

Perspective

Applications and Future Directions of Ionic Liquids in Oil Refineries

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Abstract

Ionic liquids (ILs) are salts that are liquid at or below 100 °C. They are composed entirely of ions and have unique properties like negligible vapor pressure, high thermal stability, and tunable structures. These characteristics make them a promising alternative to traditional, often volatile and toxic organic solvents in the petrochemical industry. They have broad applications in chemical and petrochemical industry processes. Ionic liquids may be applied in the following processes: desulfurization, benzene toluene xylene (BTX) separation, alkylation, and carbon capture units. Two different ionic liquid-based process configurations have been evaluated for BTX separation. It has been found that the process configuration working with 1-ethyl-3-methylimidazolium tricyanomethanide ([emim][TCM]) reduces the energy costs and capital expenditures associated with the Morphyllane process by 67 and 63%, respectively. It also reduces solvent costs, confirming it as a cleaner alternative. The hydrodesulfurization (HDS) process is operated under harsh conditions, such as high temperature and high pressure and the requirement of a noble catalyst and hydrogen. High-Temperature Hydrogen Attack (HTHA) failure occurs at high temperatures between the gaseous molecular hydrogen contained inside the steel pressure vessel and the carbon atoms located in the steel matrix or in carbides. Methane molecules are produced during this reaction. This phenomenon can consequently lead to a loss of mechanical properties due to surface decarburization and to the formation of defects caused by methane bubbles mainly located at grain boundaries. The application of ionic liquids (ILs) in oil refineries offers significant advantages, such as safety, environmental sustainability, and process efficiency, primarily by serving as versatile alternatives to hazardous traditional solvents and catalysts. Across BTX extraction, carbon capture, and desulfurization/HDS-adjacent service, the recurring barriers are high viscosity, difficult regeneration, solvent cost/inventory and uncertain long-term stability.

Keywords: petrochemical processes; ionic liquids; hydrogen sulfide; desulfurization; alkylation BTX separation; carbon capture; process safety; carbon capture



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1. Introduction

Ionic liquids (ILs) have attracted significant attention in the petrochemical industry because of their distinctive physicochemical properties, including negligible or very low vapor pressure, wide liquid-phase operating range, high thermal and chemical stability, non-flammability in many cases, and tunable solubility and functionality through cation–anion design [1]. The application of ionic liquids in oil refineries offers important potential advantages in terms of safety, environmental sustainability, and process efficiency, particularly because they can serve as versatile alternatives to contaminant removal [2]. Their

principal benefit lies in their tunable nature, which allows them to be designed for specific refinery tasks such as alkylation, desulfurization, denitrogenation, and aromatic separation [2]. In addition, many ionic liquids exhibit high thermal stability, with some systems remaining stable at temperatures above 300 °C, although this behavior is strongly dependent on ionic liquid structure [1]. This paper shows the applications of ionic liquid applications in petrochemical installations such as: desulfurization, BTX separation, alkylation, and carbon capture units. The scope of this work is to explore the current and future applications of ionic liquids in oil refineries. The structure of this paper is as follows: In Section 2.1, the applications of ionic liquids for extractive desulfurization are discussed. CFD simulation of the hydrogen sulfide extraction system is shown in Section 2.2. In Section 2.3, the applications of ionic liquids for BTX separation are discussed. Section 2.4 describes applications of ionic liquids for alkylation. The proposed CO₂ removal system using ILs is described in Section 3. Section 4 presents the BASIL™ (Biphasic Acid Scavenging Utilizing Ionic Liquids) process in refineries. Section 5 provides the status of ionic liquid applications in refineries. Section 6 covers future perspectives, advanced simulation and a commercialization roadmap.

2. Application of Ionic Liquids in Petrochemical Industry Processes

2.1. Applications of Ionic Liquids for Extractive Desulfurization

H₂S (hydrogen sulfide) is considered toxic, and it is commonly found in natural gas, crude oil, and other fossil fuels. In oil refineries it originates from two main sources: naturally occurring Sulfur compounds in crude oil and chemical reactions during the refining process.

Sources from Crude Oil

Crude oil, particularly “sour” crude, contains a variety of Sulfur compounds, which are naturally present. These compounds include:

Elemental Sulfur: Free Sulfur can be present in crude oil.

Dissolved hydrogen sulfide gas can be dissolved in crude oil itself.

Organic sulfur compounds: These are a diverse group of molecules where sulfur is bonded to a carbon chain. Examples include mercaptans (R-SH), sulfides (R-S-R), and thiophenes. These are the primary source of H₂S when broken down during refining.

Sources from Refining Processes

The high temperatures and pressures used in refining processes cause the organic sulfur compounds to decompose, releasing it as a byproduct. The main refining units that produce H₂S are:

Hydrodesulfurization (HDS) Units: This is the most significant source. HDS units use a catalyst and hydrogen gas to react with sulfur compounds, converting them into H₂S. This is a crucial step to meet environmental regulations on fuel sulfur content.

Cracking and Coking Units: Processes like catalytic cracking and delayed coking use high temperatures to break down heavy, long-chain hydrocarbons. The heat causes the sulfur compounds within these molecules to decompose, releasing H₂S.

Amine Treating Units: These units are designed specifically to “sweeten” refinery gas streams by using an amine solution to absorb and remove acid gases like H₂S and carbon dioxide. H₂S is then stripped from the amine solution and sent to the sulfur recovery unit.

Wastewater Treatment: Microbial activity in refinery wastewater treatment plants can also produce H₂S from the breakdown of sulfur-containing organic matter.

