INSTITUTO POLITÉCNICO DE BRAGANÇA
Escola Superior de Tecnologia e Gestão

Experimental Study of Thermodynamic Properties of Liquid Mixtures with Interest as Biofuels: Binary Systems: 2-Propanol, DIPE and 1 Hexene

Ana Carolina Kulik

Dissertation presented to the School of Technology and Management of Polytechnic Institute of Bragança to the Fulfillment of the Requirements for the Master of Science Degree in Renewable Energy and Energetic Efficiency

Supervisor:

Professor Ph.D. Paulo Miguel Pereira de Brito

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Dedication

To my beloved family,

Jorge Luiz Kulik, Maria de Lourdes Franco Kulik, Ana Paula Franco Köhne, Daiana Evelin Kulik Fiori, Jessica Mariana Kulik and Iasmim Poliana Kulik.

Acknowledgment

To God, for always enlightening my path.

To my parents and my sisters, who always supported me unconditionally.

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To the University of Burgos and my dear doctors Eduardo Montero, Fernando Aguilar Romero and Natalia Muñoz Rujas, who supported me and teached me not only about academic research or articles but also about life and how good are Spanish people.

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Abstract

About 25% of CO_2 emissions in the EU are originated by the transport sector. In this segment, road transport is the largest emitter, accounting for over 70% of all greenhouse gas (GHG) emissions. One of the main strategies for reducing emissions is the promotion of low emission alternative energy for transport, such as biofuels.

Some alcohols and ethers, such as oxygenate additives, are added to gasoline to reduce the emission of gases that produce environmental impact. These components can be obtained from renewable or agricultural raw materials, reducing dependence on fossil sources. The thermodynamic properties of liquid blends with interest as biofuels are of great importance to the petrochemical industry, not only because of their application in new gasoline formulations but also for refining design, purification and deposition processes.

This work reports experimental densities, speeds of sound, refractive indices of binary systems 2-propanol + di-isopropyl-ether (DIPE), 2-propanol + 1-hexene and di-isopropyl-ether (DIPE) + 1-hexene at the temperature of 298.15 K. Besides, the viscosity of the same binary systems at the temperatures of 293.15 K, 298.15K and 313.15K are also reported. Excess molar volumes, deviations in isentropic compressibility and deviations in speeds of sound were correlated by the Redlich-Kister polynomial. In total, 756 experimental measurements were collected and analyzed to scientifically contribute for the validation of new models and equations which could satisfactorily predict the liquid blend behavior of these compounds as biofuels.

Keywords: density; refraction index; speed of sound; viscosity; diisopropyl ether.

Resumo

Cerca de 25% das emissões de CO_2 na UE provêm do setor de transportes. Nesse segmento, o transporte rodoviário é o maior emissor, respondendo por mais de 70% de todas as emissões de gases de efeito estufa. Uma das principais estratégias de redução de emissões é a promoção de energia alternativa de baixa emissão para o transporte, como os biocombustíveis.

Alguns álcoois e éteres, como aditivos de oxigénio, são adicionados à gasolina para reduzir a emissão de gases que produzem impacto ambiental. Esses componentes podem ser obtidos a partir de matérias-primas renováveis ou agrícolas, reduzindo a dependência de fontes fósseis. As propriedades termodinâmicas das misturas líquidas com interesse como biocombustíveis são de grande importância para a indústria petroquímica, não apenas por sua aplicação em nova formulaçao da gasolina, mas também para o projeto dos processos de refino, purificação e deposição.

Este trabalho reporta densidades experimentais, velocidades de som, índices de refração de sistemas binários 2-propanol + éter diisopropílico (DIPE), 2-propanol + 1-hexeno e éter diisopropílico (DIPE) + 1-hexeno na temperatura de 298,15 K. Além disso, é apresentada a viscosidade dos mesmos sistemas binários nas temperaturas de 293,15 K, 298,15 K e 313,15 K. Volumes molares excessivos, desvios na compressibilidade isentrópica e desvios nas velocidades do som foram correlacionados pelo polinómio de Redlich-Kister. No total, 756 medições experimentais foram coletadas e analisadas para contribuir cientificamente na validação de novos modelos e equações que possibilitem a previsão satisfatória do comportamento da mistura líquida desses compostos como biocombustíveis.

Palavras-chave: densidade; índice de refração; velocidade do som; viscosidade; éter diisopropílico.

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Acronyms

ASTM American Society of Testing and Materials

BSFC Brake Specific Fuel Consumption

CAS Chemical Abstracts Service

DIPE Diisopropylether

EU Europe Union

GHG Greenhouse Gas

MTBE Methyl Tert Butyl Ether

NDC Nationally Determined Contribution

NIST National Institute of Standards & Technology

1 Introduction

Energy consumption from non-renewable sources, energy savings and energy efficiency, are necessary measures to reduce global greenhouse gas emissions [1]. Governments, faced with the need to control carbon dioxide emissions, encourage the use of renewable fuels as an alternative for transport.

The “biofuels” are referred to the energy-enriched chemicals generated through the biological processes or derived from the biomass of living organisms, such as microalgae, plants and bacteria [2]. The energy in biofuel is stabilized during a process of biological carbon fixation in which carbon dioxide (CO_2) is converted into sugar that is found only in living organisms and plants. [3]. In contrast with fossil fuel, biofuel is produced by, or derived from, living organisms in a relatively short period of time rather than being derived by the decomposition of organic matter over several million years [4].

Currently, there is three generation of biofuels based on different feedstocks. The “first generation” of biofuels, such as bioethanol, biobutanol and biodiesels, are produced directly from food crops like corn, wheat and soybeans. The biofuel is derived from the starch, sugar, and oil that these crops provide. [4]. The important characteristic of “first generation” biofuels include their ability to be blended with petroleum-based fuels and their efficiency in internal combustion engines, as well as the compatibility with flexible fuel vehicles [5]. The “second generation” of biofuels are made from nonfood-crops, mainly lignocellulosic feedstock such as grass, wood, and other organic wastes [4]. In a search for a viable and a cost-effective alternative to fossil fuels, past

studies have reported superior capabilities of algae-derived biomass for the production of an improved version: the third generation of biofuels [5].

Biofuels, as ecological fluids, have received much attention in recent decades. They contribute to lower greenhouse gas emissions due to their neutral carbon dioxide balance (all the carbon contained in a biofuel has been already absorbed from the atmosphere) [4]. Besides, some oxygenated compounds are used as biofuel additives as they lead to a reduction in pollutant emissions and an increase in the energy efficiency of vehicle engines [6].The biofuels study meets the main goal of the European directive «20-20-20» [7], as well as the agreement of 195 countries to adopt a new global climate agreement in Paris [8].

1.1 Problem Formulation

There is a huge amount of available thermodynamic data for pure compounds, but the thermophysical properties of biofuels and their mixtures differ from the pure compounds. The performance of fuels and biofuels in engines and other devices shows a trend of increasing pressure and temperature, which leads to the need of more reliable predictive models for complex mixtures at such conditions. Availability of high pressure and high temperature thermodynamic properties is then a requisite for the implementation of these equation and models [6].

Some alcohols and ethers, such as oxygenate additives, are added to gasoline to reduce the emission of gases that produce environmental impact. The advantages of these oxygenates can be classified into several categories

[10]. First, they can be obtained from renewable or agricultural raw materials, reducing dependence on fossil sources. Second, they increase the number of octanes, increasing the anti-knock effect of gasoline. Then, the compression ratio of the engines can be increased without the risk of crashing, leading to higher power delivery. From a combustion standpoint, the production of carbon monoxide and volatile hydrocarbons from the combustion of alcohols is lower than gasoline. Among the thermodynamic properties, the heat of vaporization of alcohols is high and leads to a reduction in the combustion temperature peak, which means lower nitrogen oxide emissions [6].

Selecting an alcohol such as propanol as oxygenate additive, it increases the number of octanes, improving the anti-knock effect of gasoline. Then the compression ratio of the engines can be increased without the risk of crashing, leading to greater power delivery. From a combustion point of view, the production of carbon monoxide and volatile hydrocarbons from the combustion of alcohols is lower than that of gasoline [6].

Di-isopropyl ether is a branched ether that has been widely used as an industrial solvent in many applications such as waxes and paints, lubricant, phenol recovery in the plastics industry and as a gasoline additive. This ether is used instead of others because it is considered environmentally benign. When released into the atmosphere, di-isopropyl ether from the vapor phase is degraded into the atmosphere by a reaction with hydroxyl radicals. When used as a fuel additive, it helps to reduce air pollution. Di-isopropyl ether (DIPE), is recommended pure or mixed with alkanes or alkanols, as gasoline engine octane rating elevators. [11].

Another short-chain olefin, 1-hexene, is a sustainable alkene attractive for biofuel development [12].

Viscosity is a transport property whose knowledge has a lot of importance in the design of transport networks, pumps, storage tanks, and most of the equipment that will be used in chemical and industrial applications.

1.1. Objectives

This work collects the results obtained from the experimentation carried out in the research laboratory of the department of electromechanical engineering of the University of Burgos from three main compounds: 2-propanol, DIPE, and 1-hexene. There is scarce or no data available in the literature for the three binary systems and reliable experimental data is necessary to optimize designs of several industry processes. Thermodynamic properties calculations, correlations and data processing after collection are also presented. The structure of the report work is detailed below, concerning the measurement procedures, equipment, presentation of the results and discussion of the results compared with the literature and predictions using the Redlich-Kister polynomial.

1.2. Document Structure

This dissertation is divided into 6 chapters in order to describe the work developed through the research.

Chapter 1 contains an introduction to biofuels, the context that it is inserted, the problem formulation and the objectives with the research.

Chapter 2 presents the bibliographic review, the theoretical framework collected from the literature which constitutes a state of the art relating to the studied field.

In Chapter 3, the materials and methods of the research are described. The methodology applied for the development of this dissertation is also described.

Chapter 4 presents the collected experimental data organized in tables and graphics complemented with a brief analysis, regarding the molar volumes of excess, refractive index and isentropic compressibility for all the binary mixtures.

In Chapter 5, the experimental data (again organized in tables and graphics) is presented, and a brief analysis for the dynamic and kinematic viscosity is carried out.

The main conclusions and suggestions for future works are presented in Chapter 6.

2 State of the Art

There is a growing demand for energy due to the increasing population which can lead to greater air pollution. On the other hand, there are limited sources of fossil-based fuels as a sustainable energy. As a result of world industrialization, the demand for oil-based fuels (fossil fuels) has increased dramatically [13]. Apart from the economic matters, the widespread use of fossil fuels is responsible for a long-term environmental problem in the form of climate changes and the global warming. The main source of energy in different forms originates from the combustion. Recently, depletion of the fossil fuels due to their continuous use has become the first priority concern for all people in the world whose lives depend on this source of energy for all their activities.

The transportation sector faces particularly strong challenges and requires a radical change and long-term policy support to confront the demand for decarbonization. Many alternatives are being investigated, ranging from energy efficiency, overall improvement of vehicle efficiency, engine downsizing, fuel efficiency, hybrid engines, plug-in hybrid vehicles, flex-fuel engine, electric vehicles, fuel cell vehicles (FCVs), etc [14].

The main source of greenhouse gas emissions are the fossil fuels [13]. The worldwide concern of the environmental pollutants has triggered intensified researches for new alternative sources of energy. Widespread applications of the fossil fuels and the environmental issues associated with their use have directed us to replace them with reasonable price, high efficiency and renewable sources. To find a proper convincing answer to this

question how to select, distribute and use the data, one needs to focus on both engine technology, fuel efficiency and biofuels.

During past decades, biofuels have been widely used as a viable alternative to fossil fuel resources, thanks to the crisis of gradual oil resources depletion, as well as due to an increase in worldwide fuel demand and consumption. The term “biofuel” refers to a fuel that is formed directly or indirectly from the biomass feedstock. Biomass is defined as biological materials that are either energy crops, wastes and byproducts from agricultural and forestry, manure or municipal solid wastes, or any other material containing microbial biomass. Charcoal, fuelwood, bioethanol, biomethane, biohydrogen, and biodiesel are some examples of biofuels that are found in continuous production [5]. Figure 1 illustrates the feedstock sources and products of biofuels.

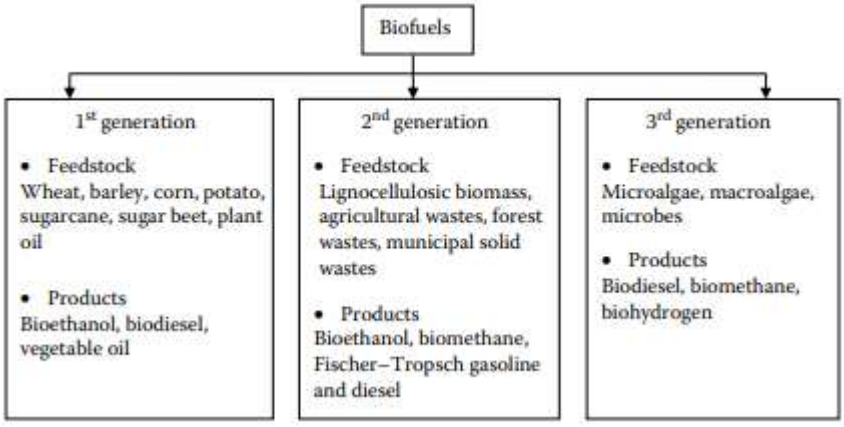

Figure 1: Classification of biofuel production: the three generations of biofuels [5].

Notably, contribution of biofuels to transport sector of global energy consumption is 0.8% only [15].

