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Estimating Density of Ionic Liquids using Equation of States and Linearized Generalized Model

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Abstract*— The need for sustainable treatment methods is evident with the increasing wastewater volume generated and more stringent environmental regulations. Deploying ionic liquids in wastewater treatment processes can be both promising and challenging. Many studies have shown that these solvents can effectively remove pollutants such as dyes, metal ions, and pharmaceutical organic compounds. However, identifying the necessary properties in engineering calculations can be rigorous and time-consuming. Two known estimation methods of parameters, such as density, are the equations of state (EOS) and generalized correlations. Ten ionic liquids with proven capability in treating specific wastewater contaminants were selected in this study, but only two were successfully predicted by Schmidt and Wenzel (SW) EOS: [OMIM]BF4 and [BMIM]BF4. Results showed that obtaining design parameters and properties through linearized generalized estimation method is more accessible, especially if time and costs are of the utmost consideration. Moreover, SW EOS can successfully predict density with better accuracy, and the generalized correlation method can still predict with acceptable accuracy and lesser computational effort.

***Index Terms*— Esmaeilzadeh-Roshanfekr EOS, ionic liquids, Schmidt and Wenzel EOS, Valderrama & Zarricueta LGM**

I. INTRODUCTION

The Philippines Statistics Authority (PSA) issued a new data set regarding generated and treated wastewater volumes in the National Capital Region (NCR) last October 2021. According to this report, the amount of wastewater generated rose by 32% while the treated volume increased from 9.7% to 14.5%, equivalent to 821.55 million cubic meters [1]. The three top water consumers in the Philippines, according to NEDA, are (i) the irrigation sector - 75.7%, (ii) the industrial sector - 14.5%, and (iii) domestic/ municipal use at 8.3% [2].

Furthermore, an updated version of the country's water quality guidelines and general effluent standards on selected parameters, known as DENR Administrative Order No. 2021-19 (DAO 2021-19), was issued on June 30, 2021. Water Quality Guidelines (WQG) refer to the level of a water constituent or numerical values used to categorize a particular water resource and its use. At the same time, General Effluent Standards (GES) means any legal constraint on the amounts, rates, or concentrations or any combination of effluent that a specific source can discharge [3]. This also covers some amendments to the previous local standard, which is the DENR Administrative Order No. 2016-08 (DAO 2016-08) [4]. DAO 2016-08 contains significant discharge quality parameters per industry category, such as mining & quarrying, textiles manufacturing, and drugs & medicines. Some prescribed values may have been eased in DAO 2021-19 compared to the earlier edition, but the fact remains that treated water must comply with these two standards.

With the increased wastewater volumes generated and stricter regulations for treated water, sustainable wastewater treatment methods are needed. Wastewater treatment with ionic liquids is gaining worldwide attention among environmentalists and industrialists [5]. Ionic liquids (ILs) are described as molten salts with melting points less than 100 $^{\circ}$C. It has negligible vapor pressure and higher thermal stability than conventional organic solvents [6]. This property of ILs translates to lower VOC emissions in its applications, qualifying it as a potential green solvent.

Some of the uses of ILs in wastewater treatment reported in the literature include the removal of dyes [7], metal ions [8], and pharmaceutical organic compounds [9]. Its application in wastewater treatment popularly takes leverage in its adaptive solubility in solid phase micro-extraction of pollutants and the combination of ultrasound-assisted dispersive methods [5].

The type and properties of ionic liquids are essential, as well as the target pollutant, volume of pollutant, and geographic conditions to ensure a successful wastewater treatment process [5]. In selecting the most suitable ionic liquid for a particular application, its physical, chemical, and thermodynamic properties are valuable to identify [10]. Numerous studies have shown the importance of estimation methods, such as providing values of critical properties with reasonable accuracies in a short time despite having many possible ILs that can be produced [11]. Of all the given properties of ILs, density is commonly attained through experiments which are also not always possible and could be quite expensive [10]. Moreover, density is the most important among the different physical and chemical properties of ILs because it is necessary for the calculations of phase equilibria, heat capacity, viscosity, amount of heat transfer, and phase change [12], which are all relevant properties for the design of wastewater treatment using ILs.

