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Comparative Modeling with Dynamic Viscosities of Pure and Crude Biodiesel Glycerol at Room Temperature using distilled Water as Modifier

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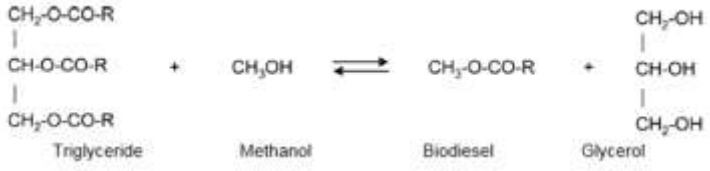
Abstract: *In material science, fluid flow plays a major role as most of the processes are dependent on the use of viscous fluids as reagents and heat transfer media or raw materials. Diverse system processes with mass transfer rates, heat transfer rates and chemical processes within two components hinge on the system's fluid dynamics phenomena. Consequently, understanding the rate phenomena in processing systems is very essential for analyzing the movement of fluids at certain conditions. Glycerol is technically adopted in most scientific applications due to its inexpensive and non-toxic biological nature. In experimental studies, aqueous glycerol solution is generally employed as its density can be altered and controlled by altering the amount of glycerol in the solution. The solutions densities of aqueous glycerol has been adequately recorded in web-based models under normal conditions. A predictive approach with distilled water from 0 to 10 liters and pure /crude biodiesel glycerol of 10 to 0 liters were proposed at 25^oC (the room temperature). Meanwhile, it is expected to be applicable at higher magnitude levels with the two fluids. Eventually, two theoretical models [y= -x+10; R^2=1]: where y denotes the distilled water fraction and x, the pure / crude glycerol fraction & [y= -1.364In(x) +16.001; R^2=0.9606]where y is the fraction of the distilled water and x, the dynamic viscosity of the pure/crude solution] were generated with the accurate computations of the fractions, densities and dynamic viscosities of pure/crude glycerol in solution at the specified ambient temperature.*

Keywords: Crude biodiesel glycerol, distilled water, dynamic viscosity, room temperature (25^oC) and cheng (2008) parameterization

1.0 INTRODUCTION

The past industrial revolution has induced the entire globe to be operating on an energy-based fossil fuel economy as the very first class of fossil fuel was coal prior to crude oil and its derivatives [1]. Presently, with growing reservations over the sustainability and environmental implications, fossil fuel still dominates the significant source of energy in all sectors. However, there are enormous demands to develop an alternative and sustainable energy supply that will meet the demands of the domestic, commercial, and industrial sectors in connection to goods and services logistics [2]. With the sources of energy transformation, the system of the economies also needs to shift with the fundamental systems that link them all. Thereby, the economic transformations are establishing new perspectives for a more sustaining and green energy structure, which will accelerate the mainstream applications in implementing new energy technologies. Biofuel is one exceptionally promising transformative source of energy [1]. Biodiesel specifically is a triglyceride fossil fuel substitute derived from biological resources from plant-based and animal fats [1]. A triglyceride interaction with primary alcohol to generate biodiesel and glycerol, or glycerin, was involved in the overall chemical reaction. The methanol removal of the R-groups of the triglycerides occurs through a catalyst, typically hydroxide of sodium or potassium. The glycerol process resulting from the processing of biodiesel is typically a dark brown viscose substance of low quality with a 60-80 percent glycerol content, some unreacted methanol, and a catalyst [1]. Purification is a required step in order to market the glycerol qualitatively for industrial value additions through established methodologies [1], [3].



Pure glycerol, however, retains 17.8°C and 290°C of melting and boiling points respectively. The availability of three groups of hydroxyl radicals makes the product hygroscopic, with a propensity of absorbing humidity from the air. The

tendency of the polyol units to form hydrogen bonds with water molecules enables glycerol easy solubility in water. Glycerol has a specific gravity of 1.26 and is slightly denser than water. That implies it will settle at the bottom when mixed with water. However, due to its solubility, it can effectively form an aqueous solution over time, often with moderate agitation [4]. The three glycerol hydroxyl groups allow ester-forming reactions with many organic acids and isocyanate-forming polyurethanes [5]. In a range of industrial procedures, glycerol is used and recycled in pharmaceuticals, cosmetics, resins, cleaning products, polyurethanes, plastics, and as a food moisturizer. The application of glycerol for commercial feedstock started with its requirement in the manufacture of explosives for the exploration and extraction of geological resources and the construction industries [5]. It, therefore, stimulated the growth of industries. Polyurethane Recent technological developments enable urethane foams to be developed with crude glycerin. In the architectural and automotive industries, polyurethane foams have an extensive range of applications as often used as insulators [6].

