ASPEN plus simulation of liquid–liquid equilibria data for the extraction of aromatics from waste tyre pyrolysis gasoline using organic and deep eutectic solvents: a comparative study

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Received: 31 July 2020 / Accepted: 11 December 2020 / Published online: 11 January 2021
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Abstract

Waste tyre pyrolysis gasoline (WTPG) contain significant amount of aromatics such as benzene, toluene and xylenes (BTX) and thus provide a good source for these value-added chemicals. Separation of aromatics from aliphatic media as obtained in WTPG and naphtha is done commercially by solvent extraction using volatile organic solvents such as sulfolane (SUF), dimethylformamide (DMF) and diethylene glycol (DEG). The high cost of this state-of-the art separation method and environmental consideration have necessitated search for non-volatile and green solvent such as deep eutectic solvent (DES). This study intends to conduct a comparative evaluation of the performance of five solvents (SUF, DMF, DEG, and two DESs) for the extraction of BTX from WTPG. The two DESs are choline chloride/ethylene glycol (DES1) and choline chloride/glycerol (DES2) in molar ratios 1:2. An ASPEN plus simulation was carried out to generate liquid–liquid equilibria (LLE) data for the pseudo-ternary systems {WTPG + BTX + solvent (SUF/DMF/DEG/DES)}. Performance evaluation was based on selectivity (S) and solute (BTX) distribution coefficient (D). The propriety of the simulation protocol was validated using literature data. The results revealed the following maximum values of selectivity and distribution coefficients for the solvents: DES2 ($S=378.283$, $D=0.656$); DES1 ($S=77.364$, $D=1.423$); SUF ($S=55.371$, $D=0.756$); DMF ($S=25.336$, $D=0.786$) and DEG ($S=17.531$, $D=0.793$). The DESs therefore performed better than the organic solvents and can suitably replace same in the extraction of BTX from waste tyre pyrolysis gasoline.

Keywords Waste tyre pyrolysis gasoline · Benzene-toluene-xylenes · Liquid–liquid extraction · Choline chloride · Ethylene glycol · Glycerol · Urea · Separation factor

Introduction

Pyrolysis is considered one of the most efficient and cost-effective methods of managing the huge amount of waste tyres generated every year across the globe. This process yields three main products, namely; non-condensable gas, pyrolysis oil, and char. Of these three products, the waste tyre pyrolysis oil (WTPO) is the most valuable. Though the proportion of each product arising from waste tyre pyrolysis vary depending on a number of operating conditions, WTPO yield of 47–58 wt % have been reported [1–3]. WTPO

contain remarkable amount of light aromatics like benzene-toluene-xylenes (BTX) and aliphatic hydrocarbons or olefins like limonene [4]. Fractional distillation of WTPO, similar to distillation of crude oil in the refinery, would yield more useful and lucrative fractions such as gasoline, kerosene, diesel and light heating oil. In a recent study, the gasoline fraction from vacuum distillation of WTPO, waste tyre pyrolysis gasoline (WTPG) obtained at boiling range < 180 °C, was reported to contain 58% aromatics [5]. WTPG is thus a good source of aromatics, just like naphtha or reformat or pyrolysis gasoline of crude oil refinery.

Separation of aromatics from its mixture with aliphatics, as obtained in WTPG and naphtha, is commercially done by solvent extraction using volatile organic solvents like sulfolane (SUF), dimethylformamide (DMF) and diethylene glycol (DEG). The high cost of this state-of-the art separation method due largely to the cost of secondary recovery of

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aromatics from the extract phase and environmental consideration have necessitated search for non-volatile and green solvent such as ionic liquid (IL) and deep eutectic solvent (DES) [6–9].