This corrosive gas may also lead to sulfur corrosion cracking (SCC). Sulfur corrosion cracking, more formally known as sulfide stress cracking (SSC), is a type of corrosion that causes brittle cracking in high-strength metals like steel, particularly in environments containing moist hydrogen sulfide (H₂S) and tensile stress. The process begins with hydrogen

sulfide reacting with water and steel, forming hydrogen atoms that diffuse into the metal. This hydrogen causes embrittlement and, under tensile stress, leads to crack initiation and propagation, resulting in spontaneous brittle failure [3].

In the hydrodesulfurization (HDS) process, which is employed in the refinery, Sulfur compounds in fuel oils react with hydrogen in presence of catalysts [4] in order to remove H_2S from hydrocarbon fuel [3]. This process is operated under harsh conditions, such as high temperature and high pressure and the requirement of a noble catalyst and hydrogen. High-Temperature Hydrogen Attack (HTHA) failure occurs at high temperatures between the gaseous molecular hydrogen contained inside the steel pressure vessel and the carbon atoms located in the steel matrix or in carbides. Methane molecules are produced during this reaction. This phenomenon can consequently lead to a loss of mechanical properties due to surface decarburization and to the formation of defects caused by methane bubbles mainly located at grain boundaries. Moreover, this conventional process is facing several challenges- with more countries limiting the Sulfur content in fuel oils in order to lower its level even to zero [5]. Ionic liquids have been proposed as an alternative to HDS (via EDS) or as downstream absorbers. They are a class of salts that are liquid at or near room temperature. They bring a new chance for extractive desulfurization [6–14]. Contrary to conventional chemical solvents, they are composed of anions and cations. They are not volatile, and have high thermal/chemical stability, tunable dissolving or extracting capabilities for inorganic or organic compounds, non-flammability, and recyclability [15]. Their physicochemical properties can be tailored [16]. These desirable properties make them suitable for extracting in EDS. Ionic liquids may be applied as solvents or absorbents for capturing and removing hydrogen sulfide from gas streams or liquid solutions. Several kinds of ionic liquids are applied for desulfurization process:

Phosphonium-Based Ionic Liquids: Ionic liquids with phosphonium cations, such as trialkylphosphonium, are also being explored. They can chemically react to form non-volatile phosphonium sulfide compounds, which can be easily separated.

Imidazolium-Based Ionic Liquids: This is one of the most widely studied classes of ionic liquids for H_2S absorption. Their structure allows for both physical and chemical absorption of H_2S . The absorption capacity can be enhanced by lengthening the alkyl chain on the cation or by selecting a basic anion, as the anion's basicity significantly influences the absorption capacity.

Polyoxometalate Based Ionic Liquids: Polyoxometalates have catalytic properties and good thermal stability. This combination may meet the needs of high-temperature wet oxidative desulfurization [17].

The effectiveness of an IL in removal largely depends on the specific cation and anion that make up its structure, as these can be “tuned” to optimize absorption.

EDS using ILs has been studied a lot. Wang and Zhang have carried altered acidity and iron (III) concentration by varying molar ratios of $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$ to 1-butyl-3-methylimidazolium chloride ([bmim] Cl) in the synthesis of iron (III)-containing ionic liquids. It has been shown that 1-butyl-3-methylimidazolium tetrachloroferrate ([bmim] Fe(III)Cl_4) is highly reactive to H_2S [18]. Abdullah et al. [19] have found that the absorption capacity of sulfur compounds in ILs is strong and depends on the chemical structures, physical properties and compactness between the cation and the anion of the ILs [20]. PETRONAS researchers, particularly at Universiti Teknologi PETRONAS (UTP), have investigated ionic liquids (ILs) for efficient, low-energy desulfurization, offering an alternative to conventional hydrotreating (HDS). Studies have focused on sulfonium-based ILs for extracting sulfur compounds from model fuels. Research indicates that cyclic sulfonium-based ionic liquids could reduce the sulfur content in the model by 50% under ambient conditions [21]. The use of ionic liquids (ILs) for the extractive desulfurization (EDS) of

fuel focuses heavily on removing dibenzothiophenes (DBTs). Because these bulky, aromatic sulfur compounds are highly resistant to conventional hydrodesulfurization (HDS), ILs serve as an excellent complementary technology due to their high extraction selectivity.

2.2. CFD Simulation of the Hydrogen Sulfide Extraction System

The simulation of the hydrogen sulfide extraction system by using ionic liquids was carried out by using COMSOL code. It solved the coupled continuity, turbulent fluid flow (by applying the RANS model), and diffusion transport equations. H_2S extraction is based on an ionic liquid system and a graphene oxide (GO) membrane. This system is shown in Figure 1 [22].

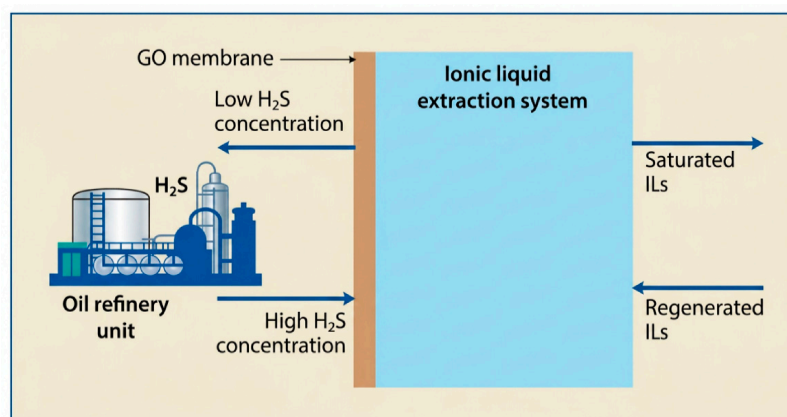


Figure 1. Schematics of the H_2S extraction system [22].

