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Volumetric and transport properties of binary liquid mixtures with 1-ethyl-3-methylimidazolium ethyl sulfate as candidate solvents for regenerative flue gas desulfurization processes

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ABSTRACT

This paper presents novel data on density, viscosity and refractive index of four binary mixtures constituted of ionic liquid 1-ethyl-3-methylimidazolium ethyl sulfate and N-methyl-2-pyrrolidone/or 1-hexanol/or liquid polyethylene glycols with molar mass 200/or 400, in the temperature range from T = 288.15 K to 333.15 K and at pressure of p = .1 MPa. Thermal conductivity has been measured for mixtures of ionic liquid and polyethylene glycol 200/or polyethylene glycol 400 in the temperature range from T = 303.15 to 323.15 K and at a pressure of p = .1 MPa. All these solutions have the potential for application in regenerative flue gas desulfurization processes. From experimental values of densities, viscosities, thermal conductivities and refractive indices, excess molar volumes and deviations in viscosity, thermal conductivity and refractive index have been calculated and correlated with Redlich-Kister polynomial equation. The values of excess and deviation functions were used for analysis of molecular interactions present in the investigated solutions. In addition, modeling of transport properties, viscosity and thermal conductivity, was carried out and the obtained results were interpreted taking into account the applied approaches and models.

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1. Introduction

The results presented in this work are a continuation of our previous studies related to volumetric and transport properties of the environmentally friendly solutions with potential application in flue gas cleaning processes [1–3].

Main pollutants contained in exhaust gasses from the industrial and power plants facilities are sulfur oxides (SO_x), among which the most abundant is sulfur dioxide (SO_2). Sulfur oxides have strong environmental impact and are considered to be the main cause of acid rains. Understanding the seriousness of the problem was followed by establishing legislation related to the discharge of pollutants into the atmosphere and development of technological procedures for flue gas purification. Regenerative flue gas scrubbing processes, using organic solvents, already have relatively long history. Due to certain limitations of current technologies, like insufficient selectivity of the solvent or large energy requirements, efforts are continually invested in finding new solvents for use in regenerative cleaning processes as effective SO_x absorbents.

Some of the solvents investigated in this study, like N-methyl-2-pyrrolidone (NMP), have already found a commercial application. The others, like ionic liquid 1-ethyl-3-methylimidazolium ethyl sulfate ([Emim][$EtSO_4$]), and liquid polymers polyethylene glycols with molar weight 200 and 400 (PEG200 and PEG400), have been suggested as possible environmentally friendly replacements [4–11]. Due to their favorable thermophysical properties (e.g. low vapor pressure, high chemical and thermal stability) ionic liquids (ILs) have been investigated as green solvents suitable as a replacement of volatile organic compounds. However, in some cases they have shown limited solute solubility, higher viscosity and many of them are more expensive than conventional solvents. The possible solution to this problem could be the use of cosolvent modified ILs. In this way it may be possible to obtain more affordable solvent with favorably modified properties. Since the ionic liquids have the advantages due to their low toxicity, it classifies them as a possible alternative or cosolvent choice for other environmentally

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friendly fluids, such as alcohols [12,13], water [14] or polyethylene glycols [15].

Polyethylene glycols (PEG) are important environmentally friendly solvents characterized by low vapor pressure, high chemical stability and low melting points. In liquid form PEG is a highly polar substance [16,17] which acts both as a proton donor and proton acceptor [18] and is capable of forming both intra- and intermolecular hydrogen bonds [19,20]. Industrial application of liquid PEG in the flue gas desulfurization processes is considered as a consequence of its advantages: the high solubility of SO_2 and relatively easy desorption, which would reduce power consumption during the phase of solvent regeneration [21].

In this study novel data on density, viscosity and refractive index, in the temperature range from T = 288.15 K to 323.15 K or 333.15 K and at pressure of p = .1 MPa, of the solutions consisting of ionic liquid [Emim][$EtSO_4$] and NMP/or 1-hexanol/or PEG200/or PEG400, have been presented. Thermal conductivity of [Emim][$EtSO_4$] and PEG200/or PEG400 binary mixtures have also been investigated in the temperature range from 303.15 to 323.15 and at a pressure of p = .1 MPa. Of all investigated solutions only the density data for [Emim][$EtSO_4$] and 1-hexanol mixture have been previously published at T = 298.15 K [13]. In addition to experimental values of densities, viscosities, thermal conductivities and refractive indices, excess molar volumes and deviations in viscosity, thermal conductivity and refractive index have been calculated for all investigated mixtures and correlated with Redlich-Kister polynomial equation [22]. The values of excess molar volumes were used for analysis of molecular interactions existing in the investigated solutions.

Viscosity modeling was done by two sets of models: group contribution UNIFAC-VISCO [23,24] and ASOG-VISCO [25] models and correlative McAllister [26], Eyring-UNIQUAC [27] and NRTL-Eyring [28] models. In addition, the approach based on the application of equations of state (EOS) was used for simultaneous modeling of excess molar volume and viscosity [29]. Thermal conductivity was correlated by Filippov [30], Jamieson [31], Baroncini [32] and Rowley [33] models.

2. Experimental

2.1. Chemicals

Data on the investigated pure chemicals, their suppliers and stated purities and purification methods are given in Table 1. The mixtures were prepared gravimetrically using Mettler Toledo balance with a stated accuracy of $1 \cdot 10^{-7}$ kg, while the standard uncertainty in mole fraction calculation is estimated to be within $\pm 1 \cdot 10^{-4}$.

Prior to use, chemicals were kept in a dry, dark place in delivery bottles. Analysis of ionic liquid using the Mettler Toledo DL 38 Karl Fisher Titrator showed that the water content was 680 ppm. Comparison of experimental values for density, dynamic viscosity and refractive index of pure compounds, with available literature data [34–50], at the atmospheric pressure and temperature of T = 298.15 K, is given in Table 2. Differences between measured density values and literature data are below 1 kg·m^{-3}, except for [Emim][$EtSO_4$] in Refs. [36,37], where the density values are approximately 6 kg·m^{-3} lower [36] or higher [37] than ours (maximum percent deviation is about 0.50%). For dynamic viscosity the difference between experimental and literature data is less than $9 \cdot 10^{-2}$ mPa·s for less viscous compounds, while for the more viscous [Emim][$EtSO_4$], PEG200 and PEG400 it goes up to 6 mPa·s. Maximum percent deviation of 6.48% is obtained for [Emim][$EtSO_4$] in comparison with Ref. [34] and for PEG200 in comparison with Ref. [48]. However, both Refs. [34,48] show very good

Table 1
Sample description.

Chemical Name	CAS Number	Source	Initial Mass Fraction Purity	Purification method
[Emim][$EtSO_4$]	342573-75-5	Merck	0.99	None
N-Methyl-2-pyrrolidone	872-50-4	Merck	0.99	None
1-Hexanol	111-27-3	Merck	0.99	None
Polyethylene glycol 200	25322-68-3	Acros Organics	0.99	None
Polyethylene glycol 400	25322-68-3	Acros Organics	0.99	None

Table 2
Densities (ρ), dynamic viscosities (η) and refractive index (n_D) of pure components at T = 298.15 K and p = .1 MPa.[a]

Component	10^{-3} ρ/(kg·m^{-3})			η/(mPa·s)			n_D		
	Exp.	Lit.	PD/(%)	Exp.	Lit.	PD/(%)	Exp.	Lit.	PD/(%)
[Emim][$EtSO_4$]	1.23627	1.23763 [34]	0.11	91.256	97.58 [34]	6.48	1.47882	1.47940 [34]	0.04
		1.23882 [35]	0.21					1.47889 [35]	0.00
		1.2296 [36]	0.54						
		1.2423 [37]	0.49						
N-Methyl-2-pyrrolidone[b,c]	1.02838	1.02872 [38]	0.03	1.6795	1.656 [38]	1.42	1.46736	1.4675 [39]	0.01
		1.02831 [39]	0.01		1.663 [39]	0.99		1.4674 [41]	0.00
		1.0283 [40]	0.01		1.67 [40]	0.57			
1-Hexanol	0.81511	0.815265 [42]	0.02	4.5296	4.439 [42]	2.04	1.41591	1.41605 [43]	0.01
		0.8151 [43]	0.00		4.50 [44]	0.66		1.4161 [47]	0.01
		0.81499 [44]	0.01		4.643 [46]	2.44			
		0.81523 [45]	0.01						
Polyethylene glycol 200	1.12118	1.12098 [48]	0.02	50.404	48.157 [48]	4.67	1.45823	1.4585 [48]	0.02
Polyethylene glycol 400	1.12253	1.12249 [48]	0.00	91.0620	92.797 [48]	1.87	1.46499	1.4650 [48]	0.00
		1.1218 [4]	0.07						
		1.12230 [49]	0.02						
		1.12162 [50]	0.08						

[a] Standard uncertainties u for each variables are $u(T)$ = ±0.01 K and $u(p)$ = ±5%, and the combined expanded uncertainties U_c are $U_c(\rho)$ = ±1.5 kg·m^{-3}, $U_{c,r}(\eta)$ = ±0.009 and $U_c(n_D) = \pm 6 \cdot 10^{-4}$ with 0.95 level of confidence ($k \approx 2$).
[b] Previously published data [1].
[c] Previously published data [2].

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