of Management of **SATHYABAMA** for their kind encouragement in doing this project and for completing it successfully. We are grateful to them.

We convey our sincere thanks to **Dr. S. SATHISH M.E., Ph.D.**, Head of the Department, Dept. of Chemical Engineering for providing us necessary support and details at the right time during the progressive reviews.

We would like to express our sincere and deep sense of gratitude to our internal Project Guide **Dr. D. VENKATESAN M.Tech., Ph.D.**, for their valuable guidance, suggestions and constant encouragement paved way for the successful completion of our project work.

We also express our thanks to all Teaching and Non-teaching staff members of the Department of Chemical Engineering who were helpful in many ways for the completion of the project.

ABSTRACT

Densities, viscosities of binary liquid mixtures composed of 1-Decanol with Pentyl acetate , Hexyl acetate and Octyl acetate were determined at 298.15, 303.15, 308.15 and 313.15 K by using the simulation software (CHEMCAD) and through EXPERIMENTAL and results were obtained. Deviation in viscosity ($\Delta\eta$), excess molar volume (V^E), excess Gibbs free energy of activation of viscous flow (ΔG^{*E}) were determined. The deviations in viscosity, excess molar volume and excess Gibbs free energy of activation of viscous flow was correlated with Redlich-Kister polynomial equation. Other parameters like Frenkel,Bingham model,Frenkel model, Hind model,Hind and ubbelohde model,Grunberg Nissan,Katti and chaudhri,Kendall model and Kendall-Monroe viscosity correlation equation were used to quantitatively analyze the interactions in the system.

Keywords : Densities, viscosities, binary liquid mixtures, deviation in viscosity, excess molar volume, excess gibbs free energy, simulation software.

TABLE OF CONTENTS

CHAPTER NO	TITLE	PAGE NO
	ABSTRACT	vi
	LIST OF TABLES	viii
	LIST OF FIGURES	ix
1	INTRODUCTION	1
	1.1 DENSITY	2
	1.2 VISCOSITY	2
	1.3 EXCESS PARAMETERS	4
	1.4 LITERATURE REVIEW	6
2	AIM AND SCOPE	10
3	THEORETICAL	12
	3.1 CHEMCAD	14
	3.1.1 CHEMCAD PRODUCTS & FEATURES	15
	3.1.1.1 CC – STEADY STATE	16
	3.1.1.2 CC – DYNAMICS	16
	3.1.1.3 CC – BATCH	16
	3.1.1.4 CC – THERM	16
	3.1.1.5 CC – SAFETY NET	17
	3.1.1.6 CC – FLASH	17
4	RESULTS AND DISCUSSION	18
5	SUMMARY AND CONCLUSION	66
	REFERENCES	69

LIST OF TABLES

FIGURE No	TITLE	PAGE NO.
4.1	Theoretical Values Of The Properties For 1-Decanol + Pentyl Acetate	18
4.2	Theoretical Values Of The Properties For 1-Decanol + Hexyl Acetate	26
4.3	Theoretical Values Of The Properties For 1-Decanol + Octyl Acetate	34
4.4	Adjustable Parameters For 1-Decanol With Pentyl Acetate, Hexyl Acetate And Octyl Acetate	47
4.5	Theoretical Values For Experimental Reading Of 1-Decanol (X1) + Pentyl Acetate(X2) At 303.15 K	53
4.6	Theoretical Values For Experimental Reading Of 1-Decanol (X1) + Hexyl Acetate (X2)At 303.15 K	55
4.7	Theoretical Values For Experimental Reading Of 1-Decanol (X1) + Octyl Acetate (X2) At 303.15 K	57

LIST OF FIGURES

TABLE No	TITLE	PAGE No.
4.1	Plots of ($\Delta\eta$) against mole fraction for 1-Decanol + Pentyl acetate	42
4.2	Plots of ($\Delta\eta$) against mole fraction for 1-Decanol + Hexyl acetate	42
4.3	Plots of ($\Delta\eta$) against mole fraction for 1-Decanol + Octyl acetate	43
4.4	Plots of (ΔG^{*E}) against mole fraction for 1-Decanol + Pentyl acetate	43
4.5	Plots of (ΔG^{*E}) against mole fraction for 1-Decanol + Hexyl acetate	44
4.6	Plots of (ΔG^{*E}) against mole fraction for 1-Decanol + Octyl acetate	44
4.7	Plots of (V_M) against mole fraction for 1-Decanol + Pentyl acetate	45
4.8	Plots of (V_M) against mole fraction for 1-Decanol + Hexyl acetate	45
4.9	Plots of (V_M) against mole fraction for 1-Decanol + Octyl acetate	46
4.10	Plots of ($\Delta\eta$) against mole fraction for 1-Decanol + Pentyl acetate found experimentally at 303.15 K	59
4.11	Plots of ($\Delta\eta$) against mole fraction for 1-Decanol + Pentyl acetate found in chemcad at 303.15 K	59

4.12	Plots of $(\Delta\eta)$ against mole fraction for 1-Decanol + Hexyl acetate found experimentally at 303.15 K	60
4.13	Plots of $(\Delta\eta)$ against mole fraction for 1-Decanol + Hexyl acetate found in chemcad at 303.15 K	60
4.14	Plots of $(\Delta\eta)$ against mole fraction for 1-Decanol + Octyl acetate found experimentally at 303.15 K	61
4.15	Plots of $(\Delta\eta)$ against mole fraction for 1-Decanol + Octyl acetate found in chemcad at 303.15 K	61
4.16	Plots of (ΔG^{*E}) against mole fraction for 1-Decanol +Pentyl acetate found experimentally at 303.15 K	62
4.17	Plots of (ΔG^{*E}) against mole fraction for 1-Decanol +Pentyl acetate found in chemcad at 303.15 K	62
4.18	Plots of (ΔG^{*E}) against mole fraction for 1-Decanol +Hexyl acetate found experimentally at 303.15 K	63
4.19	Plots of (ΔG^{*E}) against mole fraction for 1-Decanol +Hexyl acetate found in chemcad at 303.15 K	63
4.20	Plots of (ΔG^{*E}) against mole fraction for 1-Decanol +Octyl acetate found experimentally at 303.15 K	64
4.21	Plots of (ΔG^{*E}) against mole fraction for 1-Decanol + Octyl acetate found in chemcad at 303.15 K	64

LIST OF SYMBOLS AND ABBREVIATION

X_1	- Mole fraction of first component
X_2	- Mole fraction of second component
H	- Viscosity
ρ	- Density
$\Delta\eta$	- Deviation in Viscosity
V^E	- Excess molar volume
V_m	- Molar volume of mixture
ΔG^{*E}	- Excess Gibbs free energy of activation of viscous flow
d'	- Grunberg-Nissan parameter
$E_{\eta m}$	- Modified Kendall and Monroe viscosity correlation

CHAPTER 1

INTRODUCTION

In the era of increasing environmental issues, the need for sustainable greener technologies also increases day by day. Ionic liquids are one such environmentally friendly leap taken in industries replacing the volatile organic solvents. Though organic solvents are applied in sustainable areas, their increasing consumption is polluting the environment. These ionic liquids which are salts with an organic cation and either an organic or inorganic anion finds application in various areas such as lubrication, electrolytes in fuel cells and batteries, used for drug delivery in pharmaceutical industry, used in separation processes such as extraction, separation. etc. Being such a versatile technology, the market of ionic liquid that was USD 1.40 billion is expected to reach a growth of 18.4 % by 2027. This increasing market makes it a target on which a plentiful number of researches and studies are done on this non-aqueous solution in order to study its thermodynamic and transport properties that plays an important role in the application of ionic liquids in chemical and industrial applications.

Parameters such as viscosity and density of the pure chemicals and ionic liquids are studied at varying composition and temperature that helps in chemical industrial applications such as for Mass transfer operations, pipeline system transport. etc. Inter molecular interactions of the binary liquid mixtures are understood by performing studies on excess properties such as deviation in viscosity, excess molar volume, excess Gibbs free energy of activation of viscous flow and Grunberg-Nissan interaction constant of binary mixtures. This thesis is a study on the parameters and excess parameters of the binary mixtures composed of 1-Decanol with Pentyl acetate, Hexyl acetate and Octyl acetate at 298.15, 303.15, 308.15 and 313.15 K experimentally and in CHEMCAD software. Redlich-Kister polynomial equation was used for the correlation of parameters.

1.1 DENSITY

Density which is mass per unit volume and specific gravity which is the density of a substance divided by the density of water are properties that depends only on the matter type in sample and not on the amount of sample. The density of a substance can be calculated by multiplying the relative density of the substance to the density of water at that corresponding temperature. Therefore, The weight of a certain volume of a substance divided by the weight of an identical volume of water at the same temperature is the relative density. The degree of compactness of a substance, or how densely the atoms or molecules in a substance are packed together, is described by the parameter density. An broad and detailed study of density provides an experimental framework for developing, testing, and then modifying ideas for liquid mixtures and their transport properties, as well as insight into the nature of strength and the possibilities of microscopic interactions. Many engineering problems, such as process calculations, simulations, pipe design, and metering calculations, require liquid densities. The molecular volume and molar mass (MW) of the component cations and anions can be used to calculate ionic liquid densities. Molar volume (V_m) can be easily computed from density and mole fraction experimental data, making it a useful and efficient tool for studying molecular interactions. The variations of molar volume from ideality are represented by positive and negative values of excess molar volume (V^E). Several researchers have interpreted this as a culmination of three different effects: physical, chemical, and structural.

1.2. VISCOSITY

Viscosity is a transport attribute that can be defined as the resistance to flow when shear force is applied. Ionic liquids (ILs) require viscosity data for theoretical studies

or the design/development of industrial processes involving ILs; understanding the relationship between ionic structure and viscosity is also required to more rationally design and synthesize ILs with appropriate viscosity. Newtonian and non-Newtonian fluids are the two types of fluids. Non-Newtonian fluids do not obey Newton's law of viscosity, while Newtonian fluids do. The absolute viscosity is the proportionality constant in an equation that connects the shear stress to the shear rate or velocity gradient, according to Newton's law of viscosity.

$$\tau = \eta \, dv/dx$$

The shear stress (τ) is the force applied to the fluid per unit area, while the velocity gradient ' dv/dx ' is a measure of the shearing experienced by the liquid and is thus known as shear strain (γ).

The main advantage of measuring the viscosity of various materials is that you can choose the best storage method for them. Because viscosity is not a constant property, it's critical to understand how a substance will change when heated or cooled. You risk material spoiling or a poor user experience if you don't have that information. Many scholars have been interested in the viscosity of pure components as well as liquid mixtures over the years. Despite all previous efforts, a thorough explanation of the viscosity of multi-component liquid mixtures remains unattainable, owing to the difficulties of comprehending the liquids' structure. To have a comprehensive understanding of the structure of the liquid / liquid mixtures, more accurate and exact viscosity data, especially for liquid mixtures, is essential. Most fluid flow equipment requires accurate viscosity data for design. Viscosity measurement is used in the pharmaceutical business to qualify the flow behaviour of materials for a number of applications. Material characterization or finger-printing, standard testing methods to check for differences between batches, indirect way of measuring quality, product formulation, quality control, process control, design, optimization, and operation of process equipment are just some of the applications for viscometrical data. Viscometry is one of the most extensively used methods for determining polymer molecular weight since it is the simplest and fastest way to gather molecular weight-related data with the least number of instrumentation. The high viscosity of polymer solutions, especially when the amount of added polymer is tiny, is one of their most noticeable characteristics. Our laboratory has put in a lot

of effort to create a large database with precise density and viscosity of liquids and liquid mixes at various compositions and temperatures. The estimation of Gibb's free energy, free volume, internal pressure, and enthalpy, among other things, is based on extensive experimental data on viscosity combined with the analysis of ultrasonic velocity and density.

1.3. EXCESS PARAMETERS

The deviation of the solution from ideality is described by the values of the excess parameters of the binary mixtures. The excess values A^E for any parameters, can be computed using the relation,

$$A^E = A^{\text{mix}} - \sum x_i A_i \quad (i=1 \text{ to } n)$$

Where A^{mix} represent the parameter of the mixture, A_i represent the physical parameter of the pure component ' i '.

Many workers have viewed the excess parameters as a culmination of three effects:

Many workers have viewed the surplus parameters as a culmination of three effects:

(1) Physical; this is due to non-specific physical interactions.

(2) Chemical; this occurs when the liquid order of related species is broken apart.

(3) Structural; this occurs as a result of the geometrical fitting of molecules into the spaces caused by larger molecules, as well as discrepancies in the molar and free volumes of the constituents.

Thermodynamic functions that are sensitive towards the size, shape and intermolecular forces of the molecules are the ones that are mostly used to study the intermolecular forces of the Ionic Liquids. A number of researchers have used excess molar volume, viscosity deviation, and excess molar refraction to explore molecular interactions in liquid mixtures as a function of temperature and mole fraction. With the use of experimental data of sound velocity, density, and viscosity, many additional derived parameters such as Gibb's activation energy of viscous

flow, internal pressure, free volume, and so on may be estimated. Excess values of these derived metrics represent molecular unit variability and also provide important implications about the nature of interactions. Different types of intermolecular interactions between the component molecules on the basis of non-specific van der Waal's forces, hydrogen bonding, dipole-dipole interactions, donor acceptor interactions between unlike molecules, and fitting of smaller molecules into the voids created by bigger molecules can explain the values of excess parameters for binary mixtures. Physical parameters of non-ideal liquid mixes deviate significantly from linearity with respect to concentration, which has been interpreted as the presence of weak or strong interactions. Excess characteristics can be utilized to test and enhance thermodynamic models for calculating and predicting fluid phase equilibria. These extra features are crucial to comprehending intermolecular interactions.

Interactions between different molecules and the nature of molecular agitation
These functions give a notion of how far a liquid combination deviates from its ideal state. In terms of mixing factors such as excess molar volume, V^E , variations in viscosity, and so on, the nature and kind of interactions in binary organic liquid mixtures have been investigated. These characteristics can be estimated using direct density and viscosity measurements. The thermodynamic parameters of a mixture acquired from density and viscosity measurements can be used to design engineering procedures.

1.4. LITERATURE REVIEW

The Recovery And Extraction of Heavy Metal Ions Using Ionic Liquid as Green Solvent, Mas Ami Kumano, Tomoki Yabutani and Junko Motonaka* (March 2006)

Faculty of Engineering, The University of Tokushima

IL used : N,N,-diethyl-N-methyl-N-(2-methoxyethyl) ammonium bis (trifluoro methansulfonyl)imide

The sample solution is prepared by mixing 500 µl of pH 7 buffer solution containing heavy metals with 100 µl of ionic liquid containing 8-HQ. Then the solution is taken in a 2ml propylene tube and shaken mechanically for 12 hours to extract heavy metals at room temperature. Then they are centrifuged in order to separate the aqueous phase from the ionic liquid phase. Determination of metal ion concentration using ICP-AES. ICP-AES (Inductivity Coupled Plasma Atomic Emission Spectroscopy) which is an analytical technique used to find the elemental composition of the sample by de-solvating the sample into atoms/ions. The extraction efficiency is calculated by,

$$\text{Extraction efficiency(\%)} = [((C_i)_{aq} - (C_f)_{aq}) / (C_i)_{aq}] * 100$$

Where, (C_i)_{aq} and (C_f)_{aq} are conc. Of metal ions in the aqueous phase before and after extraction.

Treat Of Waste Printed Circuit Board By Green Solvent Using Ionic Liquid, P.Zhu, Y.Chen, Ly>Wang, M.Zhou , Sahngai University(2012)

IL used : [EMIM+][BF₄-]->1-ethyl-3-methylimidazolium tetrafluoroborate

The solid waste disposal centre collected waste printed circuit boards, which are mostly made of glass fibre reinforced using epoxy resin. By manually removing the welding-jointed electrical components, the recovered components can be resold. Before the experiment, the WPCB samples were broken into small pieces (15-20 cm²). IL was used as the heating media. The experiments were conducted using

self-made apparatus, which included a stainless steel cylinder, a stirrer, and a temperature-controlled furnace. The WPCBs are submerged in the IL and agitated at 50 rpm in a cylinder. TGA and FTIR tests were carried out. At 280-380 °C, WPCBs lost a significant amount of weight, showing that bromine epoxy resins are dissolving in IL at this temperature. It is found that recovering copper foils and glass fibres from WPCBs is a new process that has no negative environmental impact.