Ionic Liquids in wastewater treatment applications

A literature review was conducted to initially choose the list of ionic liquids (ILs) that were considered in this study. The twenty (20) selected ILs were based on their capability to remove: (i) heavy metals, (ii) dye, and (iii) pharmaceutical

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pollutants from previous studies and summarized in Table 1.

This study focused on these three types of pollutants because of their toxicities and possible negative environmental impacts if left untreated. Examples are the significant amounts of lead, cadmium, and mercury found in some areas in Luzon, Philippines, which are also present in fish and fishery resources around the area [13], presence of hormones such as estrogen and other endocrine disrupting chemicals in Laguna Lake that may affect aquatic organisms [14], and the expected increase of wastewater discharges with synthetic dyes which some types are found to be resistant to degradation via conventional wastewater systems [15].

In this study, density estimations are conducted for ILs with potential use for wastewater treatment, specifically those listed in Table 1. The density estimation methods assessed in this study include two equations of states, namely Schmidt and Wenzel (SW EOS) and Esmaeilzadeh-Roshanfekr (ER EOS), and one generalized linear correlation model developed by Valderrama and Zarricueta (LGM). These were used to validate the accuracies in estimating the densities of ionic liquids that can be potentially used in wastewater treatment based on the intended application conditions.

With the identification of the most suitable method for density estimation, feasibility studies for wastewater treatment design using other ILs could be conducted even without actual experimental density data. This allows treatment facilities to assess better the feasibility of utilizing ILs without the high cost of employing laboratory studies during the initial phase. This study aims to support the shift to sustainable wastewater treatment in the country where feasibility budget costs remain challenging.

II. METHODOLOGY

A. *Ionic Liquid Properties*

The properties of the ionic liquids used in this study came from the Ionic Liquids Database – ILThermo (v2.0) and in the spreadsheet for estimating several properties of ILs [16]. ILThermo is a web-based database of ionic liquids accessible for public use to provide users worldwide with recent information about experimental studies on ionic liquids, including important measurement details [17]. Currently, ILThermo contains 2,732 ionic liquids and has a total data point of 870,304 [17]. However, there are some ionic liquids included in Table 1 that were not found in either reference. Only ten (10) ILs with complete properties were subjected to density estimations using two equations of states (EOS) and the linearized generalized model (LGM).

Table 1. Initial list of Ionic Liquids for this study.

Ionic Liquid	Target Pollutant	Reference
1-Butyl-3-methylimidazolium hexafluorophosphate	Ni2+, Cu2+, Pb2+	[5]
1-butyl-3-methylimidazolium chloride	Pb2+, As3+	[5]
Glycine betaine and bis (trifluoromethyl sulfonyl) imide	Cu2+	[5]
Protonated betaine	Cu2+, Cd2+, Hg2+, Ni2+, Mn2+	[5]
3,3-(hexyl) bis (3 methylimidazolium) bromide	Heavy metals	[5]
1-aminopropyl-3-methyl imidazolium nitrate	Heavy metals	[5]
1-butyl-3-methylimidazolium dicyanamide	Heavy metals	[5]
Chloride divinylbenzene copolymer	Heavy metals	[5]
1-butyl-3-methylimidazolium acetate	Dye	[5]
1-butyl-3-methylimidazolium tetrafluoroborate	Pharmaceutical pollutant	[5]
1-methyl-3-octylimidazolium tetrafluoroborate	Zn2+, Cu2+, Cd2+, Fe2+	[18]
1-octyl-3-methylimidazolium hexafluorophosphate	Zn2+, Cu2+, Cd2+, Fe2+	[18]
1-butyl-3-methylimidazolium bis{(trifluoromethyl) sulfonyl} imide	Zn2+, Cu2+, Cd2+, Fe2+	[18]
1-octyl-3-methylimidazolium bis{(trifluoromethyl) sulfonyl} imide	Zn2+, Cu2+, Cd2+, Fe2+	[18]
methyl trioctylammonium chloride	Zn2+, Cu2+, Cd2+, Fe2+	[18]
1,3-dioctylimidazolium 2-hydroxybenzoate	Fe2+, Cob2+, Ni2+	[8]
trihexylammonium octanoate	Cu2+, Cob2+, Ni2+	[6]
trihexyl tetradecyl phosphonium chloride	As, Cr, Cd, Cu, Zn, Pb and Hg	[19]
trihexyl tetradecyl phosphonium dicyanamide	As, Cr, Cd, Cu, Zn, Pb and Hg	[19]
trihexyl tetradecyl phosphonium imide	As, Cr, Cd, Cu, Zn, Pb and Hg	[19]

