Simulation Study of Ionic Liquid Utilization for Desulfurization of Model Gasoline

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ABSTRACT: *With the increased amount of focus is being put towards reducing the emissions results from fossil fuel usually composed of hydrocarbons and impurities. The study aim at utilizing the ability of 1-octyl-3-methylimidazolium tetrafluoroborate [OMIM][BF4]. Ionic liquid as the suitable solvent for the extraction of the thiophene and its derivatives from the model gasoline. The process simulation was performed on the ASPEN plus(V8.8) with the help of UNIFAC as the thermodynamic model, previously NRTL was used as the method to calculate the interaction. The different parametric analysis was calculated for the removal of thiophene-based compounds from model gasoline. Outcomes acquired shows the significance of imidazolium-based ionic liquid(ILs) 1-octyl-3-methylimidazolium tetrafluoroborate towards the separation about S-contents from the liquid fuels at an optimum process condition of 30 °C and 2 bar pressure with the 1:1 ratio of ionic liquid and model gasoline which confirms the experimental outcomes obtained previously in the literature. By using these mild conditions, easy phase separation, high reusability and various other process parameters have been established based on the process simulation model using ASPEN plus.*

KEYWORDS *Imidazolium based ionic liquid; Unifac; Gasoline; Desulfurization; Thiophene.*

INTRODUCTION

Presently greater accentuation is begun to be put towards the control of environmental contamination [1-7, 33-34]. The significant wellspring of contamination is due to the consumption of petroleum derivative which is principal because of the excessive demand for energy [2-7, 29, 31]. So, at the same time, it has turned out to be imperative to battle the energy emergency and in addition environmental effects [30]. These measures are needed to be taken in light of the new world's ecological strategies regarding the diminishing of the sulfur-containing mixes from the fuel products [1]. In this way, the various nations have built up an extremely stringent

the approach in order to control the emission and environmental problems. The European Union likewise connected an exceptionally stringent strategy in 2005 which expressed that the sulfur content in the fossil fuel to be at most 50 ppm [8-9, 33-34]. The primary purpose of embracing these strict rules is a result of the way that sulfur discharges from various fuel items influences human well-being and furthermore greatly alter the general ecological conditions as well [4]. This sulfur content causes acid rain, ozone consumption and influences the human respiratory system [4]. Sulfur present in these fossil fuels causes the controlling system to not operate

efficiently. Considering pollution causing components refining sector needs to work towards the removal of these impurities and carry out optimization in the process which would ensure the least amount of contamination [3]. The standard technology utilized by the refineries for the sulfur expulsion is the hydrodesulphurization (HDS technology) [7, 14, 33]. This process uses the hydrogenation for the treatment of the aromatic compounds (for example, benzothiophene, dibenzothiophene, thiophene, 2-butyl benzothiophene, and their subsidiaries) since they are the ones which are available at the most astounding focus in the refinery streams contrasted with the aliphatic compounds[5-7]. These days the conditions utilized by the refineries for sulfur, content removal are usually at the elevated temperature and pressured conditions. Some alkylated components of thiophene are very impervious to hydrotreatment and hard to expel by the HDS technology which results in a decrease in the octane number of the fuel product [14, 33-34]. So, the removal of the sulfur substance from the fuel results in increasing the cost of the process. Sulfur removal by HDS technology as of now needs up gradation to the present system. Unconventional new choices have been considered for the profound desulphurization, for example, oxidative desulphurization, adsorption, etc. as an alternative to the non-hydro treating technology[2-7, 14, 33-34]. So to overcome these issues a new class of solvents has been studied widely known to be as "ionic liquids". With their unique ability to work as an environmentally friendly solvent, the Ionic liquid is generally termed as the "green solvents". This name was given due to their unique ability both physically and chemically. Ionic liquids (ILs) are the heterocyclic compounds belong to the molten salt group and mostly composed of asymmetric and bulky cations (organic) and anions (Organic/inorganic) groups [10]. They generally possess the unique property of non-flammability which makes them non-hazardous for the industrial scale. Generally, most of their ionic liquids exhibit negligible vapor pressure under common process conditions in this way they can go to regeneration easily and negligible loss to the environment so fewer pollution hazards. Generally, ionic liquid has a unique property of being thermally stable and chemically stable. They are normally in the liquid state over the wide temperature range [8, 33, 34]. They have the solvation capacity for organic and inorganic types of compounds, also

with the proper selection of the cation and anion for the IL synthesis, this unique feature can allow the scientists and engineers to tailor their solvation ability for the number of solutes. Due to their unique property of non-volatility and good stability, they are being considered for the separation process. For these properties shown by the ionic liquid emphasis is started to be put towards the use of this special class of liquids for the extraction of the sulfur impurities from the gasoline or diesel. So the efforts are being put in order to remove thiophene and its derivatives from the fuel by utilizing ionic liquid and using the extraction process. A large number of ionic liquids have been synthesized over the period and choosing a particular ionic liquid for investigating its properties are important previously the authors have utilized the same ionic liquid but with varying anions like (NTF$_2$, SCN, PF$_6$, etc)[34]. Most of the authors in their analysis of the process that ionic liquids consisiting of imidazolium base cation and tetrafluoroborate [BF$_4$] based anion are the most effective in extracting sulfur impurities from the gasoline[33].