Ionic liquids have been explored as extracting solvent for aromatic-aliphatic mixtures in numerous studies. Ferreira et al. [10] and Lyu et al. [11] provide a very comprehensive review of such works. Using both experimental liquid–liquid equilibrium data (LLE) and the conductor-like screening model for real solvents (COSMO-RS), both reviews were able to reveal the effect of such factors as aliphatic chain length, aromatic side chain, IL cation and IL anion on the distribution coefficient and selectivity. They concluded that COSMO-RS can be utilized for the preliminary design of tailor-made ILs to give desired values of distribution coefficient and selectivity in the extraction of aromatics from aliphatics. However, the key factors militating against the commercial use of ILs for this purpose are its difficulty of synthesis and high cost of production [8, 12].

Deep eutectic solvents (DESs) are analogues of ILs, which offer advantage in terms of its relative ease of synthesis, cheap cost and green nature (biodegradable and low toxicological properties) [13, 14]. Several studies have investigated the performance of DESs, synthesized from various hydrogen bond acceptors (HBA) and hydrogen bond donors (HBD), in the extraction of different aromatic-aliphatic mixtures. Hadj-Kali et al. [8] provide a comprehensive review of such studies. Other more recent works in this regard include Shekaari et al. [14–16] and Warrag et al. [17]. Drawing from the classification of some chlorine chloride-based DES (Choline chloride/urea, choline chloride/glycerol, choline chloride/ethylene glycol) as polar solvents because of their relatively higher values of the Hildebrand and Hansen solubility parameters compared to molecular solvents and ILs [18], our group recently investigated the performance of these DESs in the extraction of benzene from n-hexane [19].

The superior performance of ILs and DESs relative to the conventional solvent (Sulfolane) for extraction of aromatics from aliphatics have been well reported. For example, Guo et al. [20] investigated the capacity of two ILs, 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl) imide [EMIM][NTf₂] and 1-ethyl-3-methylimidazolium ethylsulfate [EMIM][EtSO₄], and sulfolane for the extraction of benzene from n-hexane at 303.15 K and 101.3 kPa. Their result indicates the following maximum values of selectivity and distribution coefficient for the solvents: [EMIM][EtSO₄] ($S=67.72$, $D=0.6288$); [EMIM][NTf₂] ($S=40.61$, $D=1.3613$); SUF ($S=42.38$, $D=0.7231$). Similarly, Usman et al. [19] investigated the performance of DESs in the extraction of benzene from n-hexane at 303.15 K and 101.3 kPa and reported the following values of maximum selectivity and distribution coefficient: choline chloride/glycerol (1:2) ($S=462.00$, $D=0.72$); choline chloride/urea

(1:2) ($S=126.00$, $D=0.15$); and choline chloride/ethylene glycol (1:2) ($S=31.24$, $D=0.4729$).

Though the findings of the aforementioned ILs and DESs reveal highly promising values of distribution coefficient and selectivity, they were all based on model aromatic-aliphatic mixture with only one species of each. Few studies used real mixture containing multi-component of aromatics and aliphatics. This study intends to conduct a comparative evaluation of the performance of five solvents (SUF, DMF, DEG, and two DESs) for the extraction of BTX from WTPG. An ASPEN plus simulation was carried out to generate liquid–liquid equilibria (LLE) data for the pseudo-ternary systems {WTPG + BTX + solvent (SUF/DMF/DEG/DES1/DES2)}. The two DESs are choline chloride-based (DES1: choline chloride/ethylene glycol; DES2: choline chloride/glycerol in molar ratios 1:2) as extracting solvents for the extraction of BTX from WTPG. Performance evaluation was based on selectivity (S) and solute (BTX) distribution coefficient (D).