It can be seen from Figure 1 that H_2S is diffused inside the GO membrane and absorbed by 1-ethyl-3-methylimidazolium (emim)-based ionic liquids with bis-(trifluoromethyl) sulfonylimide (NTf₂) ionic liquid (see Figure 2). It was found out that H_2S is absorbed almost completely by the 1-ethyl-3-methylimidazolium (emim)-based ionic liquids with bis-(trifluoromethyl) sulfonylimide (NTf₂) anion after a time period of 30,000 s. This time period is a function of the diffusion coefficients of H_2S in the membrane and in the ionic liquid. The CFD results obtained by using COMSOL software version 4.3b were validated against analytical results. The closed-form solution was obtained for constant surface concentration for semi-infinite medium (it is valid for a very short time). It was found that the analytical results are similar to the numerical results.

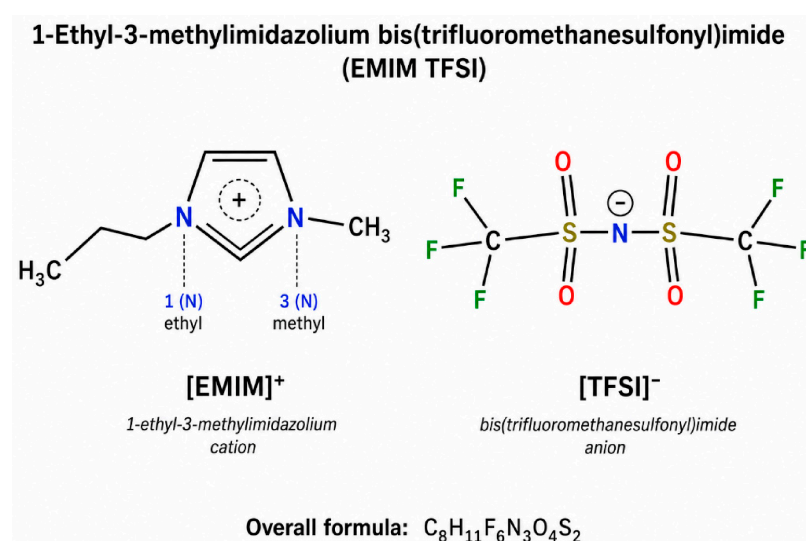


Figure 2. Chemical structure of 1-Ethyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide.

2.3. Applications of Ionic Liquids for BTX Separation

BTX stands for benzene, toluene, and xylenes. These three key aromatic hydrocarbons are produced mainly from petroleum reformate, pyrolysis gasoline, and coal tar. They are among the most important petrochemical feedstocks, with wide applications across the chemical, polymer, fuel, and materials industries. Benzene is employed for the production of phenolic and epoxy resins and styrene–butadiene rubber (SBR). Toluene is employed for the production of paints, adhesives and coatings. Mixed xylenes are used as solvents and gasoline blending components [23]. Aromatic separation stands as a challenge for the petrochemical industry.

BTX aromatics are typically produced in a refinery's catalytic reforming unit, which converts low-octane naphtha into a high-octane product called "reformate". A refinery's catalytic reforming unit transforms low-octane naphtha into high-octane gasoline components (reformate) and a valuable byproduct of hydrogen. It uses heat (endothermic reaction), pressure, and a platinum-based catalyst to convert paraffins and naphthenes into aromatics. This reformate is rich in BTX, which is then separated from other hydrocarbons for chemical production.

BTX is then separated from the reformate in a specialized unit, often called an aromatics extraction unit or BTX unit, using processes like solvent extraction or extractive distillation. In the framework of this interesting research, two different ionic liquid-based process configurations have been evaluated based on the opportunities that the use of ionic liquids enables.

The research work written by Ayuso et al. [24] explores the extractive distillation by using ionic liquids as a replacement of the Morphylane process (the Morphylane process is an extractive distillation (ED) technology that uses N-Formylmorpholine as a single-component solvent to recover high-purity aromatics like benzene and toluene from various feedstocks, including reformate, pyrolysis gasoline, and coke oven light oil). The paper covers the parametric study and techno-economic comparison of both technologies. Two different ionic liquid-based process configurations were evaluated. It was found that the process configuration working with 1-ethyl-3-methylimidazolium tricyanomethanide ([emim][TCM]) reduces the energy costs and capital expenditures associated with the Morphylane process by 67 and 63%, respectively. It also reduces the solvent costs, confirming it as a cleaner alternative.

Quijada-Maldonado carried out extractive distillation pilot plant experiments for evaluating the mass transfer efficiency decrease when using the ionic liquid 1-hexyl-3-methylimidazolium tetracyanoborate ([hmim][TCB]) as solvent for the separation of toluene and methylcyclohexane [25] (see Figure 3). It was shown that the use of the IL as solvent exhibited lower mass transfer efficiency for all the studied cases [25]. Figure 4 shows schematics of BTX separation using an ionic liquid.

The operating conditions of the toluene separation process are taken from [25]. They are shown on Table 1.

Table 1. Toluene separation process operating conditions.