Amino Acid-Functionalized Ionic Liquid Solid Sorbents for PostCombustion Carbon Capture Xianfeng Wang,^{†,‡} Novruz G. Akhmedov,[§] Yuhua Duan,[†] David Luebke,[†] David Hopkinson,[†] and Bingyun Li*,^{†,‡} [†]National Energy Technology Laboratory-Regional University Alliance (NETL-RUA), Morgantown, West Virginia 26507, United States [‡]Department of Orthopaedics, School of Medicine, West Virginia University, Morgantown, West Virginia 26506, United States [§]Department of Chemistry, West Virginia University, Morgantown, West Virginia 26506, United States (2013)

IL used : Amino acid ionic liquids (AAILs)

As new sorbents for post-combustion CO₂ removal, [EMIM][Lys] was produced and immobilised into nano porous PMMA microspheres. TGA was used to assess the CO₂ collection performance of [EMIM][AA]- impregnated PMMA sorbents. Thirty milligrammes of dried PMMA-based sorbent were deposited in the centre of a TGA microbalance quartz tube reactor and heated to 105 °C for around 60 minutes in a N₂ environment with a flow rate of 200 mL/min. The temperature was subsequently raised to 40 °F, and pure dry CO₂ was supplied at a rate of 200 mL/min until no weight gain could be seen. Desorption was achieved by injecting pure N₂ into the sample cell for 60 minutes at 100 °C. The sorbents' weight change in milligrammes was recorded, and the weight change in percentage was defined as the ratio of the amount of gas adsorbed or desorbed to the total amount of CO₂ adsorbed. The weight change of the samples during the adsorption/desorption cycles was used to calculate the adsorption capacity in mmol/(g sorbent). CO₂ adsorption in AAIL sorbents appeared to be a two-step process in which CO₂ was directly adsorbed on the surface and CO₂ diffused into the sorbent to continue reacting with amino groups. Our fitted rate constants, activation energies, and factors (related to entropy

change) revealed that the second CO₂ diffusion process was the rate-determining step for the sorbent to capture CO₂. And the adsorbent's stable multicyclic properties makes it promising for post-combustion CO₂ capture.

Ionic liquids in wood preservation, Juliusz Pernak^{1,*}, Jadwiga Zabielska-Matejuk², Aleksandra Kropacz² and Joanna Foksowicz-Flaczyk¹ (1 Poznań University of Technology, Poznań, Poland; 2 Institute of Wood Technology, Poznań), Poland (2004)

IL used : 3-alkoxymethyl-1-methylimidazolium tetrafluoroborates and hexafluorophosphates

A two-stage method was used to synthesize the ionic liquids. By nucleophilic attack of 1-methylimidazole on chloromethyl alkyl ether, quaternization yielded 3-alkoxymethyl-1-methylimidazolium chlorides in 95% yield. The final step was the high yield metathesis of isolated chloride with sodium tetrafluoroborate or potassium hexafluorophosphate in water or methanol solution. All of the 3-alkoxymethyl-1-methylimidazolium tetrafluoroborates that were prepared. The RTILs were discovered to dissolve well-known fungicides such as BAC and DDAC. It has also been tested with wood. RTILs can be used as both biocides and solvents in wood preservation. The length of the alkoxymethyl substituent determines their antifungal activity. RTILs thoroughly moisten the wood surface and penetrate to a depth of 4.8 to 6.4 mm. The depth of penetration is determined by the structure of the RTILs, specifically the type of anion.

Lignocellulosic hydrogel from recycled old corrugated container resources using ionic liquid as a green solvent, Seyed Mostafa Hashemi Sangtarashani, Mehdi Rahmaninia^{*}, Rabi Behrooz, Amir Khosravani, Wood and Paper Science and Technology Department, Faculty of Natural Resources, Tarbiat Modares University, Noor, Iran (2020)

IL used : triethylammonium acetate (TEAA)

OCC was collected locally as a primarily lignocellulosic raw material. Preparation of the pulp- Recycled OCC pulp was made from the OCC. Chemical analysis of

recycled OCC pulp- Chemical analysis was performed on the obtained fibrous OCC pulp with an average length of about 0.9 mm. The ash content of recycled pulp and the components that can be extracted using organic solvents -Ionic liquid dissolution of recycled OCC pulp. The ability of a hydrogel is to re-absorb water. To study the hydrogel structure, field emission scanning electron microscope (FESEM) images were taken using a Mira3XMU FE-SEM apparatus at an accelerating voltage of 10 kV and at various magnifications. The recycled OCC pulp was found to be composed of 84% holo- cellulose, 6% lignin, 9% ash, and about 1% extractive materials, according to preliminary analysis. Furthermore, an evaluation of the effect of different anti- solvents on water absorption revealed that hydrogel made after washing with distilled water had the best water absorption.

CHAPTER-2

AIM AND SCOPE

Theoretical and experimental studies of the excess thermodynamic properties of binary liquid systems have made significant progress in recent years depicting its importance. To predict the extent of complex formation in binary and ternary systems, excess thermodynamic functions have been used as a qualitative and quantitative guide. There is a continuing demand for thermodynamic excess properties data in the construction of separation equipment and in the testing of theories of solutions. Excess enthalpies, excess Gibbs free energy of activation for viscous flow, viscosity deviation, excess molar volume, excess internal pressure, excess free volume, molar refraction deviation, and other mixing properties derived from experimentally determined values of ultrasonic velocity, density, refractive index, and viscosity provide a better understanding of molecular interactions and molecular unit variation.

The main aim of the present work is to study the molecular interaction in various binary systems. The binary system is studied at varying temperature range such as 298.15, 303.15, 308.15 and 313.15 K and composition ranging from ($0 < x < 1$). This study on binary mixtures equips us with a precise knowledge of molecular behaviour during mixing. In many studies that have been done, the experimental results of the molecular interaction vary from the results obtained from other technique. Therefore, In order to confirm the accuracy of the results of molecular interaction of the binary mixture studies, more than one technique is performed, so that a precise correlation between microscopic structure and macroscopic properties can be established.

The three binary systems that are chose for this study are 1-Decanol with Pentyl acetate, Hexyl acetate and Octyl acetate at 298.15, 303.15, 308.15 and 313.15 K whose molecular interaction is studied and sourced in this thesis. The binary system selected is finds application in areas such as lubricants, solvents, in batteries, as coatings. Etc. The study done here is done using experimental technique and using a simulation software CHEMCAD. In the future, detailed research on molecular interactions in binary solutions may aid in the selection of binary mixtures as better

lubricants and engine oil to increase engine longevity in various industries. And this reason depicts the importance of our study.

CHAPTER - 3

THEORETICAL

CHEMCAD is process simulation software that is one of the best tools for improving engineering decisions and increasing productivity in chemical engineering calculations. CHEMCAD is used to reduce costs and capital expenditures by optimizing / bottlenecking existing processes. It also maximizes profitability by designing more efficient new processes and equipment. We will calculate the density and viscosity of the binary mixture at various temperatures using the CHEMCAD software. The values obtained from the CHEMCAD software are used in the following equations to determine the thermodynamic properties of the given system.

The Excess Molar Volume (V^E) and Viscosity Deviation ($\Delta\eta$) was obtained from equations (1) and (2)

$$V^E (\text{cm}^3 \text{mol}^{-1}) = [x_1M_1 + x_2M_2] / \rho_m - [(x_1M_1 / \rho_1) + (x_2M_2 / \rho_2)] \quad (1)$$

$$\Delta\eta (\text{m Pa s}) = \eta_m - (x_1\eta_1 + x_2\eta_2) \quad (2)$$

where x_1 and x_2 are the mole fractions calculated from mass fractions. M_1 and M_2 are molar masses, ρ_1 and ρ_2 are densities, η_1 and η_2 are the viscosities of pure components 1 and 2 respectively, ρ_m and η_m are the density and viscosity of the mixture.

The Excess Gibbs Free Energy Of Activation Of Viscous Flow was obtained from equation (3)

$$\Delta G^* E = [R \ln \eta_m V_m - (x_1 R \ln \eta_1 V_1 + x_2 R \ln \eta_2 V_2)] \quad (3)$$

where R is the universal constant of gases, T is the absolute temperature, V_1 and V_2 are the molar volumes of component 1 and 2, x_1 and x_2 represents the mole fraction of component 1 and 2. V_m is obtained from equation (4) below. η_1 , η_2 and η_m are the viscosity of component 1 and 2 and mixture respectively.

$$V_m = (x_1 M_1 + x_2 M_2) / \rho_m \quad (4)$$

where x_1 and x_2 are the mole fractions calculated from mass fractions. M_1 and M_2 are molar masses, ρ_m is the density of the mixture .

The values of V^E , $\Delta\eta$ and ΔG^{*E} were correlated by a Redlich-Kister type polynomial, equation (5)

$$\Delta Y = x_1 x_2 [0 + A_1(2 x_1 - 1)^1 + A_2 (2 x_1 - 1)^2 + A_3(2 x_1 - 1)^3 + A_4(2 x_1 - 1)^4] \quad (5)$$

The values of the parameters A_k , are obtained by fitting the equation with the least-squares method. where ΔY is the excess volume V^E , deviation in viscosity $\Delta\eta$ and excess Gibbs free energy of activation of viscous flow, ΔG^{*E}

Kendall and Monroe equation (6) for analyzing the viscosity of binary mixtures based on zero adjustable parameter and Modified Kendall-Monroe equation , (7)

$$\eta_m = (x_1 \eta_1^{1/3} + x_2 \eta_2^{1/3})^3 \quad (6)$$

$$E \eta_m = (x_1 x_2 x_1 \eta_1^{1/3} + x_2 \eta_2^{1/3})^3 \quad (7)$$

where x_1 and x_2 are the mole fractions calculated from mass fractions . η_1 and η_2 are the viscosities of pure components 1 and 2 respectively . $E\eta_m$ is the Modified Kendall-Monroe equation.

Grunberg and Nissan formulated equation (8) to determine the molecular interactions that leads to viscosity changes with one parameter to estimate the dynamic viscosity of binary liquid mixtures.

$$\ln \eta_m = x_1 \ln \eta_1 + x_2 \ln \eta_2 + x_1 x_2 d \quad (8)$$

where x_1 and x_2 are the mole fractions calculated from mass fractions. η_1 and η_2 are the viscosities of pure components 1 and 2 respectively. where d' is an interaction parameter which is a function of the composition and temperature of binary liquid mixture.

3.1 CHEMCAD

The chemical processing industry (CPI) is facing numerous challenges today, including rising fuel and feed stock costs, reduced engineering staff, shorter product life cycles, increased global competition, and increased regulation. These challenges necessitate that CPI firms seek out and implement the best tools for increasing productivity and improving engineering decisions.

CHEMCAD combines a cutting-edge graphical user interface (GUI), an extensive chemical component database, a large library of thermodynamic data, and a library of the most common unit operations to provide users with significant and measurable returns on investment. Furthermore, the program is customizable, allowing for custom chemicals, thermodynamics, unit operations, calculations, and reporting – all of which contribute to a powerful user experience.

CHEMCAD is a powerful and flexible chemical process simulation environment based on three key values: innovation, integration, and open architecture. These values provide significant benefits to CHEMCAD users:

- You have access to the most up-to-date chemical engineering techniques.
- Seamless connection to the chemical engineering computing environment, with links to tools such as MS Excel and Word and interfaces such as COM,DCOM,OPC,CAPE OPEN, and XML.

CHEMCAD can model continuous, batch, and semi-batch processes, as well as simulate both steady-state and dynamic systems. This programme is widely used worldwide for the design, operation, and maintenance of chemical processes in a

wide range of industries, including oil and gas exploration, production, and refining; gas processing; commodity and specialty chemicals; pharmaceuticals; biofuels; and process equipment manufacturing.

Chemical engineers in all of these industries use CHEMCAD on a daily basis to address a variety of challenges:

- Development of new processes from the ground up
- Existing process optimization or de-bottlenecking
- Process performance monitoring;
- Design and rating of process equipment such as vessels, columns, heat exchangers, piping, valves, and instrumentation; and
- Process performance monitoring;
- Sizing of heat exchangers
- Pressure and flow balancing of complex piping networks
- Plant data reconciliation
- Economic comparisons of process alternatives
- Plant data reconciliation
- Process scaling from lab-scale to pilot-scale and then to full-scale
- Binary interaction parameter (BIP) regression from process or lab data

CHEMCAD can deliver the results you need to stay competitive in an increasingly fast and fluid global market, regardless of how complex your process is. CHEMCAD, which is simple to use and highly customizable, can put future-proof solutions within easy reach of your engineering staff.

3.1.1 CHEMCAD PRODUCTS AND FEATURES

The CHEMCAD suite is made up of several modules that each serve a specific purpose.

You may have purchased some or all of these modules based on your specific requirements. The following sections provide brief descriptions of the various CHEMCAD modules and their most common applications.

3.1.1.1. CC-Steady State

CC-STEADY STATE, the core CHEMCAD tool, allows you to design new processes, rate existing processes, and optimize processes in steady state. It is a process simulation software that includes libraries of components, unit operations, and thermodynamic approaches for steady-state simulation of chemical processes at scales ranging from lab to full-scale. It's perfect for people who want to maintain a steady state.

3.1.1.2. CC-Dynamics

Using a dynamic simulation, the CC-DYNAMICS module allows you to design the rate of existing processes. This module is fully integrated with CHEMCAD, allowing for easy and intuitive switching between steady state and dynamics, as well as dynamic analysis of flowsheets. You may quickly model everything from simple vessel accumulation to complicated reaction rate and pressure calculations with CC-DYNAMICS. Users who want to create or rate dynamic processes will find it useful.

3.1.1.3. CC-Batch

It's a standalone or add-on programme. The CC-BATCH product allows you to construct, rate, or optimise a batch distillation column. It also contains a scheduling interface that allows you to simulate batch columns in "operational step" fashion. It's incredibly adaptable, with a variety of working modes and the capacity to mimic an unlimited number of operations. It also reduces "slop" cuts and boosts productivity, making it more adaptable.

3.1.1.4. CC-Therm

You can use the CC-THERM product to design a single heat exchanger or to test the design of a vendor's heat exchanger. It's also perfect for clients who wish to use their existing exchangers in a new service or run calculations on hypothetical scenarios. Shell-and-tube, air-cooled, plate-and-frame, and double-pipe exchangers can all be simulated with CC-THERM. For high-fidelity simulations, full integration with CHEMCAD allows you to calculate exit conditions from exchanger geometry. It

employs a variety of worldwide standards and materials to improve heat exchanger sizing accuracy.

3.1.1.5. CC-Safety Net

The CC-SAFETY NET is a simulation software for pipe and safety networks that enables for thorough study of any piping network. Its software can design and rate piping networks, as well as safety relief devices and systems, in both steady-state and dynamic systems. CC-STEADYSTATE includes the steady-state features of CC-SAFETY NET. This product allows users to create simultaneous flow and pressure-balanced simulations for single or multi-phase flow, even in reverse-flow circumstances.

3.1.1.6. CC-Flash

Physical property and phase equilibrium data, as well as property prediction and regression, are all provided by the CC-FLASH module. Customers who do not require comprehensive flow-sheet simulation tools should use CC-FLASH, which is a subset of CC-STEADY STATE. Users who want property prediction and regression, as well as physical property and phase equilibrium data, will find it useful. It is used in case of both pure components and mixtures.

CHAPTER – 4

RESULTS AND DISCUSSION

Table 4.1: Theoretical values of density ρ (kg/m³), viscosity η (mPa.s), deviation in viscosity $\Delta\eta$ (mPa.s), excess molar volumes V^E (cm³/mol), molar volume of mixture V_m (cm³/mol), excess Gibbs free energy of activation of viscous flow ΔG^{*E} (J/mol), Frenkel, Frenkel model, Hind, Hind and ubbelohde, Kendall, Bingham, Katti and chaudhri, Grunberg-Nissan parameter (d') and modified Kendall and Monroe viscosity correlation $E\eta_m$ (mPa.s) of 1-Decanol (x1) +Pentyl acetate (x2) at 298.15,303.15, 308.15 and 313.15 K.