ASPEN plus simulation

Liquid–liquid equilibria (LLE) data were simulated in Aspen plus V 9 process simulator using the activity coefficient model of non-random two liquid (NRTL). The choice of NRTL over other activity coefficient such as UNIQUAC and Wilson was informed by a number of studies that reveal the superiority of NRTL in simulation of LLE data for separation of aliphatic–aromatic systems [20–23]. Seven LLE data for different ternary systems were so simulated in this study. The first two are the n-hexane + benzene + sulfolane and n-hexane + benzene + N-formylmorpholine ternary systems whose experimental data were recently reported in the literature [14] to serve as validation for the protocol adopted in this study. The remaining five are the actual case studies for the present work, and involves the pseudo-ternary systems of WTPG-BTX-solvent (SUF, DEG, DMF, DES1, DES2). The DESs are based on choline chloride as hydrogen bond acceptor and ethylene glycol/glycerol as hydrogen bond donor in molar ratio 1:2, and named DES1 and DES2, respectively. To perform the LLE simulation, the DESs were defined as pseudo-component in the Aspen Plus V 9 process simulator. The following DES properties were added in the simulator to define the pseudo-component: density, molecular weight, normal boiling temperature and viscosity. Subsequently, viscosities, heat capacities and surface tensions of DES were estimated using the default methods implemented in the Aspen Properties system for pseudo-components. To simplify the multicomponent system in the tyre pyrolysis gasoline, hydrocarbons forming the WTPG was limited to benzene, toluene, p-xylene, n-hexane, n-heptane, and n-octane and these were selected as conventional

components from the Aspen Plus database. It was assumed that n-hexane, n-heptane, and n-octane represented the aliphatic phase while benzene, toluene and p-xylene represented the aromatic phase.

Results and discussion

Validation

Shekaari et al. [14] investigated sulfolane and N-formylmorpholine as extracting solvents for the separation of n-hexane (aliphatic) from benzene (aromatic). The experimentally generated LLE data at 303.15 K satisfied the necessary consistency data, and NRTL model was found to satisfactorily correlate the data. It was therefore considered appropriate to use these data, the LLE data for the ternary systems n-hexane(1) + benzene(2) + sulfolane(3) and n-hexane(1) + benzene(2) + N-formylmorpholine(3), for validating the simulation capacity and accuracy of ASPEN plus. Table 1 show the mole fraction of n-hexane (x_{11}) and benzene (x_{21}) in the raffinate phase from the experimental data of Shekaari et al. [14] against the Aspen simulated values at 303.15 K. Similarly, the mole fraction of n-hexane (x_{13}) and benzene (x_{23}) in the extract phase for experimental and simulated data are also presented in Table 1. The distribution coefficient (D) and selectivity (S) were evaluated using Eqs. (1) and (2), respectively.

$$D = \frac{x_{23}}{x_{21}} \quad (1)$$

$$S = \frac{x_{23} \cdot x_{11}}{x_{21} \cdot x_{13}} \quad (2)$$

D was evaluated using experimental data (D_{exp}) and simulated data (D_{sim}). Similarly, S was evaluated using

experimental data (S_{exp}) and simulated data (S_{sim}). These values are all shown in Table 1. The error in simulated values relative to the experimental values were calculated using Eqs. (3) and (4) for D and S , respectively and presented in Table 1.

$$\% \text{ error in } D = \frac{D_{\text{sim}} - D_{\text{exp}}}{D_{\text{exp}}} \times 100 \quad (3)$$

$$\% \text{ error in } S = \frac{S_{\text{sim}} - S_{\text{exp}}}{S_{\text{exp}}} \times 100 \quad (4)$$

Fig. 1a is a plot of distribution coefficient (D_{exp} , D_{sim}) against mole fraction of benzene in the extract phase (x_{23}). This figure reveals a similar pattern for both D_{exp} and D_{sim} . Figure 1b show a similar pattern with an almost perfect match between S_{sim} and S_{exp} . Figure 1c show the error in D and S , in all cases the error is less than 6%. This clearly shows that simulation is fairly accurate and the simulation protocol is good for the intended purpose.

Table 2 present the experimental and simulated LLE data for the second case study, n-hexane + benzene + N-formylmorpholine. Figure 2a show a plot of D_{exp} and D_{sim} versus x_{23} while Fig. 2b shows a plot of S_{exp} and S_{sim} against x_{23} . A similar trend was displayed by D_{exp} and D_{sim} against x_{23} . In Fig. 2b, a near perfect match between S_{sim} and S_{exp} is evident. The % error in D and S displayed in Fig. 2c indicates that the highest error is less than 10%. This is considered good enough for the comparative study intended in this work. The simulated LLE data in both case studies 1 and 2 clearly show the capacity of the Aspen plus simulation protocol adopted in this study to generate LLE data, particularly its accuracy in the determination of distribution coefficient and selectivity thus validating the simulation protocol.