B. *Density Prediction through Equations of State*

Schmidt and Wenzel (SW)

This equation of state uses critical pressure, critical temperature, and acentric factor as input parameters for low reduced temperatures with an accuracy of better than 2% in terms of molar liquid volume [20]. Equation (1) shows the SW EOS expressed in terms of the molar volume, Vm.

$$P = \frac{RT}{V_m - b} - \frac{a(T)}{V_m^2 + (1+3\omega)bV_m - (3\omega b^2)} \quad (1)$$

Where: $\alpha(T) = \Omega_{ac}\frac{\alpha_{SW}(T_r;\omega)R^2T_c^2}{P_c}$, $b = \Omega_b\frac{RT_c}{P_c}, \Omega_{ac} -= [1-\eta(1-q)]^3, \Omega_b = \eta q, \eta = \frac{1}{3(1+q\omega)}$

$q = 0.25989 - 0.0217\omega + 0.00375\omega^2$

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$$\alpha_{SW}(T_r;\omega) = \left[1 + (0.465 + 1.347\omega - 0528\omega^2)\left(1 - T_r^{\frac{1}{2}}\right)\right]^2$$

Esmaeilzadeh-Roshanfekr (ER)

This EOS is in cubic form that models the attractive interactions between molecules [12]. It is a reform of the Patel-Teja and Peng-Robinson equations of state particularly near the critical areas and offers better results compared to the two previous ones [12]. The ER EOS is expressed in Equation (2).

$$P = \frac{RT}{V_m - b} - \frac{a(T)}{V_m(V_m + c) + c(V_m - c)} \quad (2)$$

Where: $a(T) = \Omega_a \frac{\alpha_{PT}(T_r;\omega)R^2T_c^2}{P_c}$, $b = \Omega_b \frac{RT_c}{P_c}$,

$c = \Omega_c \frac{RT_c}{P_c}, \Omega_a = 3\eta^2 + \Omega_c^2 + 2\Omega_b\Omega_c + 2\Omega_c$

$\Omega_b = 2\Omega_c - 1 + 3\eta$

Smallest possible root of: $\Omega_c^3 + \left(3\eta - \frac{5}{8}\right)\Omega_c^2 + \left(3\eta^2 - \frac{3}{4}\eta\right)\Omega_c + \eta^3 - \frac{3}{8}\eta^2 = 0$

$\eta = 0.3284438 - 0.0690264\omega + 0.0078711\omega^2$

$$\alpha_{SW}(T_r;\omega) = \left[m_1 + m_2\left(1 - T_r^{\frac{1}{2}}\right)\right]^2$$

$m_1 = 0.999035 - 0.01061842\omega - 00081174\omega^2$,

$m_2 = 0.4400108 + 1.5297151\omega - 0.4710752\omega^2$

Density Estimation through generalized correlations

As equations of state utilize critical properties and introduce new factors to incorporate interaction tendencies of the substance or mixture, these could sometimes require excessive computational efforts for density predictions. At the initial stage of wastewater treatment design, this computational requirement may limit design efforts. Hence, it is also the interest of this study how a linearized correlation model would perform compared to SW and ER EOS. The proposed correlation is a linearized generalized model by Valderrama and Zarricueta (LGM). This was selected because of its relatively higher accuracy settings of 2.63 AARD% and R2 value of 0.9345 [21]. The LGM form for density prediction used in this study is shown in Equation (3).

$$\rho = \left(\frac{A}{B}\right) + \left(\frac{2}{7}\right) \cdot \left\{\frac{A \cdot \ln B}{B}\right\} \frac{(T - T_c)}{(T_c - T_b)} \quad (3)$$

Where: $A = a + b \cdot \frac{M}{V_c}$, $B = \left(\frac{c}{V_c} + \frac{d}{M}\right) \cdot V_c^{\delta}$

For ionic liquids, the values of the constants are a=0.3411, b= 2.0443, c=0.5386, d=0.0393, and δ=1.0476 [22].

Calculations

From 20 selected ILs, only 10 were used in the estimation of densities using SW EOS and ER EOS as summarized in Table 2. The molar weights, critical temperatures, critical pressures, and acentric factors of each IL needed by the equations were obtained from Valderrama, Cardona, & Rojas (2021) while the experimental values of pressure, temperature, and specific density were found in Ionic Liquids Database - ILThermo (v2.0) (2022).

The conditions in this study are under atmospheric (atm) pressures & near atm, and within the temperature range of 278.15 K to 333.15 K. This is because most of the actual wastewater treatment processes are also in these situations. The study of Farzi & Esmaeilzadeh (2016) was also conducted in ambient pressure and temperatures between 273.15 to 473.15K. Since the density, r, and the molar volume, Vm, of an ionic liquid is related to its molecular mass M by r= M/Vm, experimental molar volumes can be calculated from the given experimental densities, $\rho_{experiment}$. These experimental molar volumes became the initial values in the Microsoft Excel Solver Function to solve the calculated densities, $\rho_{calculated}$. The absolute relative deviation of density was calculated using the equation below to understand the relationship between the results:

$$\Delta\rho\ (\%) = \frac{\left|\rho_{calculated} - \rho_{experiment}\right|}{\rho_{experiment}} \times 100$$

To evaluate the accuracies of the EOS and LGM for each selected IL, the percent average absolute deviation (%AAD) given by the equation below is evaluated.

$$\%AAD = \frac{1}{N}\sum_{N} \frac{\left|\rho_{calculated} - \rho_{experiment}\right|}{\rho_{experiment}} \times 100$$

III. RESULTS AND DISCUSSION

Density Estimation using EOS

The 10 shortlisted ILs were subjected to density estimations using SW EOS and ER EOS with the number of data points as shown in Table 2. Based on the considered pressure and temperature range which are typical for wastewater treatment applications, only the densities of 2 ILs were effectively predicted through SW EOS: [OMIM]BF4 and [BMIM]BF4. The results of the density estimations of the remaining 8 ILs showed that the right-hand side of the SW EOS did not match the pressure values on the left. Hence, it can be said that SW EOS is not applicable to accurately predict the densities of the 8 ILs.

Moreover, utilizing the ER EOS did not result in converged values. It was found out in this study that ER EOS is not applicable to estimate the densities of the 10 ILs considered for wastewater treatment applications at ambient pressure and temperatures in the range of 278.15K to 333.15K.

Density Estimation for using SW EOS and LGM Correlation

Since only [OMIM]BF4 and [BMIM]BF4 were applicable for SW EOS calculations, density calculations for these ILs were also done via the linearized generalized model proposed by Valderrama and Zarricueta. Figures 1a-b shows the comparison of the experimental and calculated densities using SW EOS and LGM correlations for [OMIM]BF4 while Figures 1c-d is for [BMIM]BF4.

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Table 2. Summary of density estimations using SW EOS.

Ionic Liquid	**Synonyms**	**No. of Data points**	Applicability of SW EOS	Applicability of ER EOS
1-Butyl-3-methylimidazolium hexafluorophosphate	[BMIM]PF6	12	NA	NA
1-butyl-3-methylimidazolium chloride	[BMIM]Cl	6	NA	NA
1-butyl-3-methylimidazolium dicyanamide	[BMIM]DCA	46	NA	NA
1-methyl-3-octylimidazolium tetrafluoroborate	[OMIM]BF4	11	A	NA
1-octyl-3-methylimidazolium hexafluorophosphate	[C8MIM]PF6	5	NA	NA
1-butyl-3-methylimidazolium bis{(trifluoromethyl) sulfonyl} imide	[C4MIM] BTI	10	NA	NA
1-octyl-3-methylimidazolium bis{(trifluoromethyl) sulfonyl} imide	[C8MIM] BTI	10	NA	NA
trihexyl tetradecyl phosphonium dicyanamide	[P666,14] DCA	24	NA	NA
1-butyl-3-methylimidazolium acetate	[C4MIM]AC	21	NA	NA
1-butyl-3-methylimidazolium tetrafluoroborate	[BMIM]BF4	26	A	NA

NA - Not applicable in the given conditions
A - Applicable in the given conditions

For both ILs investigated, the experimental densities were evidently linear with respect to temperature as shown in Figure 1a and 1c, respectively. This further proves that for these ILs with potential use in wastewater treatment, the LGM developed by Valderrama and Zarricueta is also applicable.

Although the trends for calculated densities with respect to temperature in Figure 1a and 1c are in similar decreasing manner with the experimental values, its relative difference from experimental values are significantly large for those resulting from LGM compared to those resulting from SW EOS calculations as shown in Figure 1b and 1d. For [BMIM] BF4, the calculated values from SW EOS were even closer to the x-y line in Figure 1d signifying its better prediction performance than the corresponding LGM correlation.

Comparison of Density Estimation Method Performance

In comparison with other studies, Valderrama, Rea´tegui, & Rojas (2009) used a consistent hybrid method, artificial neural networks, and group contribution method (GCM+ANN) to estimate the densities of 24 ionic liquids, including [OMIM]BF4 and [BMIM]BF4. GCM+ANN uses a trained artificial neural network to study the relationship between dependent and independent variables [10].

Furthermore, the molecular mass, the mass of the groups that form the molecule, temperature, and molar volume were utilized in training the network. The calculated percent average deviation of [OMIM]BF4 using GCM+ANN is 0.63%, while [BMIM]BF4 is 0.28%. Farzi & Esmaeilzadeh (2016) also cited the results of Qi & Wang (2009) on the 4.64% AAD of [BMIM]BF4 at 288.15K-303.15K using the Prigogine-Flory-Patterson theory.

In order to assess the performance of the investigated estimation models in this study with respect to those reported in literature, a comparison of the resulting AAD values for the two ionic liquids are summarized in Table 3.

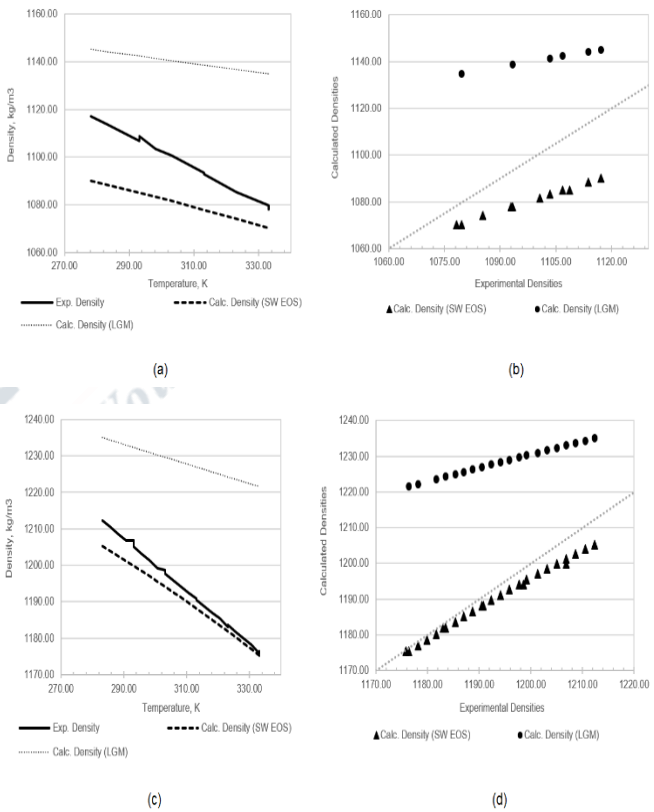

Fig 1. Comparison of Experimental Densities and Calculated Densities for [OMIM]BF4 (a, b) and [BMIM]BF4