Variable	Value
Feed Temperature	90 °C
Solvent Temperature	100 °C
Toluene concentration in feed (wt%)	70%

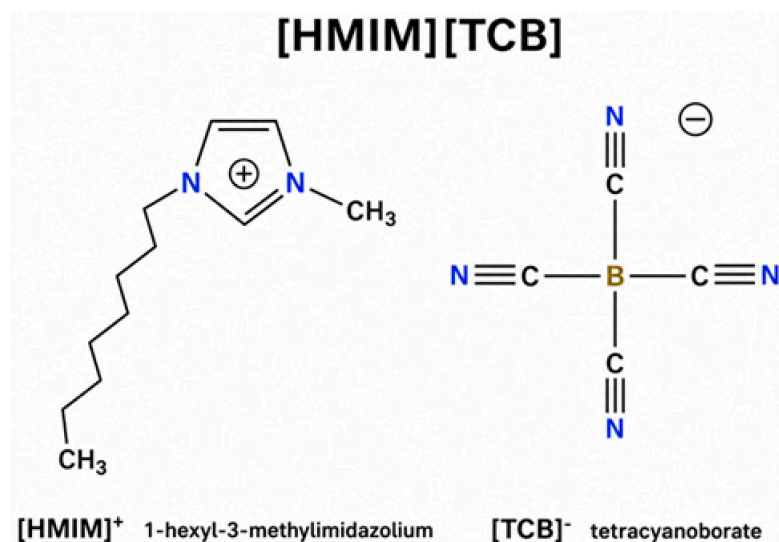


Figure 3. Chemical structure of 1-hexyl-3-methylimidazolium tetracyanoborate ([hmim] [TCB]).

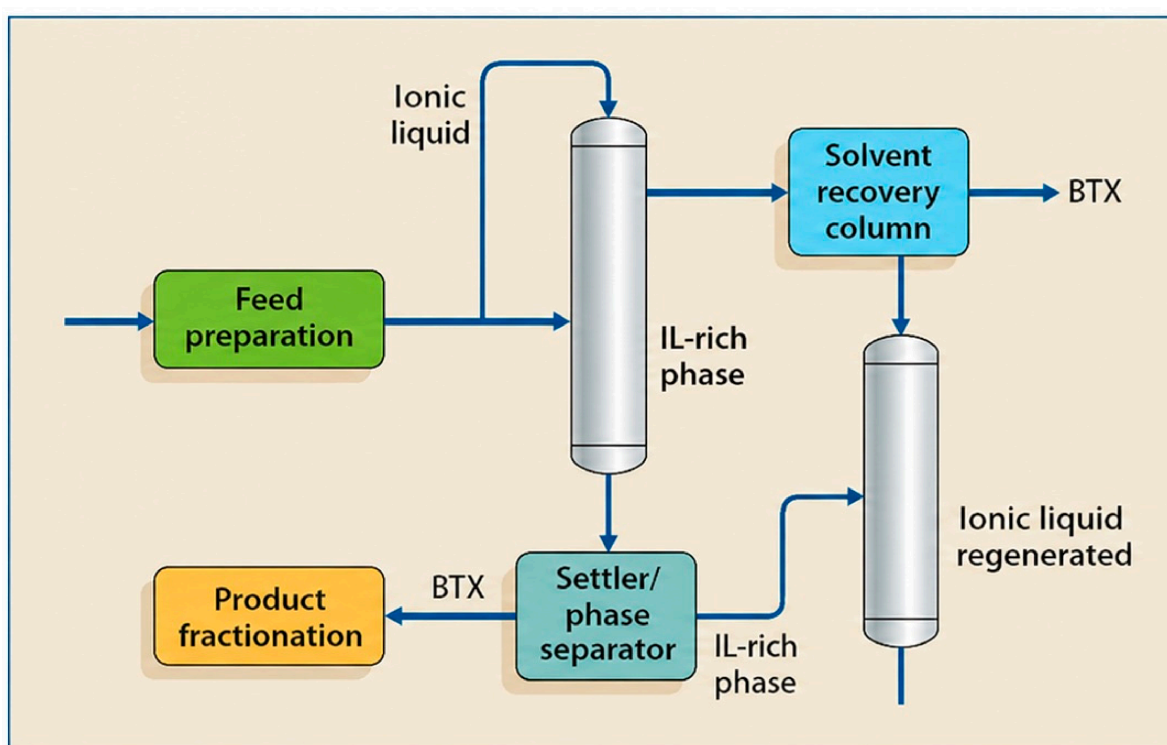


Figure 4. Schematics of the BTX extraction system.

2.4. Applications of Ionic Liquids for Alkylation

The alkylation process is a petroleum refining process that combines isobutane with light alkenes (like butylene or propylene) using a strong acid catalyst (sulfuric acid or hydrofluoric acid) to produce alkylate. However, the use of HF caused explosions at refineries. For example, a ruptured pipe in the alkylation unit at a Philadelphia refinery in June 2019 released highly toxic HF, which formed a vapor cloud before being ignited (Vapor Cloud Explosion). The US Chemical Safety Board (CSB) has published safety regulations to be updated around the use of HF [26].

Alkylate is a high-octane, low-volatility gasoline blending component that improves fuel quality and engine performance and helps reduce harmful emissions [27]. Two technologies employ ILs in alkylation processes. The first one is called Isoalky™ technology.

