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Study on micromixing and reaction process in a rotating packed bed

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ABSTRACT

The exploration on the microscale transport phenomena is of great significance to understand the mechanism of microscale mixing and chemical reaction in a rotating packed bed (RPB). In this paper, numerical investigation is carried out and compared with the experimental results. Two different scale reaction models are applied to simulate and the numerical result is in reasonable agreement with the experimental results. The fluid flow and the species transfer with a competitive and consecutive reaction are studied to obtain the evolution of the segregation index and flow field. Each environment changes and is updated continuously with the liquid film flowing outward, and the micromixing and reaction are influenced by the fractions p_1 and p_2 of different environments. It is evidenced that different factors such as rotational speeds, volume ratios and initial mixing concentration impose considerable influences on the micromixing and reaction processes. The micromixing time ranges about 5.2×10^{-2}–1×10^{-3} ms showing that micromixing performance in RPB is much better. The main product and by-product appear different evolution pattern along the package wires, which provide guideline for the optimization of RPB structure. The optimization on the RPB structure is provided and the simulation results clarify a deeper understanding on the micromixing and reaction features in RPB.

1. Introduction

Higee technology, carried out in a rotating packed bed (RPB), was originally invented by Colin Ramshow and his co-workers in 1979. In the high gravity environment provided by rotating components, the liquid is broken into tiny liquid elements including liquid films, droplets and filaments and flows chaotically through the packed bed, where large rapid updating interfacial area is generated ensuring intensive mixing so that the process of micromixing and mass transfer are greatly enhanced, and the rate of mass transfer increase 1 to 3 orders of magnitude compared with that of the traditional devices. As a highly efficient apparatus for mass transfer, separation and reaction, RPB has been widely used in chemical engineering [27,25,8,23], environmental protection [10,8,23,14,1], energy engineering [9], pharmaceutical engineering [29], and other industrial processes. In chemical engineering, Ramshaw and co-workers [27] first used Higee in distillation process. They made full use of characteristics of liquid microelements which are generated by huge shear stress, short residence time and high mass transfer coefficient compared to the traditional chemical equipment [11,20,15,16], as illustrated in Fig. 1. RPBs have been also applied to absorption [10,1], catalytic reaction [8], VOC removal [5,23,22,13] and treatment of exhaust gases [10,8,23] and wastewater [21,30]. Recently, a novel and successful application is nanomaterial preparation [6,9]. A schematic illustration of rotating packed bed is shown in Fig. 2.

As is well known, the yield, selectivity, quality of desired product and sometimes the process safety are greatly affected by efficient mixing among various species [3,38,20,16]. In RPB, the liquid is broken into micro-elements with different forms when it entered rotating package from liquid distributor. However, the degree of micromixing has a crucial impact on mass transfer in RPB. With the progress in computer science and the theory of multiphase flow, study on micromixing process is basically through the combined methods of numerical simulation with experiment. Based on the experimental data and physical model, CFD method is used in this paper to explore the performance of mixing and mass transfer in a RPB. Generally, the minimum scale of simulation by CFD is grid scale [17]. The behaviors of flow and mass transfer occurring in a sub-grid scale are difficult to describe. For the purpose of improvement in this aspect, the reaction models of both grid scale and sub-grid scale are proposed. The present study would provide a better understanding of the mechanism of micromixing, and gives a sound guideline to RPB operation.

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Nomenclature

$\overline{C_{AP}}$	passive mean concentration of species A, (mol·m^{-3})
C_{A0}	initial concentration of reactant A, (mol·m^{-3})
$\overline{C_\beta}$	mean concentration of species n, (mol·m^{-3})
C_{B0}	initial concentration of reactant B, (mol·m^{-3})
C_β	transient concentration of species β, (mol·m^{-3})
$\overline{C_0}$	mixed concentration of reactant A and B, (mol·m^{-3})
$\overline{c_{AP}^2}$	concentration deviance of species A, (mol·m^{-3})^2
c_β	fluctuation concentration of species β, (mol·m^{-3})
D_β	molecular diffusivity, (m^2·s^{-1})
k	turbulent kinetic energy, (m^2·s^{-2})
k_1, k_2	reaction coefficient, (m^3·mol^{-1}·s^{-1})
N	rotating speed, (r·min^{-1})
n	number of environment
p_n	volume fraction of environment n
r_1, r_2	reaction rate, (mol·m^{-3}·s^{-1})
s	the thickness of the unit film, (m)
$\overline{s_{\beta,n}}$	the proportion of concentration of reactants and products in environment n, (mol·m^{-3})
t_m	micromixing time, (s)
$\overline{U_i}$	mean velocity, (m·s^{-1})
V	inlet flow rate, (L·h^{-1})
Xs	segregation index
α	volume ratio of reactant A and B
β	A, B, R, S
ε	dissipation rate of turbulent kinetic energy, (m^2·s^{-1})
ν_T	turbulent dynamic viscosity, (m^2·s^{-1})
τ	mixing time, (s)
ξ	initial ratio of the feed (C_{B0}/C_{A0})
γ	parameter for micromixing

