A methodology for the selection of ionic liquids for CO_2 absorption based on thermodynamic and kinetic properties

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Ionic liquids (*ILs*) have been widely proposed as alternative solvents for CO_2 capture due to their negligible vapor pressure, high thermal stability, and structural tunability. In this context, gas–liquid contactors such as bubble column reactors are particularly attractive for IL-based CO_2 absorption because of their simple design and favorable heat and mass transfer characteristics[1,2].

However, in order to choose the appropriate ionic liquid, a purely experimental screening approach is unfeasible due to the large number of possible cation–anion combinations, exceeding 10^{14} theoretical structures. Because of this, *IL* selection frequently relies on single descriptors like absorption enthalpy or CO_2 solubility, which may not accurately reflect solvent performance under industrial absorption conditions [3].

In recent literature different computational and theoretical approaches have been used to choose the right ionic liquid. Zhang et al. [4] demonstrated that the energy demand of IL-based CO_2 capture processes is closely related to thermodynamic quantities such as Henry's law constant, CO_2 dissolution enthalpy, and working capacity, highlighting the importance of regeneration energy rather than solubility alone. Palomar et al. [5] employed a combination of *COSMO*-based screening, experimental diffusion measurements and process simulations, to show that frequently CO_2 absorption with ILs is kinetically controlled, with viscosity and diffusivity governing solvent circulation rate, column size and overall energy consumption. An additional level of complexity arises for task-specific ionic liquids (*TSILs*), for which Zhu et al. [6] demonstrated that CO_2 absorption performance depends on the interplay between diffusion and reaction kinetics rather than on thermodynamics equilibrium alone. In the present work these approaches are not used but are instead taken as a knowledge basis to define a set of experimentally accessible selection criteria for ionic liquids.

The proposed methodology is designed to be implementable using experimental thermodynamic and transport property data. The objective is to systematically exclude non-suitable candidates at an early stage by means of a minimal and coherent set of measurable properties. This framework implements recent multiscale studies into a practical, property-based pre-screening tool that supports informed decision-making and focuses experimental efforts on solvent families with realistic process potential.

Three main classes of criteria are considered. First, practical aspects such as data availability, chemical stability and compatibility with other solvents are considered. Second, the absorption mechanism and thermodynamics are evaluated by distinguishing between physical and chemical absorption in ionic liquids, using CO_2 solubility or loading and absorption enthalpy as principal descriptors to ensure industrial relevance. Third, mass-transfer limitations are explicitly incorporated through viscosity and diffusivity, reflecting the dominant role of kinetics highlighted in the literature.

This selection methodology follows a sequential approach. A literature-based pre-screening is first applied to identify well-documented *IL* families for which reliable thermodynamic and transport data are available, avoiding poorly characterized or

experimentally impractical structures (e.g.: complex structures, too expensive or toxic solvents). The selected ILs are then evaluated using combined thermodynamic, kinetic and process indicators. The main outcome is a property-based selection map that highlights critical trade-offs between CO_2 capacity, absorption enthalpy and mass-transfer limitations, defining regions of favorable and unfavorable performance.

Simultaneously, simplified process-level simulations of CO_2 absorption in bubble column systems are being carried out to qualitatively evaluate the impact of essential physicochemical properties, including liquid viscosity, diffusivity, and surface tension, on overall mass-transfer behavior. The simulations are based on a simplified liquid-side mass-transfer model, in which absorption rates are estimated from effective transport properties and interfacial area to enable qualitative comparison and sensitivity analysis to help understand experimental trends and find the most important parameters. Ongoing work focuses on validating the proposed selection strategy through experimental measurements of CO_2 solubility, viscosity and working capacity in a bubble column setup. The final objective is to provide a transferable and experimentally grounded pre-screening methodology for the rational development of ionic liquid–based CO_2 capture processes, consistent with and informed by insights from recent computational and multiscale studies.

Preliminary results suggest that ionic liquids combining moderate CO_2 capacity with favorable transport properties are better suited for absorption in bubble column systems than solvents optimized for solubility alone.

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