It was developed by Chevron and Honeywell UOP and installed in Salt Lake City [27–31]. The second one is called Ionikilatyon™ technology. This technology was developed by the China University of Petroleum [27,29]. A typical ISOALKY unit includes the following main sections (see Figure 5):

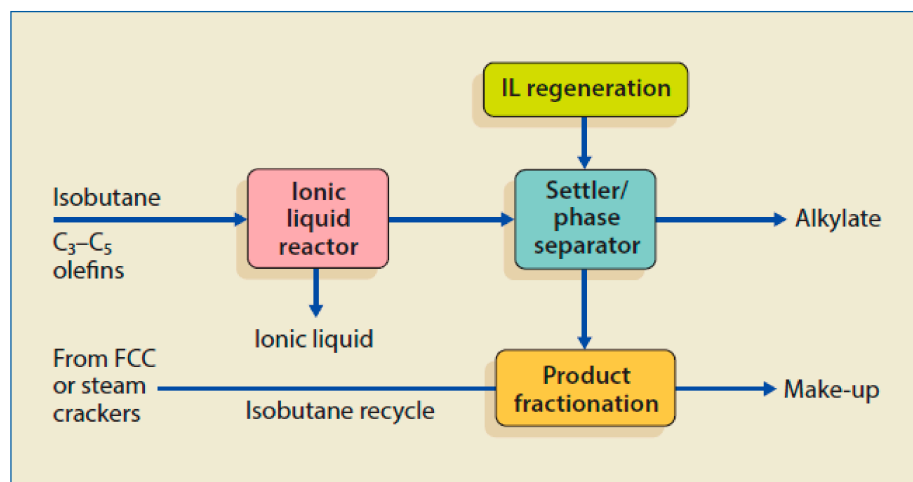


Figure 5. Schematics of ISOALKY™ process.

Feed Preparation—Isobutane and C₃–C₅ olefins (produced by FCC or steam crackers) are dried and pretreated.

Ionic Liquid Reactor—Olefins react with isobutane in the presence of an IL catalyst under mild conditions. The chloroaluminate-based IL catalyst is employed in the Isoalky™ process. ISOALKY™ technology typically uses nitrogen-containing aromatic cations combined with AlCl₃/Al₂Cl₇[−] [27]. It should be noted that chloroaluminate ILs are sensitive to moisture, which requires rigorous feed drying and an inert atmosphere (see Section 5).

Settler/Phase Separator—It separates the hydrocarbon phase (alkylate + unreacted isobutane) from the ionic liquid catalyst.

Isobutane Recycle—Unreacted isobutane is recovered and returned to the reactor.

Product Fractionation—Separation of alkylate (C₇–C₉ high-octane hydrocarbons) from lighter gases.

IL Regeneration Loop—After the reaction, the catalyst, which is a liquid, separates easily from the liquid hydrocarbon product. The catalyst is then recycled back to the reactor. The invention [32] describes the alkylation process for producing alkylate oil using ionic liquid as a catalyst, wherein during the alkylation reaction, the reaction feed is a mixture of C₄ alkene and C₄ alkane, with C₄ alkane being present in excessive amount and then separated from the alkylation product and recycled.

The operating conditions of the ISOALKY™ process are taken from [33]. They are shown on Table 2.

Table 2. ISOALKY process operating conditions.

Variable	Value
Temperature	−1–49 °C
Pressure	5.2–18.6 kg/cm ²
Olefin Conversion	>99.9%

3. Proposed CO₂ Removal System Using ILs

Oil refineries are considered among the highest carbon emitters after power plants and cement industries. The CO₂ produced in refineries comes from several different units,

such as FCC, hydrogen production (by using steam reforming technology), steam cracking, and sulfur recovery units, in addition to boilers and process heaters (combustion-related CO₂ sources). The regenerator part of Fluid Catalytic Cracker (FCC) is responsible for roughly a quarter of standard refinery CO₂ emissions at the refinery. Post-combustion technology can be retrofitted after the regenerator flue gas line using a suitable amine scrubbing technology [34]. Amine-based solvents have been mostly used so far, because of their large cyclic capacities. However, the use of these solvents is threatened by steel degradation at high temperatures and high corrosion rate (amine may cause the amine stress corrosion cracking of the steel pipes) [34,35]. Ionic liquids (ILs) represent a promising alternative to traditional amine-based solvents for CO₂ capture in oil refinery operations. These materials are salts that remain liquid at or near room temperature and offer several unique properties that make them particularly suitable for industrial carbon capture applications [36–43]. Figure 6 shows a schematic diagram of the carbon capture system based on ionic liquids for FCC.