The scientific literature published in the recent past indicates that in a life cycle analysis basis, biofuels in particular provide a net GHG benefit (30–100% compared to petroleum fuels) [14], when use of co-products are included and GHG emissions from land conversion are excluded in the analysis.

Continuous and multifarious issues associated with global biofuels demand and production, policy makers and legal advisors are figuring out guidelines by which biofuel could be produced and supplied sustainably [16]. Some aims with the policies are:

- reduce the dependency of imported fossil fuel and address energy sovereignty;
- increase the production and use of biofuels and introduce the Certificate of Efficient Production of Biofuels and Decarbonization Credits to reduce CO_2 emissions;

Sustainable biofuel is expected to impart social, economic and environmental benefits for the betterment of humanity (Fig.2). It is on a positive note that biofuel industry holistically assessed the environmental concerns related with its development [16].

Figure 2: Social, economic and environmental impacts of sustainable biofuel production

Source: [16]

The combination of various alcohols including ethanol and diesel fuel, leads to make a clean fuel [16]. In the past, there was not a stable and single-phase diesel-ethanol fuel by direct injection of the ethanol. However, this problem was solved to some extent by adding ethyl ester, octyl nitrate, methyl esters, nitro methane, nitro ethane and 2-methoxy ethyl ether as other additives or stabilizers [16].

Biogasoline usually refers to bioethanol in mixture with petrol-gasoline employed in existing combustion engine to solve the problem diminishing and hazardous-emission fuel of petroleum [17].

2.1 Oxygenated Additives - **Alcohol**

The addition of fuel oxygenates to gasoline raises combustion temperatures and improves engine efficiencies. The results are lower levels of carbon monoxide and unburned hydrocarbons in auto exhaust [18].

Adding alcohol to the fossil fuel needs a balance between the emission reduction and engine power in order to reach the optimal point. Emissions from the diesel fuel are the most critical problem using this kind of fuel. There is some researches that blended the alcohols with the gasoline to control the air pollution and improve the engine performance (Table 1). It was also focused on the emission reduction, improvement of the fuel properties and enhancement of the engine power by adding various alcohols. The most important incentives using alcohol for the purpose of emission reduction are production of oxygenated alcohols, reaching small molecular weight and the most importantly, achieving shorter molecular chain in comparison with that of the diesel fuel [13].

Table 1: Summary of emissions and performance test results from additive–gasoline blends

Researcher	Ref.	Oxygenate Additive	Additive %	Pressure(kPa)	Power (kW)	BSFC
Li et al.	[19]	Isopropanol + But+Eth	0	300	22.5	370g/kw
		Isopropanol +But+Eth	30	300	23.5	395g/kw
		Isopropanol +But+Eth	0	500	26.5	330g/kw
		Isopropanol+ But+Eth	30	500	27.8	355g/kw

Propanol and butanol have been proposed as an alternative to conventional gasoline and diesel fuels [6]. They are higher member of the series of alcohols with each molecule containing three or four carbon atoms rather

than two as in ethanol. The EN standards of the European Union (EU) and the World-Wide Fuel Charter (WWFC) for gasoline include, for example, 2-propanol, 2-methyl-2 propanol (also known as tert-butyl alcohol, TBA), and 2-methyl-1 propanol as gasoline components.

2.1.1 Engine Performance – BSFC

BSFC (brake specific fuel consumption) is affected by three parameters: 1) oxygen content of the additive. 2) Useful output power. 3) Engine speed. When the oxygenated fuels are added to the fossil fuel, the BSFC increases because blending of such fuels with the fossil fuel leads to greater oxygen content that contributes to a more complete ignition [13].

Balamurugan and Nalini [20] investigated enhancement of the engine performance by using both normal butanol and normal propanol alcohols. Their observations indicated that the engine fuel efficiency increases by adding each additive. In their experiments, the effect of the normal butanol and propanol was more than that of the normal butanol for improvement of the fuel efficiency. If the fuel could be burnt completely, it would then be possible to increase the fuel efficiency in the engine. This definition indicates that when the alcohol is oxygenated more and gets shorter branches, its properties improve the fuel efficiency in the engine at similar situations. It is clear that when blending the alcohols with the gasoline, the amount of BSFC could be significantly increased. Since the alcohols give rise to the oxygen content of the fuel, they contribute the fuel to have complete combustion.

2.1.2 Emissions - GHG

A greenhouse gas (GHG) is a gas in the atmosphere that emits and absorb radiation through the thermal infrared range. This mechanism is the basal cause of the greenhouse effect. Increasing of GHG is a result of indirect land-use change affected by cropbased biofuels as one of the most important aspects of the biofuels in terms of energy security and environment policy. The main greenhouse gases in the atmosphere of the earth are nitrogen oxides, carbon oxides, ozone, methane, and water vapor. Without the greenhouse gases, the earth temperature would be about −18 °C instead of the present average temperature of 15 °C [13].

2.1.3 Fuel Properties

Several physical-chemical fuel properties are essential for adequate combustion of a fossil fuel. Blending of the alcohols with the fossil fuel changes certain key properties such as viscosity, density, flash point and cetane or octane number. The cetane number is one of the most important properties of a diesel fuel, very similar to the octane number that is associated with the gasoline fuel. A high cetane number brings about a good starting ability in a cold weather, in addition to low combustion noise and long life of the engine. Viscosity of the fuel is one of the important characteristics of a liquid fuel. It also plays a key role in lubrication of the fuel injection systems. Blending of the alcohols to the diesel fuel causes a slight reduction in the fuel viscosity [13].

Accurate experimental data on thermodynamic properties should be available to check and develop predictive empirical equations, models and simulation programs. Industrial processes as storage, transport, separation and

mixing processes also need reliable data for its design. As a result, the experimental literature reviews on properties of pure compounds and its mixtures with characteristic hydrocarbons can provide valuable information about the fluid behavior under various temperature and pressure conditions [7].

2.1.4 Combustion

The bio-fuels blends have small effect on continuous performance of the engine and the overall combustion noise radiation. Combustion behavior and stability among the first transient cycles were mainly affected by the bio-fuel blend and reduced by the alcohols blend [13].

When the alcohols are blended into the fuel blend, a longer ignition delay is caused, due to their lower cetane number that is reliable for a further rise in the combustion noise over the pure diesel fuel operation. According to the limited tests on both genres of biofuels performed so far, more researches seem necessary, with wider variety of the biofuels and higher blending ratios, in order to attain more clear results [13].

The performance of fuels and biofuels in engines and other devices shows a trend of increasing pressure and temperature, which leads to the need of more reliable predictive models for complex mixtures at such conditions. Availability of high pressure and high temperature thermodynamic properties is then a requisite for the implementation of these equation and models. The literature review shows a lack of thermodynamic data, which serve as a basis for the development of predictive equations and models [7].

2.2 Oxygenated Additives – Diisopropyl ether

Usages of oxygenated additives have been recognized as safe, efficient, and cost-effective way to reduce the levels of mainly soot and particulate emissions and to improve combustion. During the last two decades, various ethers have become important as gasoline additives. Ethers, either alone or with other ethers or alcohols, are widely used to increase the amount of oxygen in fuel and enhance the octane rating, improving combustion and reducing emissions and the contaminant agents of automobile catalysts [22]. Methyl tert-butyl ether, MTBE, has been used as a gasoline additive to increase the octane rating and reduce air pollution. The practice of adding MTBE to gasoline started in the late 1970s and increased dramatically in the 1990s to increase combustion efficiency and reduce air pollution. But, due to its high solubility in water, mobility, and low natural biodegradation potential in the subsurface environment, MTBE has become a significant groundwater contaminant and can create a hazard to public health and the environment [22]. MTBE is classified as a potential human carcinogen by the U.S. Environmental Protection Agency. Alternative oxygenates to MTBE have been hardly studied yet. Di-isopropyl ether was suggested as one of the alternatives, which is environmentally benign.

Diisopropyl ether (DIPE) is recommended pure or mixed with alkanes or alkanols, as a gasoline engine octane rating elevators. The investigation of the thermodynamic properties of binary or ternary mixtures formed by oxygenated additives and the determination of their properties allows to know its thermodynamic behavior to model and correlate properties given prediction in

more complex mixtures and to obtain purely thermodynamic correlations for other conditions of use [23].

These mixtures are of great importance to the petrochemical industry, not only because of their application in the new gasoline but also the refining, purification and deposition processes [23].

2.3 Discussion

During the 21st Conference of the Parties, in 2015, the Paris Agreement was approved, in which one of the objectives is to keep global warming below 2°C with efforts to limit the temperature rise to 1.5°C in relation to pre-industrial levels. The agreement was considered a milestone in the climate discussions, since 195 countries signed it and 155 ratified, almost 80% (United Nations Framework Convention on Climate Change, 2017), indicating a strong global movement in the search for solutions regarding environmental impacts caused by anthropogenic action [24]. In order to achieve the objectives of the Agreement, the participating countries have presented their commitments to reduce greenhouse gas (GHG) emissions, in their Nationally Determined Contribution (NDC).

In this context of increasing concerns regarding global climate change, the reduction of greenhouse gas emissions by the transport sector is considered a priority. The sector is responsible for approximately 23% of the emissions from combustion, as shown in Figure 1, being second only to the generation of electricity and heat (42%) [24].

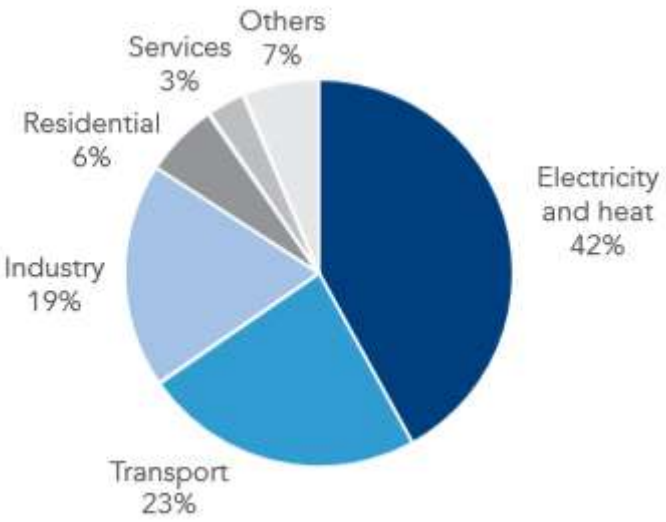

Figure 3: Global CO_2 emissions from fuel combustion by sector in 2014

Source: [25]

The global demand for energy is growing and depends largely on fossil fuels over the last decades. Approximately, 25% of world energy consumption is due to the transportation sector [25]. By 2020, this sector is expected to be responsible for one-third of global CO_2 emissions [26]. This has made human being to search for green technologies to generate clean, safe, sustainable and renewable energy resources for future generation. This consideration explains the growing interest in biofuels. This interest is also due to limited resources of fossil energies, continuous increase in crude oil prices and environmental concerns [27].

For renewable fuels generation, an alternative is the formulation of gasolines that include oxygenated compounds such as alcohols and ethers. However, the lack of experimental data is a problem due to the difficulty of making property measurements such as boiling point and volatility. For this reason, fuel reformulation and the development of alternative fuels are

currently topics of great interest. The gasoline can be reformulated for a reduction of emitted toxic pollutants. However, fossil and biofuels are of complex compositions, and reformulation can dramatically affect the physical, chemical and safety properties of the fuel [28].

To be used in gasoline engines, the thermophysical properties of biofuel must be in accordance with those established in the standards of the American Society of Testing and Materials (ASTM) D4814, for this, the purification of the product must always be carried out at the optimum conditions [29].

In this regard, the knowledge of the thermodynamic properties of biofuels such as densities, isobaric thermal expansion coefficient and the isothermal compressibility coefficient, becomes crucial not only for developing optimal biofuel production and purification processes, but also for enhancing biofuels performance in engines. In addition, modeling the flow of biofuel into petrol reservoirs and production requires reliable predictions of density [6].

Other important property in chemical industry is the viscosity. It is necessary for hydraulic calculations, fluid transport through pipes and pore surfaces, and in many mass and energy transfer. Indeed, viscosity is a fundamental characteristic of substances such as adhesives, lubricants, paintings, etc [22].

Some alcohols and ethers, such as oxygenate additives, are added to gasoline to reduce the emission of gases that produce environmental impact. The advantages of these oxygenates can be classified into several categories. First, they can be obtained from renewable or agricultural raw materials, reducing dependence on fossil sources. Second, they increase the number of

octanes, increasing the anti-knock effect of gasoline [6]. Then, the compression ratio of the engines can be increased without the risk of crashing, leading to higher power delivery. From a combustion standpoint, the production of carbon monoxide and volatile hydrocarbons from the combustion of alcohols is lower than that of gasoline. Among the thermodynamic properties, the heat of vaporization of alcohols is high and leads to a reduction in the combustion temperature peak, which means lower nitrogen oxide emissions [6].

During the last two decades, various ethers became important as gasoline additives. Ethers, either alone or with other ethers or alcohols, are widely used to increase the amount of oxygen in fuel and enhance the octane rating, improving combustion and reducing emissions and the contaminant agents of automobile catalysts [22]. Diisopropyl ether was suggested as one of the alternatives, which is environmentally benign [22].

Thermodynamic properties of liquid propanol with the hydrocarbon 1 hexene and the ether DIPE were obtained from the literature search using online library databases (Web of Science, Scopus, NIST Standard Reference Database).

