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12.3 Development of a New Correction Factor for Gas Holdup Prediction Model in Various Bubble Columns Operating in Homogeneous Regime

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KEYWORDS: bubble column, gas holdup prediction, homogeneous regime, gas holdup model.

Gas holdup is one of the crucial parameters concerning the design and operation of bubble columns (BC). Many researchers have attempted to create a reliable model for gas holdup prediction. Due to the different gas-liquid system properties, gas sparger and column dimensions and operating conditions, creation of unique model is a challenging task. Therefore the authors decided to develop a model for homogeneous in different types of BCs.

The measurements in this work have been performed in two BCs facilities both operating in air-deionized water system. The first BC (0.15 m in ID) operated with a perforated plate as a gas sparger. The second BC had 12 cylindrical nozzles arranged annularly and the annulus was strictly defined by means of an inner concentric tube. The calculations were made on the basis of a model described by Nedeltchev and Schumpe (2008) while the correction factor f_c was developed as a function of Eo depending on the BC type. Additionally the calculated values were also compared with different models to evaluate if the model fitting is competitive. For a comparison the authors calculated the bubble diameters by several correlations.

In most of the cases the model fits well in the homogeneous regime and the average relative error does not exceed the value of 20% (see Fig. 12.3.1). Furthermore this value is the lowest in comparison with the other considered models. In the heterogeneous regime it is more difficult to fit the model due to the high turbulence and more complex hydrodynamics.

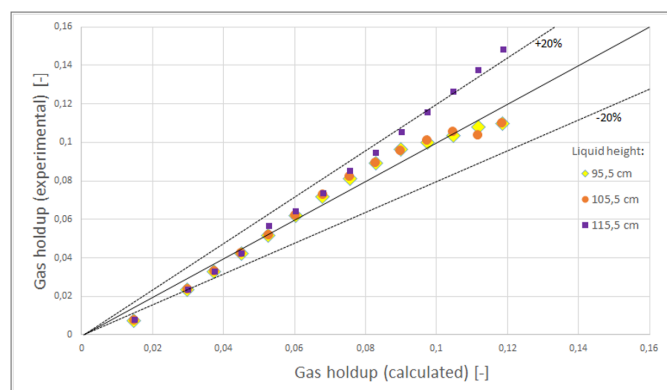


Figure 12.3.1: Parity plot of gas holdups in an annularly aerated BC operating with an air-deionized water system (clear liquid height = 0.955, 1.055, 1.155 m).

12.4 Application of proline-derived (thio)squaramide organocatalysts in asymmetric reactions

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KEYWORDS: asymmetric organocatalysis, proline, thiosquaramide, Diels–Alder reaction, conjugate addition.

In our research, we developed chiral proline-derived squaramide and thiosquaramide organocatalysts, which are capable of the dual activation in asymmetric reactions. Comparing the performance of thiosquaramide to squaramide, we examined the Diels–Alder reaction of (anthracen-9-yl)acetaldehyde and trans- β -nitrostyrene, which has been investigated in the literature using quantum chemical calculations. Moreover, their catalytic performance was compared in conjugate addition of lawsone to β,γ -unsaturated α -keto ester.

Both squaramide and thiosquaramide gave excellent yields (up to 99%) and enantiomeric excess values (up to 98%) in the Diels–Alder reaction. In the conjugate addition, the thiosquaramide catalyst has increased catalytic performance than the squaramide, which has been examined in the presence of different solvents and additives (Fig. 12.4.1).

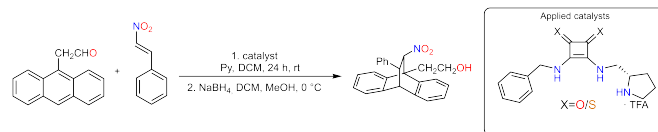


Figure 12.4.1: The Diels–Alder reaction of (anthracen-9-yl)acetaldehyde and trans- β -nitrostyrene (Py: pyridine)

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