Table 1 Experimental and simulated LLE data for n-hexane + benzene + sulfolane at 303.15 K and 1 atm

Raffinate phase				Extract phase				Distribution coefficient		Selectivity		% error	
Experimental		Simulated		Experimental		Simulated		D_{exp}	D_{sim}	S_{exp}	S_{sim}	D	S
x_{11}	x_{21}	x_{11}	x_{21}	x_{13}	x_{23}	x_{13}	x_{23}						
0.9976	0	0.968	0	0.0142	0.0082	0.0139	0						
0.9144	0.0826	0.8861	0.0843	0.0164	0.0708	0.016	0.0684	0.857	0.811	47.791	44.936	− 5.34	− 5.97
0.7619	0.2264	0.7714	0.2191	0.0224	0.1684	0.0218	0.1626	0.744	0.742	25.300	26.260	− 0.23	3.80
0.6386	0.347	0.654	0.3346	0.0302	0.2711	0.0296	0.2626	0.781	0.785	16.520	17.340	0.45	4.96
0.5539	0.4268	0.5748	0.417	0.0384	0.3315	0.0378	0.3209	0.777	0.770	11.204	11.702	− 0.92	4.45
0.4751	0.4915	0.4734	0.4786	0.0499	0.3805	0.0486	0.368	0.774	0.769	7.371	7.490	− 0.68	1.61
0.3455	0.5692	0.3552	0.5587	0.0856	0.4963	0.0833	0.4819	0.872	0.863	3.519	3.678	− 1.08	4.51
0.2949	0.5896	0.2816	0.5731	0.0919	0.5138	0.0906	0.4981	0.871	0.869	2.796	2.701	− 0.26	− 3.40

Fig. 1 **a** Distribution coefficient as function of benzene composition in the extract phase. **b** Selectivity as a function of benzene composition in the extract phase. **c** Percent error in D and S as a function of benzene composition in the extract phase

(a) Distribution coefficient as function of benzene composition in the extract phase

(b) Selectivity as a function of benzene composition in the extract phase

(c) Percent error in D and S as a function of benzene composition in the extract phase

Table 2 Experimental and simulated LLE data for n-hexane + benzene + N-formylmorpholine at 303.15 K and 1 atm

Raffinate phase				Extract phase				Distribution coefficient		Selectivity		% error	
Experimental		Simulated		Experimental		Simulated							
x_{11}	x_{21}	x_{11}	x_{21}	x_{13}	x_{23}	x_{13}	x_{23}	D_{exp}	D_{sim}	S_{exp}	S_{sim}	D	S
0.9985	0	0.9887	0	0.0002	0	0.0002	0						
0.8427	0.1123	0.8627	0.1099	0.0245	0.0713	0.0244	0.0709	0.635	0.645	21.838	22.810	1.61	4.45
0.7963	0.1492	0.8171	0.1531	0.0318	0.0977	0.0314	0.0965	0.655	0.630	16.397	16.402	− 3.74	0.03
0.7421	0.2082	0.7397	0.2279	0.0402	0.1399	0.0396	0.1379	0.672	0.605	12.404	11.303	− 9.95	− 8.88
0.5618	0.3401	0.555	0.3396	0.0684	0.2413	0.0673	0.2364	0.709	0.696	5.827	5.741	− 1.89	− 1.49
0.4722	0.3722	0.4663	0.3721	0.0823	0.2571	0.0809	0.2534	0.691	0.681	3.963	3.925	− 1.41	− 0.96
0.4231	0.3955	0.4141	0.3883	0.09	0.2738	0.089	0.2692	0.692	0.693	3.255	3.226	0.14	− 0.89
0.3913	0.4113	0.4002	0.4029	0.095	0.2851	0.0938	0.2809	0.693	0.697	2.855	2.975	0.58	4.18