Special attention is given to alcohol + hydrocarbon mixtures. As stated, 2-propanol was selected as alcohol. It increases the number of octanes, increasing the anti-knock effect of gasoline. Then the compression ratio of the engines can be increased without the risk of crashing, leading to greater power delivery [6]. As representative of hydrocarbons, 1-hexene have been chosen. It is a sustainable alkene attractive for biofuel development [12]. They represent linear, branched and cyclic alkanes, aromatics, as well as olefins, which are

regular components of gasoline [6]. Table 2 presents the list of selected compounds.

Table 2: Selected alcohol, ether and hydrocarbon.

Compound	CAS Number	Chemical Formula
Alcohol		
2-propanol	67-63-0	C_3H_8O
Ether		
DIPE	108-20-3	$C_6H_{14}O$
Hydrocarbon		
1-hexene	592-41-6	C_6H_{12}

Concerning the properties, there is a huge amount of available thermodynamic data in the literature for pure compounds, but with respect to the mixtures, the data is scarce regarding properties like density, refractive index, speed of sound and viscosity. The experimental data available in the literature are shown in Table 2 for binary mixtures alcohol (1) + ether (2), alcohol (1) + hydrocarbon (2) and ether (1) + hydrocarbon (2).

Table 3: Measured Properties and Data Sources Available - Compounds Selection

Measurement	References	Year	T/K
2- propanol (1) + DIPE (2)			
	[30]	2000	298.15
	[32]	1940	298.14
Density and derived properties - liquid	[41]	1994	298.15
	[34]	1997	298.15
Refractive Index - liquid	[30]	2000	298.15
Speed of sound - liquid	[30]	2000	298.15
Viscosity	-	-	-
2- propanol (1) + 1-hexene (2)			
Density and derived properties - liquid	[34]	1997	298.15
Refractive Index - liquid	-	-	-
Speed of sound - liquid	-	-	-
Viscosity	-	-	-
DIPE (1) + 1-hexene (2)			
Density and derived properties - liquid	-	-	-
Refractive Index - liquid	-	-	-
Speed of sound - liquid	-	-	-
Viscosity	-	-	-

Thermodynamic properties of liquid 2-propanol and DIPE and its liquid mixtures with the hydrocarbon 1-hexene have been obtained from the literature search using online library databases (Web of Science, Scopus, NIST Standard Reference Database) and high impact electronic journals. It is noticeable that there is no experimental data available regarding the viscosity. Besides, when the mixture contains the hydrocarbon 1-hexene, just one source from 1997 was found reporting a few experimental data (see appendix). As already mentioned, accurate experimental data on thermodynamic properties should be available to check and develop predictive empirical equations, models and simulation programs. Industrial processes as storage, transport, separation and mixing processes also need reliable data for its design [6].

The characteristic hydrocarbon 1-hexene presents a lack of experimental data on thermodynamic properties and for this reason it was selected to be measured with 2 propanol and DIPE. Besides, there is no experimental data for viscosity to all the compounds selected. In resume, these compounds were selected because there is a lack of experimental data available to predict their behavior like new biofuels.

3 Materials and Methods

3.1 Main Equipment

3.1.1 Densimeter DSA 5000.

The instrument used in this work, the DSA 5000 from Anton Paar USA Inc, combines two miniaturized inline cells to simultaneously measure the density and sound speed of liquid samples at ambient atmospheric pressure. The arrangement of the two measurement cells is illustrated in figure 3, and the instrument specifications, as quoted by the manufacturer [30], are listed in table 4. Both measurement cells are housed in a thermostatic block, the temperature of which is controlled with a combination of thermoelectric Peltier elements and an integrated PT-100 resistance thermometer. Although the manufacturer quotes an operating temperature range of 273 K to 343 K (table 4), the practicable lower temperature limit of the instrument is 278 K due to a significant decrease in the cooling rate of the Peltier elements below this temperature. The practicable upper temperature limit is determined by the boiling point of the liquid under study. To make a measurement, liquid sample is injected into the instrument using a syringe with a Luer tip. As is shown in figure 3, the sample first fills the sound speed cell and then the U-shaped density cell [31].

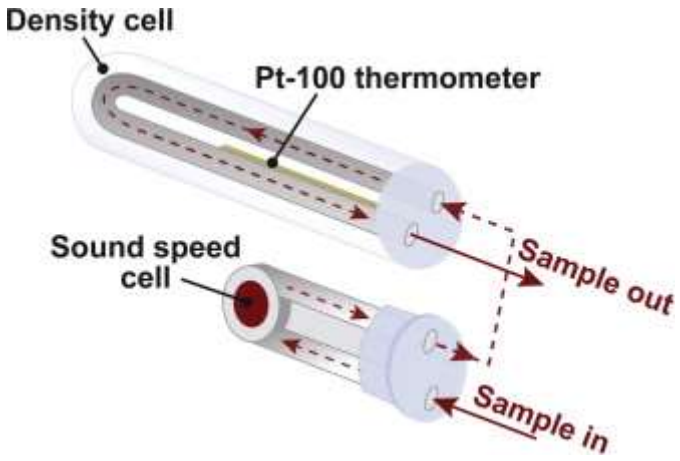

Figure 4: Schematic diagram of the measuring cells in the density and sound speed analyzer

Source: [31]

Table 4: Manufacturer's specifications for the density and sound speed analyzer.

	Density (ρ)	**Speed of Sound (u)**
Pressure range		0–0.3 MPa
Temperature range		273–343 K
Measurement range	0–3000 $kg \cdot m^{-3}$	1000–2000 $m \cdot s^{-1}$
Measurement time		1–4 min
Total sample volume		~3 cm^3
Repeatability	0.001 $kg \cdot m^{-3}$	0.1 $m \cdot s^{-1}$
Uncertainty[a]	0.005 $kg \cdot m^{-3}$	0.5 $m \cdot s^{-1}$

a – Referred to as "accuracy" by manufacturer.

The speed of sound is measured using a propagation time technique [32], [33]. The sound speed cell (see figure 4) consists of a circular cavity 8 mm in diameter and 5 mm deep. The sample is sandwiched between two piezoelectric ultrasound transducers. One transducer emits sound waves through the sample-filled cavity at a frequency of approximately 3 MHz; the second transducer receives those waves. Thus, the speed of sound (u) is obtained by dividing the known distance between transmitter and receiver by the measured propagation

time of the sound wave. The equation used by the manufacturer to determine the speed of sound is

$$W = \frac{l \times (1 + (1.6 \times 10^{-5}) \times \Delta T)}{\frac{P_S}{512} - \tau \times f_3} \quad (1)$$

where l is the path length of the sound speed cell at 293 K (~5 mm), ΔT is the temperature deviation from 293 K, PS is the measured wave propagation time, τ is an apparatus constant representing the time delay associated with the instrument's electronics, and f3 is a temperature correction term for τ [34]. Therefore, the numerator of equation (1) is the cell path length corrected for temperature effects, and the denominator is the propagation time from the transmitter to the receiver after accounting for inherent delays associated with the instrument's electronics. Measurements of air and water performed at 293 K, 313 K, and 333 K are required to adjust the apparatus constants τ and f3 in equation (1). In accordance with the International Vocabulary of Metrology, this is referred to by the manufacturer as an adjustment procedure [34].

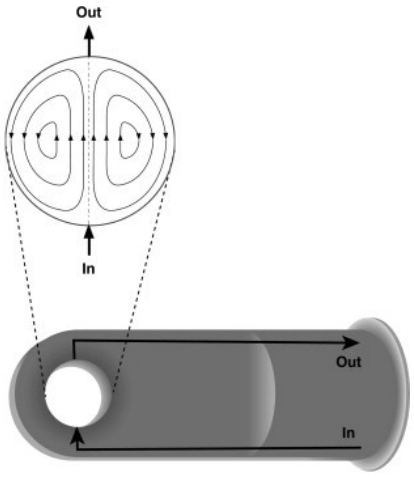

Figure 5: Schematic diagram of the speed of sound cell including streamlines representing sample flow.

Source: [34]

Density is measured using a vibrating tube densimeter. Briefly, the density is derived from the resonant frequency of a sample-filled U-shaped tube as it vibrates perpendicular to its plane in an electromagnetic field. The vibration can be regarded as a simple harmonic oscillation, thus allowing the density (ρ) to be expressed as:

$$\rho = K\tau^2 + L \tag{2}$$

where τ is the period of oscillation and K and L are defined as

$$K = \frac{C}{4\pi^2 V_t} \tag{3}$$

$$L = \frac{m_t}{V_t} \tag{4}$$

In equations (3), (4), V_t is the inner volume of the tube, m_t is its mass, and C is the constant force, which depends on the tube's size and shape and is proportional to the Young's modulus of the tube material. In the density and sound speed analyzer, the tube is made of borosilicate glass, a material whose high stiffness results in greater instrument sensitivity compared to tubes made of stainless steel or Hastelloy. Because the mechanical properties of the tube (e.g., length, radius, and stiffness) are temperature and pressure dependent, K and L must be determined via calibration with one or more liquids whose densities are well known.

The equation used by the manufacturer to determine density is a modification of equation (2). Specifically, density is obtained from

$$\rho = KA \times Q^2 \times f_1 - KB + f_2 \tag{5}$$

where KA and KB are apparatus constants, f_1 and f_2 are correction terms for temperature, viscosity, and nonlinearity, and Q is a quotient of the periods of oscillation of two tubes [31]. The density and sound speed analyzer employ a reference oscillator that is also made of borosilicate glass, is filled with a known reference substance, and is subjected to the same conditions as the measurement oscillator. By dividing the period of oscillation of the measuring cell by the period of oscillation of the reference cell, certain thermal effects are compensated for. The correction for viscosity is required because sample viscosity can have a dampening effect on the period of oscillation, which leads to an-error in the density determination [31].

3.1.2 Viscometer Stabinger SVM 3000

The Stabinger SVM 3000 viscometer is a concentric cylinder rotational viscometer built according to the modified Couette principle, with a fast-rotating outer tube and an inner measuring rotor that has a slower rotation [35]. However, this device additionally has a second cell for measuring fluid density and operates according to the principle of the U-shaped oscillating tube, said cell being a glass tube that is excited to produce resonant mechanical vibrations according to the standard DIN 51757 [36].

This device is the first instrument that meets the ASTM D 7042 precision required by the market and the viscosity measurement according to ASTM 2270 / ISO 2909 in a compact and lightweight tabletop device, which can be seen in figure 5. The SVM 3000 uses a new patented viscosity measurement principle [37] so that with only 2.5 mL of sample, it determines the dynamic and kinematic viscosity, as well as the density at ambient pressure [36].

Figure 6: The SVM 3000.

Source: [36]

The basic principle of viscosity measurement is fulfilled based on the relationship between the strain rate and the required force or vice versa. According to Stabinger's principle, the deformation or shear rate is produced by a cylinder that rotates at a constant speed, within which the sample is located, and a coaxial cylinder immersed in it. The friction between the outer cylinder and the sample rotates the inner cylinder. The device is provided with a braking pair for the rotation of the inner cylinder, through an electrical conductor, an annular element of parasitic currents inside the inner cylinder and a magnet external to the outer cylinder, to provide a magnetic field transverse to the axis of rotation. This magnet acts as a brake so that the three components do not rotate at the same speed, producing a speed difference between the outer and inner cylinder, whose value corresponds to the viscosity of the sample [36].

This induced current pair is measured with a very high resolution, which in combination with the integrated thermostatic-thermoelectric system ensures high accuracy. The resolution of the torque measurement is of the order of 50 picometers. For this reason, only one measuring cell is required, which is very compact. Due to the low density of the inner cylinder (rotor), it remains centered, by centrifugal force, rotating inside the outer cylinder and immersed

in the sample. This inner cylinder floats freely in the sample so it does not require any bearing, and if there are no bearings, consequently, there is no friction. This also makes the instrument not sensitive to vibrations. The small volume of the sample allows extremely rapid temperature changes and short equilibrium time. Shortly after the start of measurement, the rotor reaches a stable speed. This is determined by the balance between the braking effect of the induced current and the shear driving forces of the sample. Finally, dynamic viscosity is calculated using rotor speed [36]. The figure 6 shows the detail of the measuring cell of the SVM 3000.

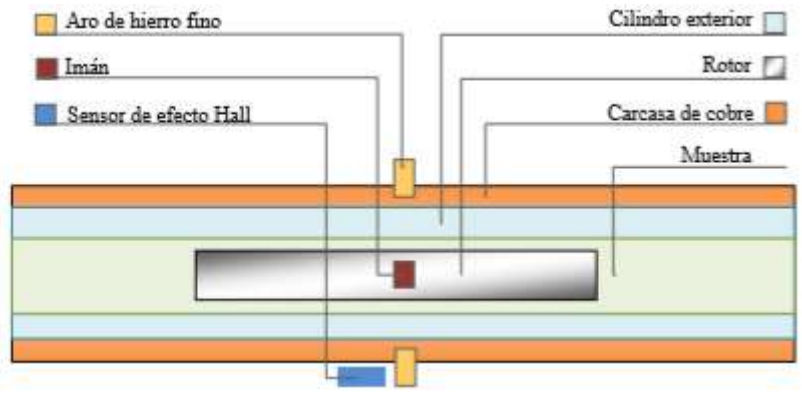

Figure 7: Detail of the measure´s viscosity cell in the SVM 3000.

Source: [36]

3.1.3 Abbemat WR digital refractometer

The Abbemat WR digital refractometer enables automatic measurements of the refractive index at different measuring wavelengths. It can be equipped with up to 8 different wavelengths in the range of 435 nm to 656 nm allowing the equipment for investigations into liquids, polymer bonds and glasses [38]. The figure 7 shows the Abbemat WR refractometer.

