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# ACCEPTED MANUSCRIPT

### Fluid Dynamics and Transport Phenomena

CFD simulation of gas-liquid flow in a high-pressure bubble column with a modified population balance model\*

Bo Zhang, Lingtong Kong, Haibo Jin\*, Guangxiang He, Suohe Yang, Xiaoyan Guo Beijing Key Laboratory of Fuels Cleaning and Advanced Catalytic Emission Reduction Technology, Beijing Institute of Petrochemical Technology, Beijing 102617, China. Email:jinhaibo@bipt.edu.cn Abstract: In this study, based on the Luo bubble coalescence model, a model correction factor  $C_{\rm e}$  for pressures according to the literature experimental results was introduced in the bubble coalescence efficiency term. Then, a coupled modified population balance model (PBM) with computational fluid dynamics (CFD) was used to simulate a high-pressure bubble column. The simulation results with and without  $C_{\rm e}$  were compared with the experimental data. The modified CFD-PBM coupled model was used to investigate its applicability to broader experimental conditions. These results showed that the modified CFD-PBM coupled model can predict the hydrodynamic behaviors under various operating conditions.

**Key words:** high-pressure bubble column; bubble coalescence; computational fluid dynamics; population balance model

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#### 1. Introduction

Bubble column reactor has simple structure, large capacity, easy operation, adequate heat and mass transfer, and small bed pressure drop <sup>[1-3]</sup>. Therefore, bubble columns are widely used in industry including chemical engineering, petrochemical, bio-engineering, environmental energy etc <sup>[4]</sup>. Many scholars have applied the population balance model in studying atmospheric bubble columns <sup>[5-7]</sup>. But bubble columns in chemical production are generally operated under high pressures and examples are hydrocracking of petroleum (*P*=5.0-21MPa), Fischer-Tropsch synthesis (*P*=2.0-5.0MPa) and benzene hydrogenation (*P*=5.0MPa) <sup>[8-11]</sup>. Although high-pressure bubble columns are widely used in chemical and biochemical processes, their fundamental hydrodynamic behaviors, which are essential for reactor scale-up and design, are still not fully understood.

The effect of pressure on the hydrodynamic behaviors of bubble columns have been experimentally investigated by many researchers. The gas holdup in high-pressure columns significantly increases due to the decreased bubble size [12-14]. The gas-liquid mass transfer and reaction performance are enhanced as the pressure rises [10, 15]. With the development of computer technology, numerical simulation of gas-liquid two-phase flow has been greatly developed. Among them, Krishna et al. [16] used a CFD model to simulate the high-pressure bubble column with the drag force between gas and liquid was considered only, and a density correction term  $\rho/\rho_0$  due to pressure change was introduced into the drag force model. Chen et al. [17] modified the gas density correction term in the drag model based on [16]. Although the radial and axial velocity

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