X1	ρ (kg/ m ³)	η (mPa.s)	V_m (cm ³ /mol)	V^E (cm ³ /mol)	$\Delta\eta$ (mPa.s)	ΔG^{*E} (kJ/mol)
298.15 K						
0	871.5036	0.0008	149.374	-0.0006	0	0
0.0798	866.8552	0.001	152.7618	-0.0008	-0.0006	27.015
0.1633	862.207	0.0012	156.3066	-0.0013	-0.0013	52.43
0.2507	857.5621	0.0016	160.0171	-0.0014	-0.0018	72.0124
0.3423	852.9196	0.002	163.9059	-0.0017	-0.0024	86.2544
0.4384	848.2803	0.0026	167.9857	-0.0019	-0.0028	93.5462
0.5393	843.6456	0.0034	172.2694	-0.0021	-0.0031	99.243
0.6455	839.0099	0.0045	176.778	-0.0024	-0.0031	95.7643
0.7574	834.3748	0.006	181.5286	-0.0027	-0.0028	84.9776
0.8754	829.7426	0.0082	186.5382	-0.0030	-0.0018	53.3426
1	825.1139	0.0113	191.828	-0.0033	0	0

Frenkel model	Frenkel	Kendall	Kendall monore	Hind	Hind and ubbelohde	Bingham	Grunberg Nissan	Katti and chaudhri
1.0008		0.0008	0.0008		0.0008	0.0008		
1.0017	0.0014	0.001	0.001	0.0014	0.001	0.001	0.1608	3.985
1.0026	0.0011	0.0012	0.0012	0.0011	0.0012	0.0012	-0.1969	3.0937
1.0034	0.0013	0.0016	0.0016	0.0013	0.0016	0.0016	0.156	3.1858
1.0043	0.0009	0.002	0.002	0.0009	0.002	0.002	0.044	2.9298
1.0055	0.0002	0.0026	0.0026	0.0002	0.0026	0.0026	0.0723	2.8879
1.0065	-0.0002	0.0033	0.0033	-0.0002	0.0033	0.0033	0.0761	2.8833
1.0076	-0.0007	0.0044	0.0044	-0.0007	0.0044	0.0044	0.0782	2.9502
1.0087	-0.0014	0.0059	0.0059	-0.0014	0.0059	0.0059	0.0512	3.0964
1.0101	-0.0023	0.0081	0.0081	-0.0023	0.0081	0.0081	0.0852	3.56
1.0114		0.0113	0.0113		0.0113	0.0113		

X1	$\rho(\text{kg/m}^3)$	$\eta(\text{mPa.s})$	$V_m(\text{cm}^3/\text{mol})$	$V^E(\text{cm}^3/\text{mol})$	$\Delta\eta(\text{mPa.s})$	$\Delta G^{*E}(\text{kJ/mol})$
303.15 K						
0	866.8871	0.0007	150.1694	-0.0152	0	0
0.0798	862.3586	0.0009	153.5583	-0.0149	-0.0005	27.23
0.1633	857.8295	0.0011	157.1043	-0.0146	-0.001	53.0124
0.2507	853.3026	0.0014	160.8159	-0.0144	-0.0015	75.2437
0.3423	848.7773	0.0018	164.7067	-0.0133	-0.0018	86.3452
0.4384	844.2537	0.0023	168.7869	-0.0139	-0.0022	95.264
0.5393	839.7337	0.0029	173.0719	-0.0134	-0.0024	100.3424
0.6455	835.212	0.0038	177.5819	-0.0131	-0.0025	97.5445
0.7574	830.6895	0.0051	182.334	-0.0128	-0.0021	87.2206
0.8754	826.1689	0.0068	187.3451	-0.0124	-0.0014	53.3025
1	821.6509	0.0093	192.6365	-0.012	0	0

Frenkel model	Frenkel	Kendall	Kendall monore	Hind	Hind and ubbelohde	Bingham	Grunberg Nissan	Katti and chaudhri
1.0007		0.0007	0.0007		0.0007	0.0007		
1.0014	0.0014	0.0013	0.0013	0.0014	0.0013	0.0013	0.6117	4.436
1.0021	0.0015	0.0021	0.0021	0.0015	0.0021	0.0021	0.2167	3.5081
1.0029	0.0011	0.0028	0.0028	0.0011	0.0028	0.0028	0.2375	3.2684
1.0036	0.0009	0.0037	0.0037	0.0009	0.0037	0.0037	0.2621	3.1479
1.0045	0.0006	0.0045	0.0045	0.0006	0.0045	0.0045	0.2258	3.0414
1.0053	0.0002	0.0053	0.0053	0.0002	0.0053	0.0053	0.1062	2.9135
1.0063	-0.0004	0.0062	0.0062	-0.0004	0.0062	0.0062	0.0957	2.9672
1.0071	-0.0005	0.0072	0.0072	-0.0005	0.0072	0.0072	0.1459	3.1916
1.0082	-0.0014	0.0082	0.0082	-0.0014	0.0082	0.0082	0.0843	3.56
1.0093		0.0093	0.0093		0.0093	0.0093		

X1	$\rho(\text{kg/m}^3)$	$\eta(\text{mPa.s})$	$V_m(\text{cm}^3/\text{mol})$	$V^E(\text{cm}^3/\text{mol})$	$\Delta\eta(\text{mPa.S})$	$\Delta G^{*E}(\text{kJ/mol})$
308.15 K						
0	862.24	0.0007	150.9788	-0.0071	0	0
0.0798	857.8328	0.0008	154.3685	-0.0078	-0.0005	27.46
0.1633	853.424	0.001	157.9153	-0.0087	-0.0009	52.96
0.2507	849.0162	0.0013	161.6278	-0.0095	-0.0012	75.4312
0.3423	844.6089	0.0016	165.5187	-0.0104	-0.0015	86.4645
0.4384	840.2025	0.002	169.6008	-0.0113	-0.0018	95.3426
0.5393	835.7986	0.0026	173.8867	-0.0123	-0.0019	101.646
0.6455	831.3919	0.0033	178.398	-0.0131	-0.002	97.7901
0.7574	826.9835	0.0044	183.1511	-0.0143	-0.0017	87.5023
0.8754	822.576	0.0058	188.1634	-0.0154	-0.0011	53.7366
1	818.1699	0.0078	193.4561	-0.0166	0	0

Frenkel model	Frenkel	Kendall	Kendall monore	Hind	Hind and ubbelohde	Bingham	Grunberg Nissan	Katti and chaudhri
1.0007		0.0007	0.0007		0.0007	0.0007		
1.0012	0.0014	0.0012	0.0012	0.0014	0.0012	0.0012	-0.8025	3.0232
1.0019	0.0011	0.0019	0.0019	0.0011	0.0019	0.0019	-0.2716	3.0198
1.0025	0.0011	0.0025	0.0025	0.0011	0.0025	0.0025	0.0777	3.1086
1.0031	0.0009	0.0032	0.0032	0.0009	0.0032	0.0032	0.0062	2.892
1.0038	0.0006	0.0038	0.0038	0.0006	0.0038	0.0038	-0.0288	2.7868
1.0045	0.0004	0.0045	0.0045	0.0004	0.0045	0.0045	0.0487	2.8559
1.0054	-0.0002	0.0052	0.0052	-0.0002	0.0052	0.0052	-0.0245	2.8475
1.0061	-0.0003	0.0061	0.0061	-0.0003	0.0061	0.0061	0.067	3.1127
1.0069	-0.0009	0.0069	0.0069	-0.0009	0.0069	0.0069	0.0376	3.5133
1.0078		0.0078	0.0078		0.0078	0.0078		

X1	$\rho(\text{kg/ m}^3)$	$\eta(\text{mPa.s})$	$V_m(\text{cm}^3/\text{mol})$	$V^E(\text{cm}^3/\text{mol})$	$\Delta\eta(\text{mPa.s})$	$\Delta G^E(\text{kJ/mol})$
313.15 K						
0	857.5618	0.0006	151.8024	-0.011	0	0
0.0798	853.277	0.0008	155.1927	-0.0115	-0.0003	27.15
0.1633	848.9894	0.0009	158.7401	-0.012	-0.0007	52.0297
0.2507	844.7021	0.0012	162.4533	-0.0125	-0.0009	75.6435
0.3423	840.4142	0.0014	166.3449	-0.013	-0.0012	87.6454
0.4384	836.1262	0.0018	170.4276	-0.0137	-0.0014	96.8724
0.5393	831.8396	0.0023	174.7143	-0.0142	-0.0015	102.846
0.6455	827.5493	0.0029	179.2262	-0.0149	-0.0015	97.8563
0.7574	823.2563	0.0038	183.9802	-0.0155	-0.0013	87.566
0.8754	818.9633	0.0049	188.9934	-0.0163	-0.0009	53.8806
1	814.6708	0.0065	194.287	-0.017	0	0

Frenkel model	Frenkel	Kendall	Kendall monore	Hind	Hind and ubbelohde	Bingham	Grunberg Nissan	Katti and chaudhri
1.0006		0.0006	0.0006		0.0006	0.0006		
1.001	0.002	0.0011	0.0011	0.002	0.0011	0.0011	1.3297	5.1526
1.0016	0.0011	0.0016	0.0016	0.0011	0.0016	0.0016	0.1201	3.4107
1.0021	0.0013	0.002	0.002	0.0013	0.002	0.002	0.5101	3.541
1.0027	0.0007	0.0026	0.0026	0.0007	0.0026	0.0026	0.1408	3.0267
1.0032	0.0008	0.0031	0.0031	0.0008	0.0031	0.0031	0.2197	3.0349
1.0038	0.0006	0.0038	0.0038	0.0006	0.0038	0.0038	0.2366	3.0439
1.0044	0.0002	0.0044	0.0044	0.0002	0.0044	0.0044	0.1643	3.0363
1.005	0.0003	0.005	0.005	0.0003	0.005	0.005	0.2237	3.27
1.0058	-0.0005	0.0058	0.0058	-0.0005	0.0058	0.0058	0.132	3.6068
1.0065		0.0065	0.0065		0.0065	0.0065		

Table 4.2: Theoretical values of density ρ (kg/m³), viscosity η (mPa.s), deviation in viscosity $\Delta\eta$ (mPa.s), excess molar volumes V^E (cm³/mol), molar volume of mixture V_m (cm³/mol), excess Gibbs free energy of activation of viscous flow ΔG^{*E} (J/mol), Frenkel, Frenkel model, Hind, Hind and ubbelohde, Kendall, Bingham, Katti and chaudhri, Grunberg-Nissan parameter (d') and modified Kendall and Monroe viscosity correlation $E\eta_m$ (mPa.s) of 1-Decanol (x1) + Hexyl acetate (x2) at 298.15,303.15, 308.15 and 313.15 K.

X1	ρ (kg/m ³)	η (mPa.s)	V_m (cm ³ /mol)	V^E (cm ³ /mol)	$\Delta\eta$ (mPa.s)	ΔG^{*E} (kJ/mol)
298.15 K						
0	868.2329	0.001	166.0959	-0.0064	0	0
0.0879	863.9142	0.0013	168.3578	-0.0061	-0.0006	38.62
0.1781	859.6017	0.0016	170.6788	-0.0059	-0.0012	68.4879
0.2709	855.2857	0.002	173.0668	-0.0055	-0.0018	86.1112
0.3663	850.971	0.0025	175.5216	-0.0052	-0.0023	103.162
0.4644	846.6583	0.0031	178.0459	-0.005	-0.0027	102.022
0.5653	842.3483	0.004	180.6423	-0.0046	-0.0028	86.6655
0.6692	838.0377	0.0051	183.3159	-0.0042	-0.0028	65.645
0.7762	833.7282	0.0066	186.0691	-0.004	-0.0024	45.264
0.8864	829.4208	0.0086	188.9048	-0.0037	-0.0013	25.2
1	825.1139	0.0113	191.828	-0.0033	0	0

Frenkel model	Frenkel	Kendall	Kendall monore	Hind	Hind and ubbelohde	Bingham	Grunberg Nissan	Katti and chaudhri
1.001		0.001	0.001		0.001	0.001		
1.0019	0.0025	0.0108	0.0108	0.0025	0.0108	0.0108	0.6147	4.3354
1.0029	0.0017	0.0209	0.0209	0.0017	0.0209	0.0209	0.2602	3.4706
1.0037	0.0018	0.0313	0.0313	0.0018	0.0313	0.0313	0.1833	3.1519
1.0048	0.0013	0.042	0.042	0.0013	0.042	0.042	0.1206	2.9617
1.0058	0.0008	0.053	0.053	0.0008	0.053	0.053	0.0213	2.8086
1.0068	0.0004	0.0643	0.0643	0.0004	0.0643	0.0643	0.0631	2.8596
1.0079	-0.0002	0.0759	0.0759	-0.0002	0.0759	0.0759	0.0298	2.9065
1.009	-0.0009	0.0879	0.0879	-0.0009	0.0879	0.0879	0.0288	3.0996
1.0102	-0.0005	0.1003	0.1003	-0.0005	0.1003	0.1003	0.2522	3.7776
1.0114		0.113	0.113		0.113	0.113		

X1	$\rho(\text{kg/m}^3)$	$\eta(\text{mPa.s})$	$V_m(\text{cm}^3/\text{mol})$	$V^E(\text{cm}^3/\text{mol})$	$\Delta\eta$ (mPa.s)	$\Delta G^{*E}(\text{kJ/mol})$
303.15 K						
0	863.8099	0.0009	166.9464	-0.1567	0	0
0.0879	859.5909	0.0011	169.2046	-0.144	-0.0005	32.261
0.1781	855.3771	0.0014	171.5218	-0.131	-0.001	71.6479
0.2709	851.1591	0.0018	173.9058	-0.1176	-0.0014	88.264
0.3663	846.9415	0.0022	176.3567	-0.1037	-0.0018	103.032 3
0.4644	842.7253	0.0027	178.8769	-0.0895	-0.0021	102.351
0.5653	838.5108	0.0035	181.469	-0.0749	-0.0021	86.3264
0.6692	834.295	0.0044	184.1382	-0.0599	-0.0021	65.9466
0.7762	830.0795	0.0056	186.887	-0.0445	-0.0018	45.661
0.8864	825.8654	0.0072	189.7181	-0.0284	-0.0011	26.022
1	821.6509	0.0093	192.6365	-0.012	0	0

Frenkel model	Frenkel	Kendall	Kendall monore	Hind	Hind and ubbelohde	Bingham	Grunberg Nissan	Katti and chaudhri
1.0009		0.0009	0.0009		0.0009	0.0009		
1.0016	0.0019	0.0016	0.0016	0.0019	0.0016	0.0016	-0.0561	3.6646
1.0024	0.0017	0.0024	0.0024	0.0017	0.0024	0.0024	0.1769	3.3873
1.0032	0.0015	0.0032	0.0032	0.0015	0.0032	0.0032	0.3063	3.2744
1.004	0.0013	0.004	0.004	0.0013	0.004	0.004	0.1654	3.006
1.0048	0.0008	0.0048	0.0048	0.0008	0.0048	0.0048	0.0563	2.8436
1.0057	0.0006	0.0057	0.0057	0.0006	0.0057	0.0057	0.1543	2.9508
1.0066	0.0002	0.0065	0.0065	0.0002	0.0065	0.0065	0.1084	2.9855
1.0074	0	0.0074	0.0074	0	0.0074	0.0074	0.0887	3.1595
1.0083	-0.0005	0.0083	0.0083	-0.0005	0.0083	0.0083	0.0924	3.6177
1.0093		0.0093	0.0093		0.0093	0.0093		

X1	$\rho(\text{kg/m}^3)$	$\eta(\text{mPa.s})$	$V_m(\text{cm}^3/\text{mol})$	$V^E(\text{cm}^3/\text{mol})$	$\Delta\eta$ (mPa.s)	$\Delta G^{*E}(\text{kJ/mol})$
308.15 K						
0	859.3605	0.0009	167.8108	-0.0118	0	0
0.0879	855.2418	0.001	170.065	-0.0122	-0.0005	33.26
0.1781	851.1274	0.0013	172.3782	-0.0127	-0.0008	72.4545
0.2709	847.0082	0.0016	174.7581	-0.0131	-0.0012	87.3543
0.3663	842.8887	0.0019	177.2047	-0.0135	-0.0015	103.2623
0.4644	838.7695	0.0024	179.7205	-0.014	-0.0017	102.6
0.5653	834.6516	0.003	182.3081	-0.0145	-0.0018	86.161
0.6692	830.5314	0.0038	184.9727	-0.0149	-0.0017	65.0321
0.7762	826.4111	0.0048	187.7166	-0.0156	-0.0015	45.855
0.8864	822.2911	0.0061	190.5427	-0.0162	-0.0009	25.2655
1	818.1699	0.0078	193.4561	-0.0166	0	0

Frenkel model	Frenkel	Kendall	Kendall monore	Hind	Hind and ubbelohde	Bingham	Grunberg Nissan	Katti and chaudhri
1.0009		0.0009	0.0009		0.0009	0.0009		
1.0015	0.0012	0.0015	0.0015	0.0012	0.0015	0.0015	-1.0536	2.6683
1.0021	0.0017	0.0021	0.0021	0.0017	0.0021	0.0021	-0.1154	3.0949
1.0028	0.0013	0.0028	0.0028	0.0013	0.0028	0.0028	-0.0491	2.919
1.0034	0.0011	0.0035	0.0035	0.0011	0.0035	0.0035	-0.1887	2.6523
1.0042	0.0008	0.0041	0.0041	0.0008	0.0041	0.0041	-0.0889	2.6984
1.0049	0.0006	0.0048	0.0048	0.0006	0.0048	0.0048	-0.068	2.7281
1.0055	0.0005	0.0055	0.0055	0.0005	0.0055	0.0055	-0.0217	2.8555
1.0062	0.0003	0.0063	0.0063	0.0003	0.0063	0.0063	-0.0127	3.0581
1.007	0	0.007	0.007	0	0.007	0.007	-0.005	3.5194
1.0078		0.0078	0.0078		0.0078	0.0078		

X1	$\rho(\text{kg/m}^3)$	$\eta(\text{mPa.s})$	$V_m(\text{cm}^3/\text{mol})$	$V^E(\text{cm}^3/\text{mol})$	$\Delta\eta(\text{mPa.s})$	$\Delta G^{*E}(\text{kJ/mol})$
313.15 K						
0	854.8836	0.0008	168.6896	-0.0165	0	0
0.0879	850.866	0.001	170.9396	-0.0166	-0.0003	33.7636
0.1781	846.8519	0.0012	173.2485	-0.0166	-0.0006	73.9817
0.2709	842.8324	0.0014	175.6239	-0.0166	-0.0009	86.1646
0.3663	838.8118	0.0017	178.0659	-0.0167	-0.0012	103.663
0.4644	834.7908	0.0021	180.5771	-0.0167	-0.0013	102.261
0.5653	830.7702	0.0026	183.1598	-0.0168	-0.0014	86.5613
0.6692	826.7468	0.0033	185.8194	-0.0168	-0.0013	65.3265
0.7762	822.7222	0.0041	188.5583	-0.0168	-0.0011	45.6196
0.8864	818.6974	0.0052	191.3791	-0.0169	-0.0007	25.326
1	814.6708	0.0065	194.287	-0.017	0	0

Frenkel model	Frenkel	Kendall	Kendall monore	Hind	Hind and ubbelohde	Bingham	Grunberg Nissan	Katti and chaudhri
1.0008		0.0008	0.0008		0.0008	0.0008		
1.0014	0.0012	0.0013	0.0013	0.0012	0.0013	0.0013	0.4863	4.2082
1.0018	0.0017	0.0019	0.0019	0.0017	0.0019	0.0019	0.2213	3.4317
1.0024	0.0013	0.0024	0.0024	0.0013	0.0024	0.0024	-0.0405	2.9281
1.0029	0.0011	0.0029	0.0029	0.0011	0.0029	0.0029	-0.0582	2.782
1.0034	0.001	0.0034	0.0034	0.001	0.0034	0.0034	-0.0314	2.7559
1.0041	0.0006	0.004	0.004	0.0006	0.004	0.004	-0.0228	2.7737
1.0046	0.0007	0.0046	0.0046	0.0007	0.0046	0.0046	0.0687	2.9458
1.0052	0.0006	0.0052	0.0052	0.0006	0.0052	0.0052	0.0461	3.1169
1.0058	0.0005	0.0059	0.0059	0.0005	0.0059	0.0059	0.148	3.6723
1.0065		0.0065	0.0065		0.0065	0.0065		

Table 4.3: Theoretical values of density ρ (kg/m³), viscosity η (mPa.s), deviation in viscosity $\Delta\eta$ (mPa.s), excess molar volumes V^E (cm³/mol), molar volume of mixture V_m (cm³/mol), excess Gibbs free energy of activation of viscous flow ΔG^{*E} (J/mol), Frenkel,Frenkel model,Hind,Hind and ubbelohde,Kendall,Bingham,Katti and chaudhri, Grunberg-Nissan parameter (d') and modified Kendall and Monroe viscosity correlation $E\eta_m$ (mPa.s) of 1-Decanol (x1) + Octyl acetate (x2) at 298.15,303.15, 308.15 and 313.15 K.

