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CFD modeling of gas–liquid mass transfer process in a rotating packed bed

Yucheng Yang [a,b], Yang Xiang [a,*], Guangwen Chu [a,b], Haikui Zou [a,*], Baochang Sun [a], Moses Arowo [a,b], Jian-Feng Chen [a,b]

[a] Research Center of the Ministry of Education for High Gravity Engineering and Technology, Beijing University of Chemical Technology, Beijing 100029, PR China
[b] State Key Laboratory of Organic-Inorganic Composites, Beijing University of Chemical Technology, Beijing 100029, PR China

HIGHLIGHTS

- CFD method was adopted to analyze mass transfer process in a rotating packed bed.
- Liquid holdup in a rotating packed bed was investigated by CFD method.
- Three optimum designs of RPBs were developed to improve mass transfer efficiency.
- The vacuum deaeration process in a RPB was studied.

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ABSTRACT

Process intensification by rotating packed bed (RPB) has attracted wide attention in the recent years. In particular, its high gas–liquid mass transfer efficiency is proved by plentiful experimental data. However, due to the complex structure of packing in the RPB, it is extremely difficult to acquire detailed information about mass transfer process inside the reactor by experiments. Therefore, this study firstly employed computational fluid dynamics (CFD) modeling technique to analyze mass transfer process in a rotating packed bed (RPB) by adding user defined function (UDF) programming to Fluent solver in order to expand its abilities to RPB. The simulation results were compared with previous correlation data on liquid holdup and the calculated values of mass transfer process were matched with experimental values of vacuum deaeration process in RPB. The results revealed liquid flow and mass transfer process inside the reactor and were also in agreement with the experimental data. Additionally, three optimum designs of RPB (kinds of packing, size of rotors and blades added in packing) were developed to improve the mass transfer efficiency. The results show high removal efficiency in the small Δd packing and the rotor with larger inner and outer diameter, and the packing with blades can improve mass transfer efficiency compared to the conventional one. The CFD technique was generally found to be an important and effective tool for analyzing and optimizing RPBs.

1. Introduction

A rotating packed bed (RPB) is a novel device that was first developed by Ramshaw and Mallinson [1] in 1981 for enhancement of mass transfer processes. This device replaces gravity with centrifugal force of up to several hundred gravitational values, and can thus achieve high volumetric mass transfer coefficients with just a small volume of the contactor. Owing to size and capital cost reductions associated with the use of RPBs, they have been extensively explored for applications in absorption [2–4], desorption [5,6], distillation [7,8], oxidation [9,10], and etc. Chen's group at Beijing University of Chemical Technology has also extended the application of RPBs in reaction processes, such as crystallization [11], production of nanoparticles [12], polymerization [13], bromination [14,15], and etc.

Some fundamental researches on hydrodynamics and mass transfer phenomena in RPBs have also been widely made. For instance, Tung and Mah [16] employed penetration theory to describe gas–liquid mass transfer process under high gravity condition, and the predicted mass transfer coefficients were found to

* Corresponding authors at: Beijing University of Chemical Technology, No. 15 Beisanhuan East Road, Beijing 100029, PR China. Tel.: +86 10 64443134; fax: +86 10 644434784.

E-mail addresses: xiangy@mail.buct.edu.cn (Y. Xiang), zouhk@mail.buct.edu.cn (H. Zou).

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Nomenclature

a	gas–liquid interfacial area, 1/m
a_c	centrifugal acceleration, m^2/s
a_t	surface area of the packing, 1/m
C	concentration of solute, kg/m^3
D	diffusion coefficient, m^2/s
d_p	spherical equivalent diameter of the packing, m
E	the removal efficiency of dissolved oxygen in liquid phase
g	centrifugal acceleration, m/s^2
g_0	characteristics centrifugal acceleration (=100 m/s^2), m/s^2
k_L	liquid-side mass transfer coefficient, m/s
k_La	volumetric liquid-side mass transfer coefficient, 1/s
L	liquid mass flux, $kg/m^2 \cdot s$
P	pressure, $kg/m \cdot s^2$
N	rotational speed, rpm
Q_L	liquid flow rate, L/h
r_i	inner radius of the bed, mm
r_o	outer radius of the bed, mm
t	time, s
T	temperature, K
u'	fluctuating velocity, m/s
U	Liquid flow rate per unit area, cm/s
U_i	the mean velocity, m/s
U_{inlet}	the inlet velocity of liquid, m/s
U_0	characteristics flow rate per unit area (=1 cm/s), cm/s
V_i	volume inside the inner radius of the bed, m^3
V_0	volume between the outer radius of the bed and the stationary housing, m^3
V_t	total volume of the RPB, m^3
x	x-coordinate, m
Z	axial depth of the packing, mm

Greek letters

α_q	volume fraction of phase q
ε_L	liquid holdup
μ	viscosity of fluid, Pa·s
v	kinematic viscosity of the liquid, m^2/s
v_0	characteristic kinematic viscosity (=1.0×10^{-6} m^2/s), m^2/s
ρ	density of fluid, kg/m^3
Φ	vacuum degree, MPa
σ	liquid surface tension, N/m
δ	thickness of bed, mm
ω	angular velocity, rad/s

be in agreement with the experimental results. Munjal et al. [17] assumed that liquid flow in rotating blades and disk is laminar flow, and that liquid randomly distributes on the surface of a rotating bed. Comparison between the penetration theory and the complete convection–diffusion model showed that the former is more reasonable at low rotational speed than the latter. Additionally, Munjal et al. [18] reported for the first time gas–liquid interfacial areas and liquid-side mass-transfer coefficients in a rotating bed based on chemical absorption of CO_2 into NaOH solution. In 1990, Kumar and Rao [19] proposed a correlation for pressure drop in RPB with a wire mesh as the packing. They further used the correlation proposed by Tung and Math to predict liquid-film mass transfer coefficient for chemical absorption, and the results compared well with the experimental data. Liu et al. [20] reported the overall gas-phase mass transfer coefficient based on experiments about the stripping of ethanol from the ethanol–water mixture. Further, Chen et al. [21–23] examined the effects of various radii of a packed bed, packing's size, shape, material, surface property and viscosity of liquid on mass transfer efficiency, and observed that k_La increased with decreasing volume of the packed bed and viscosity of liquid, and that the wire mesh has higher mass transfer efficiency as compared to other various shapes of packings such as Rasching rings and intalox saddles. Additionally, Chen et al. [21] proposed an empirical correlation based on experimental data from the literature which proved feasible for predicting the experimental coefficients of RPB. Moreover, Luo et al. [24] developed a model based on the Danckwerts surface renewal theory to predict the liquid-side volumetric mass transfer coefficient in rotor, and the predicted values of mass transfer coefficient were in agreement with the experimental values with deviations within ±15%.

It is evident that all the above studies employed experimental approach to analyze mass transfer phenomena in RPBs. However, this method is costly to optimize, involves tedious processes and hardly reveals comprehensive information. It is thus necessary to develop an efficient and economical technique for analysis of mass transfer phenomena in RPBs. Fortunately, the advent and improvement in computer capacity has enabled the application of computational fluid dynamics (CFD) as an efficient and economical tool to simulate the hydrodynamics and mass transfer behavior of various industrial processes [25–27]. CFD has been employed in the recent past to study hydrodynamics in RPBs. For instance, Llerena-Chavez and Larachi [28] simulated 3D single-phase flows in RPB, which used a porous model to describe packing, and they and Yang et al. [29] proposed some optimum designs of RPB to reduce gas maldistribution. Based on Llerena-Chavez's results, Martinez et al. [30] simulated multiphase flow of water-SO_2 in an RPB; however, the results did not reveal the flow pattern and distribution of liquid in the RPB. Yang et al. [31] utilized foursquare obstacles to simplify the packing and systematically investigated the effect of flow rates and rotational speeds on single-phase flow in RPB while Shi et al. [32] employed the Yang's geometrical model and developed 2D CFD computational model to study the mutiphase flow RPBs. In order to clearly reveal the gas–liquid distributions in RPBs, various models including the volume of fluid (VOF) multiphase model, sliding model (SM) and the Reynolds stress model (RSM) were used to compute the velocity, distribution and residence time of liquid phase. However, to the best of our knowledge, there is hitherto scarce information on the analysis of mass transfer in RPB by CFD method.

This study therefore employed the CFD method for the first time to analyze mass transfer process in RPB, and the results were validated with those of experiments on vacuum deaeration process. The effects of various operating parameters such as rotational speed and liquid flow rate on the mass transfer efficiency were investigated, and the distribution of dissolved oxygen along radial position was illustrated. Additionally, three optimum designs of RPB (packing porosity, size of rotors and blades added in packing) were developed to improve the mass transfer efficiency.

2. CFD model

2.1. Geometrical model

A reasonable geometrical model of RPB leads to a fair multiphase flow simulation, and the accuracy of multiphase flow simulation leads to a fine gas–liquid mass transfer simulation.