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Single-Bubble Aspect Ratio: A Novel DNS-Based Correlation with Application to Ionic Liquid-Water Systems

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Introduction. The increasing concentration of atmospheric greenhouse gases, especially CO_2, is a key contributor to climate change, with a large portion of emissions originating from industrial activities. As a result, CO_2 capture has gained significant attention in recent years. Ionic liquids have emerged as promising solvents for CO_2 absorption due to their negligible vapor pressure, high thermal stability, and tunable physicochemical properties [1]. Bubble columns are an attractive reactor configuration for large-scale CO_2 absorption processes, due to their simple design, lack of moving parts, efficient gas–liquid mass transfer, and ease of scale-up. However, their reactor-scale performance is strongly governed by bubble-scale dynamics [2]. In particular, the overall mass transfer rate is governed by the bubble interfacial area, which is directly related to bubble size and shape. Therefore, an accurate characterization of bubble shape is essential for a reliable estimation of CO_2 absorption performance. In this context, the present study introduces a correlation derived from direct numerical simulations for the bubble aspect ratio, applicable over a broad range of fluid properties. The correlation is then used to predict the influence of concentration of 1-butyl-3-methylimidazolium tetrafluoroborate ([Bmim][BF_4]) in water on bubble aspect ratio.

Methods. The simulations were performed using the volume-of-fluid method, as implemented in the "*Fujin*" code [3], in a three-dimensional rectangular domain of size $6d_B/\times 6d_B \times 12d_B$, where d_B is the bubble diameter. The optimal spatial grid resolution was found to be $d_B/\Delta x = d_B/\Delta y = d_B/\Delta z = 30$.

Results and Discussion. The simulation results were combined with available experimental data on single bubbles to obtain a comprehensive correlation for the bubble aspect ratio. The functional form of the proposed correlation follows that of Besagni and Deen (2016) [4], namely $E = f(Re, Eo)$, where Re and Eo are the bubble Reynolds and Eötvös numbers. The novel proposed correlation reads as

$$E = \frac{1}{(1 + 0.02EoRe)^{0.18}}. \quad (1)$$

Eq. 1 is plotted in Fig. 1 together with the calibration data for single bubbles, both numerical and experimental, as well as the correlation proposed by Besagni and Deen (2016) [4]. It is important to note that the behavior differs significantly, especially at high $EoRe$, where the present correlation exhibits a much steeper trend compared to that of Besagni and Deen (2016) [4], in agreement with the single-bubble data. This discrepancy arises because the Besagni and Deen (2016) [4] correlation was calibrated using both single-bubble and swarm data. Given its applicability across a wide range of fluid systems, the correlation is here applied to [Bmim][BF_4]

over a volumetric concentration range from 1% to 100%, as shown in Fig. 2. As the [Bmim][BF_4] concentration decreases, the aspect ratio systematically decreases over the entire range of bubble diameters, indicating increased bubble deformation due to the corresponding reduction in surface tension.

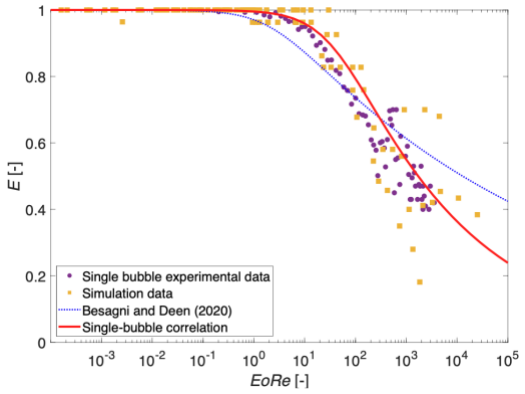


Figure 1: Bubble aspect ratio E vs $EoRe$ for single bubbles: comparison of data with the proposed correlation (Eq. (1)) and that of Besagni and Deen (2016) [4].

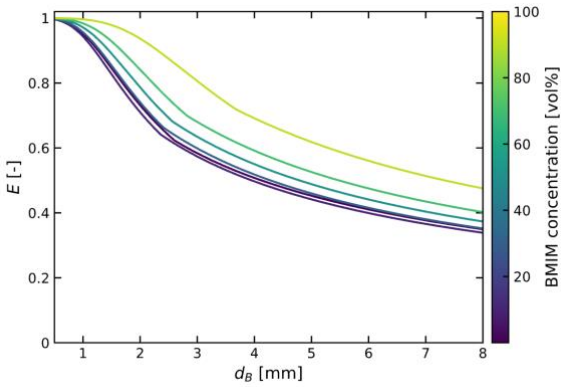


Figure 2: Bubble aspect ratio E vs. bubble diameter d_B for single bubbles in BMIM–water mixtures at volumetric concentrations ranging from 1% to 100%.

Conclusions. A novel correlation for the bubble aspect ratio has been developed by combining direct numerical simulations and experimental data. The proposed formulation accurately captures bubble shape over a wide range of conditions and shows improved agreement with single-bubble data compared to existing models. Moreover, the effect of [Bmim][BF_4] concentration has been highlighted, showing increased bubble deformation at lower concentrations. These results will be validated in future studies through comparison with experimental data.

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