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A review of ionic liquids and deep eutectic solvents design for CO_2 capture with machine learning

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A R T I C L E I N F O

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A B S T R A C T

Ionic liquids (ILs) and deep eutectic solvents (DESs) are regarded as the next generation solvents for carbon capture which consist of cations and anions. Thousands of combinations of cations and anions can lead to varied properties of ILs/DESs, which makes it difficult to screen such ILs/DESs for CO_2 in experiments. Computer-aided molecular design (CAMD) saves time and cost by reversing the search for the structure of ILs that are suitable for carbon capture. Compared with other thermodynamic models, machine learning (ML) models have the advantages of efficiency and accuracy in CAMD; hence, the number of studies on the application of ML models in the field of CAMD is growing each year. In this paper, a concise review of the application of ML to ILs/DESs-based CO_2 capture technology is provided. The development process of ML models in (1) the prediction of the properties of ILs/DESs using their structure; and (2) the prediction of the carbon capture effect using process parameters is discussed. Perspectives on future research directions are proposed and key challenges are identified for screening suitable ILs/DESs using the capture effectiveness of a specific carbon capture process as an evaluation criterion.

1. Introduction

The negative effects of climate change caused by anthropogenic CO_2 emissions are becoming more prominent in our society—for example, more frequent extreme weather, rising sea levels, and the destruction of ecosystems (Baker et al., 2018; Bokhorst et al., 2011). To combat this trend, reducing CO_2 emissions through carbon capture, utilization, and storage (CCUS) is widely considered as a critical solution (Chen et al., 2022; Jiang et al., 2020). Capturing CO_2 from point sources (e.g., coal-fired power plants, iron-steel, and cement industry) is one of the most economically feasible approaches to curb carbon emissions (Gao et al., 2020). In several industrial-scale CCUS projects, more than one million tons of CO_2 is captured and stored per year; however, the solvent-based CO_2 scrubbing technologies used in these projects are too expensive to deploy on a large scale (Burns et al., 2020; Koytsoumpa et al., 2018). Currently, the most developed commercial carbon capture technology is thermal amine scrubbing, which allows the formation of carbamate adducts through chemical bonding with carbon dioxide (Said et al., 2020). Nevertheless, a large thermal input is required to dissociate the adducts and to achieve the desorption of CO_2 because of the high sorption heat and high heat capacity of the absorbent (Varghese and Karanikolos, 2020). Moreover, amine-based solvents encounter challenges, such as thermal adsorbent degradation, process equipment corrosion, and evaporative loss.

Ionic liquids (ILs), which are a class of room-temperature molten salt composed of anions and cations, are one of the most promising materials for CO_2 capture (Nematollahi and Carvalho, 2019; Sun et al., 2023). The advantages of ILs include the high absorption of CO_2, negligible vapor pressure during absorbent regeneration, high thermal stability, and adjustable solvent properties (Haider et al., 2020; Hospital-Benito et al., 2020). The tunability of the ILs structure makes it possible for solvents to be synthesized with specific desired properties. By varying the combination of anion and cation species, as well as their ratios, ILs exhibit diverse properties. It is estimated that there are approximately 10^{18} potential combinations (Liu et al., 2021). CO_2 capture performance is also sensitive to both the characteristics of ILs and operating conditions (Aghaie et al., 2018). Howbeit, there are thousands of possible CO_2 capture materials and different combinations of operating conditions,

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