Extraction of BTX from WTPG

The performance evaluation of three organic solvents (SUF, DEG, DMF) and two deep eutectic solvents (DES1, DES2) in the extraction of pseudo-component (BTX) from WTPG was done, based on the Aspen simulated LLE data at 323.15 K for each solvent, using distribution coefficient (D) and selectivity (S) as metrics as defined by Eqs. (1) and (2). As used in the referred equations, x_{11} and x_{13} represent mole fraction of WTPG in the raffinate and extract phase, respectively while x_{21} and x_{23} represent the mole fraction of BTX in raffinate and extract phase, respectively.

Performance of organic solvents (SUF, DEG, DMF)

Tables 3, 4 and 5 show the simulated LLE data for the pseudo-ternary systems of WTPG-BTX-organic solvent (SUF/DMF/DEG), respectively. The distribution coefficient for BTX (D) and selectivity (S) values are also displayed in the Tables and plotted in Figs. 3, 4 and 5 against the composition of BTX in the extract phase. These tables and figures reveal decreasing values of selectivity as the composition of BTX in the extract phase increases. Similar trend was reported in the extraction one component aromatic from one component aliphatic [12, 24]. The highest value of S for the organic solvents is in the following decreasing order: SUF (55.371) > DMF (25.336) > DEG (17.531), thus sulfolane outperformed DMF and DEG in this regard. The BTX distribution coefficient for all the organic solvents are generally less than 1, with no marked difference between the values obtained for the three organic solvents. Sulfolane is therefore regarded as the best organic solvent for BTX extraction from WTPG, no wonder it is the commonly used extracting solvent for aromatics in the industries. It is insightful to compare the values obtained in this study with literature values for sulfolane. Tripathy et al. [24] reported S values varying

from 30 to 2 and D values varying from 0.48 to 0.7 in the extraction of toluene from n-heptane using sulfolane as extracting solvent at 323.15 K. In another study using sulfolane to extract benzene from n-hexane, Mahmoudi and Lotfollahi [6] reported the following values: D (0.49–0.72) and S (7.12–20.14). In a recent study, Guo et al. [20] reported the following values: D (0.7722–0.9129) and S (42.07–1.35) in the extraction of benzene from n-hexane using sulfolane at 323.15 K. The relatively higher values of D and S in the present study may be attributed to multi-component extraction in addition to simulation error. Sulfolane will be used as benchmark for the comparative analysis in this study.

Performance of deep eutectic solvents (DES1, DES2)

Tables 6 and 7 show the simulated LLE data, BTX distribution coefficient (D) and selectivity (S) for the pseudo-ternary systems of WTPG + BTX + DES1 (ChCl:EG) and WTPG + BTX + DES2 (ChCl:Gly) at 323.15 K, respectively and plotted in Figs. 6 and 7. The D values for the WTPG + BTX + DES1 system are greater than 1 for all compositions while it is less than 1 for the WTPG + BTX + DES2 system. The ethylene glycol based DES does better than the organic solvents and the glycerol-based DES on this account. However, Alkhaldi et al. [22] affirmed that D value greater than 0.4 is acceptable standard to achieve feasible separation for liquid–liquid extraction process. The S values are significantly greater than 1 for both systems, and it decrease with increasing composition of BTX in the extract phase. The S values for DES2 is remarkably higher than the values for DES1. The maximum value of S for DES2 is 378.283 while the value for DES1 is 77.364. The glycerol-based DES therefore show superior performance as extracting solvent for aromatics (BTX). This is in agreement with the findings of our earlier work [19].

