Numerical investigation of bubble columns with ionic liquids for CO_2 absorption

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The increasing concentration of greenhouse gases in the atmosphere, particularly CO_2, is one of the main causes of climate change, with a significant fraction of global emissions deriving from the industrial sector. In recent year, increasing attention has been paid to CO_2 capture. Ionic liquids (ILs) are increasingly investigated as solvents for CO_2 absorption. Compared with conventional solvents, they combine several advantages such as negligible vapour pressure with high thermal stability and tunable physicochemical properties [1].

Bubble columns are an attractive reactor option for gas liquid absorption processes because they offer simple operation, compact design, low maintenance, and efficient heat and mass transfer [2]. Nevertheless, the flow in bubble columns is governed by multi-scale interactions that span a wide range of scales. In the case of ILs, current understanding of the associated fluid dynamics and mass transfer remains limited, and numerical studies addressing these systems are still scarce. On this basis, the AURIGA project lays the groundwork for the study and characterization of bubble column reactors for CO_2 absorption using IL.

The present work provides a comprehensive numerical investigation of a bubble column operating with an IL and CO_2 in batch mode presenting a homogeneous flow regime. Different closures for drag, bubble-induced turbulence (BIT), and mass transfer are compared. Simulations were performed for the comparison of two distinct IL solvents. The solvents were 1-butyl-3-methylimidazolium tetrafluoroborate ([Bmim][BF_4]) and 1-ethyl-3-methylimidazolium acetate ([Emim][Ac]). CO_2 absorption in [Bmim][BF_4] was modelled as purely physical, while [Emim][Ac] was modelled with a simplified reaction mechanism which captures the primary enhancement effect of chemical absorption.

Three-dimensional transient simulations were performed using a customized version of OpenFOAM v10, in which the drag, BIT, diffusive, and reactive mass transfer models were implemented. The computational domain consists of a vertical cylindrical bubble column discretized with a structured mesh. The results were time-averaged for 220 seconds, starting after the initial 20 seconds. The effect of co-current and counter-current liquid flow on CO_2 absorption is also studied.

Model predictions were validated against experimental global gas holdup data from [4] and established correlations for the volumetric mass transfer coefficient (k_la). Among the different formulation of the drag coefficient considered in this study, the model proposed by [5] provided the best agreement with the experimental data concerning global gas holdup, with a deviation less than 5% for all the cases considered (Figure 1).

All the investigated mass transfer models provided reasonable predictions, but the ones that depend on turbulent properties are more sensitive to local flow conditions. The assessment of BIT models revealed that not explicitly accounting for viscosity effects in the formulation reflected in k_la with deviations over 150% with respect to the correlations, caused by a overprediction of turbulence in the liquid phase and gas holdup.

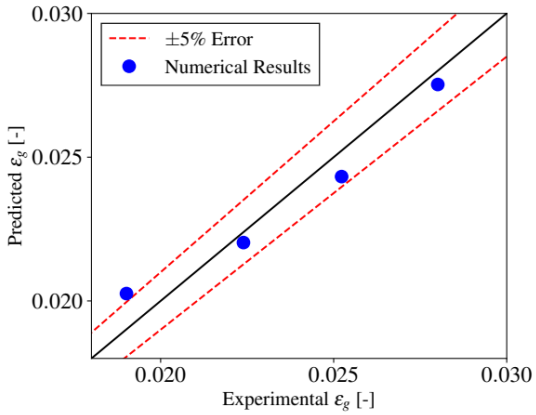

Figure 1: Parity graph comparing experimental gas holdup values from [4] and numerical results from the CFD model, with ±5% error lines For batch operating mode and superficial gas velocities varying from 0.0045 to 0.006 m/s, using [Bmim][BF_4] as the solvent.

In conclusion, the simulations results confirm that closure selection governs the accuracy of gas holdup and $k_l a$ in IL bubble columns. Using drag correlations developed for ILs and accounting for viscosity in BIT are necessary to avoid overpredicting turbulence and holdup. The comparison between [Bmim][BF_4] and [Emim][Ac] highlights the expected contrast between a physical absorption system and a reactive solvent, chemical absorption provides an additional enhancement beyond diffusion. The counter current operation gives the highest absorption performance because it increases holdup and interfacial area.

References:

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Acknowledgments:

This work has been financed by the Italian Ministry of University and Research (Ministero dell'Università e della Ricerca) within the FIS2 call. In particular, This work has been conducted within the AURIGA ("Unvealing the RIddles of GAs liquid fluid dynamics: towards novel carbon dioxide absorption systems") project. Project number FIS-2023-00204, CUP D53C25000730001, funded within the FIS2 call (Decreto Direttoriale n. 1236 del 1-08-2023).