Figure 8: Abbemat MW digital refractometer

Source: [38]

3.2 Procedure

The sound velocities and densities of the mixtures and pure compounds were measured with a liquid vibrating tube densimeter DSA-5000-M, with a measuring range: 0-3 g/cm^3, 1000-2000 m/s, 0-70ºC, 0-3 bar, resolution 1.10^{-6} g/cm^3, 0.1 m / s, and accuracy ± 5 · 10^{-6}, ± 0.5 m/s.

The refractive indices were measured with an Abbemat WR model automatic refractometer, with a measuring range 1.30 - 1.72, resolution 1.10^{-6} and accuracy ± 4 · 10^{-5}.

The viscosity was measured using the equipment Viscometer Stabinger SVM 3000, detailed in the section 3.1.2. Calibrations of both the refractometer and the densimeter were performed periodically (once a week), with air and double-distilled water, taking three references of both water and air for each device [32].

During the first weeks of work, there was a training for handling each equipment described. The DSA 5000 densimeter and the Abbemat WR refractometer were calibrated once a week according to the manufacturers' instructions for their proper functioning.

To all the samples, glasses tubes of 22mL was used. The mass of the samples was weighed with a Mettler Toledo brand scale, model MS204S, with a resolution of 0.0001 g, and with an uncertainty of 0.0001 g. Three weights were recorded. First, the tubes were weighed empty, after with the volume of the first component and then, with the volume of the both components.

In sequence, the samples were degassed for a period of 10 minutes by an ultrasonic bath, P-Selecta brand, Ultrasons-H model, frequency of 40 kHz and at a power of 150 W.

Once the samples were degassed, a volume of about 4 cm^3 of the sample was taken with a syringe with a hypodermic needle and introduced into the densimeter described in 2.1. There was special care to avoid air bubbles in the process of filling the densimeter DSA 5000. It could falsify the measurement. The remaining liquid into the syringe was discharged into a proper container. From the sample remaining in the vial, enough quantity was collected with a micropipette to be taken to the refractometer and measured [32].

Other volume of about 10cm^3 was collected with another syringe and introduced into the viscometer described in 3.1.2. This sample was enough to record the viscosity to three temperatures: 293.15 K, 298.15K and 313.15K.

3.2.1 Calibration of the densimeter DSA 5000 and Abbemat WR refractometer

Every week, a sample of about 100mL of distilled water was collected from the chemistry laboratory and then, about 10mL of the sample, was inserted into a clean, dry 14mL glass vial and sealed, in order to avoid evaporation.

The samples were then degassed for a period of 5 minutes in an ultrasound bath, brand P-Selecta, model Ultrasons-H, frequency of 40 kHz and a power of 150 W.

Once degassed and using a syringe, a volume of 4 cm^3 of the sample was introduced into the densimeter and giving special care to avoid air bubbles that could distort the measure. From the remaining sample in the field, enough liquid was collected with a micropipette to be taken by the refractometer and measured. The experimental values were collected three times and compared with the literature.

The atmospheric pressure data was also checked and recorded. Three measurements of the DSA 5000 were collected without any liquid inside. This is the calibration for the "air" of the equipment. Then, the syringe sample was introduced and three more measurements for the equipment's "water" calibration were recorded in a measure's table. Just after the week calibration, the measures began. To start each new measure, the DSA 5000 was completely dried and cleaned with acetone.

3.3 Literature NIST

To begin the research, the data from NIST (National Institute of Standards and Technology) was consulted. The report was extracted from Thermodynamics Research Center, Applied Chemicals and Materials Division. The completed report generated is in the appendix section of this document. Properties from three components measured was searched: 2-propanol, di-isopropyl ether and 1-hexene. The components studied can be checked in the figure 8. To generate the report, 4 properties was consulted: density and derived properties for the liquid, refractive index for the liquid, speed of sound for the liquid and viscosity for the liquid. The generation of this document was important to check all the scientific literature related with the compounds studied. These three compounds were selected because there was not experimental data to describe their behavior as new biofuels.

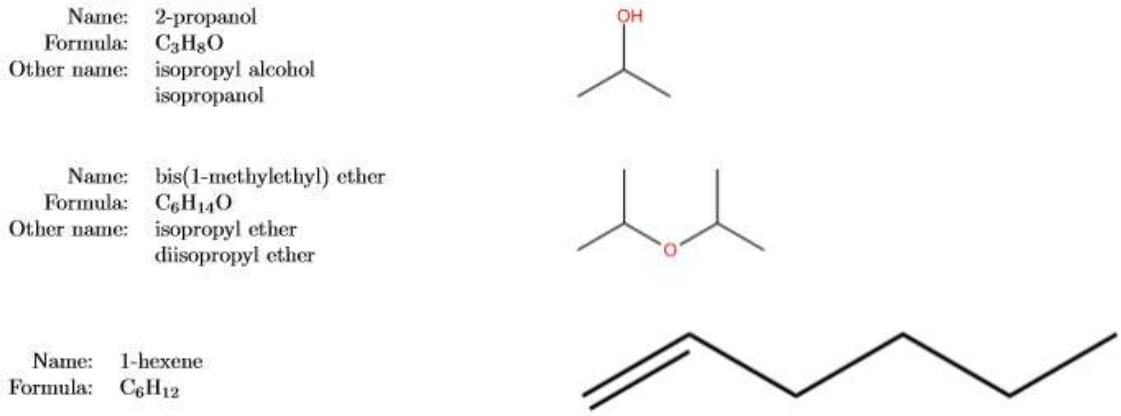

Figure 9: Detail of the compounds studied.

Source: NIST Report. Generated on November 12th.

The first step to begin the measures, was compare the experimental measures to the pure components with the literature. The table 5 shows the comparison.

Table 5: Comparison of measured experimental values for pure compounds at 298.15 K with data collected from literature.

	ρ / (g · cm^{-3})		n_D		u / (m · s^{-1})	
component	experimental	literature	experimental	literature	experimental	literature
2-propanol	0.78144	0.78126[a] 0.78095[b] 0.78483[d]	1.374984	1.3752[a] 1.37501[b] 1,3591[d]	1140.63	1139[b] 1141[c]
deviation		0.12%		0.38%		0.055%
DIPE	0.71847	0.71854[a] 0.71845[b] 0.71789[d]	1.365076	1.3655[a] 1.36512[b] 1.36513[d]	998.09	-
deviation		0.025%		0.013%		
1-hexene	0.66847	-	1.384988	-	1065.74	-

a [39]. b [23] c [31]. d [41]

When comparing the density, refractive index and sound velocity results obtained for 2-propanol and DIPE with those found in the literature, the relative maximum deviation between the experimental data and those reported by RIDDICK [39] - 1986, ARCE [18] - 2000, AMINABHAVI [40] – 1993, BLANCO [41] – 1994, values of: 2-propanol 0.12% (density), 0.38% (refractive index) and 0.055% (sound velocity), respectively and DIPE 0.025% (density) and 0.013% (refractive index) were obtained.

4 Results and Discussion - Density

4.1 Density, Sound Velocity and Refractive Index at 298.15K

According the table 5, the experimental values of the pure components, compared with the literature, are very close, which means that the measuring equipment and the procedure adopted for obtaining the experimental data are adequate. The experimental results of densities, sound velocities and refractive indices for all binary samples at the temperature of 298.15 K and atmospheric pressure are shown in tables 6, 7 and 8, as well as molar excess volumes, variations in the index of refraction of the mixture, and variations in isentropic compressibility.

Molar volumes of excess and derived properties (variations in refractive index and variations in isentropic compressibility) were evaluated for each point of composition by using equations 6 to 9 [23].

$$V_m^E = \sum_{i=1}^{N} x_i M_i(\rho^{-1} - \rho_i^{-1}) \quad (6)$$

$$\Delta n_D = n_D - \sum_{i=1}^{N} x_i n^0{}_{Di} \quad (7)$$

$$\Delta k_S = k_S - \sum_{i=1}^{N} x_i k_{Si} \quad (8)$$

$$k_S = \rho^{-1} u^{-2} \quad (9)$$

where ρ is the density, n_D is the index of refraction, k_S is the isentropic compressibility, calculated using the Laplace equation (see eq. 9), and $\rho^0{}_i$ and $n_D{}^0{}_i$ are the density and refractive index of the pure components.

The algebraic representation of thermodynamic properties and the classification of solutions is given by Redlich–Kister polynomial equation. This equation can be used to fit activities in two component mixtures over the entire

concentration range and to calculate the activities (molecular level) of both components. This method provides an immediate distinction between various types of solutions [21]. The values of excess properties, and derived properties were correlated by the Redlich-Kister polynomial equation (10) for each binary mixture [23].

$$\Delta Q_{ij} = x_i x_j \sum_{p=0}^{M} Ap\,(x_i - x_j)^p \qquad (10)$$

Tables 6, 7, and 8 show the experimental thermodynamic properties obtained with the binary mixtures at temperature of 298.15K.

Table 6: Thermodynamic properties of binary system 2 prop + DIPE at 298.15 K.

x1	ρ / kg m $^{-3}$	V^E_m / cm^3 mol $^{-1}$	n_D	Δn_D	u / m s $^{-1}$	k_S / TPa $^{-1}$	Δk_S / TPa^{-1}
2-propanol (1) + DIPE (2)							
0.0498	720.82	-0.118	1.36561	0.00004	1004	1377	1
0.0988	723.17	-0.221	1.36615	0.00009	1008	1360	4
0.1483	725.55	-0.302	1.36667	0.00012	1012	1345	9
0.2003	728.05	-0.366	1.36718	0.00012	1017	1329	15
0.2499	730.47	-0.410	1.36765	0.00010	1021	1313	19
0.2993	732.99	-0.452	1.36814	0.00010	1026	1297	23
0.3478	735.53	-0.480	1.36864	0.00012	1031	1280	27
0.3991	738.29	-0.499	1.36912	0.00008	1036	1261	29
0.4474	741.03	-0.510	1.36960	0.00009	1042	1243	31
0.4982	744.04	-0.524	1.37014	0.00013	1049	1223	31
0.5487	747.21	-0.534	1.37067	0.00016	1056	1201	31
0.5992	750.50	-0.531	1.37121	0.00019	1063	1179	29
0.6468	753.71	-0.517	1.37167	0.00018	1071	1157	27
0.6989	757.41	-0.494	1.37225	0.00025	1080	1133	24
0.7483	761.06	-0.460	1.37274	0.00025	1089	1109	21
0.7980	764.93	-0.419	1.37323	0.00025	1099	1083	16
0.8489	769.08	-0.364	1.37376	0.00027	1109	1057	11
0.8990	773.36	-0.296	1.37423	0.00025	1120	1031	5
0.9493	777.78	-0.205	1.37465	0.00017	1132	1004	-1

Table 7: Thermodynamic properties of binary system 2 prop+1hexene at 298.15 K.

x1	ρ / kg m $^{-3}$	V^E_m / cm^3 mol $^{-1}$	n_D	Δn_D	u / m s $^{-1}$	k_S / TPa $^{-1}$	Δk_S / TPa^{-1}
2-propanol (1) + 1-hexene (2)							
0.0499	670.92	0.1946	1.38417	-0.00032	1060	1326	25
0.0998	674.14	0.2684	1.38351	-0.00047	1058	1326	42
0.1485	677.44	0.3359	1.38293	-0.00057	1057	1323	55
0.1984	680.98	0.3992	1.38238	-0.00061	1056	1317	66
0.2467	684.82	0.4150	1.38184	-0.00066	1056	1310	75
0.2972	688.95	0.4400	1.38134	-0.00066	1057	1300	83
0.3466	693.28	0.4489	1.38089	-0.00061	1058	1289	88
0.3980	698.10	0.4430	1.38045	-0.00054	1060	1275	91
0.4489	703.15	0.4261	1.38002	-0.00045	1063	1260	92
0.4991	708.45	0.4025	1.37956	-0.00041	1066	1242	92
0.5480	713.89	0.3736	1.37918	-0.00030	1070	1224	90
0.5974	719.75	0.3337	1.37879	-0.00019	1074	1204	86
0.6472	725.93	0.2967	1.37842	-0.00006	1080	1182	81
0.6968	732.48	0.2543	1.37798	0.00000	1086	1158	74
0.7487	739.72	0.2076	1.37755	0.00009	1093	1132	65
0.7989	747.20	0.1572	1.37710	0.00015	1101	1105	55
0.8489	754.99	0.1163	1.37662	0.00017	1110	1077	43
0.8983	763.19	0.0739	1.37608	0.00013	1118	1048	30
0.9490	772.12	0.0286	1.37553	0.00009	1129	1016	15

Table 8: Thermodynamic properties of binary system DIPE+1hexene at 298.15 K.

x1	ρ / kg m $^{-3}$	V^E_m / cm^3 mol $^{-1}$	n_D	Δn_D	u / m s $^{-1}$	k_S / TPa $^{-1}$	Δk_S / TPa^{-1}
DIPE (1) + 1-hexene (2)							
0.0511	671.28	0.0589	1.38379	-0.00018	1062	1322	1
0.0992	673.88	0.1082	1.38269	-0.00032	1058	1327	2
0.1505	676.64	0.1543	1.38154	-0.00045	1054	1331	3
0.2001	679.24	0.1925	1.38043	-0.00057	1049	1337	4
0.2501	681.88	0.2247	1.37935	-0.00066	1046	1341	5
0.2988	684.38	0.2502	1.37832	-0.00072	1042	1346	5
0.3503	687.05	0.2707	1.37725	-0.00076	1038	1350	5
0.4004	689.62	0.2845	1.37624	-0.00077	1035	1354	6
0.4508	692.16	0.2923	1.37521	-0.00080	1031	1359	6
0.4992	694.57	0.2942	1.37425	-0.00080	1028	1363	6
0.5491	697.06	0.2903	1.37327	-0.00078	1025	1366	5
0.6007	699.59	0.2802	1.37229	-0.00074	1021	1370	5
0.6501	702.01	0.2648	1.37135	-0.00069	1018	1374	5
0.7012	704.46	0.2430	1.37037	-0.00066	1015	1378	5
0.7499	706.79	0.2168	1.36949	-0.00057	1012	1381	4
0.8003	709.24	0.1841	1.36856	-0.00049	1009	1385	3
0.8497	711.52	0.1466	1.36772	-0.00036	1006	1388	2
0.8997	713.85	0.1032	1.36683	-0.00025	1003	1391	2
0.9493	716.12	0.0548	1.36598	-0.00011	1001	1394	1

In the Redlich-Kister equation (see eq. 10), ΔQij is the property of excess, x is the molar fraction, A is the adjustment parameter, and M is the degree of expansion of the polynomial. The parameters to be calculated with this

equation are shown in table 9. The curves adjusted for the excess and derivative properties are shown in figures 10 to 12. The molar volumes of excess are negative to the binary 2 propanol + DIPE, obtaining lower values with shorter chain lengths of alkanol.