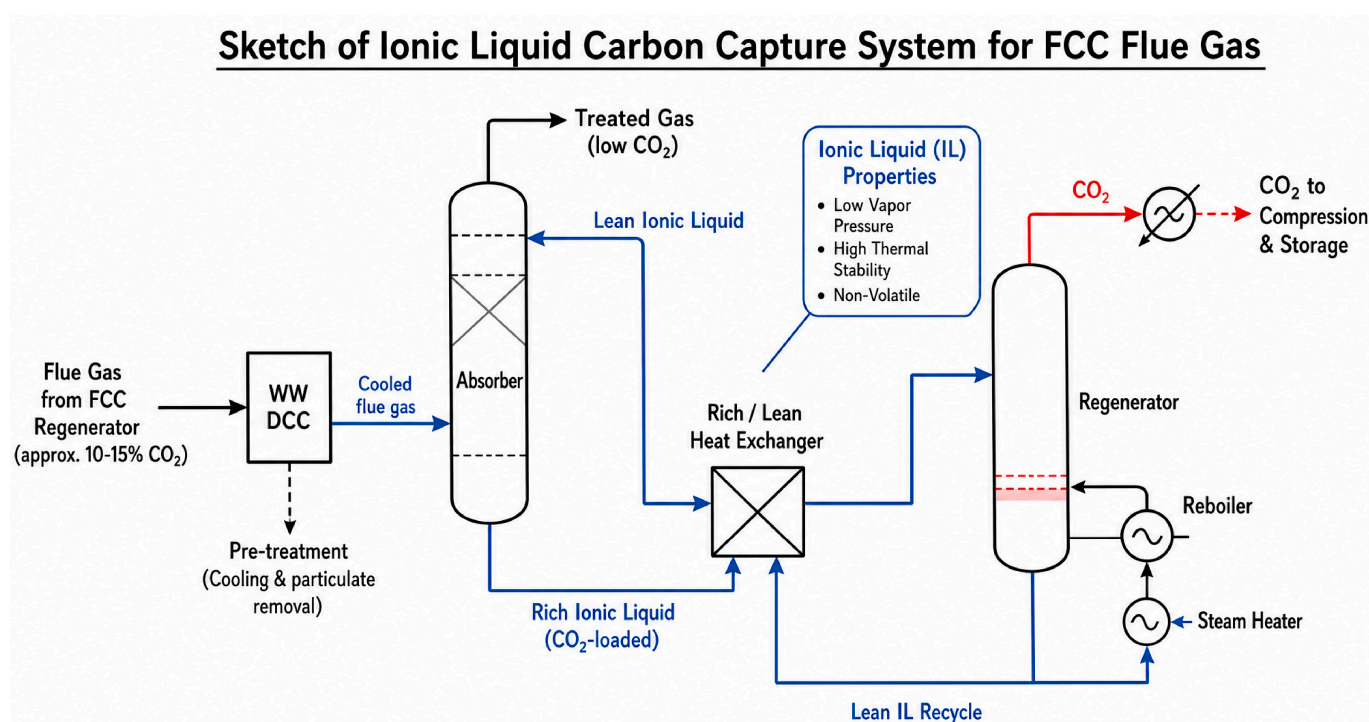


Figure 6. Schematic diagram of carbon capture system based on ionic liquids for FCC.

The ionic liquid (IL) carbon capture system for a Fluid Catalytic Cracking (FCC) unit is typically integrated as a post-combustion capture process. It is composed of four sub-systems: pretreatment, absorber, heat exchanger and regenerator.

The pretreatment treats the flue gas exiting the FCC regenerator, which contains a relatively high concentration of CO₂. Before entering the capture unit, the FCC regenerator flue gas is cleaned. Then the cooled flue gas enters the bottom of the absorber column. The rich IL is pumped through a lean/rich heat exchanger. It is pre-heated by the hot lean IL returning from the regenerator. A reboiler located at the bottom uses steam to heat the IL. The heat supplied by the reboiler breaks the bond between the IL and CO₂. Then the CO₂ gas is released and exits from the top of the regenerator.

It may be possible to develop a CO₂ removal system by using 1-ethyl-3-methylimidazolium dicyanamide ([emim][DCA]) ionic liquid [44]. The General Electric Company (GE) and the University of Notre Dame have issued a patent dealing with CO₂ capture that applies Phase Change Ionic Liquid (PCIL). This patent describes a method for removing from mixed gas streams (like

flue gas) using Phase-Change Ionic Liquids (PCILs). Unlike traditional liquid absorbents, these materials exhibit a unique phase behavior. The PCIL is initially a solid. Upon reacting with CO₂, it transforms PCIL-CO₂ into a liquid complex. When the liquid complex is heated, it releases the CO₂ gas and reverts back to its original solid form for reuse [45]. The overall increase in the cost of electricity is about 4.1 ¢/kWh for the PCIL process compared with 5.7 ¢/kWh for the MEA process [46].

4. The BASIL™ (Biphasic Acid Scavenging Utilizing Ionic Liquids) Process in Refineries

The BASIL™ (Biphasic Acid Scavenging Utilizing Ionic Liquids) process is a landmark chemical technology developed by BASF, originally highlighted by the American Chemical Society's C&EN [47]. It revolutionized how strong acids are scavenged in reactions by using 1-methylimidazole to create a reusable ionic liquid. 1-MIM selectively reacts with the generated HCl, forming 1-methylimidazolium chloride. This newly formed compound is an ionic liquid (IL). Because it is essentially a room-temperature molten salt, it forms a clear, distinct liquid phase separate from the organic product.

5. Limitation and Status of Applying Ionic Liquid Applications in Refineries

In refinery applications, ionic liquids (ILs) are technically promising; however their main limitation is that they often solve one separation problem while creating a solvent-handling and regeneration problem elsewhere. Across BTX extraction, carbon capture, and desulfurization/HDS-adjacent service, the recurring barriers are high viscosity, difficult regeneration, solvent cost/inventory, uncertain long-term stability, and incomplete industrial-scale proof.