Rheological parameters could provide a clearer understanding of device output in terms of its dynamic viscosity relative to temperature. Dynamic viscosity is the estimation of the intrinsic resistance of the fluid with respect to flow. The internal friction within a fluid to flow indicates the responsibility of a force in the displacement of a fluid at a definite condition. The force (F) is directly proportional to the following: Shear Rate, Surface Area, and Dynamic Viscosity (Á) [13]. Dynamic viscosity operates as the constant factor of proportionality existing between the stress (F / A) and the distortion or shear rate, according to Newton's viscosity law. It is considered a more fundamental property as sophisticated viscometers depend on calculating the shear stress at a particular shear rate that provides complete viscosity profile characterizations [7]. In order to optimize the chemical processes and the energy requirement with the pipeline transport and pump operations, the theoretical knowledge of fluid viscosities is essential. In the laboratory studies of flow phenomena, aqueous glycerol is commonly employed [8]. Generally, glycerol – water mixtures are being used to regulate the moisture content of a system at equilibrium [9]. Based on the glycerol proportion, the equilibrium state of the solutions is modified from 0.0 to 1.0 with the simplicity of blending glycerol and water. This mechanism was well investigated empirically and analytically from different perspectives like the molecular structure, dynamics, and hydrogen bond network [10] [11]. However, in most studies, the physicochemical properties have been studied as a feature of glycerol molar fraction, and there are few claims about the relationship with water at the same equilibrium state. As glycerol is a standard biologically compatible solution [12]. It will be rational to justify the interaction of water and glycerol molecules from a dynamic viewpoint to demonstrate the rheological performance of glycerol both at pure and crude grades. Differential calorimetric scanning (DSC) measurements of water-glycerol mixtures showed that water in a higher concentration of glycerol solutions enters a super-cooling state, and it was discussed that this physical solution is Water property is possibly connected to the hydrogen-bonding framework of the water molecules and their interaction with the solutes [11]. The physiological characteristics of water are biochemically favorable in the glycerol – water mixtures [9], [12]. A variety of techniques, including completed attenuated reflection FTIR spectroscopy (ATR-IR)[13], nuclear magnetic resonance (NMR)[14], broadband dielectric spectroscopy[15], electron spin resonance[16], neutron diffraction[9], thermodynamic analysis[17], and molecular dynamics simulation[18] and investigating the properties of glycerol-water mixtures with qasi-elastic incoherent method with neutron scattering as a promising model for examining the molecular dynamics of glycerol-water mixtures[19]. These techniques explore how biomaterials and foods deal with water and its properties. IQENS examines a single particle's correlation for designing the dynamics of molecules. In IQENS, the hydrogen atom has a wide cross-section which In addition, the hydrogen cross-section is greater in magnitude than that of deuterium. Thus, allowing the molecular dynamics of a single molecule in a multi-component system to be conducted individually by isotope labeling with deuteration [9].The goal of this work is to formulate a temperature-dependent mathematical predictive model of the mixture of crude glycerol (biodiesel)-water mixtures to estimate the management of viscosity in aqueous systems as may be needed in polyurethane production we have modeled the thermodynamics and molecular dynamics of glycerol-water solutions in relation to the effects of viscosities at standard ambient temperature.

2.0 METHODOLOGY

The model estimations is fundamentally based on the web based computed parameterizations cheng et al 2018 [20].

3.0 RESULTS AND DISCUSSION

Table 1. Selected physicochemical properties

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Property	Crude glycerol	Treated glycerol	Pure/standard glycerol	
			Value	Reference
Color	Brown	Colorless	Colorless	[21]
pH	11.24	6.57	6.84	[21]
Relative density	1.0504	1.2120	1.2613	[21]
Refractive index	2.4185	1.4540	1.4720	[21]
Viscosity(Cp)	1026	940	954	[21]
Moisture content (%)	9.27	0.23	0	[21]
Ash content (%)	6.14	0.04	0	[21]
Glycerol content (%)	15.56	95.96	99.90	[21]

Table 2. Outputs from aqueous pure glycerol modeling

Water(L)	Pure glycerol(L)	Pure glycerol fraction (L)	Pure glycerol fraction (kg)	Mixture density(Kg/m^3)	Mixtures dynamic Viscosity (×10^{-2})
0	10	1.0	1.00	1258	90568.00
1	9	0.9	0.92	1237	20813.00
2	8	0.8	0.84	1214	6664.60
3	7	0.7	0.75	1190	2684.60
4	6	0.6	0.65	1165	1275.80
5	5	0.5	0.56	1139	685.59
6	4	0.4	0.46	1112	404.64
7	3	0.3	0.35	1084	256.93
8	2	0.2	0.24	1055	172.88
9	1	0.1	0.12	1026	121.89
10	0	0	0	9970	89.00

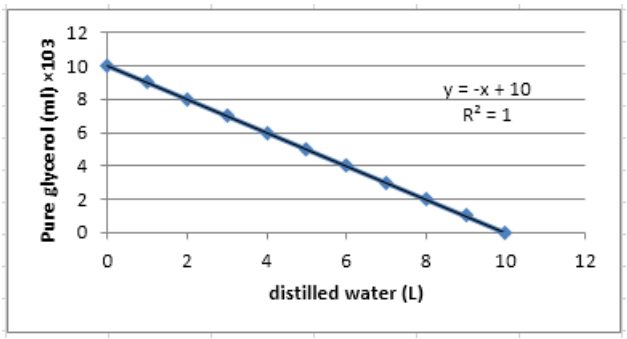

Figure 1. Relationship between pure glycerol and distilled water

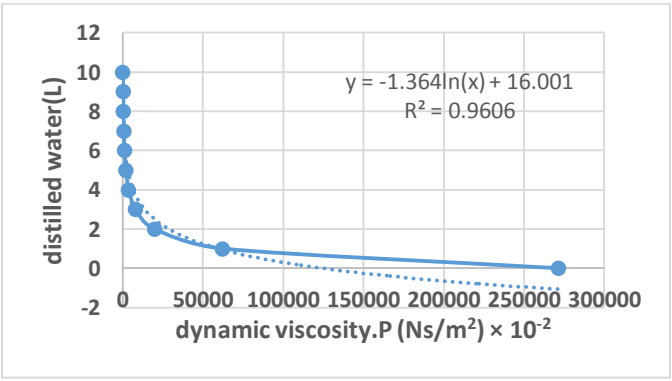

Figure 2. Distilled water and dynamic viscosity with pure glycerol

Table 3. Outputs from aqueous crude glycerol modeling

Water(ml)	Pure glycerol (L)	Crude glycerol fraction.(L)	Pure glycerol fraction(kg)	Mixture density(×10^{-2})	Mixtures dynamic Viscosity (Ns/m^2)(×10^{-2})
0	10	1.00	1.00	37740	271704.00
1	9	0.90	0.92	37110	62439.00
2	8	0.80	0.84	36402	19983.80
3	7	0.70	0.75	3570	8053.80
4	6	0.60	0.65	34950	3827.40

5	5	0.50	0.56	34170	2056.77
6	4	0.40	0.46	33360	1213.92
7	3	0.30	0.35	32520	770.79
8	2	0.20	0.24	31650	518.64
9	1	0.10	0.12	30780	365.67
10	0	0	0	99700	89.00

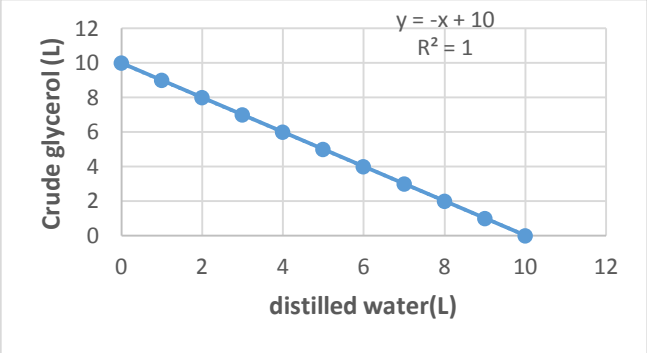

Figure 3.Crude glycerol and distilled water

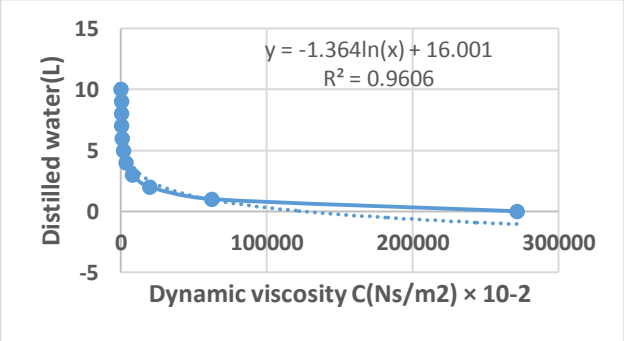

Figure 4.Distilled water and dynamic viscosity with crude glycerol

Revealed in Tables 1, 2, and 3 are the relevant and selected physicochemical parameters of crude glycerol from homogenously and alkaline trans esterified waste groundnut oil [21]. Similarly, figures 1, 2, 3, and 4 define the relationship between the distilled water/pure glycerol, distilled water/dynamic viscosity with pure glycerol, distilled water/crude glycerol, and distilled water/dynamic viscosity with crude glycerol respectively. The two distinct models [y= -x+10; R^2=1] and [y= -1.3641In(x) + 16.001; R^2= 0.9606] establish some intrinsic relationships between the distilled water modifier (y) and the viscosity (x) which are thermodynamic parameters that are directly relevant to the molecular dynamics [21].

4.0 CONCLUSIONS

As fluids, the dynamic viscosities of glycerol-water mixtures were modeled with respect to the thermodynamic and molecular dynamics of water –glycerol molecules via an internet-based predictive approach at a constant 25^{o}C room temperature. Based on this, the absolute viscosities of both the pure and crude glycerol-water mixtures can be calculated directly with water as a singular non-toxic parametric modifier. The computed model data are assumed to be a good approach that explains the molecular interaction at that state.

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