This reflects the type of interactions that take place in the mix. The longer the chain length of alcohol, the lower is the packaging effect. The ethers participate in cross-association effects with the hydrogens present in the alcohols, so that the values of the excess volumes will be negative, unlike in the ether + alkane mixtures, in which the excess volumes will be positive, which indicates a greater packing effect in the ether + alkanol mixtures or a less effective packaging in the ether + alkane mixtures. It explains the positive excess volume in the figure 10 when the 1-hexene is one component of the binary system.

The variations in the refractive index in the case of the 2-propanol + 1-hexene is sigmoidal, with a negative initial region followed by a smaller positive region when the molar faction is 0.7. The curve in the case of the 2-propanol + DIPE mixture is totally positive

The deviation in isentropic compressibility is positive for all the binary mixtures.

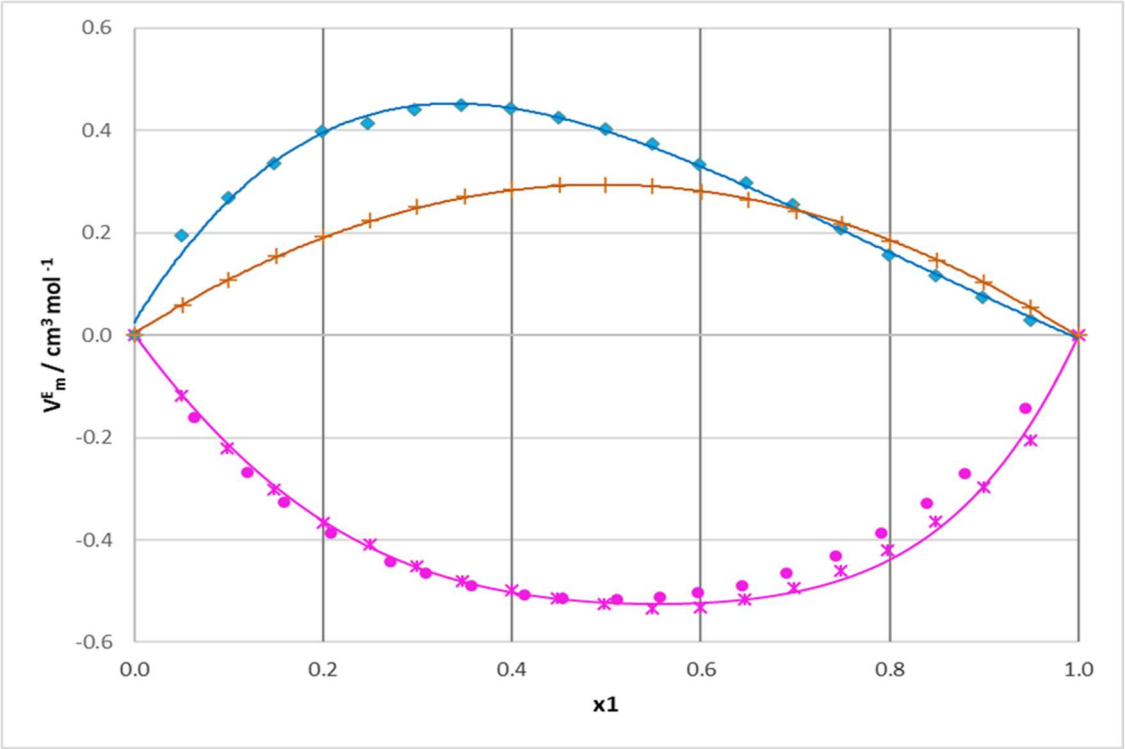

Figure 10: Experimental values of the molar volumes of excess at 298.15 K of the binary systems: 2-propanol (1) + DIPE (2) ( ) this work, 2-propanol (1) + DIPE (2) ( ), [Arce, A., et al.]; 2-propanol (1) + 1-Hexene (2) ( ) this work; DIPE (1) + 1-Hexene (2) ( ) this work. The solid lines (-) show the values calculated from the Redlich-Kister equation.

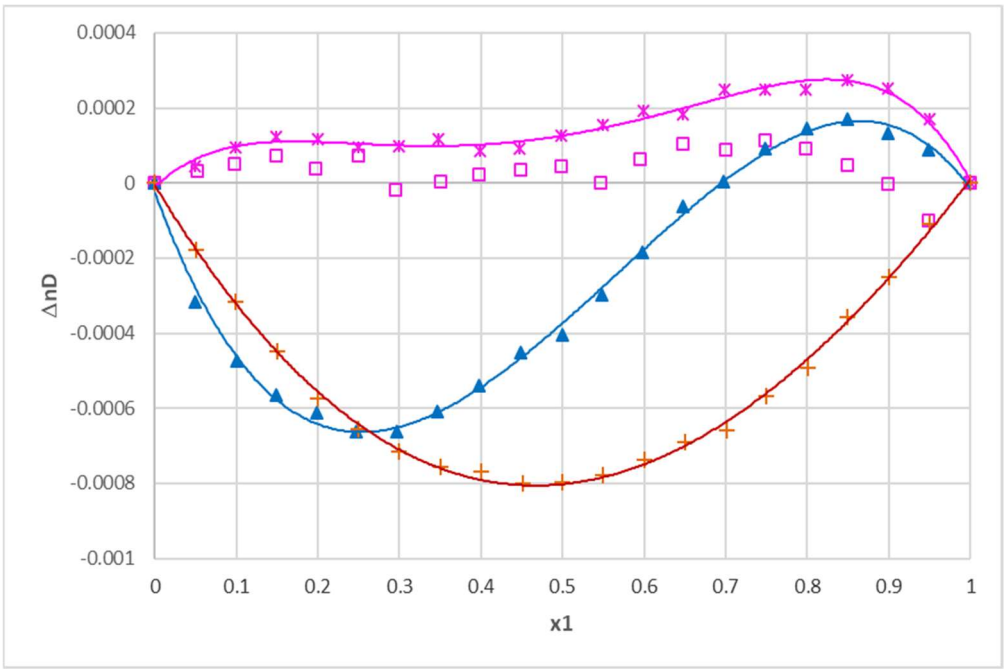

Figure 11: Experimental values of the variations in the refractive index at 298.15 K of the binary systems: 2-propanol (1) + DIPE ( ) this work; 2-propanol (1) + DIPE (2) ( ) [Muñoz-Rujas, N. et al.], 2012; propanol (1) + 1-Hexene (2) ( ), this work, DIPE (1) + 1-hexene (2) ( ), this work. The solid lines (-) show the values calculated from the Redlich-Kister equation.

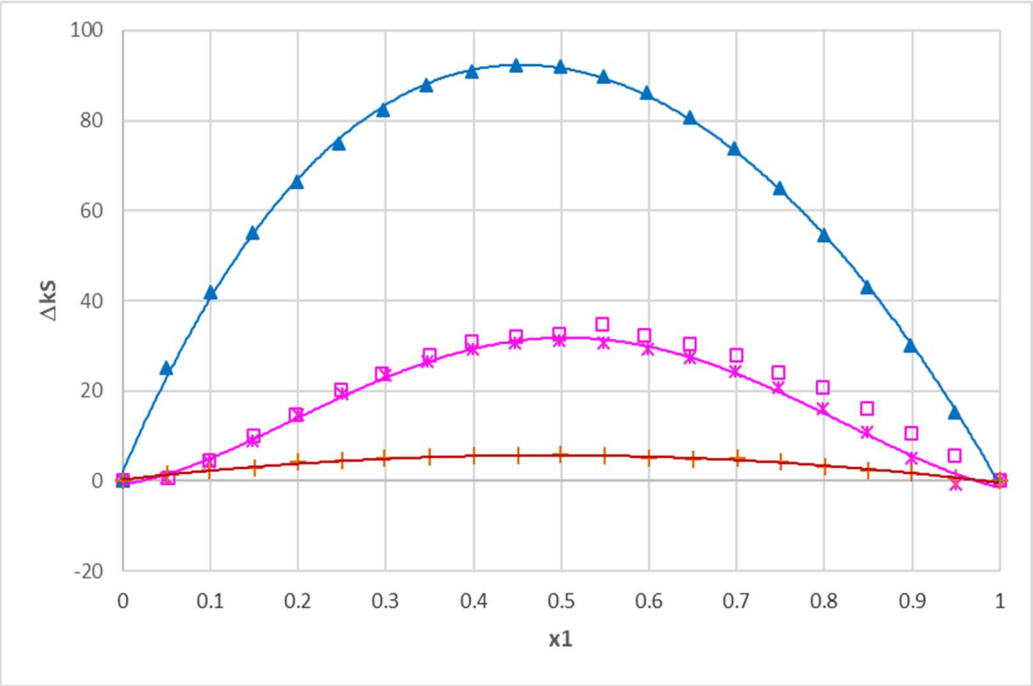

Figure 12: Experimental values of deviations in isentropic compressibility ΔkS at 298.15 K of binary systems: 2 propanol (1) + DIPE (2) (✱) this work; 2-propanol (1) + DIPE (2) [Muñoz-Rujas, N. et al]; 2- propanol (1) + 1-hexene (2) (▲) this work; DIPE + 1-Hexene (+) this work. The solid lines (-) show the values ΔkS calculated from the Redlich-Kister equation.

Table 9: Adjustment coefficients to the Redlich-Kister equation of excess properties and results.

	A_0	A_1	A_2	A_3	σ
2-propanol (1) + DIPE (2)					
V^E_m / cm^3 mol^{-1}	-5.4597	0.2283	-0.0098	7.86×10^{-5}	1.14×10^{-5}
Δn_D	1.3651	0.0095	0.0018	-0.0014	0.0005
Δk_S / TPa^{-1}	1392.31	-282.9964	-117.1778	-13.6543	29.0978
2- propanol + 1-Hexene (2)					
V^E_m / cm^3 mol^{-1}	1.5901	-1.0123	0.4417	-0.6681	0.0003
Δn_D	1.3849	-0.01530	0,0131	-0,0078	2.14×10^{-5}
Δk_S / TPa^{-1}	1392.47	-287.07	-108.03	-19.05	1.0551
DIPE (1) + 1-Hexene (2)					
V^E_m / cm^3 mol^{-1}	1.1766	-0.0425	0.0015	-5.14×10^{-5}	1.61×10^{-7}
Δn_D	1.3849	-0.02345	0.0043	-0.0008	1.24×10^{-5}
Δk_S / TPa^{-1}	1316.36	106.6258	-30.5270	5.0546	0.1844

$$\sigma = \left(\sum_{i}^{N} (Z_{\exp} - Z_{calc})^2 / N\right)^{1/2}$$

5 Results and Discussion - Viscosity

5.1 Viscosity at temperatures 293.15K, 298K and 313.15K.

Transport properties are important in the design of efficient engineering processes. These characterize the response of the fluid to change the temperature, flow rate or composition, and their knowledge should normally be acquired by experimental measurements or by theoretical estimation. The viscosity of a material reflects the underlying microscopic interactions between the material's molecules and is especially important in the food, oil and plastics industries, vital in fluid transport processes, in the control food quality and product composition analysis [43].

The viscosity is of great importance in liquid fuels for the purposes of its storage and transport, since it is needed for the calculation of pressure losses in pipelines and for the specification of pumps and exchangers [42]. Viscosity is one of the most important properties of diesel car fuels because it influences the design of injectors and the spraying process in compression ignition engines (diesel engines) [43].

The process to develop new biofuels begins into laboratory. The first step is to measure new compounds with interest as biofuels and study their behavior and properties. The new data collected can be used by other researches to develop new equations and models to predict their behavior as new biofuels. One of the objectives of this thesis is the determination of experimental data to develop and study new compounds to biofuels and for this, it is necessary to evaluate the viscosity of the fluids studied.

In this chapter, the viscosities of three pure compounds and three mixtures were measured with a commercial Stabinger SVM 3000 viscometer at ambient pressure up to a temperature of 313.15 K. The experimental values show a decreasing trend in viscosity with temperature. There is no experimental data available relating to these compounds in the literature.

The data obtained are presented in tables 10, 11 and 12. When comparing the experimental values of the viscosities, it is observed that the addition of alcohol considerably increases this property. When the binary system contains the ether and 1- hexene, the viscosity decreases significantly.