Fig. 2 **a** Distribution coefficient as function of benzene composition in the extract phase. **b** Selectivity as a function of benzene composition in the extract phase. **c** Percent error in D and S as a function of benzene composition in the extract phase

(a) Distribution coefficient as function of benzene composition in the extract phase

(b) Selectivity as a function of benzene composition in the extract phase

(c) Percent error in D and S as a function of benzene composition in the extract phase

Table 3 Simulated LLE composition, Distribution coefficient (D) and Selectivity (S) for WTPG + BTX + SUF system at 323.15 K

Raffinate phase		Extract phase		D	S
x_{11}	x_{21}	x_{13}	x_{23}		
0.8518	0.1063	0.0100	0.0691	0.650	55.371
0.7371	0.2127	0.0130	0.1384	0.651	36.894
0.6201	0.3183	0.0280	0.2086	0.655	14.514
0.5006	0.4215	0.0560	0.2812	0.667	5.964
0.3781	0.5192	0.1060	0.3593	0.692	2.468
0.2503	0.6033	0.2120	0.4510	0.748	0.883
0.2012	0.7288	0.3170	0.5512	0.756	0.480

Table 4 Simulated LLE composition, Distribution coefficient (D) and Selectivity (S) for WTPG + BTX + DMF system at 323.15 K

Raffinate phase		Extract phase		D	S
x_{11}	x_{21}	x_{13}	x_{23}		
0.9706	0.0294	0.0301	0.0231	0.786	25.336
0.8843	0.0307	0.0528	0.0241	0.785	13.148
0.7988	0.0335	0.1074	0.0251	0.749	5.573
0.7142	0.0378	0.1640	0.0269	0.712	3.099
0.6301	0.0442	0.2230	0.0299	0.676	1.911
0.5461	0.0533	0.2849	0.0342	0.642	1.230
0.4615	0.0667	0.3505	0.0407	0.610	0.803
0.3747	0.0874	0.4213	0.0508	0.581	0.517

Table 5 Simulated LLE composition, Distribution coefficient (D) and Selectivity (S) for WTPG + BTX + DEG system at 323.15 K

Raffinate phase		Extract phase		D	S
x_{11}	x_{21}	x_{13}	x_{23}		
0.9589	0.0518	0.0434	0.0411	0.793	17.531
0.9087	0.0608	0.0541	0.0449	0.738	12.404
0.8557	0.1210	0.0681	0.0509	0.421	5.286
0.7987	0.1801	0.0866	0.0598	0.332	3.062
0.7356	0.2374	0.1113	0.0729	0.307	2.030
0.6632	0.2921	0.1457	0.0929	0.318	1.448
0.5732	0.3427	0.1979	0.1264	0.369	1.068
0.4124	0.3811	0.3212	0.2185	0.573	0.736

Comparative analysis

Considering its current usage as solvent for the extraction of aromatics from aliphatics in the industries and its superior performance relative to the other two organic solvent (DMF and DEG), it is reasonable to use sulfolane as benchmark for this comparative analysis with the DESs. The BTX distribution coefficient (D) value is the following order DES1 > SUF > DES2, while the S values is in the following order DES2

Fig. 3 Distribution coefficient and Selectivity as function of BTX composition in the extract phase for WTPG + BTX + SUF **Fig. 4** Distribution coefficient and Selectivity as function of BTX composition in the extract phase for WTPG + BTX + DMF **Fig. 5** Distribution coefficient and Selectivity as function of BTX composition in the extract phase for WTPG + BTX + DEG

Table 6 Simulated LLE composition, Distribution coefficient (D) and Selectivity (S) for WTPG+BTX+DES1 (ChCl:EG) system at 323.15 K

Raffinate phase		Extract phase		D	S
x_{11}	x_{21}	x_{13}	x_{23}		
0.8906	0.1094	0.0151	0.1435	1.312	77.364
0.8599	0.1193	0.0301	0.1604	1.345	38.410
0.8267	0.1310	0.0595	0.1798	1.373	19.070
0.7903	0.1450	0.0880	0.2025	1.397	12.542
0.7495	0.1623	0.1155	0.2295	1.414	9.176
0.7023	0.1847	0.1416	0.2629	1.423	7.060
0.6443	0.2161	0.1659	0.3073	1.422	5.523
0.5579	0.2719	0.1862	0.3799	1.397	4.186

