

Ionic Liquids for Carbon Capture: A Comprehensive Review of Absorbents, Mechanisms, and Process Applications

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Abstract- — The escalating atmospheric CO₂ concentration and its contribution to global climate change have driven intensive research into carbon capture technologies. Ionic liquids (ILs) have emerged as promising alternatives to conventional amine-based absorbents, offering unique advantages including negligible vapor pressure, exceptional thermal stability, and tunable physicochemical properties through rational cation-anion design. This comprehensive review examines the full spectrum of ionic liquid applications in CO₂ capture, from fundamental absorption mechanisms to process-scale implementations. Physical absorption in conventional ILs, chemisorption in task-specific ILs incorporating amine, carboxylate, and amino acid functionalities, and IL-based mixed absorbents are systematically analyzed. Structure-property relationships governing CO₂ solubility—including the influence of cation alkyl chain length, anion basicity, and functional group incorporation—are critically evaluated against experimental and computational data. Supported ionic liquid membranes (SILMs) and ionic liquid-based mixed matrix membranes for CO₂ separation are reviewed, highlighting permeability-selectivity trade-offs and stability considerations. Process configurations including IL-based absorption-desorption cycles, membrane contactors, and hybrid systems are assessed for energy consumption and economic viability. Recent advances in computational screening, machine learning-guided IL design, and process intensification are presented. Key challenges including high viscosity, long-term stability under operating conditions, absorbent regeneration energy, and scale-up economics are addressed. Finally, future directions toward industrial implementation are discussed, emphasizing the integration of ILs with renewable energy sources and the development of sustainable, cost-effective capture technologies.

Keywords: Ionic liquids; carbon capture; CO₂ absorption; task-specific ionic liquids; gas separation; supported ionic liquid membranes; process intensification; machine learning

I. INTRODUCTION

The Global Challenge of Carbon Emissions

Atmospheric carbon dioxide concentrations have risen from pre-industrial levels of approximately 280 ppm to exceed 420 ppm in 2025, primarily driven by fossil fuel combustion and industrial activities [1]. This increase correlates strongly with global temperature rise, ocean acidification, and climate instability, making CO₂ mitigation one of the most urgent technological challenges of the twenty-first century. The Intergovernmental Panel on Climate Change (IPCC) scenarios consistent with limiting warming to 1.5°C require rapid deployment of carbon capture, utilization, and storage (CCUS) technologies at unprecedented scale [2].

Carbon capture encompasses three primary contexts: post-combustion capture from flue gases (typically 5-15% CO₂ at near-atmospheric pressure), pre-combustion capture from syngas (15-60% CO₂ at elevated pressure), and oxy-fuel combustion (high-purity CO₂ stream) [3]. Each application

imposes distinct requirements on capture materials regarding CO₂ partial pressure, temperature, and contaminant tolerance.

Limitations of Conventional Capture Technologies

Aqueous amine scrubbing, particularly using monoethanolamine (MEA), remains the benchmark technology for post-combustion CO₂ capture despite several inherent limitations [4]. Amine-based processes suffer from:

- **High regeneration energy:** The strong chemical bonding between CO₂ and amines requires significant thermal energy (3.5-4.5 GJ/t CO₂) for absorbent regeneration, reducing power plant efficiency by 20-30% [5].
- **Solvent degradation:** Amines undergo oxidative and thermal degradation in the presence of O₂, SO_x, and NO_x, requiring continuous solvent makeup and generating corrosive degradation products [6].

- **Equipment corrosion:** Amine solutions corrode carbon steel equipment, necessitating expensive construction materials and corrosion inhibitors [7].
- **Volatile losses:** Amine volatility leads to solvent losses and potential environmental release of degradation products [8].
- These limitations have motivated extensive research into alternative capture materials, among which ionic liquids have attracted particular attention.

Ionic Liquids: Definition and Relevance to Carbon Capture

Ionic liquids are salts composed entirely of ions with melting points below 100°C, many remaining liquid at room temperature (room temperature ionic liquids, RTILs) [9]. Their relevance to carbon capture derives from several distinctive properties:

- **Negligible vapor pressure:** ILs exhibit immeasurably low volatility, eliminating solvent losses to the gas stream and enabling regeneration without evaporative losses [10].
- **Exceptional thermal stability:** Most ILs remain stable above 300-400°C, allowing operation at elevated temperatures and thermal regeneration without decomposition [11].
- **Tunable CO₂ affinity:** Through rational selection of cations (imidazolium, ammonium, phosphonium, pyridinium) and anions (halides, tetrafluoroborate, hexafluorophosphate, bis(trifluoromethylsulfonyl)imide, acetate, amino acid anions), CO₂ solubility can be optimized over four orders of magnitude [12].
- **Dual absorption mechanisms:** ILs can capture CO₂ through physical absorption (Henry's law solubility) or chemical absorption via functional groups (amines, carboxylates, azolates) incorporated into the ionic structure [13].
- **Designer solvent capability:** The estimated 10⁶-10⁸ possible cation-anion combinations enable systematic optimization for specific capture conditions [14].

