Reactive CFD modeling of CO_2 absorption in a gas-liquid vortex reactor

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Highlights

- CFD simulation, coupling interphase mass transfer, population balance model and kinetics for CO_2 capture.
- Deviation between simulation results and experimental data within ±20%.
- Internal transport phenomenon and CO_2 absorption process revealed.
- Guideline provided for reactor design including energy-efficient CO_2 capture.

1. Introduction

In light of growing concerns about global warming, the focus on the development of energy-efficient technologies that aim at mitigating greenhouse gas emissions increases. Chemical absorption, a mature and cost-effective method, plays a pivotal role in this context. Efficient gas-liquid contact in absorbers and desorbers is crucial for enhancing process efficiency and reducing capital and operational costs. The gas-liquid vortex reactor (GLVR) (Figure 1), a novel process intensification device developed at Laboratory for Chemical Technology (LCT, Ghent University), stands out for simple structure, low cost, easy scale-up, and high micromixing and mass transfer efficiencies[1,2]. As depicted in Figures 1(a) and 1(b), a GLVR operates by introducing gas and liquid flows tangentially into a cylindrical chamber, creating a highly turbulent vortex and a centrifugal force field. Understanding interphase mass transfer within GLVRs is essential for optimizing operating conditions and reducing energy consumption.

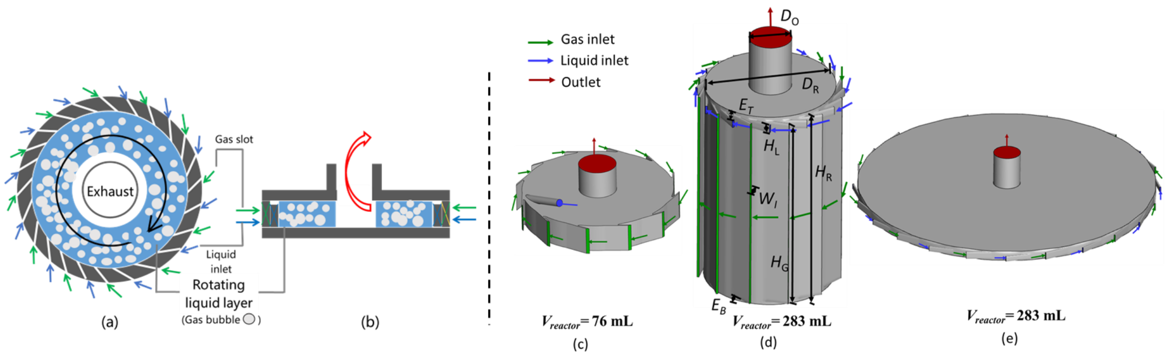

Figure 1. Schematic diagram of a GLVR: (a) top view; (b) side view. Schematic diagram of the studied GLVRs: (c) baseline geometry; optimized designs: (d) cylinder-shaped geometry, (e) pancake-shaped geometry.

Computational fluid dynamics (CFD) is a powerful tool to reveal the gas-liquid flow patterns and detailed transport processes in the reactor. In this study, a 3D CFD model is developed to study the gas-liquid hydrodynamics and interphase mass transfer behavior in GLVRs. In addition, the relationship between the CO_2 absorption rate and the total energy input in a GLVR is explored.

2. Methods

In this study, the Euler-Euler approach for multiphase flow modeling is used, coupled with the SST k-ω turbulence model for capturing the dynamics of turbulent flows. The Population Balance Model (PBM) is employed to include the effects of bubble aggregation and breakage on the bubble size distribution. Additionally, a reaction mass transfer model is used to simulate CO_2 absorption into a MEA solution. This is done by incorporating a user-defined function (UDF) for CO_2 mass transfer rate calculations: $S^{CO_2} = k_l a \times E \times M_{CO_2} \times (c^*_{CO_2} - c_{CO_2})$, where k_l is the liquid-side mass transfer coefficient, E is an enhancement factor, a is specific interfacial area, M_{CO_2} is the molecular weight of CO_2, $(c^*_{CO_2} - c_{CO_2})$ is the concentration driving force. A computational grid size of 1.5 mm ensures grid-independent results. Three GLVR geometries are investigated, as shown in Figures

2(c), 2(d) and 2(e). CO_2 concentration in the gas phase at the GLVR outlet is recorded to calculate CO_2 absorption efficiencies ($E_{absorption} = \frac{1-m_{CO_2,outlet}}{m_{CO_2,inlet}}$, where $m_{CO_2,inlet}$ and $m_{CO_2,outlet}$ represent the mole fractions of CO_2 in the gas phase at the GLVR inlet and outlet, respectively). Experimental data for CO2 absorption efficiencies are used to validate the computational approach.

3. Results and discussion

The relationship between total energy input and the CO_2 absorption rate in three GLVRs is explored. An optimized GLVR design exhibits higher CO_2 absorption rates compared to the baseline geometry due to their expanded chamber volumes and prolonged gas-liquid contact times. The cylinder-shaped geometry, in particular, achieves superior absorption rates with a relatively lower energy input, attributed to its lowest pressure drop[3]. For all three GLVR configurations, the relationship between total energy input and CO_2 absorption rate is not linear. The significant increase in CO_2 absorption rate with increased total energy input at lower gas velocities points to a relatively stable energetic efficiency. Figure 2 presents a comparative analysis of the absorption factor (absorption factor $= \frac{CO_2 \text{ absorption rate}}{\text{volume of the absorber}}$) for different absorption technologies. The GLVR absorption factor outperforms that of bubble columns and packed columns, as well as intensified equipment including rotating disc reactors and rotating packed beds (RPB), but is slightly inferior to that of microreactors. Overall, the GLVR is an effective CO_2 absorber with high absorption rates in a small reactor volume.

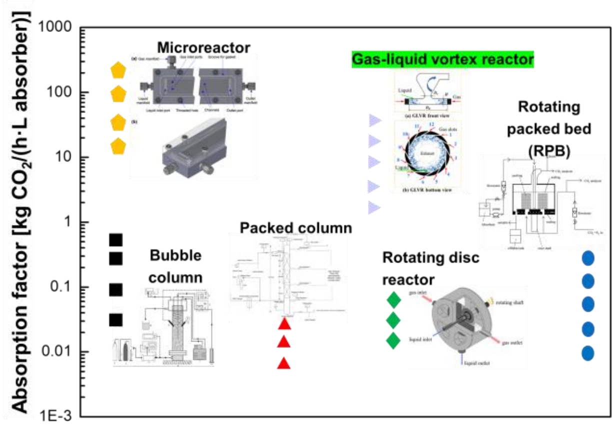

Figure 2. comparative analysis of the absorption factor for CO_2 absorption in MEA solution among various reactor technologies

4. Conclusions

A CFD-PBM model is developed and validated for simulating CO_2 chemical absorption in MEA solution in a GLVR. Optimized GLVR geometries, especially the cylinder-shaped configuration, demonstrate enhanced CO_2 absorption rates with lower energy input compared to a baseline GLVR geometry. The GLVR outperforms conventional devices and intensified devices like RPBs, and is comparable to microreactors.

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Keywords

CO_2 Capture, Vortex Unit, CFD simulation, Mass Transfer