Figures 13, 14 and 15 present the values for dynamic viscosity for all binary systems. Comparing figures 13 and 14 with figure 15, it can be observed that the dependence of the dynamic viscosity with the composition of the alcohol is not linear. At the temperatures of 293.15K and 298.15K, the viscosity increases as the alcohol composition is increased in the binary mixture (see figures 13 and 14), while when the temperature is increased to 313.15K, the viscosity does not increase significantly (figure 15).

Dynamic and cinematic viscosities were measured at temperatures of 293.15K, 298.15K and 131.15K. The data obtained are present in tables 10, 11 and 12. There is no experimental data already published for these mixtures.

Table 10: Viscosity of binary system 2 prop + DIPE at 293.15 K, 298.15K and 313.15K.

	T = 293.15K			T=298.15K			T=313.15K		
x1	μ / mPa.s	ρ / g cm $^{-3}$	νy / mm^2.s^{-1}	μ / mPa.s	ρ / g cm $^{-3}$	νy/ mm^2.s^{-1}	μ / mPa.s	ρ / g cm $^{-3}$	νy / mm^2.s^{-1}
2-propanol (1) + DIPE (2)									
0.0498	0.33832	0.7262	0.46590	0.32555	0.7210	0.45156	0.26867	0.7050	0.38109
0.0988	0.35085	0.7284	0.4817	0.33672	0.7232	0.46562	0.28934	0.7073	0.40908
0.1483	0.36336	0.7309	0.49711	0.33806	0.7258	0.4658	0.24683	0.7099	0.34769
0.2003	0.38395	0.7333	0.52363	0.36646	0.7282	0.50327	0.27815	0.7124	0.39043
0.2499	0.40299	0.7357	0.54776	0.38883	0.7306	0.53221	0.31174	0.7149	0.43605
0.2993	0.42028	0.7375	0.56988	0.3992	0.7324	0.54503	0.31529	0.7168	0.43983
0.3478	0.45257	0.7407	0.61101	0.42777	0.7356	0.58149	0.34725	0.7202	0.48215
0.3991	0.4789	0.743	0.64458	0.44888	0.7379	0.60831	0.33324	0.7226	0.46117
0.4474	0.51723	0.7460	0.69338	0.47401	0.741	0.63969	0.36589	0.7257	0.50418
0.4982	0.56196	0.7489	0.75039	0.52346	0.744	0.70359	0.39148	0.7288	0.53716
0.5487	0.6162	0.7520	0.81942	0.57065	0.7471	0.7638	0.42873	0.7321	0.58559
0.5992	0.67899	0.7552	0.8991	0.62746	0.7504	0.83617	0.45885	0.7356	0.62379
0.6468	0.75746	0.7582	0.99899	0.68983	0.7537	0.91528	0.49833	0.739	0.67435
0.6989	0.85951	0.762	1.1279	0.77793	0.7574	1.0272	0.55423	0.7429	0.74608
0.7483	0.93951	0.7657	1.227	0.8838	0.761	1.1613	0.62018	0.7467	0.83056
0.7980	1.1346	0.7694	1.4747	1.0138	0.7649	1.3253	0.73938	0.7508	0.98482
0.8489	1.3231	0.7735	1.7105	1.1523	0.7691	1.4982	0.82811	0.7552	1.0966
0.8990	1.5994	0.7778	2.0564	1.3853	0.7734	1.7913	0.97265	0.7597	1.2803
0.9493	1.9464	0.7821	2.4887	1.6868	0.7778	2.1687	1.1331	0.7644	1.4825

Table 11: Viscosity of binary system 2 prop+1-hexene at 293.15 K, 298.15K and 313.15K.

	T = 293.15K			T=298.15K			T=313.15K		
x1	μ / mPa.s	ρ / g cm $^{-3}$	νy / mm^2.s^{-1}	μ / mPa.s	ρ / g cm $^{-3}$	νy / mm^2.s^{-1}	μ / mPa.s	ρ / g cm $^{-3}$	νy / mm^2.s^{-1}
2-propanol (1) + 1-hexene (2)									
0.0499	0.27933	0.6753	0.41408	0.27327	0.6706	0.40892	0.20771	0.6561	0.37301
0.0998	0.28977	0.6787	0.42696	0.28050	0.67390	0.41624	0.18178	0.6592	0.27575
0.1485	0.29897	0.6819	0.43843	0.28918	0.6771	0.42706	0.21885	0.6624	0.33037
0.1984	0.31229	0.6855	0.45554	0.30081	0.6807	0.4419	0.22507	0.6661	0.3379
0.2467	0.32803	0.6894	0.47583	0.31654	0.6846	0.46238	0.2239	0.6694	0.33426
0.2972	0.33766	0.6937	0.48675	0.3198	0.6888	0.46426	0.22379	0.674	0.33202
0.3466	0.36759	0.6979	0.52667	0.34079	0.6931	0.49169	0.26454	0.6783	0.38999
0.3980	0.40314	0.7027	0.57372	0.37107	0.6979	0.53171	0.25877	0.6831	0.3788
0.4489	0.44176	0.7077	0.62418	0.41218	0.703	0.58634	0.44152	0.6883	0.44152
0.4991	0.49511	0.7131	0.69432	0.44235	0.7084	0.62445	0.3071	0.6936	0.44274
0.5480	0.5426	0.7185	0.75522	0.49304	0.7137	0.69081	0.35132	0.6991	0.50254
0.5974	0.60978	0.7245	0.84163	0.5607	0.7196	0.77922	0.38244	0.7051	0.54242
0.6472	0.69065	0.7306	0.94532	0.61798	0.7258	0.85145	0.44017	0.7111	0.619
0.6968	0.78147	0.7369	1.0604	0.70005	0.7323	0.95594	0.49938	0.7181	0.69547
0.7487	0.91669	0.7441	1.232	0.82065	0.7396	1.1095	0.56613	0.7254	0.78046
0.7989	1.0729	0.7515	1.4277	0.95262	0.7471	1.2752	0.61662	0.733	0.84118
0.8489	1.2717	0.7593	1.6748	1.1207	0.7549	1.4846	0.75201	0.741	1.0148
0.8983	1.53	0.7676	1.9932	1.3468	0.7631	1.7648	0.86408	0.7495	1.1529
0.9490	1.8902	0.7763	2.435	1.6376	0.772	2.1213	1.0954	0.7587	1.4439

Table 12: Viscosity of binary system DIPE+1-hexene at 293.15 K, 298.15K and 313.15K.

	T = 293.15K			T=298.15K			T=313.15K		
x1	μ / mPa.s	ρ / g cm $^{-3}$	□νy / mm^2.s^{-1}	μ / mPa.s	ρ / g cm $^{-3}$	νy / mm^2.s^{-1}	μ / mPa.s	ρ / g cm $^{-3}$	□νy / mm^2.s^{-1}
DIPE (1) + 1-hexene (2)									
0.0511	0.27699	0.6757	0.40994	0.26912	0.671	0.40109	0.18722	0.6566	0.28514
0.0992	0.2787	0.6783	0.41085	0.26908	0.6736	0.39947	0.19986	0.6591	0.30321
0.1505	0.28167	0.6811	0.41352	0.27398	0.6764	0.40505	0.21453	0.6619	0.32411
0.2001	0.28418	0.6838	0.41561	0.27599	0.679	0.40647	0.21321	0.6643	0.32093
0.2501	0.28669	0.6865	0.41764	0.27866	0.6816	0.40881	0.22074	0.6669	0.33098
0.2988	0.28859	0.689	0.41887	0.2803	0.6841	0.40973	0.20139	0.6693	0.30088
0.3503	0.29135	0.6917	0.42122	0.2827	0.6868	0.41162	0.20133	0.6719	0.29964
0.4004	0.29373	0.6942	0.42304	0.28265	0.6893	0.41002	0.2033	0.6744	0.30147
0.4508	0.29646	0.6968	0.42544	0.28725	0.6919	0.41516	0.21505	0.6769	0.3177
0.4992	0.29858	0.6993	0.42699	0.28946	0.6943	0.4169	0.19715	0.6792	0.29028
0.5491	0.30138	0.7018	0.42945	0.29172	0.6968	0.41866	0.19953	0.6816	0.29274
0.6007	0.30407	0.7043	0.43171	0.29439	0.6993	0.42097	0.20036	0.684	0.29291
0.6501	0.30686	0.7068	0.43418	0.29697	0.7017	0.42319	0.21471	0.6864	0.31282
0.7012	0.30967	0.7093	0.43661	0.29942	0.7042	0.42519	0.2389	0.6888	0.34686
0.7499	0.31207	0.7116	0.43855	0.29947	0.7065	0.42386	0.22597	0.691	0.32701
0.8003	0.31428	0.714	0.44019	0.30377	0.7089	0.42853	0.23029	0.6933	0.33215
0.8497	0.31721	0.7164	0.4428	0.30528	0.7112	0.42926	0.22896	0.6956	0.32916
0.8997	0.32066	0.7188	0.44613	0.30926	0.7136	0.43338	0.22417	0.6979	0.32121
0.9493	0.32303	0.721	0.44801	0.31182	0.7159	0.43559	0.22348	0.7001	0.31922

Figures 13, 14 and 15 show the variation of the dynamic viscosity in function of x1 for the three different temperatures. As the molar volume of the alcohol (2-propanol) increases in the sample, the liquid blend become more viscous (see figures 13 and 14). Unlike adding alcohol to the mixture, by increasing the temperature, the mixture becomes, in all cases, less viscous.

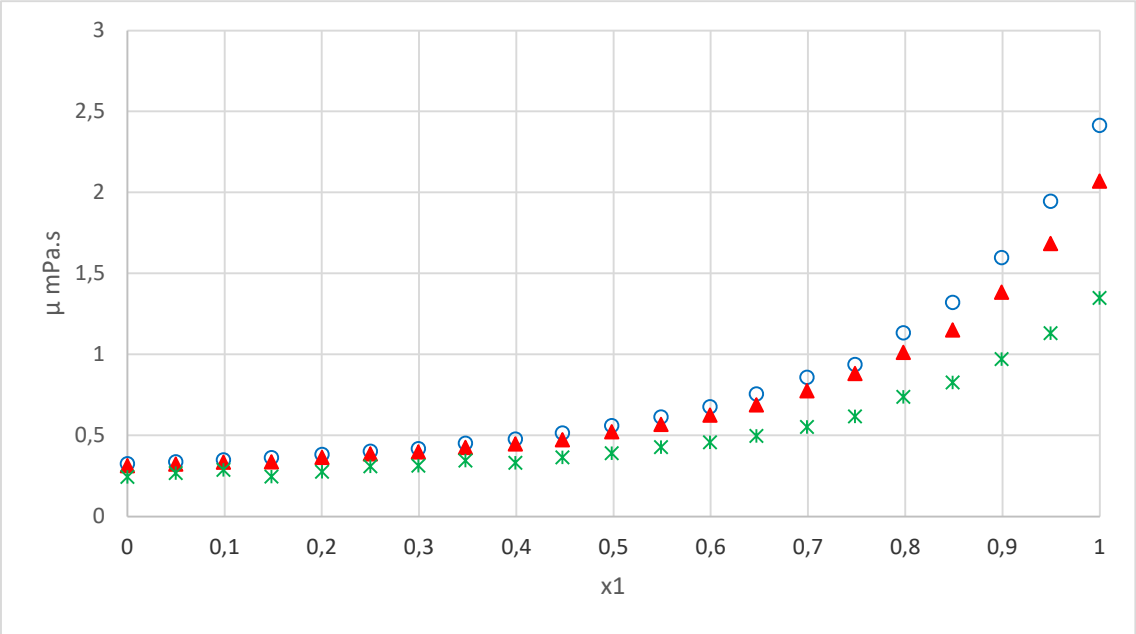

Figure 13: Dynamic viscosity at 293.15 K, 298.15K and 313.15K of the binary systems: 2-propanol + DIPE. 2-propanol (1) + DIPE (2) (○) 293,15K; 2-propanol (1) + DIPE (2) (▲) 298.15K, 2- propanol (1) + DIPE (2) (✳) 313.15K.

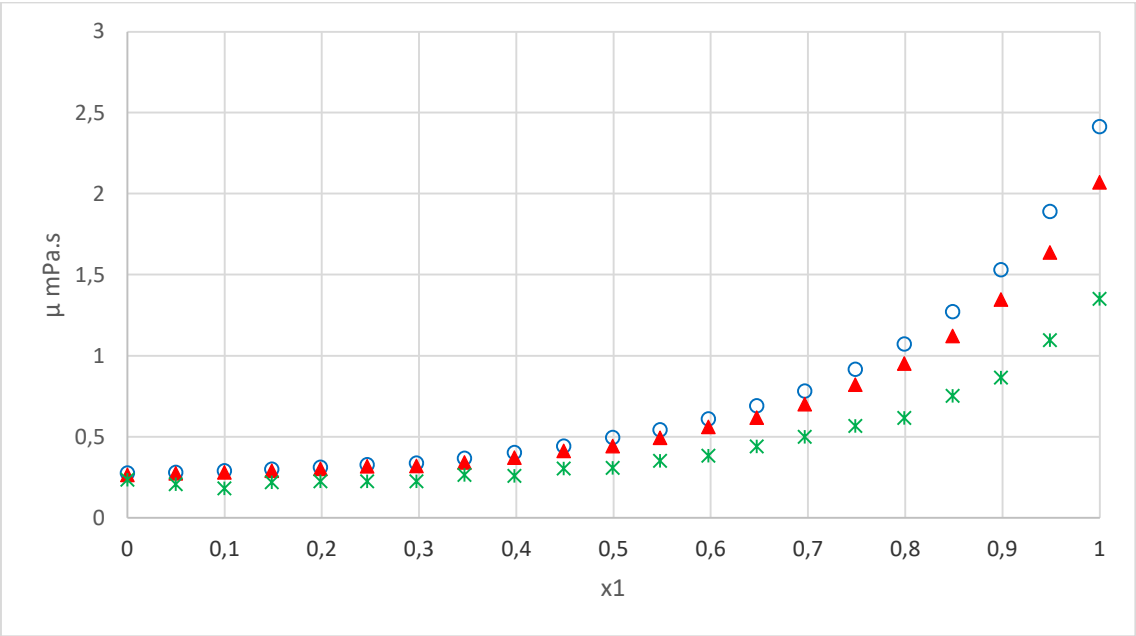

Figure 14: Dynamic viscosity at 293.15 K, 298.15K and 313.15K of the binary systems: 2-propanol + 1-Hexene. 2-propanol (1) + 1-hexene (2) (○) 293,15K; 2-propanol (1) + 1-hexene (2) (▲) 298.15K, 2- propanol (1) + 1-hexene (2) (✳) 313.15K.