X1	ρ (kg/m ³)	η (mPa.s)	V_m (cm ³ /mol)	V^E (cm ³ /mol)	$\Delta\eta$ (mPa.s)	ΔG^{*E} (kJ/mol)
298.15 K						
0	864.5071	0.0017	199.258	-0.0017	0	0
0.1037	850.866	0.001	170.9396	-0.0166	-0.0003	33.7394
0.2066	846.8519	0.0012	173.2485	-0.0166	-0.0006	62.2266
0.3087	842.8324	0.0014	175.6239	-0.0166	-0.0009	95.3644
0.4099	838.8118	0.0017	178.0659	-0.0167	-0.0012	110.662
0.5102	834.7908	0.0021	180.5771	-0.0167	-0.0013	108.5623
0.6098	830.7702	0.0026	183.1598	-0.0168	-0.0014	86.6326
0.7085	826.7468	0.0033	185.8194	-0.0168	-0.0013	62.3563
0.8065	822.7222	0.0041	188.5583	-0.0168	-0.0011	30.6162
0.9036	818.6974	0.0052	191.3791	-0.0169	-0.0007	13.2626
1	814.6708	0.0065	194.287	-0.017	0	0

Frenkel model	Frenkel	Kendall	Kendall monore	Hind	Hind and ubbelohde	Bingham	Grunberg Nissan	Katti and chaudhri
1.0017		0.0017	0.0017		0.0017	0.0017		
1.0027	0.0027	0.0027	0.0027	0.0027	0.0027	0.0027	-0.3649	3.2228
1.0037	0.0027	0.0036	0.0036	0.0027	0.0036	0.0036	-0.0348	3.0738
1.0047	0.0026	0.0047	0.0047	0.0026	0.0047	0.0047	-0.0783	2.8187
1.0056	0.0025	0.0056	0.0056	0.0025	0.0056	0.0056	0.0054	2.8041
1.0065	0.0022	0.0066	0.0066	0.0022	0.0066	0.0066	-0.062	2.7119
1.0076	0.0019	0.0076	0.0076	0.0019	0.0076	0.0076	0.0029	2.815
1.0085	0.0017	0.0085	0.0085	0.0017	0.0085	0.0085	-0.0044	2.9186
1.0094	0.0013	0.0094	0.0094	0.0013	0.0094	0.0094	-0.0263	3.1217
1.0104	0.0011	0.0104	0.0104	0.0011	0.0104	0.0104	-0.0161	3.6246
1.0114		0.0113	0.0113		0.0113	0.0113		

X1	$\rho(\text{kg/m}^3)$	$\eta(\text{mPa.s})$	V_m (cm^3/mol)	$V^E(\text{cm}^3/\text{mol})$	$\Delta\eta$ ($\text{mPa.s})$	ΔG^{*E} (kJ/mol)
303.15 K						
0	860.3346	0.0015	200.2244	-0.0081	0	0
0.1037	856.46	0.0018	199.4375	-0.0085	-0.0005	33.6594
0.2066	852.585	0.0022	198.6567	-0.0089	-0.0009	65.5666
0.3087	848.7098	0.0027	197.8819	-0.0094	-0.0012	96.632
0.4099	844.8386	0.0032	197.114	-0.0098	-0.0015	110.326
0.5102	840.972	0.0038	196.353	-0.0102	-0.0017	107.5623
0.6098	837.1027	0.0046	195.5972	-0.0105	-0.0017	85.2632
0.7085	833.2385	0.0055	194.8483	-0.011	-0.0016	64.6263
0.8065	829.3724	0.0066	194.1047	-0.0113	-0.0013	31.2653
0.9036	825.5123	0.0079	193.368	-0.0116	-0.0007	12.6316
1	821.6509	0.0094	192.6365	-0.12	0	0

Frenkel model	Frenkel	Kendall	Kendall monore	Hind	Hind and ubbelohde	Bingham	Grunberg Nissan	Katti and chaudhri
1.0015		0.0015	0.0015		0.0015	0.0015		
1.0023	0.0027	0.0023	0.0023	0.0027	0.0023	0.0023	-0.0861	3.4995
1.0031	0.0027	0.0031	0.0031	0.0027	0.0031	0.0031	0.0232	3.1318
1.0039	0.0026	0.0039	0.0039	0.0026	0.0039	0.0039	0.0993	2.9967
1.0048	0.0023	0.0048	0.0048	0.0023	0.0048	0.0048	0.0223	2.8214
1.0055	0.002	0.0055	0.0055	0.002	0.0055	0.0055	-0.0276	2.7463
1.0063	0.0019	0.0063	0.0063	0.0019	0.0063	0.0063	0.0063	2.8184
1.0071	0.0017	0.0071	0.0071	0.0017	0.0071	0.0071	-0.0048	2.9186
1.0079	0.0013	0.0079	0.0079	0.0013	0.0079	0.0079	0.0096	3.1576
1.0087	0.0011	0.0086	0.0086	0.0011	0.0086	0.0086	0.0344	3.6762
1.0094		0.0094	0.0094		0.0094	0.0094		

X1	$\rho(\text{kg/m}^3)$	$\eta \text{ (mPa.s)}$	V_m (cm^3/mol)	V^E (cm^3/mol)	$\Delta\eta$ (mPa.s)	ΔG^{*E} (kJ/mol)
308.15 K						
0	856.141	0.0014	201.2051	0.0097	0	0
0.1037	852.34	0.0016	200.4015	-0.0104	-0.0005	32.6213
0.2066	848.538	0.002	199.6041	-0.0112	-0.0007	63.6163
0.3087	844.7353	0.0024	198.813	-0.0118	-0.001	94.233
0.4099	840.9362	0.0028	198.0288	-0.0126	-0.0012	108.62
0.5102	837.1412	0.0033	197.2515	-0.0133	-0.0014	106.2664
0.6098	833.3429	0.004	196.4797	-0.0139	-0.0013	86.6326
0.7085	829.5492	0.0047	195.7149	-0.0146	-0.0012	63.16493
0.8065	825.7531	0.0056	194.9555	-0.0153	-0.001	30.643
0.9036	821.9625	0.0066	194.2031	-0.0159	-0.0006	13.6323
1	818.1699	0.0078	193.4561	-0.0166	0	0

Frenkel model	Frenkel	Kendall	Kendall monore	Hind	Hind and ubbelohde	Bingham	Grunberg Nissan	Katti and chaudhri
1.0014		0.0014	0.0014		0.0014	0.0014		
1.0021	0.0022	0.0021	0.0021	0.0022	0.0021	0.0021	-0.4812	3.1066
1.0027	0.0024	0.0027	0.0027	0.0024	0.0027	0.0027	0.0116	3.1202
1.0034	0.0023	0.0034	0.0034	0.0023	0.0034	0.0034	0.0408	2.9377
1.004	0.0021	0.004	0.004	0.0021	0.004	0.004	-0.0451	2.7536
1.0046	0.002	0.0047	0.0047	0.002	0.0047	0.0047	-0.0756	2.6983
1.0053	0.0019	0.0053	0.0053	0.0019	0.0053	0.0053	0.0097	2.8222
1.0059	0.0017	0.0059	0.0059	0.0017	0.0059	0.0059	-0.0286	2.8949
1.0066	0.0013	0.0066	0.0066	0.0013	0.0066	0.0066	0.0064	3.1544
1.0072	0.0011	0.0071	0.0071	0.0011	0.0071	0.0071	-0.0172	3.6246
1.0078		0.0078	0.0078		0.0078	0.0078		

X1	$\rho(\text{kg/m}^3)$	$\eta(\text{mPa.s})$	V_m (cm^3/mol)	V^E (cm^3/mol)	$\Delta\eta$ (mPa.s)	ΔG^{*E} (kJ/mol)
313.15 K						
0	851.9258	0.0013	202.2007	-0.0061	0	0
0.1037	848.1987	0.0015	201.38	-0.0073	-0.0003	34.663
0.2066	844.47	0.0018	200.5657	-0.0084	-0.0006	64.2643
0.3087	840.7403	0.0021	199.7577	-0.0095	-0.0008	95.2625
0.4099	837.0135	0.0025	198.9568	-0.0107	-0.001	109.2623
0.5102	833.2903	0.0029	198.1631	-0.0117	-0.0011	107.163
0.6098	829.5633	0.0035	197.3749	-0.0128	-0.001	86.2362
0.7085	825.8406	0.0041	196.5938	-0.0139	-0.001	63.4313
0.8065	822.1148	0.0048	195.8183	-0.0148	-0.0008	32.6324
0.9036	818.3939	0.0056	195.0499	-0.0159	-0.0005	12.462
1	814.6708	0.0066	194.287	-0.017		0

Frenkel model	Frenkel	Kendall	Kendall monore	Hind	Hind and ubbelohde	Bingham	Grunberg Nissan	Katti and chaudhri
1.0013		0.0013	0.0013		0.0013	0.0013		
1.0018	0.0022	0.0019	0.0019	0.0022	0.0019	0.0019	-0.2734	3.3132
1.0024	0.0021	0.0024	0.0024	0.0021	0.0024	0.0024	-0.0622	3.0464
1.0029	0.0021	0.0029	0.0029	0.0021	0.0029	0.0029	-0.1026	2.7943
1.0035	0.0019	0.0035	0.0035	0.0019	0.0035	0.0035	-0.05	2.7487
1.004	0.0018	0.004	0.004	0.0018	0.004	0.004	-0.106	2.6675
1.0046	0.0017	0.0045	0.0045	0.0017	0.0045	0.0045	-0.0017	2.8108
1.005	0.0017	0.0051	0.0051	0.0017	0.0051	0.0051	-0.0121	2.9109
1.0055	0.0016	0.0056	0.0056	0.0016	0.0056	0.0056	-0.0256	3.1224
1.0061	0.0011	0.0061	0.0061	0.0011	0.0061	0.0061	-0.0884	3.5534
1.0066		0.0066	0.0066		0.0066	0.0066		

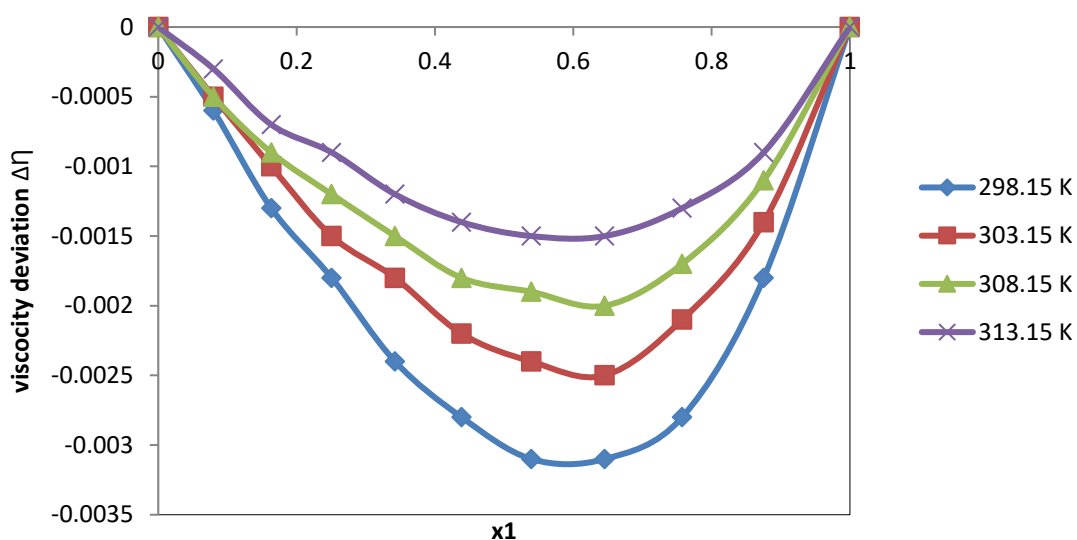


Fig 4.1 Plots of deviation in viscosity ($\Delta\eta$) against mole fraction for the system 1-Decanol (x_1) + Pentyl acetate (x_2) at different temperatures 298.15 K, 303.15 K, 308.15 K and 313.15 K.

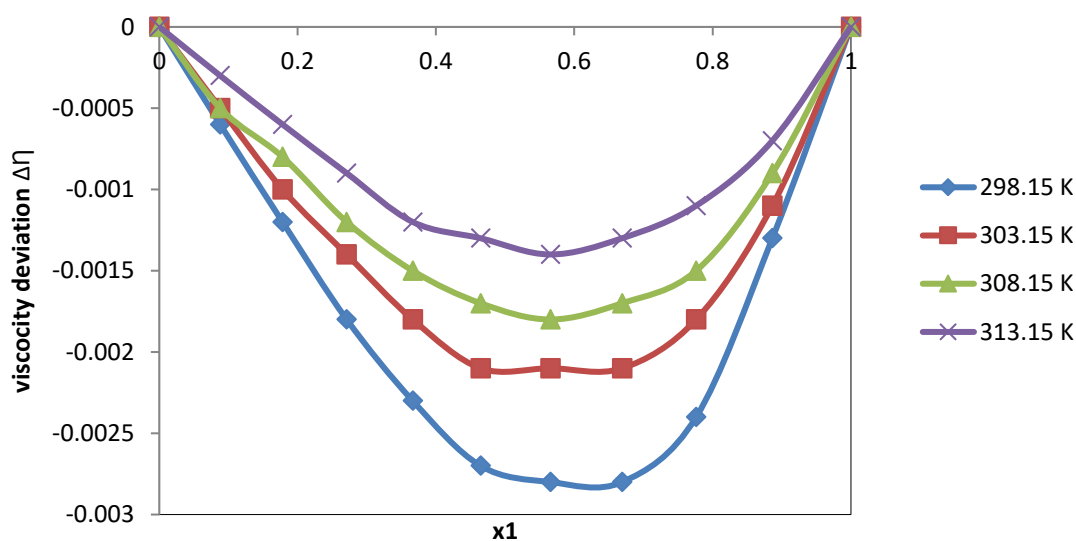


Fig 4.2 Plots of deviation in viscosity ($\Delta\eta$) against mole fraction for the system 1-Decanol (x_1) + Hexyl acetate (x_2) at different temperatures 298.15 K, 303.15 K, 308.15 K and 313.15 K.

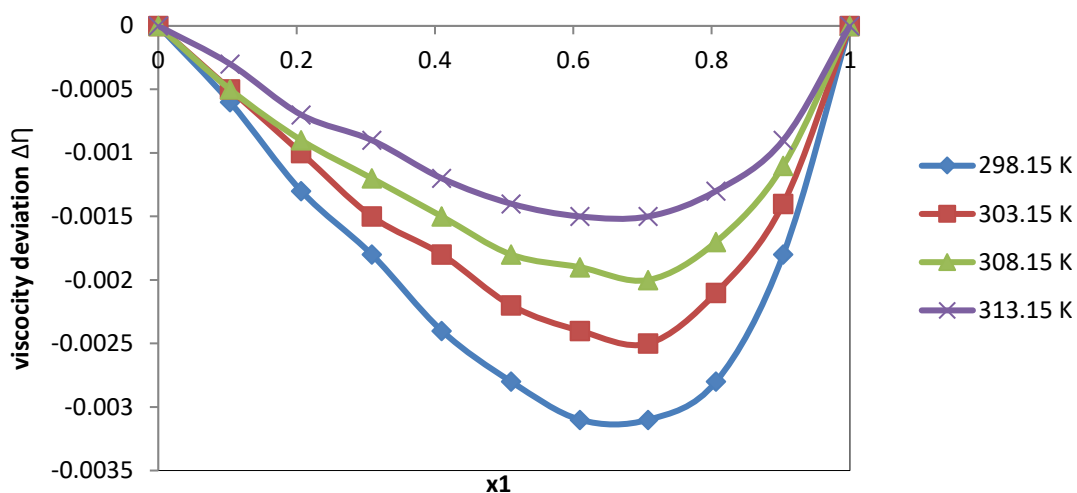


Fig 4.3 Plots of deviation in viscosity ($\Delta\eta$) against mole fraction for the system 1-Decanol (x_1) + Octyl acetate (x_2) at different temperatures 298.15 K, 303.15 K, 308.15 K and 313.15 K.

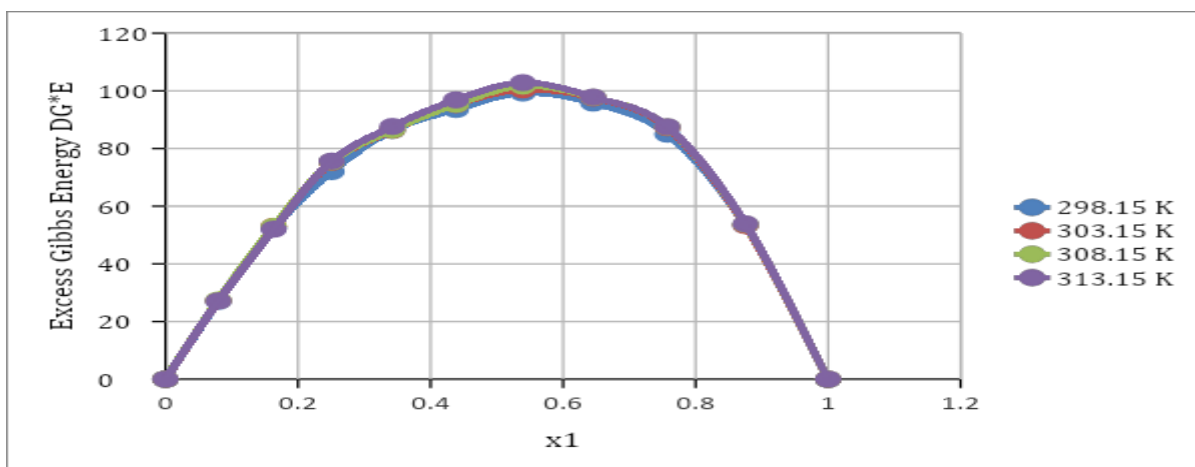


Fig 4.4 Plots of Excess Gibbs free energy of activation of viscous flow (ΔG^{*E}) against mole fraction for the system 1-Decanol (x_1) + Pentyl acetate (x_2) at different temperatures 298.15 K, 303.15 K, 308.15 K and 313.15 K.

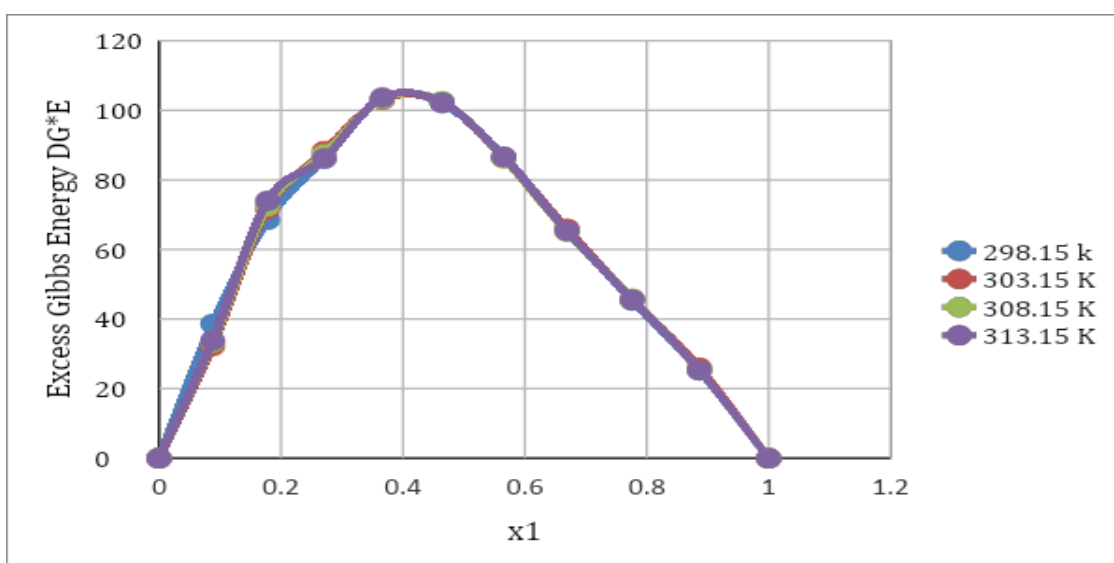


Fig 4.5 Plots of Excess Gibbs free energy of activation of viscous flow (ΔG^*E) against mole fraction for the system 1-Decanol (x_1) + Hexyl acetate (x_2) at different temperatures 298.15 K, 303.15 K, 308.15 K and 313.15 K.

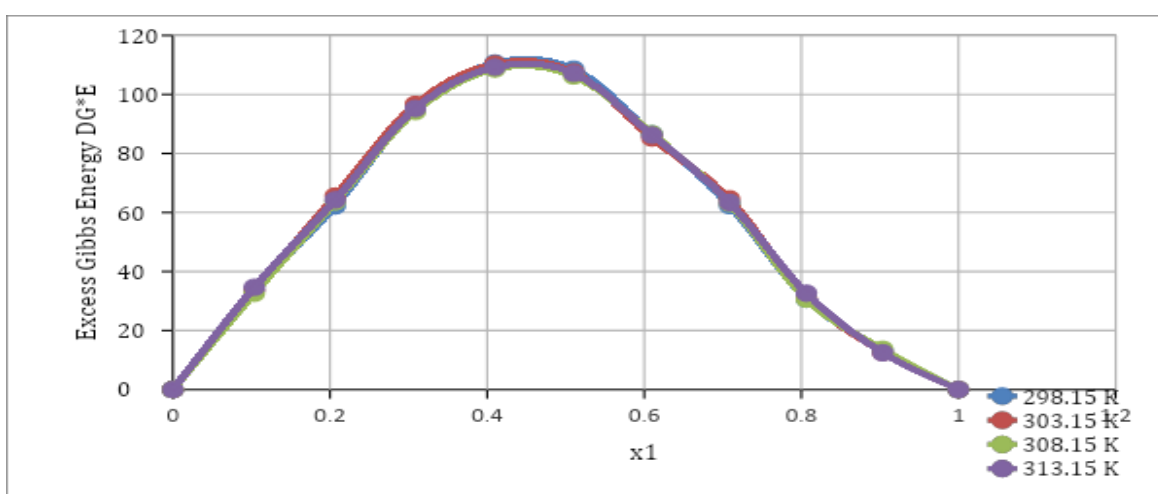


Fig 4.6 Plots of Excess Gibbs free energy of activation of viscous flow (ΔG^*E) against mole fraction for the system 1-Decanol (x_1) + Octyl acetate (x_2) at different temperatures 298.15 K, 303.15 K, 308.15 K and 313.15 K.

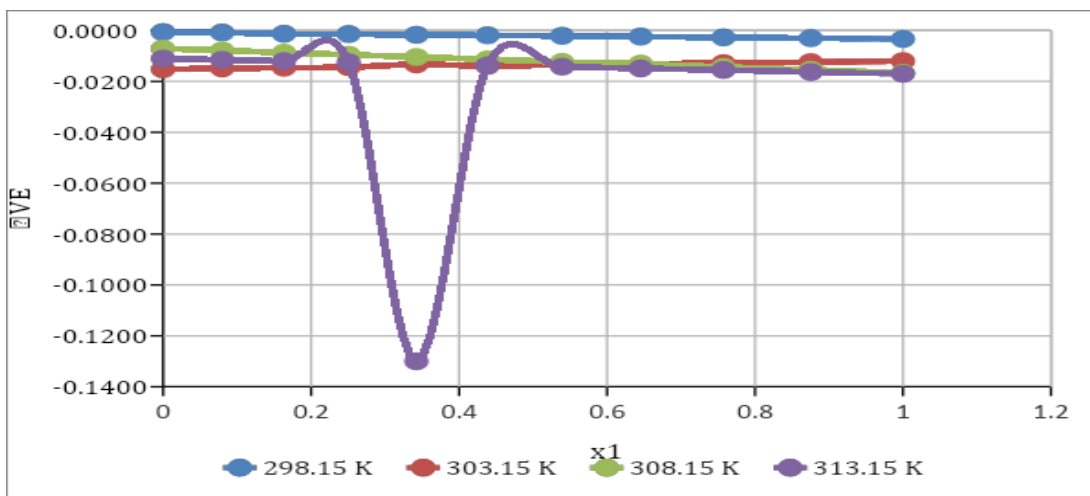


Fig 4.7 Plots of Molar volume against mole fraction for the system 1-Decanol (x1) + Pentyl acetate (x2) at different temperatures 298.15 K, 303.15 K, 308.15 K and 313.15 K.

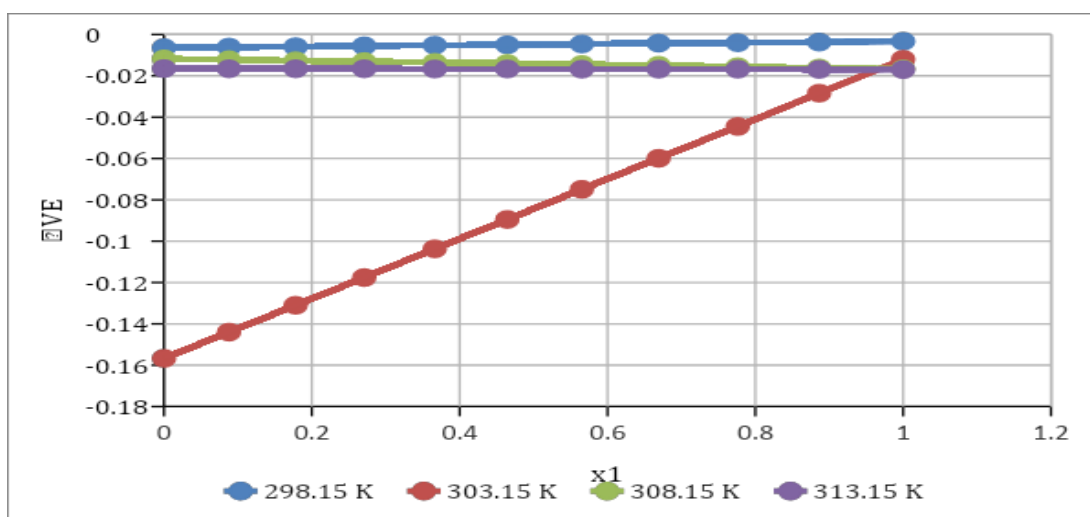


Fig 4.8 Plots of Molar volume against mole fraction for the system 1-Decanol (x1) + Hexyl acetate (x2) at different temperatures 298.15 K, 303.15 K, 308.15 K and 313.15 K.

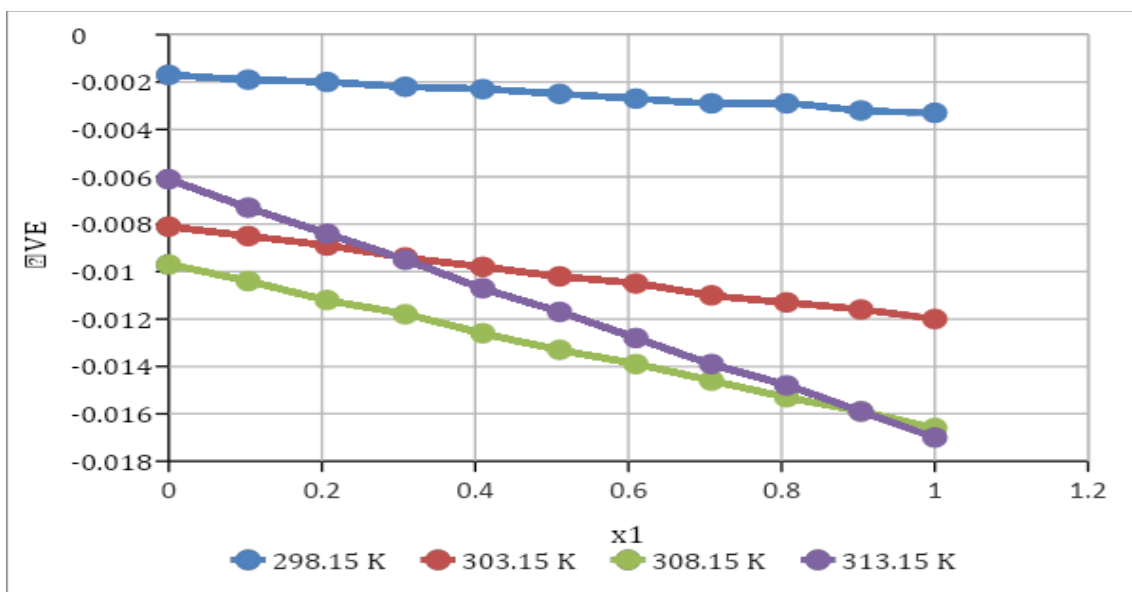


Fig 4.9 Plots of Molar volume against mole fraction for the system 1-Decanol (x_1) + Octyl acetate (x_2) at different temperatures 298.15 K, 303.15 K, 308.15 K and 313.5 K

Table 4.4 Adjustable parameters A_i , for deviation in viscosity ($\Delta\eta$), Excess volume (V^E), and Excess Gibbs free energy (ΔG^E), for binary mixtures at various temperatures.

1-Decanol (1) + Pentyl acetate (2)						
<i>Temp 298.15 K</i>						
	<i>a0</i>	<i>a1</i>	<i>a2</i>	<i>a3</i>	<i>a4</i>	<i>S</i>
$\Delta\eta$	-0.0119437	-0.0052103	-0.002997	0.0001601	0.00305	0.00101
VE	-0.0080384	-0.0027846	-0.008478	-0.0159781	-0.01794	0.0022
ΔG^E	358.10626	60.2327313	-1697.804	101.97973	2588.49	1299.25
Temp 303.15 K						
	a0	a1	a2	a3	a4	S
$\Delta\eta$	-0.0093753	-0.0039255	-0.001471	0.0002659	0.00085	0.00109
VE	-0.0568986	-0.0059538	0.0179973	0.0490412	-0.26468	0.0547
ΔG^E	562.849766	-234.18795	-1102.465	-498.65066	2488.7	896.4828

Temp 308.15 K						
	a0	a1	a2	a3	a4	S
$\Delta\eta$	-0.0075592	-0.0032622	-0.001195	0.0017074	-0.00033	0.00064
VE	-0.0488186	-0.0155984	-0.009254	-0.0439542	-0.04395	0.0067
ΔG^*E	40.8619696	-391.74173	1632.7842	2156.4914	-4452.05	644.6526
Temp 313.15 K						
	a0	a1	a2	a3	a4	S
$\Delta\eta$	-0.0058362	-0.0017345	-0.001308	-0.0012805	0.00065	0.00108
VE	-0.1656475	0.35531191	0.3395007	-0.6726248	-0.56822	0.859
ΔG^*E	796.743784	487.719373	-2910.771	-2675.6546	6656.96	2706.402

	1-Decanol (1) + Hexyl acetate (2)						
	Temp 298.15 K						
<i>Xi</i>		a0	a1	a2	a3	a4	S
	$\Delta\eta$	-0.0109848	-0.0052193	-0.002147	0.0030346	0.00531	0.00114
	VE	-0.0201326	0.00217398	0.003704	0.0250445	-0.0909	
	$\Delta\mathbf{G^*E}$	176.336875	-134.99022	55.14973	-1034.8166	1314.4	395.0857
	Temp 303.15 K						
<i>Xi</i>		a0	a1	a2	a3	a4	S
	$\Delta\eta$	-0.0084023	-0.0029091	-0.001076	-6.192E-05	0.00101	0.0008
	VE	-0.3595101	0.12097753	0.1749728	1.0888091	-1.78158	
	$\Delta\mathbf{G^*E}$	312.366726	-575.21903	1560.101	1171.0337	-2803.51	629.5333

	Temp 308.15 K						
<i>Xi</i>		a0	a1	a2	a3	a4	S
	$\Delta\eta$	-0.0070484	-0.002704	0.0005272	0.0012175	-0.00212	0.00103
	VE	-0.0584568	-0.0090638	-0.005366	-0.0196273	-0.23325	
	ΔG^*E	-358.9795	-403.59089	3477.9835	2560.8816	-7451.54	1235.2193
	Temp 313.15 K						
<i>Xi</i>		a0	a1	a2	a3	a4	S
	$\Delta\eta$	-0.0054691	-0.0014436	0.0008233	-0.0009739	-0.00118	0.00045
	VE	-0.0696406	-0.0060533	0.0036012	0.0163389	-0.29043	
	ΔG^*E	-65.285565	468.794532	544.90586	-1490.9649	1261.17	429.7451

	1-Decanol (1) + Octyl acetate (2)						
	Temp 298.15 K						
<i>Xi</i>		a0	a1	a2	a3	a4	S
	$\Delta\eta$	-0.008649	-0.0024478	0.0004828	6.972E-05	-0.00276	0.00089
	VE	-0.0104448	-0.0015059	0.0020698	-0.0117264	-0.04676	
	ΔG^*E	-82.476595	-158.53399	581.44419	1061.7186	-1874.18	514.2603
	Temp 303.15 K						
<i>Xi</i>		a0	a1	a2	a3	a4	S
	$\Delta\eta$	-0.006612	-0.0029351	-0.00105	0.0019188	0.00134	0.00057
	VE	-0.0419828	-0.0032742	-0.001497	-0.0298307	-0.16746	
	ΔG^*E	3.47622672	-381.37632	616.66655	914.01607	-1180.43	273.0927

	Temp 308.15 K						
		a0	a1	a2	a3	a4	S
<i>Xi</i>	$\Delta\eta$	-0.0053775	-0.0019404	0.0019183	0.0015166	-0.00488	0.0009
	VE	-0.0545866	-0.0056092	-0.001868	-0.0521624	-0.22041	
	ΔG^*E	-509.85724	-356.06052	1821.8309	3209.964	-5565.29	650.7451
	Temp 313.15 K						
<i>Xi</i>		a0	a1	a2	a3	a4	S
	$\Delta\eta$	-0.0042305	-0.0008785	-0.000231	-0.0010688	-0.00022	0.00067
	VE	-0.0483245	-0.0099167	0.0026786	-0.0780268	-0.20101	
	ΔG^*E	-184.17565	126.199838	871.10881	262.19539	-2060.5	429.3935

Table 4.5 :Theoretical values of density ρ (kg/m³), viscosity η (mPa.s), deviation in viscosity $\Delta\eta$ (mPa.s), excess molar volumes V^E (cm³/mol), molar volume of mixture V_m (cm³/mol), excess Gibbs free energy of activation of viscous flow ΔG^{*E} (J/mol) for experimental reading of 1-Decanol (x1) + Pentyl acetate (x2) at 303.15 K.