Table 3. Comparison of %AAD with other studies

Ionic Liquid	Temperature range (K)	Number of data points	%AAD	Model	Reference
1-methyl-3-octylimidazolium tetrafluoroborate or [OMIM]BF4	317K – 322K	6	0.63	GCM+ANN	[10]
	278.15K – 333.15K	11	1.62	SW EOS	This study
		6	3.53	LGM	
1-butyl-3-methylimidazolium tetrafluoroborate or [BMIM]BF4	288.15K – 303.15K	4	4.64	PFP	[25]
	278K – 313K	6	0.15	GCM+ANN	[10]
	283.15K – 333.15K	26	0.28	SW EOS	This study
		20	2.82	LGM	

From Table 3, it can be noted that the GCM+ANN model has higher accuracy and precision for [OMIM]BF4 densities. However, the resulting AAD values for SW EOS and LGM correlations investigated in this study is still less than 5% showing promise if typical usage of resulting data would be for quick preliminary design calculations. For estimating density of [BMIM]BF4, on the other hand, GCM+ANN model still has higher accuracy and precision at 0.15% AAD but SW EOS is not that far behind at 0.28%. In comparison to the PFP model, the LGM model has better performance at 2.82% AAD but already relatively higher than GCM+ANN and SW EOS models. Nonetheless, the resulting AAD from LGM models are still less than 5%. This further supports Valderrama and Zarricueta guarantee that their LGM model has 78% probability of deviation below 5% from experimental values [22].

Given the extent of calculations required, the more complex models like GCM+ANN and SW EOS performed relatively more accurate and precise than the generalized linear correlation investigated. If the ease of calculations is to be factored in and the 5% deviation would be deemed acceptable for preliminary design basis, then the use of LGM model would be quicker yet still accurate to use.

Importance of Present Work in relation to wastewater treatment

Recent technological development shows that liquid membrane (LM) has identified as one of the feasible separation processes appropriate for different applications such as wastewater treatment [23]. LM has been noted as a flexible method because it blends the principle of membrane technology and solvent extraction [24]. The latter process involves several process parameters to design the appropriate equipment such as density and viscosity. This study shows how to acquire density values of two ionic liquids, [OMIM]BF4 and [BMIM]BF4, through reliable estimation methods in a shorter period. Researchers can utilize these kinds of methods to further study the application of ionic liquids in wastewater treatment especially on process design.

IV. CONCLUSION

This study has used two equations of states, namely Schmidt & Wenzel (SW EOS) and Esmaeilzadeh-Roshanfekr (ER EOS), and a generalized correlation by Valderrama & Zarricueta (LGM) to estimate the densities of ten ionic liquids for wastewater treatment. These ten selected ILs are found to be effective by other studies in the removal of metal ions, dyes, and pharmaceutical organic compounds in wastewater. Density estimations using the two EOS showed that only two of the ten ILs could be accurately predicted by SW EOS, while ER EOS was found not applicable at ambient pressure and within the temperature range of 278.15 to 333.15K conditions. Based on the 11 experimental data points of 1-methyl-3-octylimidazolium tetrafluoroborate/ [OMIM]BF4, estimates through SW EOS yielded 1.62% AAD, while the 26 experimental data points of 1-butyl-3-methylimidazolium tetrafluoroborate or [BMIM]BF4 resulted to 0.28% AAD. On the other hand, the Linearized General Model could predict the densities of all ten ILs with slightly higher values of %AAD, such as 3.53% and 2.82% for [OMIM]BF4 and [BMIM]BF4, respectively. Overall, this study showed that predicting the densities of ionic liquids for wastewater treatment application through a linearized generalized method is more convenient to use, especially if time and costs are of the utmost consideration and that density can be successfully predicted through the SW EOS method with better accuracy than generalized correlation. Moreover, the generalized correlation method offers lesser computational effort than SW & ER EOS and still with acceptable accuracy.

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