Advantages of desulfurization using ionic liquids lead us to the performance under mild conditions, easy phase separation, high reusability, and adjustable extraction ability. So a process model is designed for the selective removal of sulfur based impurities from the model gasoline [33]. In the context of this article, the aim is to incorporate the recently proposed and calculation of the ionic liquid on experimental bases into the process simulation software and thus enabling us to design the process scheme to be used industrially and study various feasibility and the process constraints to scale up the process and its viability for the industry.

THEORITICAL SECTION
Selection of the ionic liquid

To select an ionic liquid for the desulphurization process certain factors are required. First of all, the solvent that is to be utilized can be easily regenerated. Secondly, the components of the fuel apart from the sulfur-based compounds should be negligibly soluble in the extracting solvent. 1-octyl-3-methyl imidazolium tetrafluoroborate [OMIM][BF$_4$] was selected as the possible solvent to be used in this simulation study. It is considered because they are being capable of efficiently extract the sulfur contents like dibenzothiophene (DBT) from fuel oils because during the extraction process

it forms the π-π interaction between the aromatic and the thiophene ring of the sulfur-containing compound [10-12]. Also while selecting ionic liquid hydrophobic and hydrophilic nature of the solvent is also important to be known because it affects the solvation capacity of the ionic liquid. The other reason for the selection of specific this ionic liquid is because of the fact that to model ionic liquid on software ASPEN Plus (v8.8) various physical and chemical properties are required as well as the binary interaction parameter. So based on all these factors this class of ionic liquid was chosen. The process was modeled on the ASPEN plus software using the thermodynamic model UNIFAC. To validate the experimental results previously obtained using [OMIM][BF$_4$] for the extraction of impurities from the gasoline [13].

Thermodynamics properties prediction

The thermodynamic properties of the ionic liquid are modeled on the basis of the UNIFAC. Such a model has generally described the ionic liquid well. They depend on the binary interaction parameters for each part of he species present in the system. UNIFAC is a thermodynamic model which computes the activity coefficient of liquid in terms of the constants which shows the area and size of the different functional groups present in the liquid mixture. The size and area data are usually obtained from the molecular structure data as shown in Table 3, and binary interaction parameters are calculated from the equilibrium data are shown in Table 2 which is based on the functional groups incorporated to make the molecule. Table 1 highlights the different functional groups contributed (representation of each group in the molecule) for the molecules used in this simulation work for the UNIFAC model [12]. Since we are using the UNIFAC functional group based approach so the functional groups contributed to the molecules also need to be specified on the ASPEN plus(v8.8) platform since mostly the UNIFAC model works on the functional group contributions.

The ionic liquid is decomposed into various functional groups and there binary interaction parameters were established which is already defined in the UNIFAC model [12]. The volume parameter and surface area parameters are also specified in Table 3 which depends on the molecular van dar Waals volume and surface area [12].

Since ionic liquids are not yet included in the database of the ASPEN plus platform. So to perform
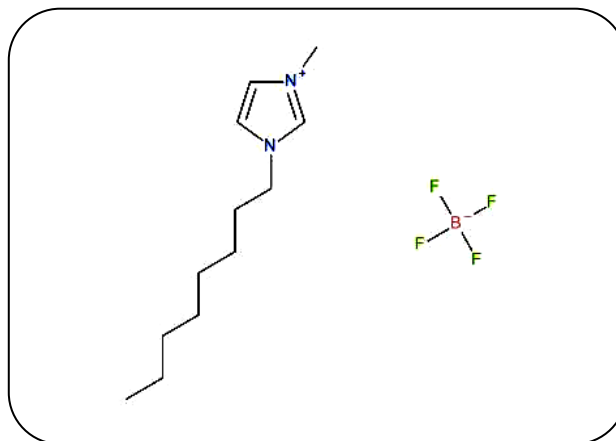

Fig. 1: structural representation of [OMIM][BF$_4$].

simulation the scalar and temperature dependent properties of the ionic liquid need to be specified into the software platform.