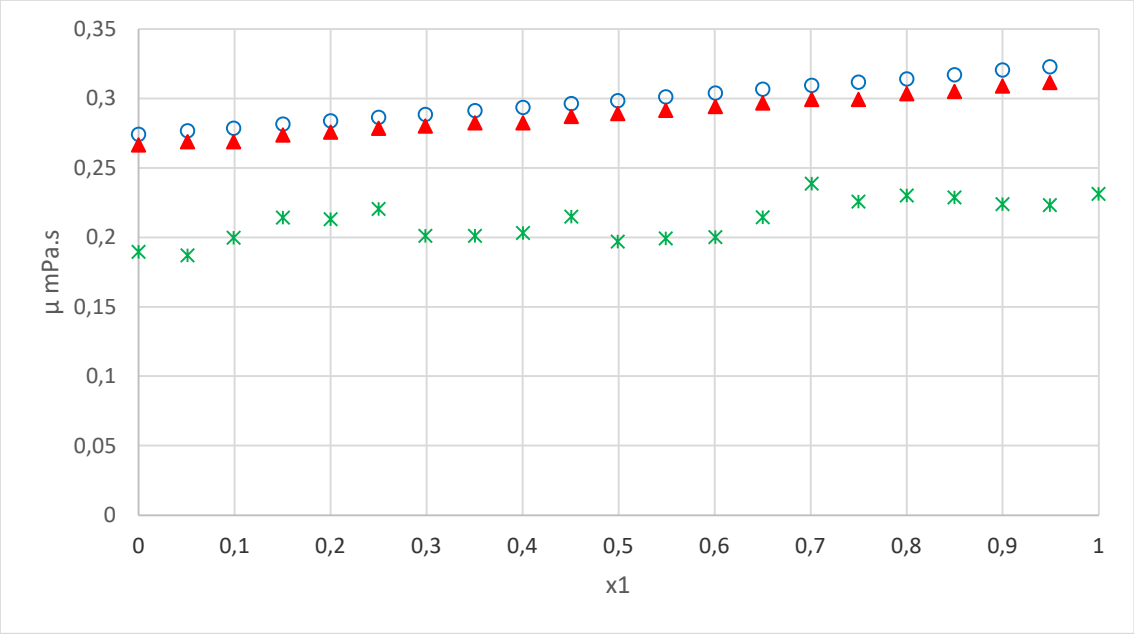

Figure 15: Dynamic viscosity at 293.15 K, 298.15K and 313.15K of the binary systems: DIPE + 1-Hexene. DIPE (1) + 1-hexene (2) (○) 293.15K; DIPE (1) + 1-hexene (2) (▲) 298.15K; DIPE (1) + 1-hexene (2) (✳) 313.15K.

When there is no alcohol in the mixture, but only DIPE and 1-hexene (figure 15), the liquid mixture also remains more viscous as the concentration of the ether increases, however, this behavior only occurs at temperatures of 293.15K and 298.15K. When the temperature reaches 313.15K, the viscosity behavior becomes unstable when the ether concentration is increased. This occurs because the viscosity is very low and its value is below of the measurement scale and calibration of the equipment used – viscosimeter SVM 3000.

Unfortunately, there is no experimental data to compare the results obtained. It is important that new experimental data are collected for these

compounds at high temperatures, for a better evaluation and analysis of the viscosity behavior for these studied compounds.

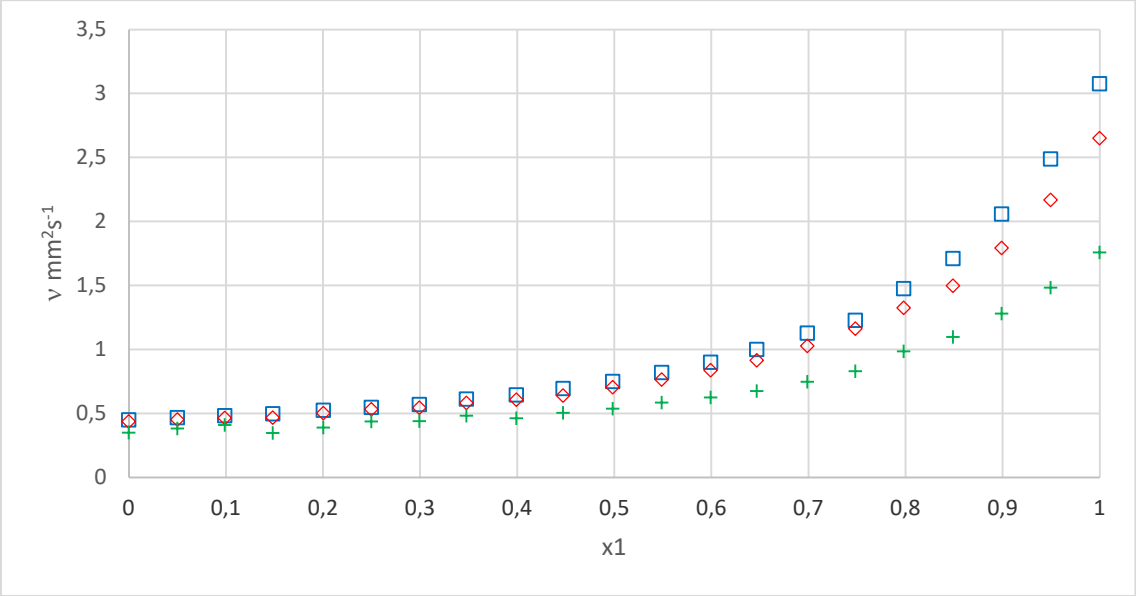

Figure 16: Kinematic viscosity at 293.15 K, 298.15K and 313.15K of the binary systems: 2-propanol + DIPE. 2-propanol (1) + DIPE (2) (□) 293.15K; 2-propanol (1) + DIPE (2) (◇) 298.15K, 2- propanol (1) + DIPE (2) (+) 313.15K.

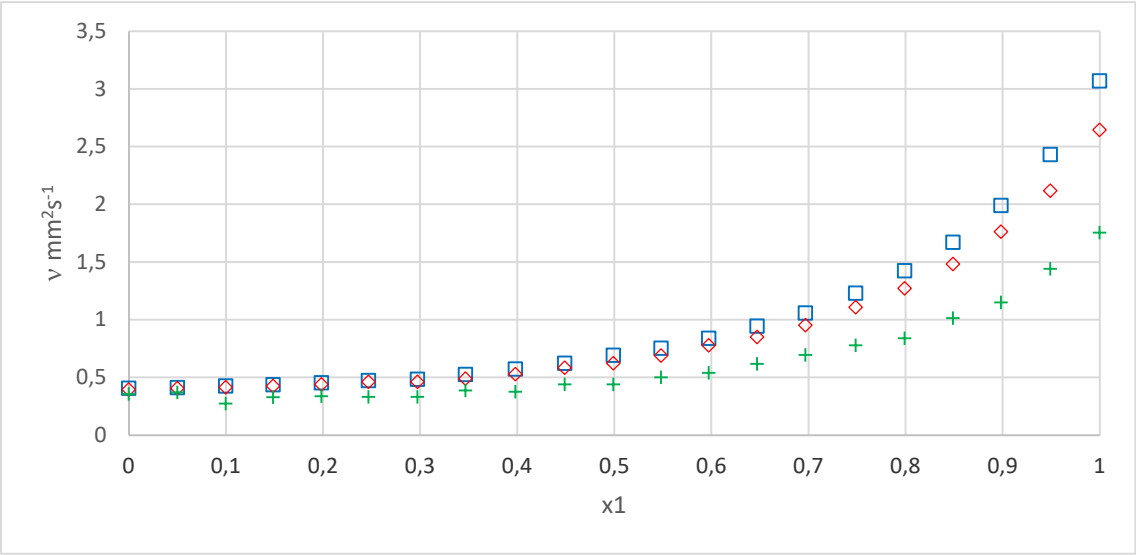

Figure 17: Kinematic viscosity at 293.15 K, 298.15K and 313.15K of the binary systems: 2-propanol+1-hexene. 2-propanol (1) + 1- hexene (2) (□) 293.15K; 2-propanol (1) + 1- hexene (2) (◇) 298.15K, 2- propanol (1) + 1- hexene (2) (+) 313.15K.

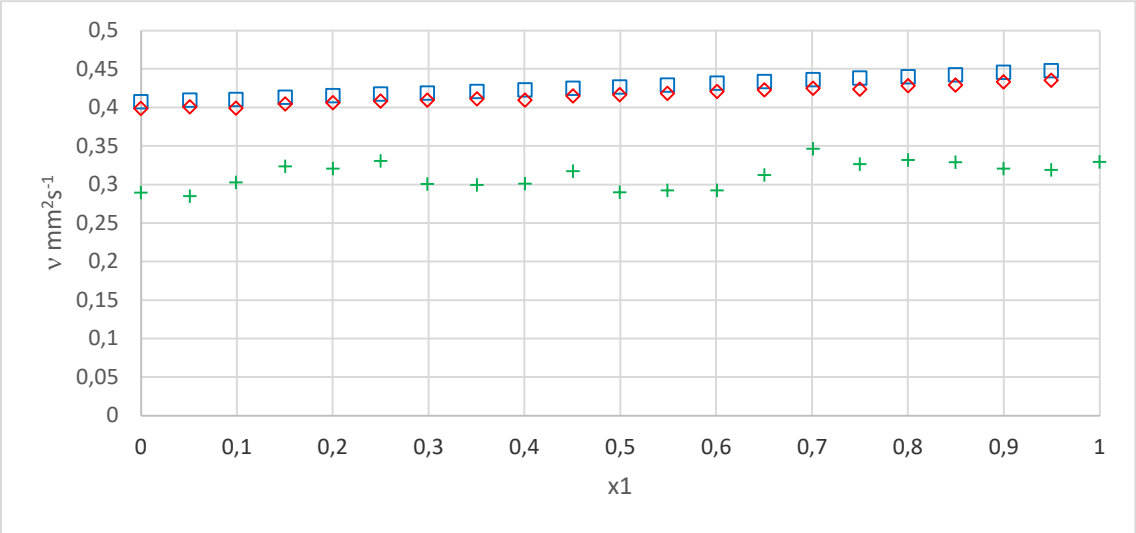

Figure 18: Kinematic viscosity at 293.15 K, 298.15K and 313.15K of the binary systems: DIPE+1-hexene. DIPE (1) + 1- hexene (2) (□) 293.15K; DIPE (1) + 1- hexene (2) (◇) 298.15K, DIPE (1) + 1- hexene (2) (+) 313.15K.

Figures 16, 17 and 18 show the kinematic viscosity in function of x1 for the three different temperatures. The behavior of the kinematic viscosity is like the dynamic viscosity. For this reason, the comments respect the figures analysis are the same already exposed.

In figures 19, 20 and 21, the experimental data in dynamic viscosity was compared with experimental data of pure compounds. In the figures 18, 19 and 20, the experimental data was compared with viscosity of pure compounds from Shell Chemicals, 2016 [44], Riddick, 1986 [39] and the doctoral thesis Ollarves, 2014 [36].

The variation in dynamic viscosity is calculated according to formula 11.

$$\Delta\mu = \mu\,\mathrm{exp} - (x_i * \mu p1 + x_j * \mu p2) \qquad (11)$$

Where $\Delta\mu$ is the variation in dynamic viscosity, μ exp is the experimental value of dynamic viscosity, x_i is the molar fraction of the first compound, $\mu p1$

is the pure dynamic viscosity of the first component. x_j is the molar fraction of the second compound and $\mu p2$ is the pure dynamic viscosity of the second component. In summary, the variation in dynamic viscosity is calculated by the difference between the measured viscosity value and the sum of the molar fractions of each compound multiplied by the value of the pure component according to the current literature.

Variations in the dynamic viscosity of the sample are negative in case of the 2-propanol + DIPE and 2-propanol + 1-hexene.

In the case of DIPE + 1-hexene, at the temperature of 293.15K the curve is linear, with an initial positive region and when the mole fraction is almost 0.5, as the mole fraction of DIPE increases, the curve becomes negative. In the temperature of 298.15K, the curve is also linear with a positive initial region followed by a greater negative region at low mole fractions of the alkanol. Variations in the dynamic viscosity are negative in the case of the DIPE + 1-hexene at temperature of 313.15K.