Scope and Organization

This review comprehensively examines ionic liquid applications in CO₂ capture, focusing on developments from 2010-2025. Section 2 establishes fundamental principles of CO₂-IL interactions, including experimental measurement techniques and computational modeling approaches. Section 3

analyzes physical absorption in conventional ILs, detailing structure-property relationships governing CO₂ solubility. Section 4 reviews chemisorption in task-specific ionic liquids incorporating reactive functional groups. Section 5 covers IL-based membranes for CO₂ separation. Section 6 addresses process configurations and engineering considerations. Section 7 presents computational design strategies including machine learning. Section 8 discusses challenges, economic considerations, and future directions.

II. FUNDAMENTALS OF CO₂ CAPTURE IN IONIC LIQUIDS

Mechanisms of CO₂ Absorption

CO₂ absorption in ionic liquids proceeds through two primary mechanisms, alone or in combination:

- **Physical absorption:** CO₂ dissolves in ILs through weak van der Waals and Lewis acid-base interactions without chemical bond formation [15]. The absorption follows Henry's law, with solubility proportional to CO₂ partial pressure. Physical absorption dominates in conventional ILs with weakly coordinating anions ([BF₄]⁻, [PF₆]⁻, [NTf₂]⁻) and is characterized by rapid kinetics, complete reversibility, and moderate absorption enthalpies (10-20 kJ/mol) [16].
- **Chemical absorption:** CO₂ reacts chemically with basic sites in task-specific ILs, forming carbamates, carbonates, or carboxylates [17]. Chemical absorption achieves higher capacities, particularly at low CO₂ partial pressures, but requires greater energy for regeneration (40-80 kJ/mol) and may exhibit slower kinetics [18].
- **The absorption mechanism can be tuned through IL design:** introducing amine, azolate, or phenoxide functionalities promotes chemisorption, while maintaining inert anions maintains physisorptive behavior [19].

Thermodynamic and Kinetic Considerations

CO₂ absorption thermodynamics are characterized by the absorption isotherm, typically measured using gravimetric or volumetric methods [20]. The absorption capacity (mol CO₂/mol IL or mol CO₂/kg IL) varies with pressure and temperature according to:

- **Henry's law regime (low pressure):** $C = H \times P$, where H is the Henry's law constant (typically 30-100 bar for physisorption) [21].

Langmuir-type behavior (higher pressure): $C = (C_{\text{max}} \times K \times P) / (1 + K \times P)$, where C_{max} is saturation capacity and K is the equilibrium constant [22].

Absorption enthalpy (ΔH_{abs}) determines regeneration energy requirements and is obtained from temperature-dependent solubility measurements via the van't Hoff equation [23]. For physisorption, ΔH_{abs} typically ranges from -10 to -20 kJ/mol, while chemisorption exhibits ΔH_{abs} from -40 to -100 kJ/mol [24].

Kinetic parameters including absorption rate constants and diffusion coefficients influence contactor design and cycle times. IL viscosity, typically 10-500 times higher than conventional solvents, often limits mass transfer rates [25].

Analytical Methods for CO₂-IL Systems

Solubility measurements: Gravimetric methods using magnetic suspension balances provide accurate absorption isotherms under controlled pressure and temperature [26]. Volumetric methods measure pressure decay in constant-volume cells [27]. In situ FTIR and NMR spectroscopy identify absorbed CO₂ species and reaction products [28].

- **Spectroscopic characterization:** FTIR reveals carbamate formation (absorption bands at 1650-1680 cm⁻¹ for amine-functionalized ILs) and bicarbonate/carbonate species (1350-1450 cm⁻¹) [29]. ¹³C NMR identifies chemical environments of absorbed CO₂ [30].
- **Computational methods:** Molecular dynamics simulations elucidate CO₂ distribution and transport in ILs [31]. Density functional theory (DFT) calculations predict reaction pathways and binding energies [32]. COSMO-RS (Conductor-like Screening Model for Real Solvents) screens ILs for CO₂ solubility based on thermodynamic calculations [33].