Scalar properties

Scalar properties include the critical and the volumetric properties of the model gasoline as well as an ionic liquid, the normal boiling, accentric factor which then can be utilized in various thermodynamics relations. The detailed scalar properties of the [OMIM][BF$_4$] is illustrated in Table 5. These properties are calculated using the group contribution method as described by *Valderrama* [15] as follows.

$$Tb = 198.2 + \sum n\Delta TbM \tag{1}$$

$$Tc = \frac{Tb}{\left[0.5703 + 1.121\sum n\Delta TM - \left(\sum n\Delta TM\right)^2\right]} \tag{2}$$

$$P_c = \frac{M}{\left(0.2573\left(\sum n\Delta TM\right)^2\right)} \tag{3}$$

$$V_c = 6.75 + \sum\sum n\Delta T_M \tag{4}$$

$$\omega = \frac{(Tb-43)(Tc-43)}{(Tc-Tb)(0.7Tc-43)}\log\left(\frac{Pc}{Pb}\right) - \tag{5}$$

$$\left(\frac{(Tc-43)}{(Tc-Tb)}\right)\log\left(\frac{Pc}{Pb}\right) + \log\left(\frac{Pb}{Pc}\right) - 1$$

Where T_b is normal boiling temperature, T_{bM} is a contribution to normal boiling temperature, T_c is critical temperature, n is number of times that a group appears in a molecule Table 1, T_M is a contribution to the critical temperature, P_c is critical pressure, M is molecular mass, P_M is a contribution to critical pressure, V_c is critical volume,

Table 1: Different functional group present in each of the components involved in the simulation based on UNIFAC MODEL[12].

Components	Function groups						
	C	CH	CH_2	CH_3	ACH	C_4H_4S	$MIMBF_4$
Hexane	0	0	4	2	0	0	0
i-Octane	1	1	1	5	0	0	0
Cyclohexane	0	0	4	2	0	0	0
Toulene	0	0	0	1	6	0	0
Pentane	0	0	3	2	0	0	0
Thiophene	0	0	0	0	0	1	0
Dibenzothiophene	0	0	0	0	8	1	0
OMIMBF4	0	0	7	1	0	0	1

Table 2: Binary interaction between the functional groups involved in this simulation according to UNIFAC model[12].

m/n	$MIMBF_4$	C	CH	CH_2	CH_3	ACH	C_4H_4S
$MIMBF_4$	0	145.8	145.8	145.8	145.8	-163.26	175.06
C	400.89	0	0	0	0	61.13	92.99
CH	400.89	0	0	0	0	61.13	92.99
CH_2	400.89	0	0	0	0	61.13	92.99
CH_3	400.89	0	0	0	0	61.13	92.99
ACH	602.87	-11.12	-11.12	-11.12	-11.12	0	-39.16
C_4H_4S	240.9	-8.479	-8.479	-8.479	-8.479	23.93	0

V_M is a contribution to the critical volume, P_b is normal boiling pressure and is an accentric factor. The values of T_{bM}, T_M, P_M and V_M are listed in Table 4.

Temperature dependent properties

Usually, the temperature dependent properties are evaluated with the set of empirical equations which are based on the experimental evaluations. These properties are important in simulation on the ASPEN plus (v8.8) as these will guide us to analyze the different energy necessity of the system. The temperature dependent properties of the ionic liquid are extracted from the NIST database for ionic liquids and then incorporated into the simulation platform Table 5 [17-28].

Process simulation
Selection of model gasoline and sulfur species

Real gasoline contains a wide range of chemical constituents mainly are the hydrocarbons in the range of C_5-C_{10} with a negligible amount of further other organic components. Since the availability of the data for all the components is impossible so we selected hexane, cyclohexane, i-octane, toluene as the constituents to represent the model gasoline for the simulation because not all the functional groups' interaction parameters are available to be incorporated into the ASPEN Plus. These compounds are most commonly been used for the representation of the gasoline. There are also many types of thiophene-based derivatives that can be found in the gasoline but for this simulation study, we have chosen thiophene and dibenzothiophene (DBT) as the key compound to target during the extraction process.

A thermodynamic model for simulation

UNIFAC commonly called the UNIQUAC which is utilized for the estimation of the nonelectrolyte movement in the nonideal mixture[12]. UNIFAC consolidates the idea of the functional group interaction

Table 3: Volume and surface area parameters of the functional groups according to UNIFAC[12].

Functional Group	R	Q
MIMBF$_4$	6.5669	4.005
C	0.2195	0
CH	0.4469	0.228
CH2	0.6744	0.54
CH3	0.9011	0.848
ACH	0.5313	0.4
C$_4$H$_4$S	2.8569	2.14

Table 4: Parameters in group contribution method.

group	ΔT_{bM}	ΔT_M	ΔP_M	ΔV_M
Without rings				
-CH$_3$	23.58	0.0275	0.3031	66.81
-CH$_2$	22.88	0.0159	0.2165	57.11
-B	-24.56	−0.0264	0.0348	22.45
-F$^-$	−0.03	0.0228	0.2912	31.47
With rings				
=CH-	26.73	0.0114	0.1693	42.55
>N-	68.16	0.0063	0.0538	25.17
=N-	57.55	−0.0011	0.0559	42.15

Table 5: some scalar properties calculated of [OMIM][BF$_4$].