X	DENSITIES (g/cc) (ρ)			(η) VISCOSITIES (mPa.s)			Vm(cm ³ /mol)		
	LIT	CHEM CAD	EXP	LIT	CHEM CAD	EXP	LIT	CHEMCAD	EXP
0	0.8672	0.8668	0.867	0.805	0.8021	0.8032	150.115	150.184	150.149
0.0798	0.8632	0.8627	0.8629	1.6144	1.6116	1.6127	153.408	153.497	153.462
0.1633	0.8592	0.8586	0.8588	2.4238	2.4211	2.4222	156.853	156.963	156.926
0.2507	0.8552	0.8545	0.8547	3.2332	3.2306	3.2317	160.459	160.59	160.553
0.3423	0.8512	0.8504	0.8506	4.0426	4.0401	4.0412	164.237	164.391	164.352
0.4384	0.8472	0.8463	0.8465	4.852	4.8496	4.8507	168.2	168.378	168.339
0.5393	0.8392	0.8422	0.8424	5.6614	5.6591	5.6602	173.181	172.565	172.524
0.6455	0.8352	0.8381	0.8383	6.4708	6.4686	6.4697	177.584	176.969	176.927
0.7574	0.8235	0.834	0.8342	7.2802	7.2781	7.2792	183.925	181.61	181.566
0.8754	0.8312	0.8299	0.8301	8.0897	8.8087	8.0897	186.211	186.502	186.457
1	0.8235	0.8216	0.8223	9.708	9.752	9.7074	192.204	192.648	192.484

$V^E(\text{cm}^3/\text{mol})$			$\Delta\eta(\text{mPa.s})$			$\Delta G^E(\text{kJ/mol})$		
LIT	CHEM CAD	EXP	LIT	CHEM CAD	EXP	LIT	CHEM CAD	EXP
-0.0003	-0.0006	-0.0009	0	0	0	-0.0286	0	0
-0.066	-0.0762	-0.0662	0.0989	-0.0005	-0.0007	1258.0885	27.23	28.2623
-0.1354	-0.1559	-0.1372	0.1649	-0.001	-0.0015	1762.371	53.0124	54.261
-0.2079	-0.2403	-0.2102	0.1962	-0.0015	-0.0019	1942.9952	75.2437	75.4626
-0.2853	-0.329	-0.2882	0.1901	-0.0018	-0.0024	1932.8828	86.3452	86.8626
-0.367	-0.4228	-0.3704	0.1439	-0.0022	-0.0028	1789.8411	95.264	96.13
0.3673	-0.5204	-0.416	0.055	-0.0024	-0.003	1556.3617	100.3424	100.92
0.3004	-0.626	-0.5499	-0.0811	-0.0025	-0.0026	1223.7585	97.5445	96.9316
1.9317	-0.7367	-0.6481	-0.2679	-0.0021	-0.0018	837.239	87.2206	86.2631
-0.7488	-0.8555	-0.7526	-0.509	-0.0014	-0.001	320.0191	53.3025	52.863
0	-0.0005	-0.0005	0	0	0	0.0191	0	0

Table 4.6 :Theoretical values of density ρ (kg/m³), viscosity η (mPa.s), deviation in viscosity $\Delta\eta$ (mPa.s), excess molar volumes V^E (cm³/mol), molar volume of mixture V_m (cm³/mol), excess Gibbs free energy of activation of viscous flow ΔG^{*E} (J/mol) for experimental reading of 1-Decanol (x1) + Hexyl acetate (x2) at 303.15 K.

X	DENSITIES (g/cc) (ρ)			(η) VISCOSITIES (mPa.s)			V_m (cm ³ /mol)		
	LIT	CHEM CAD	EXP	LIT	CHEM CAD	EXP	LIT	CHEM CAD	EXP
0	0.8636	0.8638	0.8646	0.782	0.7786	0.7804	166.987	166.948	166.793
0.0879	0.86	0.86	0.8607	1.5935	1.5902	1.5919	169.124	169.124	168.986
0.1781	0.8564	0.8562	0.8568	2.405	2.4018	2.4034	171.316	171.357	171.237
0.2709	0.8528	0.8524	0.8529	3.2165	3.2134	3.2149	173.571	173.652	173.55
0.3663	0.8492	0.8486	0.849	4.028	4.025	4.0264	175.887	176.012	175.929
0.4644	0.8456	0.8448	0.8451	4.8395	4.8366	4.8379	178.268	178.437	178.374
0.5653	0.842	0.841	0.8412	5.651	5.6482	5.6494	180.717	180.931	180.888
0.6692	0.8384	0.8372	0.8373	6.4625	6.4598	6.4609	183.236	183.499	183.477
0.7762	0.8348	0.8334	0.8334	7.274	7.2714	7.2724	185.83	186.142	186.142
0.8864	0.8312	0.8296	0.8295	8.0855	8.083	8.0839	188.5	188.864	188.886
1	0.8235	0.8216	0.8223	9.708	9.7061	9.7074	192.204	192.648	192.484

$V^E(\text{cm}^3/\text{mol})$			$\Delta\eta(\text{mPa.s})$			$\Delta G^{*E}(\text{kJ/mol})$		
LIT	CHEM CAD	EXP	LIT	CHEM CAD	EXP	LIT	CHEM CAD	EXP
0	-0.0004	-0.0009	0	0	0	0.0389	0	0
-0.0796	-0.0834	-0.0661	0.0269	-0.0005	-0.0008	1236.9188	32.261	32.7363
-0.1622	-0.1686	-0.1324	0.0333	-0.001	-0.0013	1702.1692	71.6479	72.312
-0.2473	-0.2585	-0.2035	0.0164	-0.0014	-0.0018	1845.884	88.264	88.7664
-0.337	-0.3503	-0.2754	-0.0236	-0.0018	-0.0023	1806.8965	103.0323	103.5316
-0.4298	-0.4465	-0.3506	-0.0877	-0.0021	-0.0025	1645.8127	102.351	102.564
-0.5252	-0.5456	-0.4288	-0.1769	-0.0021	-0.00267	1394.4426	86.3264	86.9346
-0.6262	-0.6479	-0.509	-0.2928	-0.0021	-0.0022	1071.1431	65.9466	66.4613
-0.7304	-0.7548	-0.5929	-0.4364	-0.0018	-0.0015	687.4075	45.661	46.3133
-0.8394	-0.865	-0.68	-0.6085	-0.0011	-0.0009	251.4601	26.022	26.3496
0	-0.0005	-0.0005	0	0	0	0.0191	0	0

Table 4.7 :Theoretical values of density ρ (kg/m³), viscosity η (mPa.s), deviation in viscosity $\Delta\eta$ (mPa.s), excess molar volumes V^E (cm³/mol), molar volume of mixture V_m (cm³/mol), excess Gibbs free energy of activation of viscous flow ΔG^{*E} (J/mol) for experimental reading of 1-Decanol (x1) + Octyl acetate (x2) at 303.15 K.

X	DENSITIES (g/cc) (ρ)			(η) VISCOSITIES (mPa.s)			V_m (cm ³ /mol)		
	LIT	CHEM CAD	EXP	LIT	CHEM CAD	EXP	LIT	CHEM CAD	EXP
0	0.8612	0.8603	0.8607	0.7582	0.762	0.7569	200.023	200.232	200.139
0.1037	0.8578	0.8568	0.8571	1.5718	1.5751	1.5706	199.125	199.358	199.288
0.2066	0.8544	0.8533	0.8535	2.3854	2.3882	2.3843	198.234	198.49	198.443
0.3087	0.851	0.8498	0.8499	3.199	3.2013	3.198	197.349	197.628	197.604
0.4099	0.8476	0.8463	0.8463	4.0126	4.0144	4.0117	196.471	196.773	196.773
0.5102	0.8442	0.8428	0.8427	4.8262	4.8275	4.8254	195.602	195.927	195.95
0.6098	0.8408	0.8393	0.8391	5.6398	5.6406	5.6391	194.737	195.085	195.131
0.7085	0.8374	0.8358	0.855	6.4534	6.4537	6.4528	193.88	194.251	189.889
0.8065	0.834	0.8323	0.8319	7.267	7.2668	7.2665	193.027	193.421	193.515
0.9036	0.8306	0.8288	0.8283	8.0806	8.0799	8.0802	192.183	192.6	192.717
1	0.8235	0.8216	0.8223	9.708	9.7061	9.7074	192.204	192.648	192.484

$V^E(\text{cm}^3/\text{mol})$			$\Delta\eta(\text{mPa.s})$			$\Delta G^E(\text{kJ/mol})$		
LIT	CHEM CAD	EXP	LIT	CHEM CAD	EXP	LIT	CHEM CAD	EXP
-0.0002	-0.0005	-0.0004	0	0	0	0.0612	0	0
-0.0874	-0.088	-0.0576	-0.1145	-0.0005	-0.001	1170.1013	33.6594	34.636
-0.1738	-0.1756	-0.1149	-0.2218	-0.0009	-0.0014	1559.1504	65.5666	66.0463
-0.2604	-0.2633	-0.1723	-0.322	-0.0012	-0.0017	1641.8117	96.632	97.236
-0.3471	-0.3508	-0.2287	-0.4141	-0.0015	-0.0019	1561.2657	110.326	110.7624
-0.4319	-0.4361	-0.2839	-0.4982	-0.0017	-0.0021	1381.0255	107.5623	107.9366
-0.5181	-0.5228	-0.3404	-0.576	-0.0017	-0.0018	1132.6592	85.2632	84.552
-0.6033	-0.6082	-4.8269	-0.6457	-0.0016	-0.0014	836.6344	64.6263	64.2355
-0.69	-0.695	-0.4507	-0.7092	-0.0013	-0.001	504.7675	31.2653	30.8622
-0.7748	-0.7796	-0.5054	-0.7646	-0.0007	-0.0006	146.9744	12.6316	12.0325
0	-0.0005	-0.0005	0	0	0	0.0191	0	0

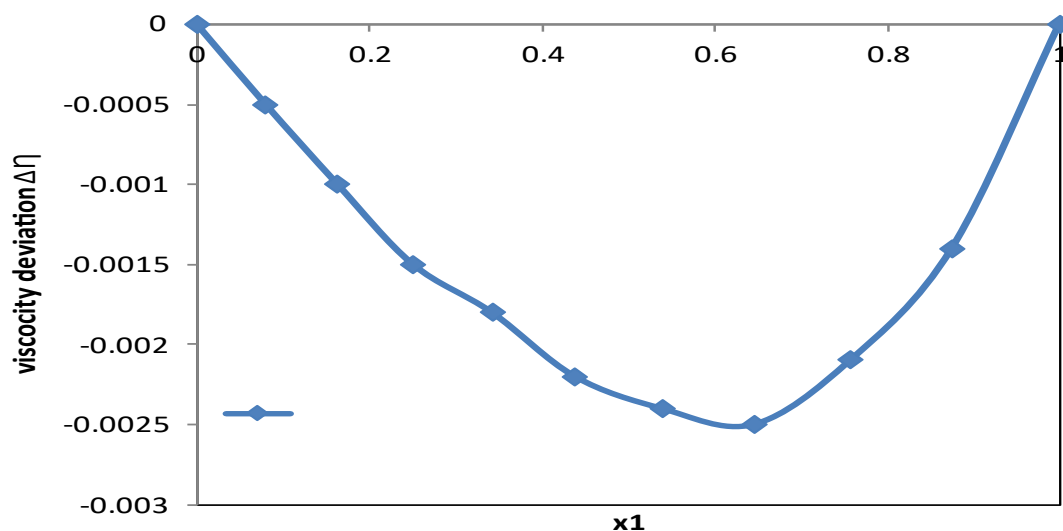


Fig 4.10 Plots of deviation in viscosity ($\Delta\eta$) against mole fraction for the system 1-Decanol (x_1) + Pentyl acetate (x_2) using Chemcad at temperature 303.15 K .

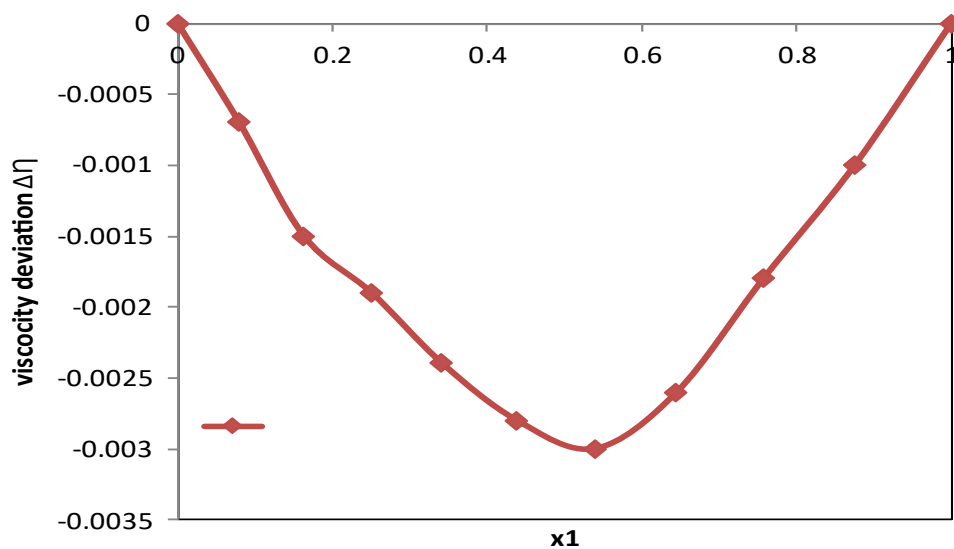


Fig 4.11 Plots of deviation in viscosity ($\Delta\eta$) against mole fraction for the system 1-Decanol (x_1) + Pentyl acetate (x_2) by experiment at temperature 303.15 K .