5.1. BTX/Aromatic Extraction: Main Limitations

For BTX or aromatics extraction from refinery streams, the biggest practical problem is often solvent recovery, not initial selectivity. Several ionic liquids look excellent in lab equilibrium data, but recovery from real refinery feeds can become the bottleneck. In one refinery-oriented study, regeneration by stripping was unsuccessful for real feeds, and flash recovery required very high vacuum (~0.001 MPa) and elevated temperature, which the study describes as difficult to realize at refinery scale. A second major drawback is high viscosity, which increases the pressure loss, mixing, and mass transfer in extraction equipment. The same source notes that many literature ionic liquids are poorly suited to large-scale service because they combine high viscosity with corrosiveness or moisture instability. In practice, this means bigger equipment penalties, slower phase contact, and a narrower operating window than refinery process engineers want. There is also a selectivity-versus-capacity trade-off. Some IL structures give strong aromatic selectivity but low loading; others improve capacity but sacrifice selectivity. This matters because a refinery solvent must not only separate BTX well but also do so with reasonable solvent circulation rates and manageable column sizes. Real refinery feeds are also more difficult than model benzene/paraffin mixtures because multiple aromatics, aliphatics, and hetero-compounds compete simultaneously. A further limitation is chemical robustness. Halogen-containing ionic liquids can be corrosive (may cause stress corrosion cracking) or moisture-sensitive; decomposition may form acids such as HCl or HF, which is a major materials-of-construction and process safety concern. Some high-performing ILs are also water-insoluble and high in molecular weight, meaning that refiners may need large solvent inventories, which decreases the project economics [48].

5.2. Carbon Capture: Main Limitations

For carbon capture, the most cited drawback is very high viscosity, and it often becomes worse after CO₂ loading. A review manuscript claims that viscosity can increase dramatically upon absorption, which directly penalizes gas–liquid mass transfer, pumping, and absorber/desorber design [49]. There is also a difficult capacity-versus-regeneration trade-off. Reactive/chemical ILs usually capture more CO₂, but they pay for it with energy-intensive regeneration because the CO₂ is more strongly bound. Physical ILs are easier conceptually, but they generally have lower driving force and may require deeper vacuum or more energy to desorb CO₂ effectively. A membrane regeneration study found that a physical IL needed higher vacuum than a reactive IL to reach comparable desorption performance, increasing overall energy use and cost [49,50]. Water management is another limitation. Adding water can reduce viscosity and improve diffusion for some physical ILs, but for chemical ILs, it can reduce reaction-driven capture performance. So, the process window becomes narrow: the same change that helps mass transfer may hurt capture chemistry [50]. From a refinery deployment perspective, the commercial barriers are still significant: high solvent cost, limited availability of low-cost IL families, unresolved corrosion/toxicity questions, and uncertain long-term stability. Reviews also report that some IL approaches are not attractive for low-pressure CO₂ streams unless specially designed, which is important because refinery flue gas is typically dilute and has low partial pressure [49]. Applying PCILs from controlled laboratory settings to rugged industrial processes introduces several severe operational bottlenecks. These challenges generally stem from their high viscosity, low thermal conductivity, and material handling issues. Even when converted to liquid phase, PCILs tend to be significantly more viscous than conventional organic solvents or water [51]. Moving, pumping, and spraying a liquid with high viscosity significantly elevates pressure losses. During the reverse process (e.g., stripping CO₂ or discharging heat), the ionic liquid solidifies. Managing a flowing fluid that transitions into a crystalline or amorphous solid means that systems face severe clogging and piping blockages. Like most organic salts and ionic liquids, PCILs possess relatively low thermal conductivity. When acting as a latent heat storage material, the solid layers that freeze directly onto heat exchanger surfaces act as thermal insulators. This drastically drops the heat transfer rate over time, requiring expensive design remedies [52].

5.3. Hydrodesulfurization/Deep Desulfurization: Main Limitations

In Sulfur removal, the first limitation is conceptual: ionic liquids usually do not replace conventional hydrodesulfurization (HDS) in a simple, drop-in way. Most successful IL schemes are extractive or oxidative desulfurization steps used for deep polishing, especially for refractory sulfur molecules such as dibenzothiophenes. That means they often complement HDS rather than substitute for the refinery's core hydrogen-based desulfurization system. The second limitation is recycling and solvent durability. Reviews report that IL-based desulfurization can be reused, but performance often declines with cycle number because oxidation products accumulate and some IL is lost during separation. This is a serious refinery issue because economics depend on stable solvent performance over many cycles, not just a few laboratory experiments. Third, many IL desulfurization routes add a new burden: extra chemistry and extra separations. Oxidative desulfurization generally needs an oxidant plus separation of sulfones/sulfoxides from the IL phase. So, although IL methods can run under milder conditions than HDS, they may replace reactor severity with more complicated downstream separation and solvent cleanup [53].

5.4. Alkylation: Main Limitation

The major limitations of ionic liquids in alkylation are: strong sensitivity to water and other feed impurities, catalyst deactivation, and narrow operating window.

Chloroaluminate ionic liquids can be deactivated by water, methanol, and ethers. Water hydrolyzes active AlCl_3 species and can form HCl , while methanol and diethyl ether tie up the active Lewis-acid sites by complexation. In practice, this means that the unit needs very dry feed and tight impurity control, not just good catalyst chemistry [54].

One study on chloroaluminate ionic liquids found that only about half of the total AlCl_3 is catalytically active, and deactivation occurs once that active fraction is consumed. Activity can be restored by adding fresh anhydrous AlCl_3 , but this means that catalyst management is continuous and tied to impurity ingress and side reactions [54].

Ionic liquid alkylation performance is very sensitive to cation/anion choice, halide composition, and acidity level. In one alkylation study, stronger acidity improved activity, but highly acidic formulations deactivated rapidly because of higher moisture sensitivity. At higher temperature, activity and TMP selectivity also dropped because of decomposition of imidazolium ions. So, the catalyst must be tuned carefully [55].