Scalar properties of [OMIM][BF$_4$]			
Molecular weight	Mw	282.1	-
Normal boiling point	Tb	313.55	C
Critical temperature	Tc	463.85	C
Critical pressure	Pc	16.02	bar
Critical volume	Vc	883.4	cm³/mol
Acentric factor	ω	1.0287	-
Specific gravity	S.G	1.11088	-

the idea and the UNIQUAC idea for the estimation of the binary interaction parameters[12]. UNIFAC additionally gives us the comprehension of the size and surface range of the individual components identified with the atomic structure of the parts. The anticipated movement coefficients can be utilized to produce double cooperation parameters in any abundance Gibbs energy model. In expansion to this, UNIFAC parameters are accessible for a large portion of the utilitarian gatherings in the blends so it can be chosen over the COSMO-RS display as it has better outcomes and the model can without much of a stretch be connected with the ASPEN plus®.

Simulation details

It has been substantially reported inside the previous results for the removal of sulfur impurities

Table 6: Temperature dependent properties of IL [OMIM][BF₄]

COMPONENT	[OMIM][BF₄]	[OMIM][BF₄]	[OMIM][BF₄]	[OMIM][BF₄]	[OMIM][BF₄]
Physical property	Ideal gas heat capacity	Liquid molar density	Liquid heat capacity	Liquid thermal conductivity	Liquid viscosity
Temperature units	C	C	C	C	C
Property name	CPIG	DNLTMLPO	CPLTMLPO	KLTMLPO	MULNVE
Property units	cal/mol-K	mol/cc	cal/mol-K	kcal-m/hr-sqm-K	cP
Polynomials for equation	-1.0540031	0.003968	115.5946	0.143098	-12.0742
	0	-2.23E-06	0.129243	-8.56E-05	11060.3
	0	-7.47E-10	0.000357	0	-3486590
	0	0	-5.02E-06	0	5.31E+08
	0	3	3.63E-08	2	-0.15
	0	-0.15	5	21.05	90
	-273.15	120	-77.27	61.25	
	726.85		94.74		

from the liquid fuels using an ionic liquid in the form of aromatics impurities located in the fuels and assist to achieve the focused separation of the extremely low sulfur gasoline. The principle concept of this simulation is to take a look at the impact of the usage of an ionic liquid for the elimination of sulfur impurities and to compare the experimental data with the simulation results. Since the ionic liquid is not available on the database of the ASPEN Plus (v8.8) so we need to rigorously define the structural aspects of the ionic liquid which include the volume and the surface area of the functional groups involved in the ionic liquid. The functional group numbers of the various functional groups of which ionic liquid constituents showed in Table 8 needs to be input into the ASPEN Plus due to the fact that ionic liquids are not present so every aspect needs to be specified in detail.

The temperature dependent properties for the selected ionic liquid such as ideal gas heat capacity parameters "CPIG-1", the heat of vaporization "DHVLDP-1", liquid viscosity "MULNVE", thermal conductivity "KLTMLPO-1", liquid vapour pressure "PLXANT-1/PLTDEPOL" calculated based on the experimental results [17-28]. Since ionic liquids are nonvolatile there Antoine equation should represent that value so for this, we are setting a value of -1×10^{10}. In addition of defining the temperature dependent properties some other physical property information are also needed to be specified such as normal boiling point "T_b", critical temperature "T_c", critical pressure "Pc", critical volume "V_C", andacentric

Table 7: Composition of the model gasoline used in the simulation.

Feed Components	COMPOSITION (wt %)
Hexane	30
Cyclohexane	25
i-octane	29
Toluene	10
Thiophene	100 ppm
DBT	100 ppm

factor "ω". These properties were calculated by the group contribution method as shown in Table 5 [13]. After defining the properties and binary interactions of the components, we will move towards the simulation environment and uses the extraction column with 10 stages working at 30⁰C and 2 bar Fig. 2. The effect of varying process parameters such as no of stages, temperature and pressure have also been studied and discussed later on The compositionsof the model gasoline selected for this simulation are as shown in Table 7.

RESULT AND DISCUSSION:
Sensitivity analysis
Number of stages in the extractor and ionic liquid

It has been known that as the stage number of the separation column increases the interaction between

Table 8: UNIFAC group ID and group number of the functional groups in the database of Aspen plus.