III. PHYSICAL ABSORPTION IN CONVENTIONAL IONIC LIQUIDS

Imidazolium-Based Ionic Liquids

Imidazolium cations with weakly coordinating anions constitute the most extensively studied class for CO₂ physisorption [34]. The benchmark IL 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([C₄mim][NTf₂]) exhibits CO₂ solubility of approximately 0.025 mole fraction at 25°C and 1 bar, increasing to 0.6-0.7 mole fraction at 50-100 bar [35].

Anion effects: Anion choice dominates CO₂ solubility in imidazolium ILs. Solubility increases with anion fluorination and follows the order: [NTf₂]⁻ > [PF₆]⁻ > [BF₄]⁻ > [DCA]⁻ > halides [36]. The [NTf₂]⁻ anion provides optimal balance of CO₂ affinity and low viscosity due to its delocalized charge and flexible structure [37].

- **Cation alkyl chain length:** Increasing alkyl chain length from ethyl to hexyl enhances CO₂ solubility through increased free volume and dispersive interactions, though gains diminish beyond C₈ due to viscosity increases [38]. The relationship follows: [C_nmim][NTf₂] with n = 2, 4, 6, 8 showing progressive solubility enhancement [39].
- **Cation functionalization:** Ether-functionalized side chains reduce viscosity while maintaining CO₂ solubility [40]. Nitrile-functionalized cations introduce specific CO₂ interactions [41].

Phosphonium and Ammonium Ionic Liquids

Phosphonium-based ILs offer advantages including higher thermal stability and different solvation characteristics compared to imidazolium analogues [42]. Trihexyl(tetradecyl)phosphonium-based ILs ([P₆₆₆₁₄][NTf₂]) achieve CO₂ solubilities comparable to imidazolium ILs with lower viscosity at elevated temperatures [43].

Quaternary ammonium ILs, particularly with long alkyl chains, provide additional design options though generally exhibit higher viscosity than imidazolium or phosphonium analogues [44].

Pyrrolidinium and Other Cation Classes

Pyrrolidinium cations yield higher viscosity but improved electrochemical stability relevant to integrated capture-conversion processes [45]. Pyridinium-based ILs offer aromatic character with different charge distribution compared to imidazolium [46].

Structure-Property Relationships

Comprehensive analysis of CO₂ solubility in physisorptive ILs reveals:

Free volume theory: CO₂ dissolves preferentially in IL free volume, with solubility correlating with molar volume and expansivity [47]. Fluorinated anions increase free volume through weak interionic interactions [48].

Lewis acid-base interactions: CO₂ acts as a Lewis acid, interacting preferentially with basic anions [49]. Anion basicity scales with CO₂ solubility among physisorptive anions [50].

Viscosity-solubility trade-off: ILs with highest CO₂ solubility often exhibit highest viscosity, creating mass transfer challenges [51]. Optimal ILs balance these competing factors.

IV. CHEMISORPTION IN TASK-SPECIFIC IONIC LIQUIDS

Amine-Functionalized Ionic Liquids

Incorporating amine groups into ionic liquid structures enables chemical reaction with CO₂ analogous to aqueous amines but without volatility [52]. Two approaches dominate:

- **Cation-tethered amines:** Amine groups attached to the cation via alkyl spacers [53]. Primary amines form carbamates with 0.5 mol CO₂/mol amine stoichiometry (two amines required per CO₂), while secondary amines exhibit variable stoichiometry depending on steric factors [54].
- **Anion-tethered amines:** Amino acid anions provide naturally occurring amine functionality [55]. Amino acid ILs (AAILs) combine the green credentials of biological feedstocks with effective CO₂ capture, achieving capacities of 0.5-1.0 mol CO₂/mol IL [56].
- **Dual-functionalized ILs:** Incorporating amines on both cation and anion maximizes amine density but increases viscosity significantly [57].

Carboxylate-Based Ionic Liquids

Acetate-based ILs ([C_nmim][OAc]) exhibit enhanced CO₂ solubility through formation of reversible carbene-CO₂ adducts [58]. The mechanism involves deprotonation of the imidazolium C2 proton by acetate, generating an N-heterocyclic carbene that reacts with CO₂ [59]. This chemistry achieves capacities approaching 0.3-0.4 mol CO₂/mol IL at 1 bar, significantly exceeding physisorption [60].

Azolate Ionic Liquids

ILs incorporating pyrazolide, imidazolide, triazolide, and tetrazolide anions demonstrate exceptional CO₂ capacities through formation of carbonate-like species [61]. These "azolate" ILs achieve near-stoichiometric CO₂ absorption (0.9-1.0 mol CO₂/mol IL) at 1 bar with moderate absorption enthalpies (40-60 kJ/mol) enabling reversible capture [62].