Based on the NASA website [56], an approximate TRL status of applications of ionic liquid in oil refineries has been developed. It should be noted that there is not a single universally published TRL table for all ionic liquid refinery applications, so this is a synthesis from public evidence mapped to the standard TRL scale, where TRL 9 means commercial use, TRL 5–6 means pilot/prototype demonstration, and TRL 3–4 means lab proof of concept and component validation. The Technology Readiness Level (TRL) status for the processes provided in this work is shown in Table 3.

Table 3. TRL status of applications of ionic liquids in oil refineries.

<i>Ionic Liquid Application in Refining Processes</i>	<i>Estimated TRL</i>	<i>Practical Usage</i>
Alkylation	9	Commercially deployed
BTX separation	4–5	Lab-validated, with some pilot work in related aromatic/aliphatic separations but not broadly commercial for refinery BTX service
Carbon capture	5–6 for hybrid IL/amine systems; ~4–5 for pure/refinery-specific IL use	Pilot/demo stage, not mainstream refinery deployment
Desulfurization	3–4	Mostly lab and process-design stage

6. Future Perspectives, Numerical Simulations and Commercialization Roadmap of IL

The research and development of new ionic liquids is carried out by applying Quantum Chemistry (such as: Variational Quantum Eigensolver) and Density Functional Theory (DFT) computational tools [57]. Quantum chemistry, Density Functional Theory (DFT) and COSMO-RS (Conductor-like Screening Model for Real Solvents) may be applied to design and optimize ionic liquids (ILs) for various refinery applications. These tools provide molecular-level insights into interaction energies, geometries, and electronic structures, allowing for the pre-screening of ILs with tailored properties. Quantum chemistry simulates

reaction pathways, intermediate states, and transition states in catalysis, helping optimize ILs for catalytic processes. Variational Quantum Eigensolver (VQE) strategies have already been combined with chemically relevant solvent distribution models, suggesting a route toward treating correlated electronic structure in condensed ionic environments beyond the standard DFT paradigm [58].

The coupling of Variational Quantum Eigensolvers (VQEs) and Tensor Networks (TNs) with Density Functional Theory (DFT) is a promising hybrid, multi-scale, quantum–classical approach designed to tackle the simulation of large, strongly correlated ionic liquid molecular systems. This framework, often referred to as DFT-TN-VQE or quantum-enhanced DFT (QEDFT), aims to overcome the “curse of dimensionality” in quantum simulations by using tensor networks to compress the quantum state and DFT to manage the surrounding environment. Variational Quantum Eigensolver (VQE) is used to calculate the exact ground state energy. Tensor networks (like Matrix Product States—MPSs) are used to efficiently represent, compress, and simulate the quantum wave function, reducing the number of qubits and the depth of the quantum circuit needed [59].

Harrow–Hassidim–Lloyd (HHL) and quantum singular-value transformation (QSVT) may be applied for ionic liquid multi-physics simulations. They are applied for solving linear systems of equations, offering potential speedups for solving the main transport partial differential equations (momentum, energy and diffusion with chemical kinetics terms) [60,61].

7. Conclusions

Ionic liquids (ILs) have attracted significant attention in the petrochemical industry because of their unique physicochemical properties such as negligible vapor pressure, wide liquid range, high thermal stability, and tunable solubility/chemical functionality. In the framework of this paper, four applications of ILs in refinery processes have been described. They may be applied in desulfurization, BTX separation, alkylation and carbon capture processes. Several kinds of ionic liquids are applied for the desulfurization process.

It has been found that the process configuration working with 1-ethyl-3-methylimidazolium tricyanomethanide ([emim][TCM]) reduces the energy costs and capital expenditures associated with the Morphyllane process by 67 and 63%, respectively. It also reduces the solvent costs, confirming it as a cleaner alternative.

Currently there are two examples of the use of ILs in alkylation plant refineries. The first one is Isoalky™ technology, developed by Chevron and Honeywell UOP and installed in Salt Lake City. The second one is Ionikilatyon™ technology, developed by the China University of Petroleum.

It may be possible to develop a CO₂ removal system by using 1-ethyl-3-methylimidazolium dicyanamide ([emim][DCA]) ionic liquid.

In refinery applications, ionic liquids (ILs) are technically promising; however, their main limitation is that they often solve one separation problem while creating a solvent-handling and regeneration problem elsewhere. Across BTX extraction, carbon capture, and desulfurization/HDS-adjacent service, the recurring barriers are high viscosity, difficult regeneration, solvent cost/inventory, uncertain long-term stability, and incomplete industrial-scale proof.

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Abbreviations

[bmim] Cl	1-butyl-3-methylimidazolium chloride
BTX	Benzene, toluene, xylene
CFD	Computational Fluid Dynamics
ED	Extractive distillation
EDS	Extractive desulfurization
[emim][DCA]	1-ethyl-3-methylimidazolium dicyanamide
[emim][TCM]	1-ethyl-3-methylimidazolium tricyanomethanide
FCC	Fluid Catalytic Cracker
HDS	Hydrodesulfurization
HTHA	High-Temperature Hydrogen Attack
IL	Ionic liquid
NFM	N-Formylmorpholine
PCIL	Phase Change Ionic Liquid
SCC	Stress corrosion cracking
SSC	Sulfide stress cracking
TRL	Technology Readiness Level
VQE	Variational Quantum Eigensolver

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