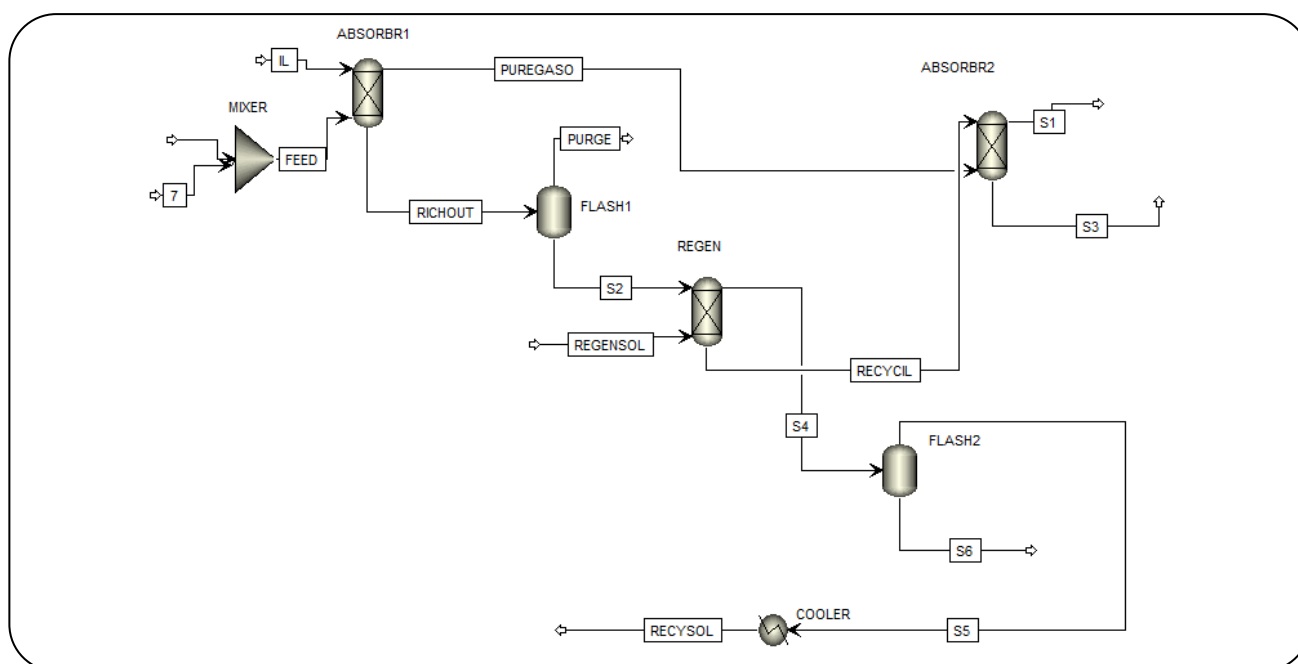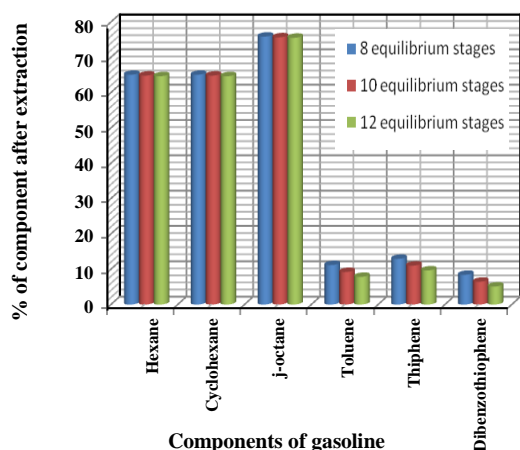| GROUP ID	GROUP NUMBER
C	1000
CH	1005
CH_2	1010
CH_3	1015
ACH	1105
C_4H_4S	3750

Fig. 2: Process simulation of gasoline desulfurization with ionic liquid [omim][bf4] at 30ᵒC ,2 bar and 1:1 of IL to gasoline.

the counter currently interacting liquid also increases. This was also evident from the simulation results obtained and the same pattern could be seen in the graphical Fig. 3. The results correspond well with the experimental results performed as shown in Table 9 [13]. So it was observed that adding more trays has an effect on the separation of the sulfur based impurities from the model gasoline up to a certain limit. So ultimately an adequate 8 stages absorber column is selected which would result in an efficient stage for separation as shown by the simulation result around 10% thiophene and <10% of dibenzothiophene remains in the stream after absorption with the ionic liquid shown in Fig. 3. Further increasing the stages would add up to increase the cost of the absorber while the removal efficiency does not improve significantly.

The operating temperature of the extraction column was also varied in the simulation to observe the various aspects of it on the separation efficiency and regeneration. On the removal of sulfur based impurities from the gasoline in the absorption column. Both Fig. 4a & 4b show that initially as we increase the temperature it does not affect the separation of DBT but further increase in the temperature results in an increasing amount of both thiophene and DBT in the extracted gasoline. So working at a lower temperature would be ideal for the process. Although higher temperature reduces the viscosity of the IL which results in better efficiency of the extraction according to the mass transfer principle. But in our case higher temperature significantly decreases the interaction between sulfur impurities and selected ionic liquid which ultimately decreases removal efficiency. So (30-40)ᵒC

Table 9: Comparison between the experimental and simulation result of %wt reduction in the thiophene and dibenzothiophene at various stages.