Phenoxide and Alkoxide Ionic Liquids

Phenoxide-based ILs capture CO₂ through formation of aryl carbonate species [63]. The basicity of the phenoxide determines reactivity, with electron-withdrawing substituents

moderating absorption enthalpy [64]. Alkoxide-functionalized ILs exhibit high reactivity but may suffer from stability limitations [65].

Reversible Ionic Liquids

"Switchable" ionic liquids that transform between molecular and ionic states upon CO₂ exposure offer novel process configurations [66]. Amidines and guanidines react with CO₂ to form ionic alkylcarbonate salts, reverting upon heating or purging [67]. These systems enable CO₂-triggered property changes for separations and reactions.

V. IONIC LIQUID MEMBRANES FOR CO₂ SEPARATION

Supported Ionic Liquid Membranes (SILMs)

SILMs consist of ionic liquid immobilized within porous support materials (polymeric, ceramic, or metallic) by capillary forces [68]. CO₂ transports through the IL phase by solution-diffusion mechanism, with permeability determined by CO₂ solubility and diffusivity in the IL [69].

- **Selectivity:** SILMs achieve high CO₂/N₂ selectivities (20-60) and CO₂/CH₄ selectivities (10-30) depending on IL choice [70]. Anion fluorination enhances both solubility and selectivity [71].
- **Stability:** The primary limitation of SILMs is IL displacement from pores under transmembrane pressure [72]. Matching IL hydrophobicity to feed composition and optimizing pore structure improves stability [73].

Polymerized Ionic Liquid Membranes

Polymerized ionic liquids (PILs) combine IL properties with polymer mechanical stability [74]. PIL membranes exhibit enhanced CO₂ solubility through IL character while maintaining structural integrity under pressure [75]. Block copolymers with IL and structural segments optimize permeability and selectivity [76].

Mixed Matrix Membranes

Incorporating ILs into polymer matrices creates mixed matrix membranes with tunable properties [77]. ILs plasticize polymer chains, increasing free volume and CO₂ diffusivity while maintaining selectivity through CO₂-philic character [78]. IL-filled metal-organic frameworks (MOFs) within polymer matrices represent emerging composite materials [79].

Facilitated Transport Membranes

Incorporating reactive carriers (amines, carbonates) into IL membranes enables facilitated CO₂ transport through reversible reactions [80]. Mobile or fixed-site carriers enhance CO₂ flux while maintaining high selectivity over non-reactive gases [81].

VI. PROCESS CONFIGURATIONS AND ENGINEERING

Absorption-Desorption Cycles

The conventional process configuration for IL-based CO₂ capture parallels amine scrubbing: CO₂ absorption in an absorber column followed by thermal regeneration in a stripper [82]. Key differences include:

- **Operating temperature:** ILs enable absorption at higher temperatures (50-80°C) without solvent loss, reducing cooling requirements [83].
- **Regeneration energy:** Physisorptive ILs require 2.0-3.0 GJ/t CO₂ compared to 3.5-4.5 GJ/t CO₂ for MEA, offering significant energy savings [84].
- **Flowsheet modifications:** IL properties enable novel configurations including pressure-swing regeneration and hybrid temperature-pressure swings [85].

Membrane Contactors

Membrane contactors using ILs as absorbents combine membrane gas-liquid contact with IL nonvolatility [86]. Microporous membranes provide high interfacial area without flooding or entrainment limitations [87]. IL-filled membrane contactors achieve high CO₂ removal efficiency with compact equipment [88].

Hybrid Processes

Integrating IL absorption with membrane separation or cryogenic distillation enables optimized process schemes [89]. Hybrid processes exploit complementary strengths: absorption for bulk removal, membranes for polishing, and IL properties for both functions [90].

Process Modeling and Simulation

Rate-based process models incorporating IL thermodynamics and transport properties guide scale-up [91]. Aspen Plus and gPROMS simulations with customized property packages predict column performance and energy requirements [92]. Validation at pilot scale (10-100 kg CO₂/day) confirms model predictions [93].

VII. COMPUTATIONAL DESIGN AND MACHINE LEARNING

COSMO-RS Screening

COSMO-RS (Conductor-like Screening Model for Real Solvents) predicts CO₂ solubility in ILs from quantum chemical calculations without experimental input [94]. Screening of virtual IL libraries identifies high-performance candidates, reducing experimental effort by orders of magnitude [95]. COSMO-RS accurately ranks ILs by CO₂ affinity and predicts absorption selectivity [96].

Molecular Dynamics Simulations

Molecular dynamics simulations reveal CO₂ distribution, diffusion pathways, and interactions at atomic resolution [97]. Free energy calculations predict absorption thermodynamics [98]. Simulations guide IL design by identifying structural features controlling CO₂ solubility and transport [99].