2. Physical picture

2.1. The physical description of the fluid flow in RPB

In RPB, the layers of the package wires are taken to be circular in the cross section and woven according to the pattern shown in Fig. 3. The non-premixed liquid reactants are sprayed in the form of thin liquid films from the center of RPB at the same radial speed with the azimuth velocity being zero and form a sheet of liquid before they come onto the first layer of the wire. During the procedure that they flow toward the first layer of package, the two liquid films contact with each other to form a single liquid sheet. The reactants of A and B would diffuse and react at the interface between the two liquid films. Upon impact with the first layer of the package wires, the initial single liquid sheet is divided into two sheets flowing around on the package wire upper semi-sphere and lower semi-sphere respectively and obtains the circular speed of the package while it continues to flow towards the outer package wires under the action of centrifugal force. The mixing and reaction between the species continue within the two liquid sheets. Upon leaving the wires, the two liquid sheets merge again and flow outward in the void space. The process keeps going on until the liquid sheet leaves the last layer of the package wire.

2.2. The main assumptions

In order to explore the fluid flow, mixing and chemical reaction within the liquid films, the basic assumptions are adopted:

(1) All the layers of the package wires are identical in structure.
(2) The film is in a continuous flow.
(3) The gravity in RPB is much weaker than the centrifugal effect and is ignored.
(4) The liquid films are captured by every layer of the package wires during the process flowing outward and divided into two sheets, which flow around on the surface of the package wire. Though the thicknesses of the two sheets of liquid would be different, it is omitted in present study.

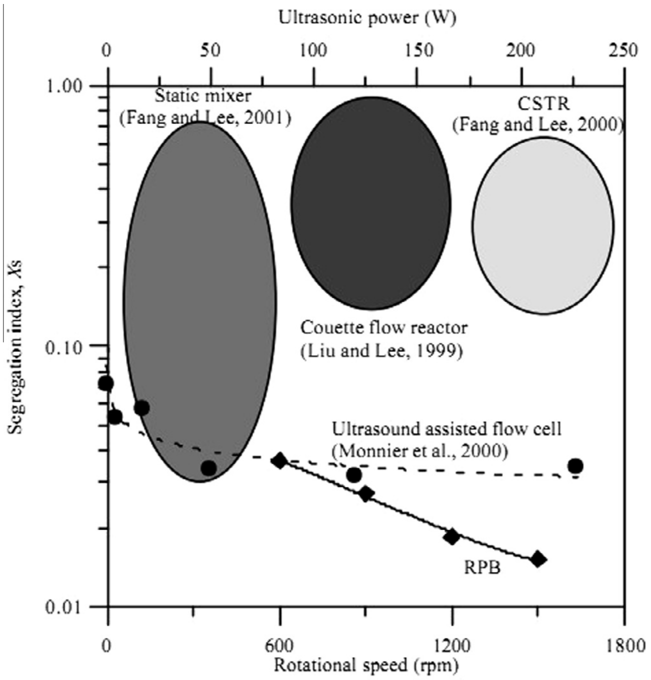

Fig. 1. Contrast of segregation index in different mixing devices.

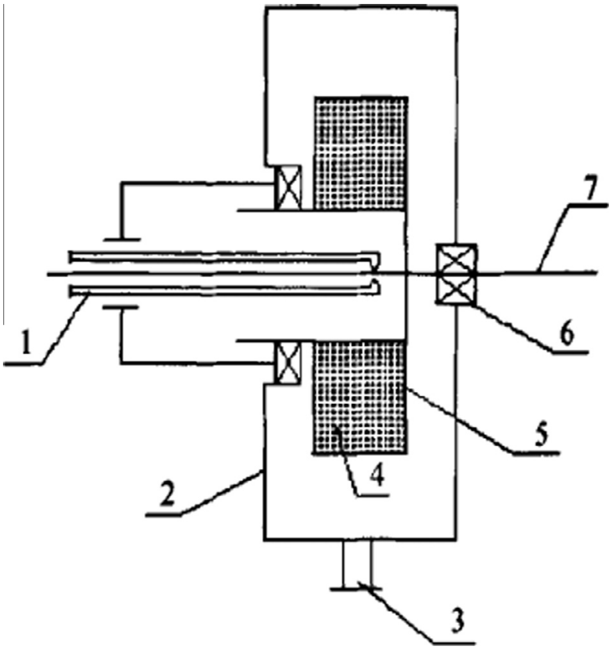

Fig. 2. Main structure of an RPB.