Extraction stages	Experimental Result		Simulation Result	
	thiophene	DBT	thiophene	DBT
1	40 wt %[13]	70 wt %[13]	60 wt%	20 wt%
2	60 wt %[13]	79 wt%[13]	87 wt%	40 wt%
3	79 wt%[13]	87 wt %[13]	94 wt %	55 wt%

Fig. 3: Represents the % composition of the components of the model gasoline and impurities after absorption with ionic liquid [OMIM][BF₄] at 30 ⁰ C ,2 bar and 1:1 of IL to gasoline.

can be considered as an optimal temperature to work with. Pressure has a very little effect on the extraction efficiency of the impurities so it does not account for affecting the process efficiency as shown in Fig. 5a, 5b & 5c at various equilibrium stages.

Regeneration of [OMIM][BF₄]:

Ionic liquid used during this simulation after extraction needs to be regenerated to be reused and recycled back into the process. Regeneration column with 5 equilibrium stages is selected and the solvent is chosen for the regeneration of [OMIM][BF₄] is pentane due to its favorability and immiscibility with the ionic liquid. Also, it has been stated previously in the literature that on a mass basis pentane has a better performance and there is not much difference between the other solvents [16]. So pentane was chosen as the better choice for the regeneration process. The solvent was simulated and the performance of the pentane was evaluated at different ratios with the ionic liquid to remove the thiophene and

its derivatives from the model gasoline efficiently. The result is evaluated at different equilibrium stages the amount of IL regenerated in the process as shown in Fig. 6.

Flash drum pressure

During the process, we require two flash columns one at the top stream of the extraction column and another after regeneration column for the recovery of the ionic liquid and the solvent for it to be recycled back into the process. It was observed that increasing the pressure of the flash column at the top stream of the extraction column the number of ionic liquid falls which is being regenerated using the flash column. The same effect can also at the flash column after the regeneration column.

Effect of alkyl cation length

Since the UNIFAC parameters were available so we checked the performance of [OMIM][BF4] against the other ionic liquids by changing the cations of the imidazolium based ionic liquids having the same type of anion. We can see the performance of the EMIMBF4 and BMIMBF4 against the ionic liquid we used for the simulation i.e. OMIMBF4. The simulation's results revealed that as the alkyl chain of the ionic liquid increases the sulfur removal ability of the ionic liquid also further enhances the potential efficiency of the extraction of sulfur to reach the ultra-low sulfur gasoline i.e. >10ppm Fig. 8.