Machine Learning Approaches

Machine learning has emerged as a powerful tool for IL discovery and optimization [100]. Key applications include: Property prediction: Neural networks and random forests trained on experimental data predict CO₂ solubility, viscosity, and thermal stability with high accuracy [101].

- **High-throughput screening:** ML models screen millions of hypothetical ILs to identify promising candidates for experimental validation [102].
- **Process optimization:** Reinforcement learning optimizes process conditions and IL selection simultaneously [103].
- **Structure-property relationships:** ML identifies non-intuitive correlations between IL structure and performance [104].

Integration of ML with robotic synthesis and testing platforms accelerates the design-build-test-learn cycle [105].

VIII. CHALLENGES AND FUTURE DIRECTIONS

Viscosity and Mass Transfer

High IL viscosity (typically 10-500 times higher than water or amines) limits mass transfer rates and increases pumping energy [106]. Strategies to mitigate viscosity include:

- Elevated operating temperatures [107]
- Low-viscosity ILs with ether-functionalized cations or asymmetric anions [108]
- IL-solvent mixtures (organic solvents or water) with optimized composition [109]
- Process intensification using Higee rotating packed beds [110]

Long-Term Stability

IL stability under realistic flue gas conditions requires evaluation of:

- **Thermal stability:** ILs must withstand regeneration temperatures (100-150°C for physisorption, 120-200°C for chemisorption) without decomposition [111].
- **Oxidative stability:** O₂ (3-6% in flue gas) may oxidize ILs at elevated temperatures [112].
- **Contaminant tolerance:** SO_x, NO_x, and particulates may degrade IL performance or accumulate in the absorbent [113].
- **Hydrolytic stability:** Some ILs ([BF₄]⁻, [PF₆]⁻) hydrolyze in the presence of water, releasing HF [114].
- **Economic Considerations**
- IL cost remains a barrier to commercial deployment. Current IL prices (\$50-1000/kg) exceed amines (\$1-5/kg) by orders of magnitude [115]. Cost reduction strategies include:
 - Simplified synthesis routes [116]
 - Bulk production scaling [117]
 - IL recycling and extended lifetime [118]
 - High-value coproducts offsetting capture costs [119]

Economic analyses suggest IL capture costs of \$40-80/t CO₂, competitive with amines (\$60-100/t CO₂) when IL lifetime and performance advantages are considered [120].

Integration with Renewable Energy

Future carbon capture systems must integrate with intermittent renewable energy sources [121]. IL properties enabling flexible operation include:

- Rapid response to variable CO₂ loads [122]
- Low thermal mass for start-stop operation [123]
- Compatibility with solar thermal regeneration [124]
- Electrochemically-mediated capture using IL electrolytes [125]

Direct Air Capture Applications

Direct air capture (DAC) of CO₂ (~400 ppm) requires exceptionally high CO₂ affinity materials [126]. Task-specific ILs with strong chemisorption achieve sufficient capacity at ambient CO₂ concentrations [127]. IL-based DAC systems offer advantages including nonvolatility and thermal stability for sorbent regeneration [128].

CO₂ Conversion and Utilization

Integrated capture-utilization processes employ ILs as both capture media and reaction solvents [129]. CO₂ captured in ILs can be directly converted to fuels, chemicals, or materials without intermediate desorption [130]. Electrocatalytic and photocatalytic conversion in IL electrolytes represents an emerging frontier [131].

IX. CONCLUSIONS

Ionic liquids have demonstrated exceptional potential as next-generation materials for carbon capture, offering unique combinations of properties unavailable in conventional solvents. Key advances include:

- Fundamental understanding of CO₂-IL interactions guiding rational design
- Task-specific ILs achieving high capacity through chemisorption
- IL-based membranes with tunable permeability-selectivity
- Computational screening and machine learning accelerating discovery
- Process designs exploiting IL nonvolatility for energy-efficient capture

Despite significant progress, challenges remain in viscosity management, long-term stability validation, and cost reduction. The path to commercial deployment requires continued integration of materials development with process engineering, economic analysis, and sustainability assessment. As global carbon management scales to meet climate targets, ionic liquids are positioned to play an increasingly important role in the portfolio of capture technologies.

The coming decade will likely see:

- First commercial-scale IL-based capture demonstrations
- Integration of IL capture with renewable energy
- Machine learning-designed ILs optimized for specific sources

- Hybrid capture-utilization processes
- Sustainable, bio-derived ILs with minimal environmental footprint
- With continued research and development, ionic liquids can contribute substantially to the carbon management infrastructure required for climate stabilization.

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