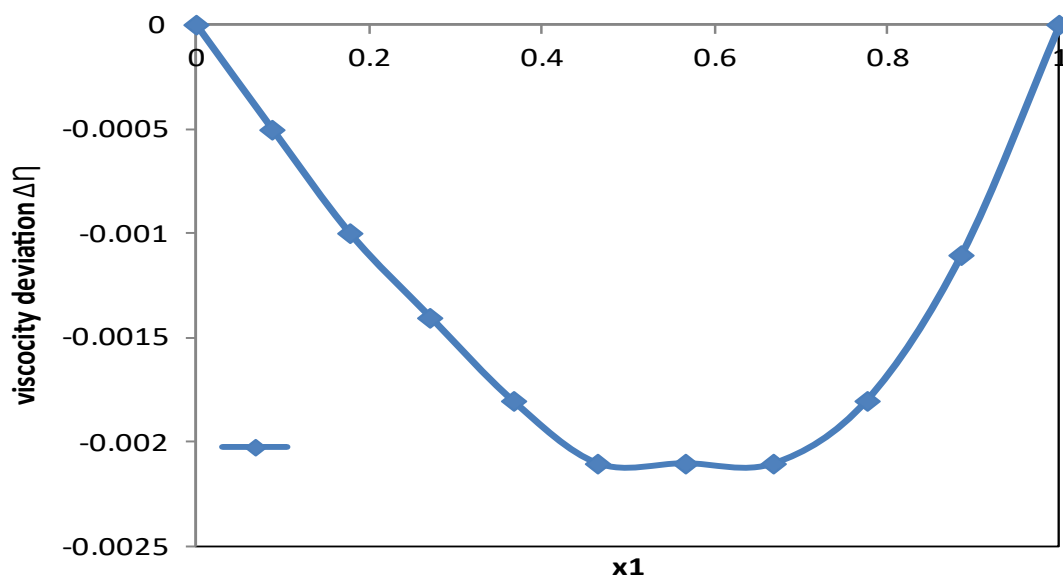


Fig 4.12 Plots of deviation in viscosity ($\Delta\eta$) against mole fraction for the system 1-Decanol (x_1) + Hexyl acetate (x_2) using Chemcad at temperature 308.15 K .

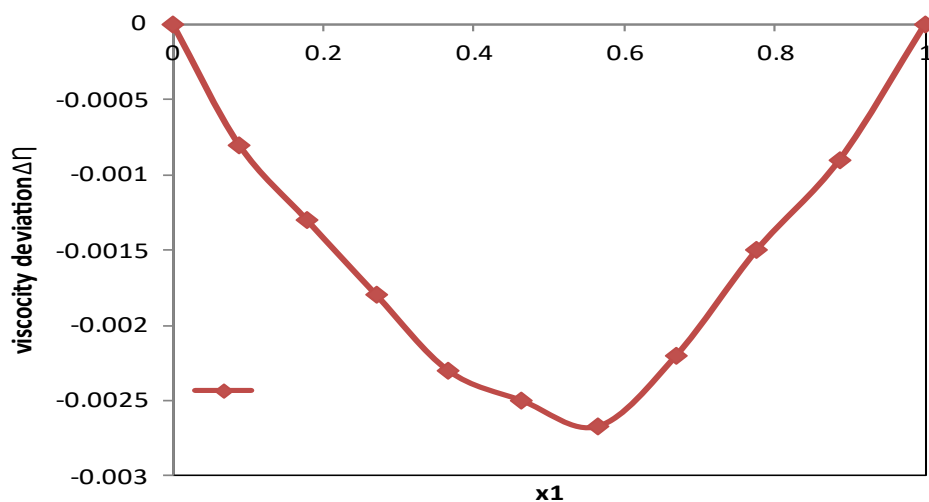


Fig 4.13 Plots of deviation in viscosity ($\Delta\eta$) against mole fraction for the system 1-Decanol (x_1) + Hexyl acetate (x_2) by experiment at temperature 313.15 K .

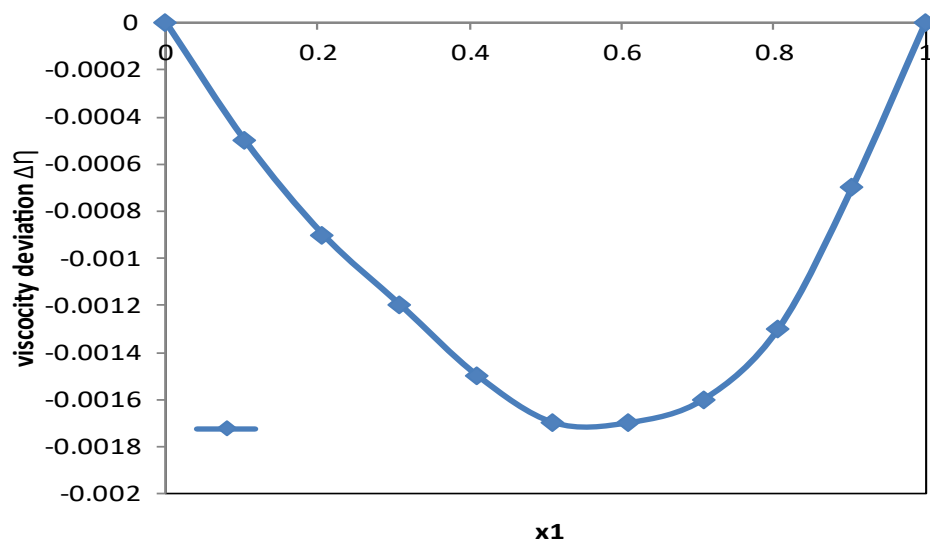


Fig 4.14 Plots of deviation in viscosity ($\Delta\eta$) against mole fraction for the system 1-Decanol (x_1) + Octyl acetate (x_2) using Chemcad at temperature 303.15 K .

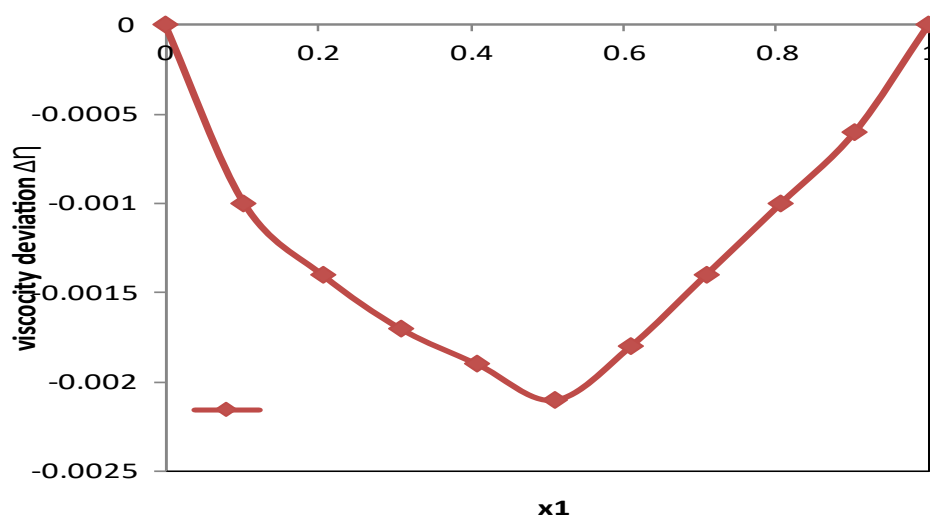


Fig 4.15 Plots of deviation in viscosity ($\Delta\eta$) against mole fraction for the system 1-Decanol (x_1) + Octyl acetate (x_2) by experiment at temperature 303.15 K .

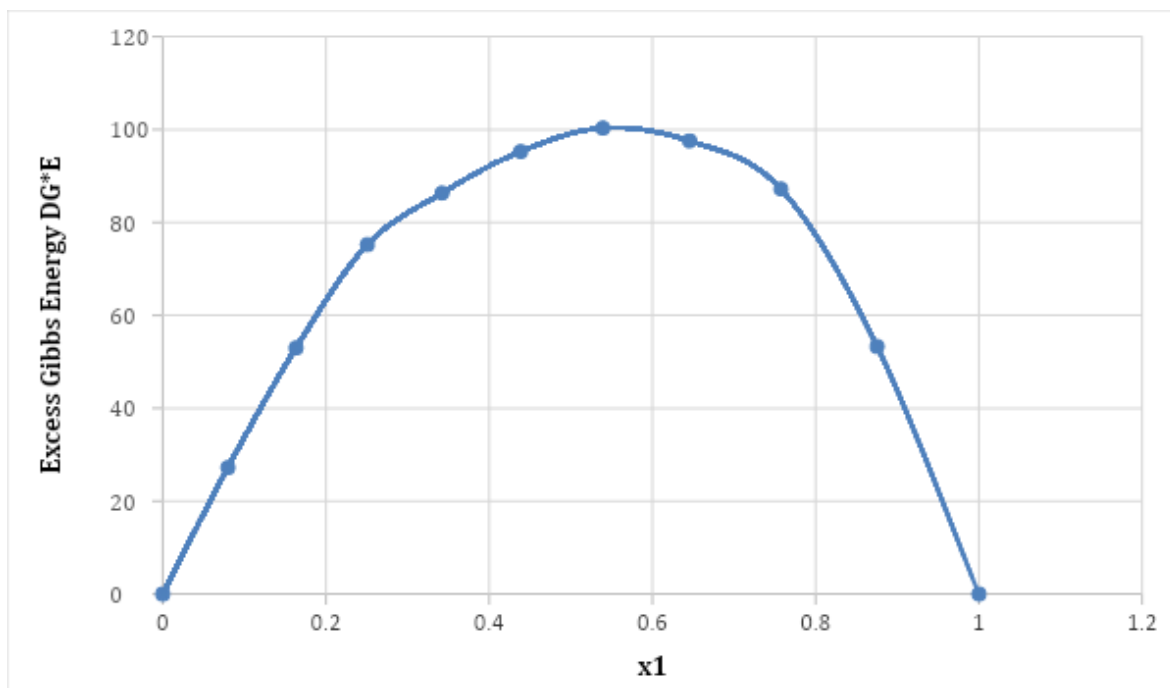


Fig 4.16 Plots of Excess Gibbs free energy of activation of viscous flow (ΔG^*E) against mole fraction for the system 1-Decanol (x_1) + Pentyl acetate (x_2) using Chemcad at temperature 303.15 K .

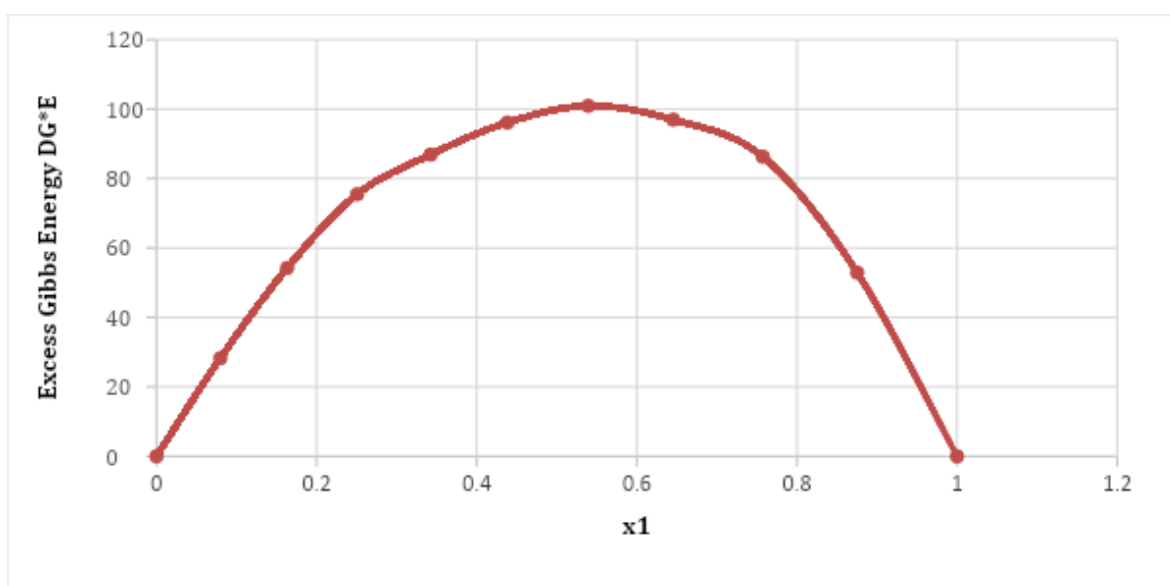


Fig 4.17 Plots of Excess Gibbs free energy of activation of viscous flow (ΔG^*E) against mole fraction for the system 1-Decanol (x_1) + Pentyl acetate (x_2) by experiment at temperature 303.15 K

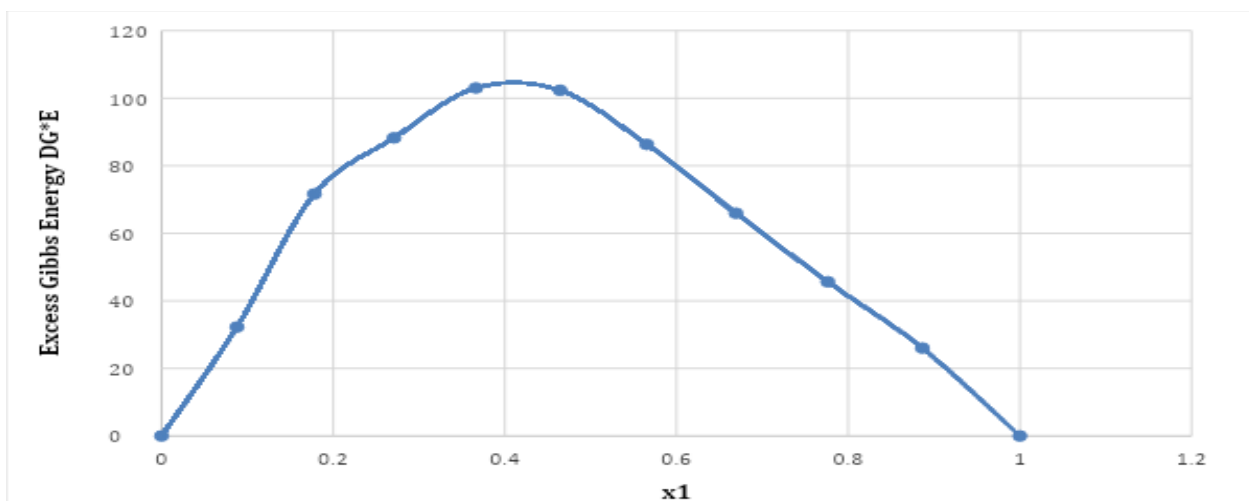


Fig 4.18 Plots of Excess Gibbs free energy of activation of viscous flow (ΔG^*E) against mole fraction for the system 1-Decanol (x_1) + Hexyl acetate (x_2) by using Chemcad at temperature 303.15 K

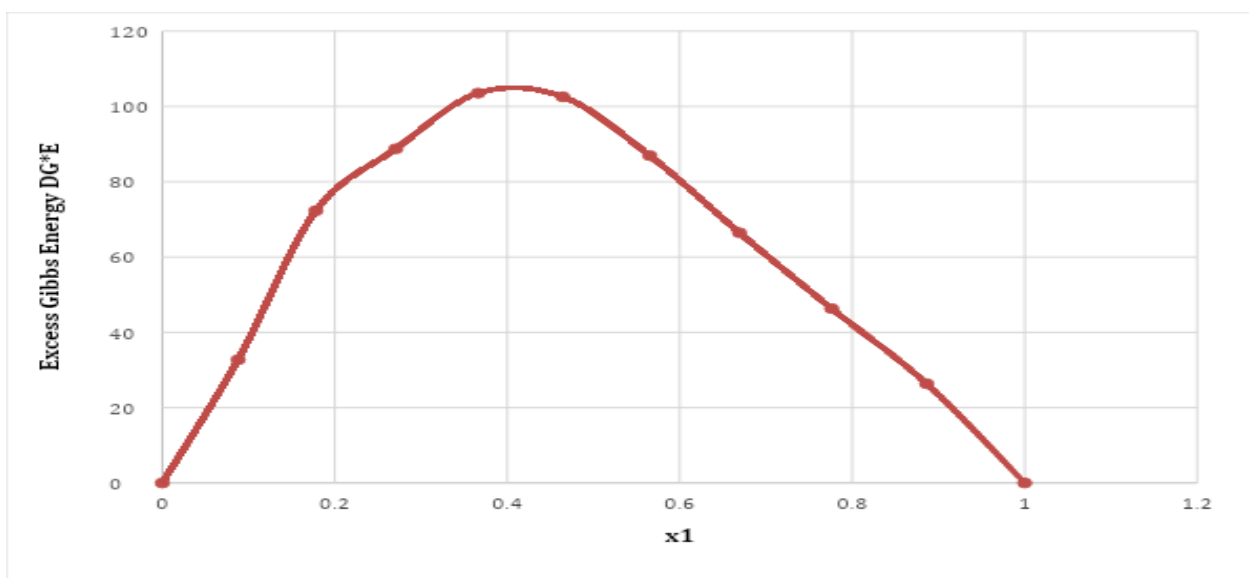


Fig 4.19 Plots of Excess Gibbs free energy of activation of viscous flow (ΔG^*E) against mole fraction for the system 1-Decanol (x_1) + Hexyl acetate (x_2) by experiment at temperature 303.15 K