Comparison between experimental and simulation results

A comparative analysis was done against the simulation results of the model gasoline for the UNIFAC simulation model and the experimental outcomes obtained by NRTL model [13]. The results in Fig. 8 show that the simulation findings support the experimental
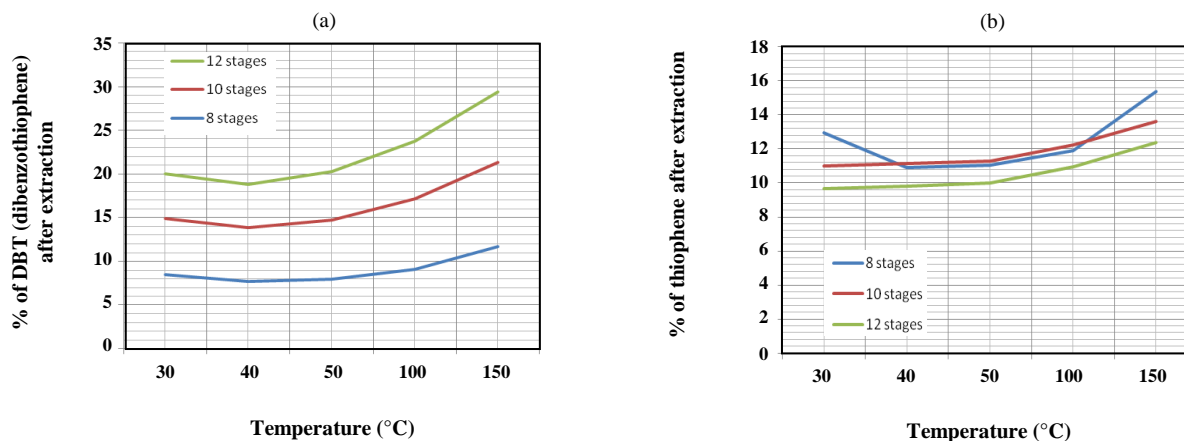
Fig. 4: (a) Effect of the temperature on the extraction of DBT(dibenzothiophene) at different temperatures as well as different equilibrium stages operating at 2 bar with an IL:gasoline ratio of 1:1. (b) Effect of the temperature on the extraction of thiophene at different temperatures as well as different equilibrium stages operating at 2 bar with an IL: gasoline ratio of 1:1.
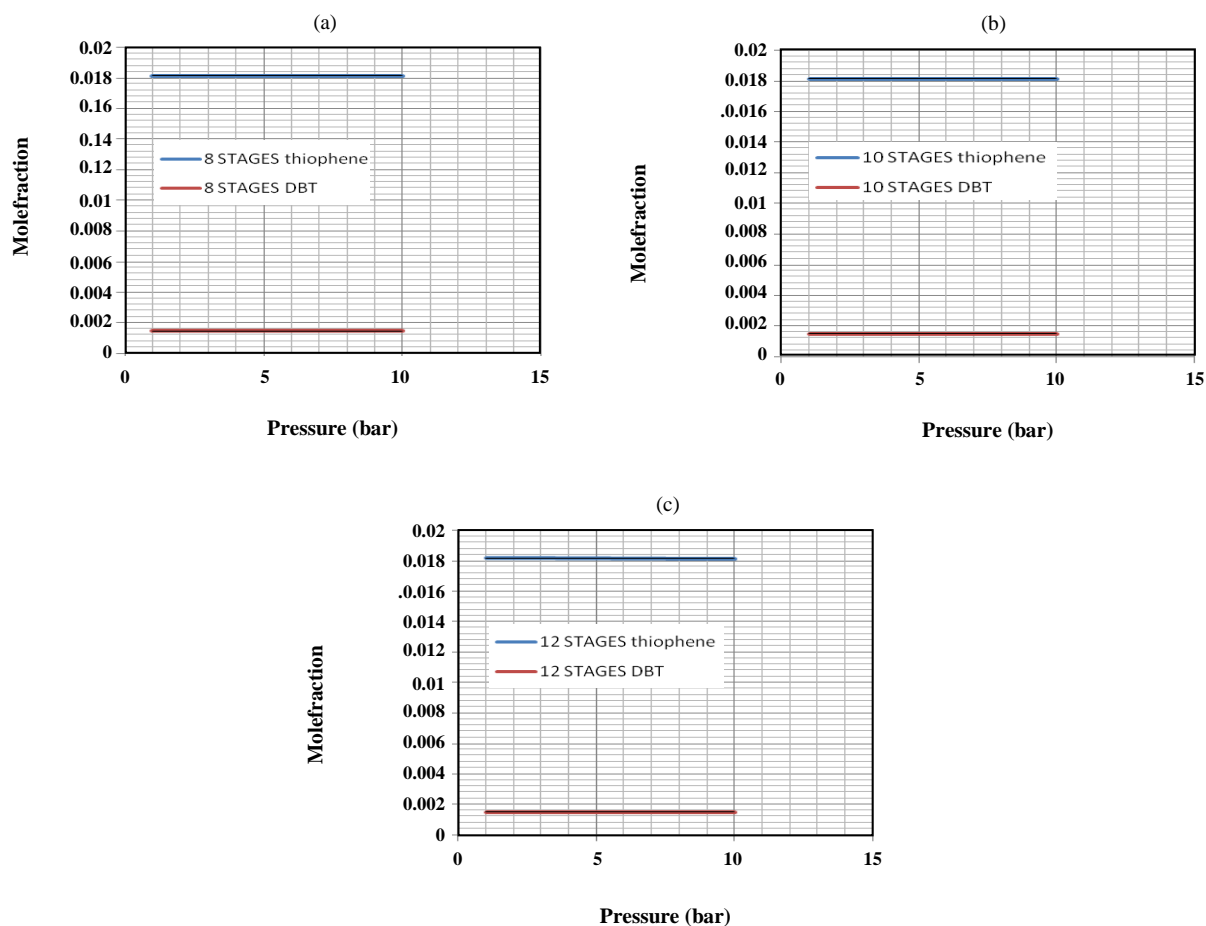

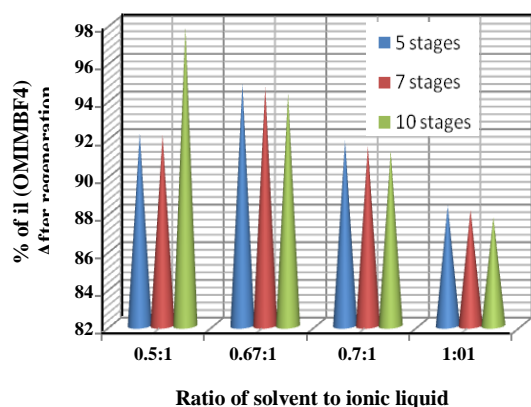*Fig. 5: (a) Effect of the pressure on the extraction of thiophene and dibenzothiophene(DBT) at different pressure at 8 equilibrium stages with an IL: gasoline ratio of 1:1. (b) Effect of the pressure on the extraction of thiophene and dibenzothiophene(DBT) at different pressure at 10 equilibrium stages with an IL: gasoline ratio of 1:1. (c) Effect of the pressure on the extraction of thiophene and dibenzothiophene(DBT) at different pressure and at 12 equilibrium stages with an IL: gasoline ratio of 1:1.*