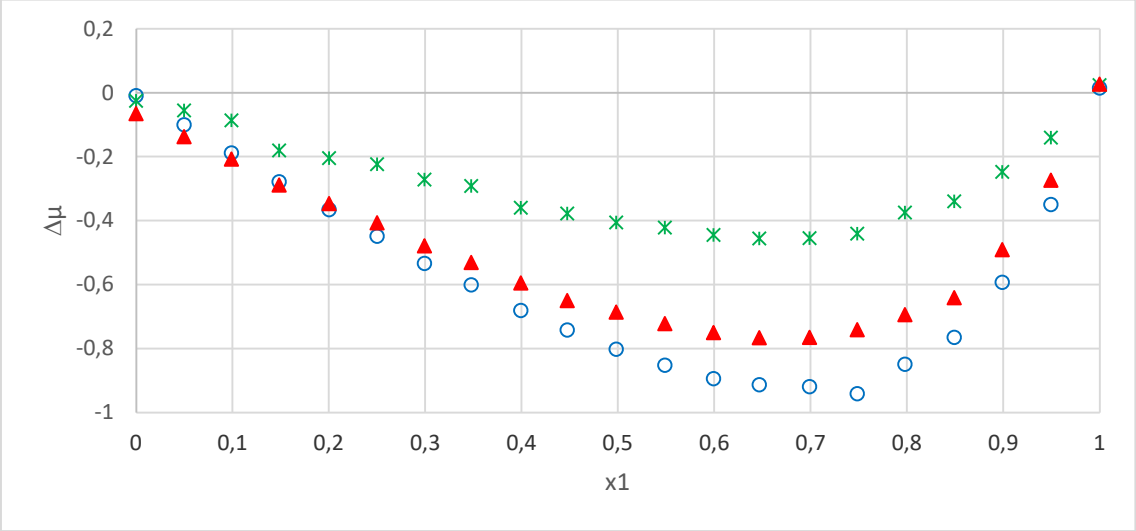

Figure 19: Experimental values of deviations in dynamic viscosity Δμ at 293.15 K (○), 298.15K (▲), 313.15K (✳) of binary system: 2 propanol (1) + DIPE (2).

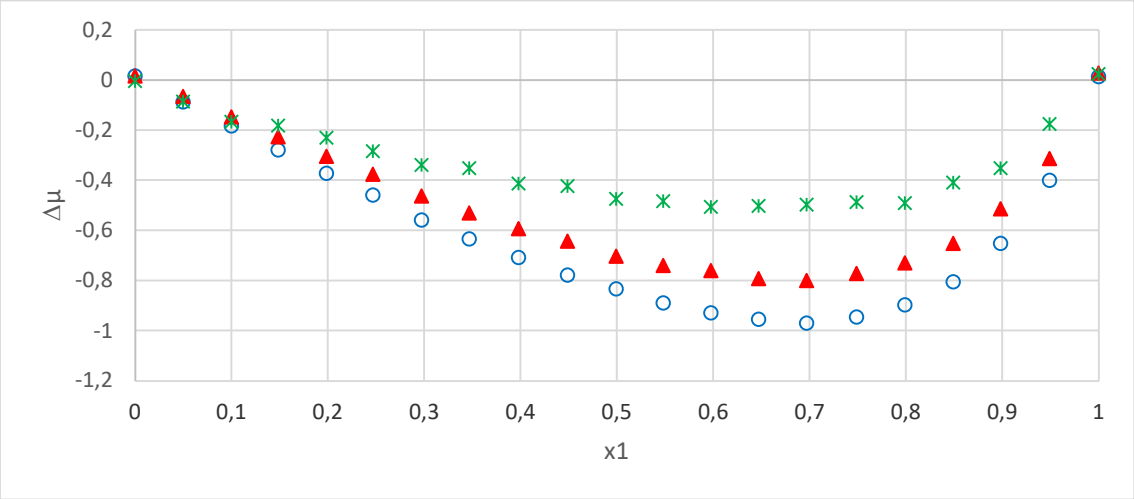

Figure 20: Experimental values of deviations in dynamic viscosity Δμ at 293.15 K (○), 298.15K (▲), 313.15K (✳) of binary system: 2 propanol (1) + 1-hexene (2).

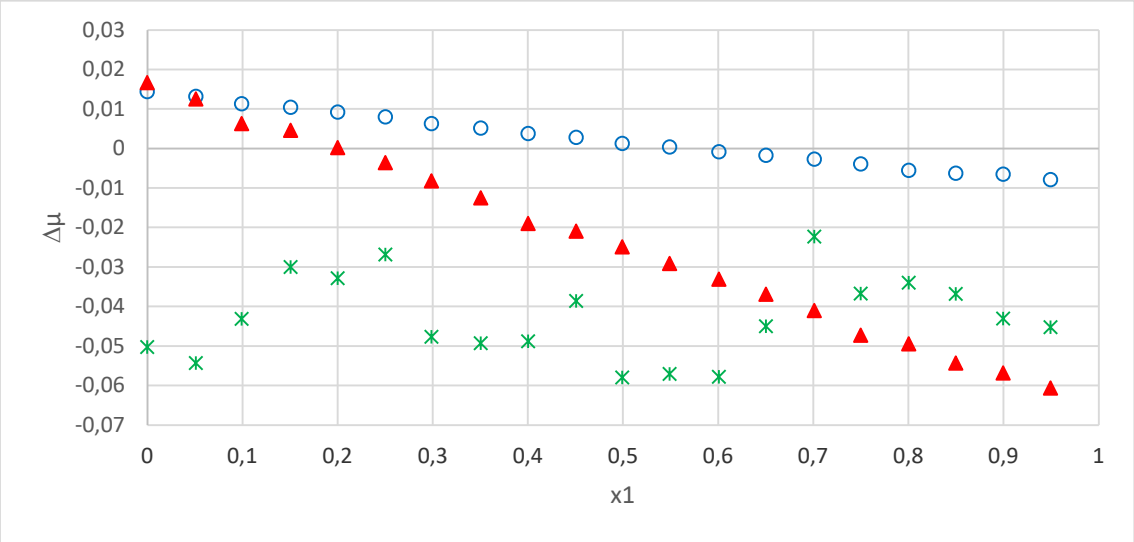

Figure 21: Experimental values of deviations in dynamic viscosity Δμ at 293.15 K (○), 298.15K (▲), 313.15K (✳) of binary system: DIPE (1) + 1-hexene (2).

6 Conclusions and Future Work

6.1 Conclusions

Some thermophysical properties of three binary systems containing oxygenated additives have been studied.

From density measurements, excess volumes at 0.1 MPa and 298.15 K have been determined, having positive values except for the mixture 2-propanol + DIPE.

Isentropic compressibility has been obtained from density and speed of sound experimental values at 0.1 MPa and 298.15 K.

Refractive indices have been measured at 0.1 MPa and 298.15 K. The highest values are found for the mixture 1-hexene + DIPE.

Dynamic viscosities were obtained by using a Stabinger viscometer at 0.1 MPa and at 293.15, 298.15 and 313.15 K.

This work provides firstly, 189 experimental values of density, refractive index and speed of sound at a temperature of 298.15K using two high precision equipment - DSA 5000 and Abbemat MW digital refractometer. Then, 567 experimental values of dynamic, kinematic viscosity were collected and, again, density at temperatures of 293.15K, 298.15K and 313.15K using the SVM 3000 viscometer. This equipment is suitable for the research with biogasolines/biofuels.

In total, 756 experimental measurements were collected and analyzed as a way to scientifically contribute to the use of biofuels. All the experimental data measured were presented, both numerically and graphically, the results

were discussed from the thermodynamic point of view and compared with the currently literature available and Redlich-Kister polynomial with good results.

Finally, with these research report, an experimental knowledge of the thermodynamic functions of liquid mixtures for their application to the production, design and use of new generation fuels with renewable components was provided.

6.2 Future Work

There are few scientific articles available using these compounds as components (2 propanol, DIPE and 1-hexene). In terms of viscosity, there is nothing published. This work launches the study of the pure and binary mixtures of these compounds. Future works that would deepen the analysis of these compounds as future biofuels would be the experimental data of the ternary mixtures of the same compounds.

In addition, viscosity was measured up to a temperature of 313.15K. As already mentioned, the viscosity plays a key role in lubrication of the fuel injection systems. The results of the behavior of viscosity changes significantly when reaching 313.15K. Unfortunately, these values are below than the limits of our viscosimeter SVM 3000 and there is no experimental data to compare the behavior of these property in this temperature. Acquire new experimental data to the same compounds in high temperatures would be important to develop the knowledge to new biofuels.

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APPENDIX

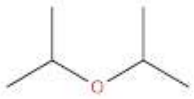
NIST Literature Report

Thermodynamics Research Center
Applied Chemicals and Materials Division
National Institute of Standards and Technology
Document generated on November 12, 2019 at 2:01:44 AM.

Compounds

Name: 2-propanol
Formula: C_3H_8O
Other name: isopropyl alcohol
isopropanol

Name: bis(1-methylethyl) ether
Formula: $C_6H_{14}O$
Other name: isopropyl ether
diisopropyl ether



Name: 1-hexene
Formula: C_6H_{12}

Chemical Systems, Measured Properties, and Data Sources

Compounds: 2-propanol
bis(1-methylethyl) ether

Measurement: Density and derived properties for the liquid

6 data sources are listed in the NIST SOURCE Data Archive.

1. Wichterle, I.
Isothermal vapor-liquid equilibria in the ternary system propan-2-ol + diisopropyl ether+ 2,2,4-trimethylpentane and the three binary subsystems at 330 K and 340 K
ELDATA: The International Electronic Journal of Physico-Chemical Data, 1999, 5, 179-189
Temperature: 298.15 K
Pressure: 101 kPa

2. Arce, A.; Arce, A.; Martinez-Ageitos, J.; Rodil, E.; Rodriguez, O.; Soto, A.
Physical and equilibrium properties of diisopropyl ether + isopropyl alcohol + water system
Fluid Phase Equilib., 2000, 170, 113-126
Temperature: 298.15 K
Pressure: 101.3 kPa

3. Miller, H. C.; Bliss, H.
The system isopropyl ether - isopropanol vapor-liquid equilibrium
Ind. Eng. Chem., 1940, 32, 123-5
Temperature: 298.14 K
Pressure: 101 kPa

4. Blanco, S. T.; Embid, J. M.; Otin, S.
Excess volumes of (2,2,4-trimethylpentane + methanol or ethanol or propan-2-ol or di-1-methylethyl ether or 1,1-dimethylethyl methyl ether) and of (methanol or ethanol or propan-2-ol + di-1-methylethyl ether or 1,1-dimethylethyl methyl ether) at the temperature 298.15 K
J. Chem. Thermodyn., 1994, 26, 23-28
Temperature: 298.15 K
Pressure: 101.3 kPa

5. Letcher, T. M.; Govender, P. U.
The excess molar volumes of (an alkanol + a branched chain ether) at the temperature 298.15 K and the application of hte ERAS model
Fluid Phase Equilib., 1997, 140, 207-220
Temperature: 298.15 K
Pressure: 101.3 kPa

6. Kammerer, K.; Lichtenthaler, R. N.
Excess properties of binary alkanol-ether mixtures and the application of the ERAS model
Thermochim. Acta, 1998, 310, 61-67
Temperature: 298.15 K
Pressure: 101 kPa

Compounds: 2-propanol
bis(1-methylethyl) ether

Measurement: Refractive Index for the liquid

1 data source is listed in the NIST SOURCE Data Archive.

1. Arce, A.; Arce, A.; Martinez-Ageitos, J.; Rodil, E.; Rodriguez, O.; Soto, A.
Physical and equilibrium properties of diisopropyl ether + isopropyl alcohol + water system
Fluid Phase Equilib., 2000, 170, 113-126
Temperature: 298.15 K
Pressure: 101.3 kPa

Compounds: 2-propanol
bis(1-methylethyl) ether

Measurement: Speed of sound for the liquid

1 data source is listed in the NIST SOURCE Data Archive.

1. Arce, A.; Arce, A.; Martinez-Ageitos, J.; Rodil, E.; Rodriguez, O.; Soto, A.
Physical and equilibrium properties of diisopropyl ether + isopropyl alcohol + water system
Fluid Phase Equilib., 2000, 170, 113-126
Temperature: 298.15 K
Pressure: 101.3 kPa

Compounds: 2-propanol
bis(1-methylethyl) ether

Measurement: Viscosity for the liquid

No experimental data in the NIST SOURCE Data Archive

Compounds: 2-propanol
1-hexene

Measurement: Density and derived properties for the liquid

1 data source is listed in the NIST SOURCE Data Archive.

1. Letcher, T. M.; Mercer-Chalmers, J.; Govender, U. P.; Radloff, S.
Excess molar enthalpies and excess molar volumes of binary mixtures of 1- alkenes with 1-propanol and 2-propanol
Thermochim. Acta, 1993, 224, 33-8
Temperature: 298.15 K
Pressure: 101.3 kPa

Compounds: 2-propanol
1-hexene

Measurement: Refractive Index for the liquid

No experimental data in the NIST SOURCE Data Archive

Compounds: 2-propanol
1-hexene

Measurement: Speed of sound for the liquid

No experimental data in the NIST SOURCE Data Archive

Compounds: 2-propanol
1-hexene

Measurement: Viscosity for the liquid

No experimental data in the NIST SOURCE Data Archive

Compounds: bis(1-methylethyl) ether
1-hexene

Measurement: Density and derived properties for the liquid

No experimental data in the NIST SOURCE Data Archive

Compounds: bis(1-methylethyl) ether
1-hexene

Measurement: Refractive Index for the liquid

No experimental data in the NIST SOURCE Data Archive

Compounds: bis(1-methylethyl) ether
1-hexene

Measurement: Speed of sound for the liquid

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Measurement: Density and derived properties for the liquid

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