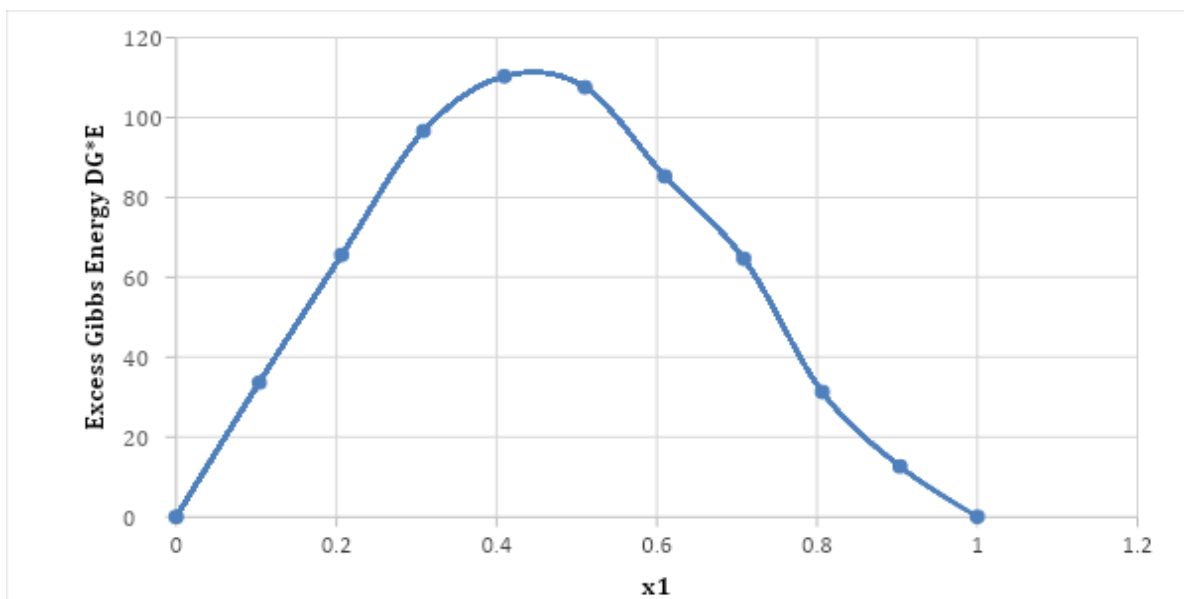


Fig 4.20 Plots of Excess Gibbs free energy of activation of viscous flow (ΔG^{*E}) against mole fraction for the system 1-Decanol (x_1) + Octyl acetate (x_2) by using Chemcad at temperature 303.15 K

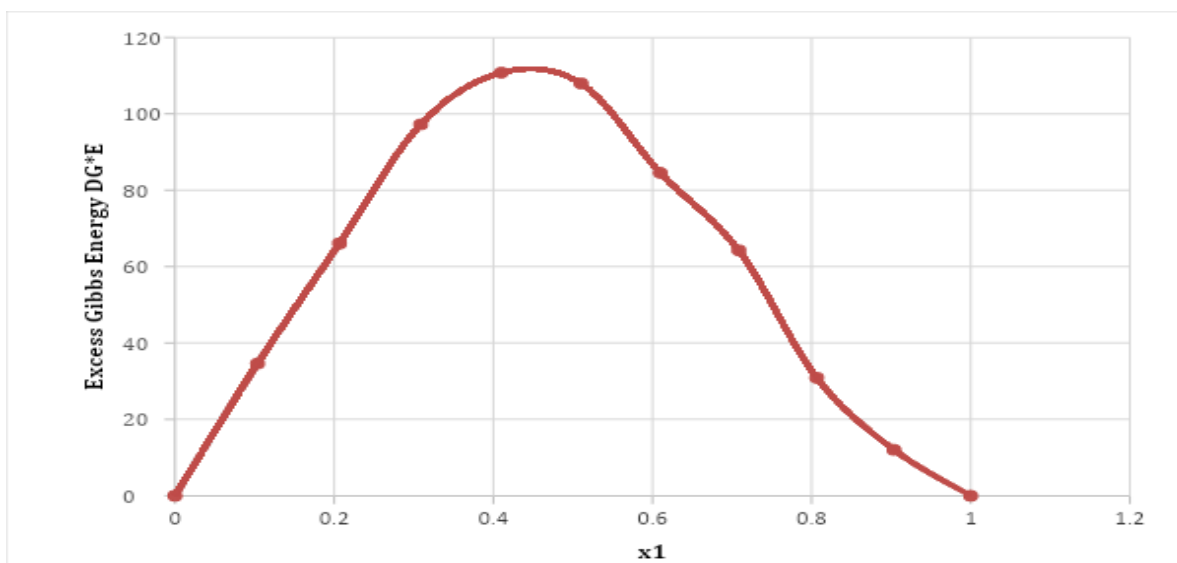


Fig 4.21 Plots of Excess Gibbs free energy of activation of viscous flow (ΔG^{*E}) against mole fraction for the system 1-Decanol (x_1) + Octyl acetate (x_2) by experiment at temperature 303.15 K

Densities, viscosities of binary liquid mixtures composed of 1 Decanol with pentyl acetate, hexyl acetate and octyl acetate were determined at 298.15, 303.15, 308.15 and 313.15 K by using the simulation software (CHEMCAD). From results were obtained, deviation in viscosity ($\Delta\eta$), excess molar volume (V^E), excess Gibbs free energy of activation of viscous flow (ΔG^{*E}), were determined. The deviation in viscosity ($\Delta\eta$), molar volume (V_m), excess Gibbs free energy of activation of viscous flow (ΔG^{*E}), And modified Kendall Monroe viscosity ($E\eta m$) is plotted against mole fraction as shown in the figures above. For all the systems negative deviation is observed for the viscosity deviation. The negative values of the deviation in viscosity ($\Delta\eta$) suggest the existence of weak intermolecular interactions upon mixing. It is clear from the graph that the deviation magnitude decreases as the temperature of the system increases. The maximum magnitude of negative deviation for viscosity deviation is observed at the temperature of 313.15K, and the maximum magnitude is exhibited by the 1 Decanol + Pentyl acetate system. The magnitude of (ΔG^{*E}) represents the strength of interaction between unlike molecules. Excess Gibbs free energy of activation of viscous flow was found to be positive for all plots. From the plots it is observed that the magnitude of (ΔG^{*E}) increases with the increase in the temperature for all the systems. This indicates that the strength of interaction increases with the increase in the temperature. The plot of molar volume (V_m) versus the mole fraction shows a linear curve, which indicates the binary mixture almost behaves ideally. The Kendall- Monroe viscosity plots moves from larger magnitude curves to lower magnitude curve with the increase in the temperature. All the Kendall-Monroe viscosity plots are positive in nature. The Grunberg-Nissan parameter (d') is an interaction parameter, which gives an idea about the interaction within the system. The positive value indicates the strong interaction within the system, and the negative value indicates the weak interaction in the systems. The deviations in viscosity, excess molar volume and excess Gibbs free energy of activation of viscous flow were correlated with Redlich- Kister polynomial equation, which correlates the various deviation parameters with the mole fraction of the components

CHAPTER – 5

SUMMARY AND CONCLUSIONS

5.1.SUMMARY

Densities, viscosities of binary liquid mixtures composed of 1 Decanol with pentyl acetate, hexyl acetate octyl acetate were determined at 298.15, 303.15, 308.15 and 313.15 K. By using the simulation software (CHEMCAD) results were obtained, deviation in viscosity ($\Delta\eta$), excess molar volume (V^E), excess Gibbs free energy of activation of viscous flow (ΔG^{*E}), were determined. The plots of deviation in viscosity, molar volume, Excess Gibbs free energy, Kendall-Monroe viscosity correlation against mole fraction is obtained for the each system at different temperatures. For all the systems negative deviation is observed for the viscosity deviation. The negative values of the deviation in viscosity ($\Delta\eta$) suggest the existence of weak intermolecular interactions upon mixing . The strength of the specific forces is not the factor influencing the viscosity deviation in the liquid mixture. This leads to suggestions that combinations of an interactive and non interactive force are responsible in these positive and negative deviations. The ($\Delta\eta$) values are in general negative and large over the entire range of alcohol mole fraction. The curves are skewed toward the alcohol rich regions. An increased temperature is found to enhance the mixture viscosity contribution to the overall viscosity deviations. The large negative viscosity deviations suggest that in these mixtures, the forces between pairs of unlike molecules are less than the forces between like molecules. The magnitude of (ΔG^{*E}) represents the strength of interaction between unlike molecules. Excess Gibbs free energy of activation of viscous flow was found to be positive for all plots. The excess Gibbs free energy of activation of viscous flow attains a maximum between (0.34 – 0.6) of the mole fraction. The plot of modified Kendall-Monroe viscosity gives positive values. The inverse relationship between the temperature and viscosity is clearly understood from the plots. For every system, as the temperature increases, the Kendall-Monroe viscosity value decreases. Kendall-Monroe equation is a cubic empirical equation which is very helpful in finding the viscosity data in many applications like blending, mixing etc. The Kendall-Monroe viscosity plots moves from larger magnitude curves

to lower magnitude curve with the increase in the temperature. The peak point of viscosity shifts from the mole fraction range (0.7-0.4) as the chain length of the hydrocarbon chain increases. For the lower chain hydrocarbons the peak point of viscosity is observed nearly at the mole fraction range of 0.8, e.g. 1 Decanol + Pentyl acetate system. As the chain length increases the peak point shifts nearly the mole fraction range of 0.6, e.g. 1 Decanol + Octyl acetate system. The Grunberg-Nissan parameter (d') is an interaction parameter which is a function of the composition and temperature of binary liquid mixture. Grunberg-Nissan interaction parameters are both positive and negative for the systems. The positive value of Grunberg-Nissan parameter indicates the strong interaction of molecules within the system and the negative value indicated the weak interaction among the molecules. The plot between the molar volume vs mole fraction gives a linear line for all the systems. These plots are studied for determining the ideality of the binary mixture. The linear nature shows that the system is nearly behaving ideally. The Redlich-Kister equation is used to correlate the various deviation parameters with the mole fraction and the coefficients are determined for the correlation.

5.2 CONCLUSION

Densities, viscosities of binary liquid mixtures composed of 1 Decanol with pentyl acetate, hexyl acetate octyl acetate were determined at 298.15, 303.15, 308.15 and 313.15 K. By using the simulation software (CHEMCAD) results were obtained, deviation in viscosity ($\Delta\eta$), excess molar volume (V^E), excess Gibbs free energy of activation of viscous flow (ΔG^{*E}), were determined. The plots of deviation in viscosity, molar volume, Excess Gibbs free energy, Kendall-Monroe viscosity correlation against mole fraction is obtained for the each system at different temperatures. A comparison of experimental thermodynamic data of multicomponent mixtures with that calculated by means of various predictive methods is very useful from different points of view:

It suggests which model is more appropriate to the characteristics of the system

It may indicate which parameters should be improved when the model involves group contributions

It may allow the identification of some model as a convenient reference for the interpretation of the deviations observed

It allows us to use the data for various design purposes which are used in the process industries

The thermodynamics and transport properties of the system are determined through a study of the system at various temperatures, and the deviation parameters are derived. An itemized analysis of the experimental Grunberg-Nissan interaction parameter (d') against temperature and composition can provide precise information on future molecular interactions, structural changes, and independent parameters of other models correlating viscosity in binary liquid mixtures. Also, as a result of our research on the chosen systems, we have come to the following conclusion: As the size of the alkyl group grows larger, the magnitude of the viscosity divergence decreases. Pentyl acetate > Hexyl acetate > Octyl acetate is the order in which the magnitude of viscosity deviation increases for the current system. As a result, it is obvious that as the alkyl group increases, the amount of the variation in viscosity decreases. Both systems have a linear connection based on the data acquired from the molar volume vs mole fraction data. It is obvious from the linearity relationship that the system behaves in a near-ideal manner.

REFERENCES

Akl M. Awwad And Kifah A. J Bara, Excess volumes of n-pentylacetate with alkanes, cycloalkanes and aromatics at 303.15 K , Fluid Phase Equilibria, Volume 46, 1989, Pages 259-265

Belda .R, A proposed equation of correlation for the study of thermodynamic properties (density, viscosity, surface tension and refractive index) of liquid binary mixtures, Fluid Phase Equilibria, Volume 282, 2009 , Pages 88-99

Bhajan Lal, Melike Sahin, Erol Ayranci, Volumetric studies to examine the interactions of imidazolium based ionic liquids with water by means of density and speed of sound measurements, The journal of chemical thermodynamics, Volume 12, 2012, Pages 142-147

Giro . F, Gonçalves . M.F, Ferreira. A.G.M, Fonseca . I.M.A, Viscosity and density data of the system water + n-pentyl acetate + methanol Calculations with a modified Redlich–Kwong–Soave equation of state, Fluid Phase Equilibria, Volume 204, 2003, Pages 217-232

Hiannie Djojoputro and Suryadi Ismadji, Density and Viscosity for a Binary Mixture of cis-3-Hexenyl Formate, Butyl Acetate, trans-2-Hexenyl Acetate, and cis-3-Hexenyl Acetate with Ethanol at Several Temperatures, Journal of chemical and engineering data , Volume 50, 2000, Pages 1009-1013

Mohamed M. El-Banna, Densities and Viscosities for Mixtures of Pentyl Acetate and Hexyl Acetate with Normal Alkanols at 298.15 K, Journal of chemical and engineering data , Volume 42, 1997, Pages 31-34

Mohammed Taghi Zafarani-Moattar* and Roghayeh Majdan-Cegincara, Viscosity, Density, Speed of Sound, and Refractive Index of Binary Mixtures of Organic Solvent + Ionic Liquid, 1-Butyl-3-methylimidazolium Hexafluorophosphate at 298.15 K, Journal of chemical and engineering data , Volume 52, 2007, Pages 2359-2364

Montañó .D.F, Martí'n .S, P. Cea, Lo'pez .M.C, and Artigas.H, Volumetric, Acoustic, and Refractive Properties of Isomeric Chlorobutanes with Diisopropyl Ether, Journal of chemical and engineering data , Volume 55 ,2010, Pages 5953-5959

Nani Indraswati, Mudjijati, Filicia Wicaksana, and Herman Hindarso, Density and Viscosity for a Binary Mixture of Ethyl Valerate and Hexyl Acetate with 1-Pentanol and 1-Hexanol at 293.15 K, 303.15 K, and 313.15 K, Journal of chemical and engineering data , Volume 46 ,2001, Pages 134-137

Nicolás F. Gajardo-Parra, Matías I. Campos-Franzani, Ariel Hernández, Néstor Escalona, and Roberto I. Canales, Density and Viscosity of Binary Mixtures Composed of Anisole with Dodecane, Hexadecane, Decalin, or 1,4-Dioxane: Experiments and Modeling, Journal of chemical and engineering data , Volume 107, 2007, Pages 2411-2502

Prolongo. M.G, Masegosa .R.M, Herniindez-Fuente . I, Horta. A, Viscosities and Excess Volumes of Binary Mixtures Formed by the Liquids Acetonitrile, Pentyl Acetate, 1-Chlorobutane, and Carbon Tetrachloride at 25 C, Journal of chemical and engineering data , Volume 46, 2001, Pages 141-155

Ramesh L. Gardas,‡ Mara G. Freire,‡ Pedro J. Carvalho,‡ Isabel M. Marrucho,‡ Isabel M. A. Fonseca,§ Abel G. M. Ferreira,*,§ and João A. P. Coutinho, *PpT* Measurements of Imidazolium-Based Ionic Liquids, , Journal of chemical and engineering data , Volume 53, 2008, Pages 805-811

Sastry .N.V & Valand .M.K, Volumetric Behaviour of Acrylic Esters (Methyl-, Ethyl-, and Butyl Acrylate) + 1-Alcohol (Heptanol, Octanol, Decanol and Dodecanol) at 298.15 K and 308.15 K, Physics and chemistry of liquids, Volume 38, 2000, Pages 30-76

Shahram Ranjbar , Zahra Fakhri & Jahan B. Ghasemi, Studies of dynamic viscosity

& gibbs energy of activation of binary and ternary mixtures of benzylchloride + nitrobenzene + isobutanol from $t = (288.15 \text{ to } 313.15)\text{K}$, Chemical engineering communications, Volume 198, 2011, Pages 815-836

Tiancheng Mu and Buxing Han, Structures and Thermodynamic Properties of Ionic Liquids, Cheminform, Volume 46, 2013, Pages 20-26

Venkatesan.D, Joshua Amarnatha.D , and Saravanakumar.K, Thermophysical Properties of Binary Mixtures of Diisopropyl Ether with Methyl Benzoate, Ethyl Benzoate, and Benzyl Acetate at Various Temperatures, Russian journal of physical chemistry, Volume 94, 2020, Pages 1573-1580

Venkatesan .D, Joshua Amarnath .D, Sinduri .E and Saravanakumar .K, Physical Properties of Butyronitrile Mixtures with Pentane, Hexane, Heptane, and Octane, Russian journal of physical chemistry , Volume 93, 2019, Pages 1489-1496

Venkatesan.D , Joshua Amarnath D, Srinivasa Krishna .T , Piyashi Biswas , Ranjan Dey, Densities, viscosities and excess parameters of octanol with alkyl(C1 – C4) acetates at varying temperatures, Journal of Molecular liquids, Volume 107, 2007, Pages 2411-2502

Zhibo Zhang,^{†,‡} Qing Zhou,[‡] Xingmei Lu,[‡] Congzhen Qiao,^{*,†} and Suojian Zhang^{*}, Densities and Viscosities of Binary Mixtures Containing 1,3-Dimethylimidazolium Dimethylphosphate and Alcohols, Journal of Chemical engineering , Volume 59, 2014, Pages 2377-2388.