Fig. 6: Effect of the ratio of the ionic liquid and solvent on the regeneration ability of [OMIM][BF$_4$] at 30^{0}C and 2 bar.
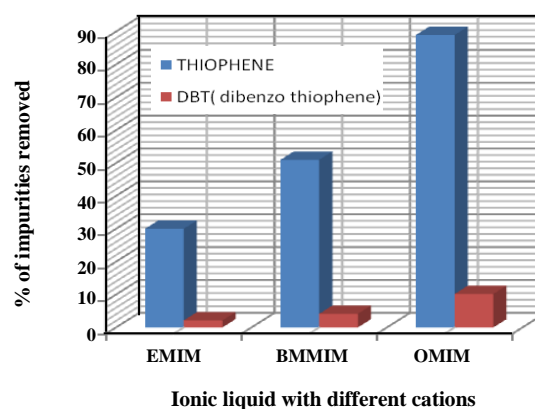

Fig. 8: Comparison between different ionic liquids for the removal of sulfur components at 30^{0}C, 2bar and 8 theoretical equilibrium stages.
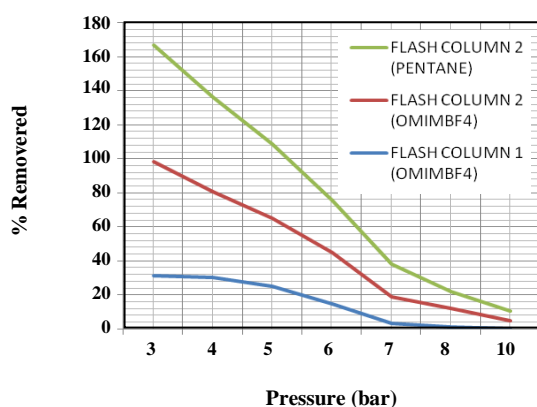

Fig. 7: effect of the pressure in flash column 1 and flash column 2 at different pressures for the recovery of ionic liquid and solvent.
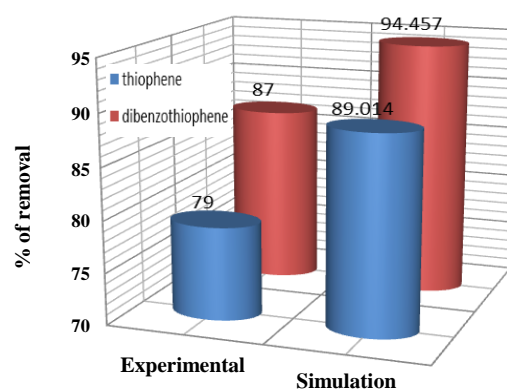

Fig. 9: comparison between the experimental and simulation results using ionic liquid [OMIM][BF$_4$] at 25ºc with 1:1 ration between IL and gasoline.

conclusions and it is reasonably accurate within the selected experimental conditions. For the components, we have studied in this simulation model the ionic liquid desulfurization efficiency is higher around 10-15% comparative to the experimental results. This would suggest that the number of extraction stages is somewhat higher than indicated by the experimental results. As it was previously been stated that by raising the alkyl chain length the sulfur removal ability increases and this result can be seen and both the simulation results as well as shown in Fig. 8 [16]. So, by observing the outcomes of the simulation model it is concluded that the selected UNIFAC model is not only accurate but also, validates the experimental findings. The experimental result uses NRTL as the thermodynamic model whereas

the simulation model is based on the UNIFAC model [13]. So, the unifac approach used here is reasonably comparable and it turns to be a suitable predictive method for the design of the desulfurization process using ionic liquid.

CONCLUSIONS

It was successfully established in this study that 1-octyl-3-methylimidazolium tetrafluoroborate [OMIM][BF4] ionic liquid be used for the efficient desulfurization of the gasoline. The process shows that almost 90% of thiophene has been removed by the ionic liquid, although it has a little effect in the removal of DBT but with the further experimental study and the calculation of the binary interactions between the DBT and ionic liquid

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it can also be possible to increase the removal of DBT. Results in this study show that the selected process can be used for the desulfurization of gasoline in accordance with the legislative requirement imposed by the authorities. UNIFAC thermodynamic model for process calculation is successfully validated in agreement with the experimental result evaluated by NRTL model. It is concluded that UNIFAC is the suitable thermodynamic model for process simulation of Gasoline desulfurization. Further rigorous study on the UNIFAC model and economic aspects of the process can enhance the efficiency of the selected process scheme can enhance the efficiency of the process and could lead us to an economically feasible process　model for its commercial scale implemented in the future.

Nomenclature

UNIFAC	UNIVERSAL functional group activity coefficient method
OMIMBF$_4$	1-octyl-3-methylimidazolium tetrafluoroborate
R_K	UNIFAC volume parameter of the functional groups of components
Q_K	UNIFAC surface area parameter of the functional groups of components
IL	Ionic liquid
DBT	Dibenzothiophene
T_b	Normal boiling point
T_C	Critical temperature
P_c	Critical pressure
V_C	Critical volume
P_b	Normal boiling pressure
T_{bM}	Contribution to normal boiling temperature
T_M	Contribution to critical temperature
M	Molecular mass
P_M	Contribution to critical pressure
V_M	Contribution to critical volume
ω	Eccentric factor

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