Table 7 Simulated LLE composition, Distribution coefficient (D) and Selectivity (S) for WTPG+BTX+DES2 (ChCl:Gly) system at 323.15 K

Raffinate phase		Extract phase		D	S
x_{11}	x_{21}	x_{13}	x_{23}		
0.9325	0.0659	0.0015	0.0401	0.608	378.283
0.8560	0.1398	0.0233	0.0917	0.656	24.098
0.7687	0.2214	0.0323	0.1275	0.576	13.705
0.6673	0.3111	0.0415	0.1550	0.498	8.011
0.5412	0.4108	0.0497	0.2058	0.501	5.455
0.4916	0.4921	0.0562	0.2356	0.479	4.188

Fig. 6 Distribution coefficient and Selectivity as function of BTX composition in the extract phase for WTPG+BTX+DES1 (ChCl:EG) system

> DES1 > SUF. The maximum value of S for the solvents as follows: 378.283 (DES2); 77.364 (DES1); and 55.371 (SUF). Both DES1 and DES2 outperform SUF in terms of selectivity; they are therefore very suitable replacement for sulfolane in the extraction of aromatics from aliphatics.

Fig. 7 Distribution coefficient and Selectivity as function of BTX composition in the extract phase for WTPG+BTX+DES2 (ChCl:Gly) system

There is also the need to consider their physicochemical properties as the best extracting solvents have good selectivity and capacity, high thermal stability, good availability, low cost, high surface tension, and low to moderate viscosity [25]. Table 8 show some physical properties of the five solvents considered in this study. Compared to sulfolane, the viscosities of DES1 and DES2 are significantly higher. This has implication for the cost of pumping; hence there is the need to add a co-solvent to temper the viscosity of these DESs. On the other hand, the surface tensions of the DESs are relatively higher than that of sulfolane.

Conclusion

The performance of three commonly used organic solvents for extraction of aromatics from aliphatics, namely, sulfolane, dimethylformamide, diethylene glycol was compared with two choline chloride-based deep eutectic solvents in the extraction of benzene-toluene-xylene from waste tyre pyrolysis gasoline. Aspen plus simulation of the pseudo-ternary liquid–liquid equilibria data for the systems {WTPG + BTX + solvent (SUF/DMF/DEG/DES1/DES2)} was carried out at 323.15 K. The results revealed the following maximum values of selectivity and distribution coefficients for the solvents: DES2 ($S=378.283$, $D=0.656$); DES1 ($S=77.364$, $D=1.423$); SUF ($S=55.371$, $D=0.756$); DMF ($S=25.336$, $D=0.786$) and DEG ($S=17.531$, $D=0.793$). The DESs therefore performed better than the organic solvents and can suitably replace same in the extraction of BTX from waste tyre pyrolysis gasoline. There is however the need to reduce the viscosity of the deep eutectic solvents using co-solvent. It can be concluded that deep eutectic solvent formed by mixing choline chloride and glycerol or ethylene glycol are suitable replacement for sulfolane in the extraction of BTX from waste tyre pyrolysis gasoline.

Table 8 Physicochemical properties of solvents considered in this study

Solvent	MW (g/mol)	T _m (K)	ρ (g/cm ³)	μ (mPa.s)	P ^{vap} (Pa)	σ (mN/m)	References
SUF	120.17	301.55	1.26	10.35	9.1	47.95	[25]
DMF	73.09	212.75	0.94	0.90	370	35.83	[25]
DEG	106.12	262.85	1.11	30.2	17	27.93	[25]
DES1	107.93	239.68	1.19	281	1.5	58.07	[26]
DES2	263.76	236.89	1.12	45		58.74	[27]

Acknowledgements The authors would like to thank “Professor Ayo Francis Ogunye Trust Foundation, University of Lagos” for the research grant (VC/OA/E.29/Vol. 9).

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