Advanced Designer Amines for CO₂ Capture: Interrogating Speciation and Physical Properties

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Abstract

The emission of carbon dioxide from fossil fuel has attracted attention since awareness of global climate change emerged. Post combustion carbon capture (PCC) with amine solvent is considered to be the most viable technology to reduce CO₂ emission effectively in the short and medium term¹. However, the wide application of this technology is limited by the high cost of CO₂ capture while the large scale economic benefit of the pure CO₂ product is still waiting to be exploited. In this case, efficient amine solvent, which possesses superior chemical reactivity, and energy efficiency and stability, compared to the industrial standard monoethanolamine (MEA), is in urgent need to reduce cost of carbon capture. Accordingly, a series of purpose designed diamines (termed designer amines throughout) containing two reactive nitrogen amine groups into one molecule have been developed². It has been demonstrated recently that designer amines combining many desirable advantages have great potential to reduce cost of CO₂ capture³. However, there is still a necessity to further comprehend the inherent CO₂ capture properties and behaviour of designer amine solvents.

In this work, the chemical speciation of 2.0 M solutions of designer amine solvents during CO₂ absorption has been investigated using NMR spectroscopy. The general structure of the designer amines is shown in Figure 1. For comparison purposes, 4.0 M monoethanolamine (MEA) and 2.0 M piperazine (PZ) have been investigated in this work.

A plot of the concentration of the various dissolved species as a function of total dissolved CO₂ loading can be used to guide the interpretation of the mechanism for CO₂ absorption by designer amines. A plot of CO₂ speciation, in the form of carbamate and bicarbonate, in 4-amino-1-propylpiperidine (4A1PPD) solution, is shown in Figure 2. The amines were selected to investigate and confirm the influence of chain type and functionality on the speciation of the parent designer amine skeleton. The results confirm there is no significant influence of the chain type on the speciation given the similarity in the structure and the molecular location of the chains relative to the active primary amine group (towards CO₂ directly). Such relationships between amine structure and their chemical behaviour and speciation during CO₂ absorption as demonstrated here could provide guidelines for molecular modification to improve amine solvent performance. Additionally, the effect of speciation on the physical properties of amines (i.e. density and viscosity) and the ability to tune the composition of the absorbent to achieve a compromise between the chemical and physical properties is under investigation.
Figure 1. Molecular structure of designer amines (Rs = hydrogen, alkyl or hydroxyl-alkyl etc.)

Figure 2. Speciation plot of 4A1PPD versus CO\textsubscript{2} loading

References: