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Short communication

# A structured packed-bed reactor designed for exothermic hydrogenation of acetone

Yanjun Duan[a,b], Min Xu[a], Xiaoming Zhou[a], Xiulan Huai[a,*]

[a] Institute of Engineering Thermophysics, Chinese Academy of Sciences, Beijing 100190, China
[b] University of Chinese Academy of Sciences, Beijing 100049, China

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ABSTRACT

Fixed-bed reactors randomly packed with catalysts have many disadvantages that may adversely affect the desired chemical reaction. The increasingly used monolithic reactor, in contrast, has many operational advantages; however, for a kinetically-controlled reaction, it does not contain sufficient catalyst to sustain the reaction. To address the problems associated with both randomly packed-bed reactor and the monolithic reactor, a structured packed-bed reactor was proposed and mathematical models were built for randomly packed-bed reactor and structured packed-bed reactor. Their respective performances were compared when applied to the exothermic reaction of the isopropanol–acetone–hydrogen chemical heat pump system. The results showed that the structured packed-bed reactor performed better in terms of pressure drop and heat transfer capacity, and had a lower radial temperature gradient, indicating that this reactor had a higher effective heat conductivity. Isopropanol on the catalyst particle surfaces was more concentrated near the tube wall because a wall effect existed in the boundary layer around the particle-wall contact points.



## 1. Introduction

A chemical heat pump (CHP) is a device that can be employed for low-temperature heat upgrading and energy storage. It can provide the high temperatures required for industrial sectors by taking advantage of the heat of reversible catalytic reactions (Cacciola, Anikeev, Recupero, Kirillov, & Parmon, 1987). As a new energy-saving device, the CHP has developed rapidly in recent years because of its advantages of having zero theoretical power consumption, high energy efficiency (Raldow & Wentworth, 1979) and no pollutant emission. Among the many CHP systems proposed to date, the isopropanol–acetone–hydrogen CHP system (IAH-CHP) is highly promising (KlinSoda & Piumsomboon, 2007).

Research on the exothermic IAH-CHP reactor has mainly adopted the traditional packed-bed reactor. This type of reactor is randomly filled with catalyst particles, and it usually suffers from the disadvantages of high thermal resistance, high pressure drop, and low heat transfer coefficient. These disadvantages may lead to hot spots and side reactions, and hence decrease the selectivity of the reaction.

The monolithic reactor is increasingly being used, developed, and evaluated in many new reactor applications (Williams, 2001), and has many operational advantages compared to the conventionally used packed-bed reactor in several aspects, such as energy input, efficiency, safety, and reactant–catalyst separation (Nijhuis et al., 2001). However, the thin wash-coat of monolithic reactor which is usually only 20–150-μm thick results in a lack of catalyst for kinetically-controlled reactions. To solve the problems of both the randomly packed-bed reactor and monolithic reactor, we propose a new structured packed-bed reactor.

The catalyst-assisted IAH-CHP absorbs heat at about 353 K by isopropanol dehydrogenation and releases heat at about 473 K by acetone hydrogenation. In this process, working fluids are cycled in a closed system. The pressure is the most important process variable that affects the stability of the system (Kitikiatsophon & Piumsomboon, 2004), and temperature is the most important process variable that affects the efficiency of the system. Moreover, the exothermic reaction temperature is more important than the endothermic reaction temperature because it is affected to a much greater extent by the reaction temperature (Chung, Kim, Yeo, & Song, 1997). Thus, it is necessary to study the pressure and temperature in the system, especially in the exothermic reactor.

The purpose of this paper is to build mathematical models of the structured packed-bed reactor and the randomly packed fixed-bed reactor with spheres, and to compare the performances

* Corresponding author. Tel.: +86 10 82543035; fax: +86 10 82543033.
*E-mail address:* hxl@iet.cn (X. Huai).

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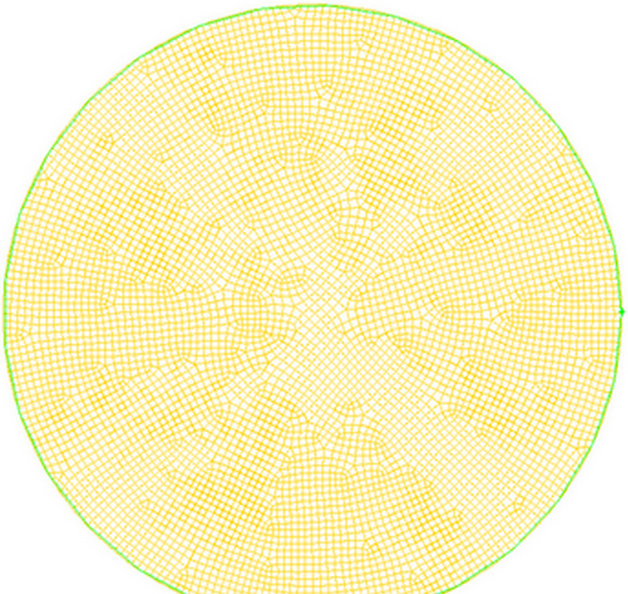


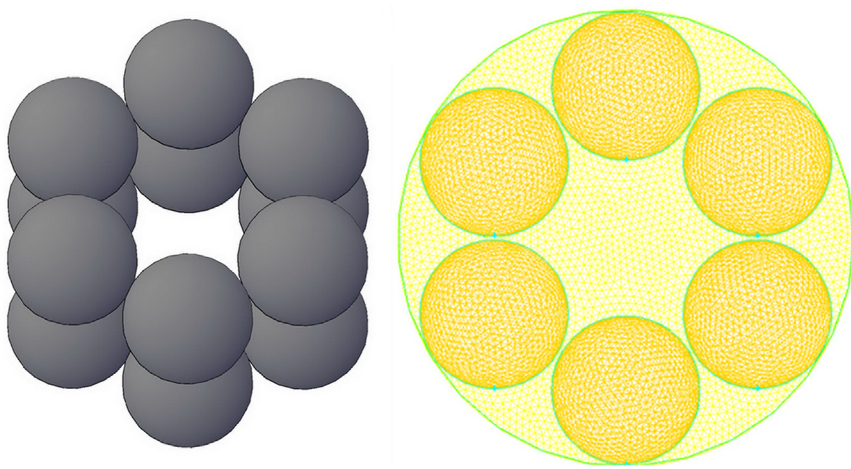
**Fig. 1.** Cross-sectional view of randomly packed-bed reactor.

of these two kinds of reactors for acetone hydrogenation in terms of pressure drop, reaction rate, conversion, velocity, and species distributions, as well as temperature distributions and heat transfer.

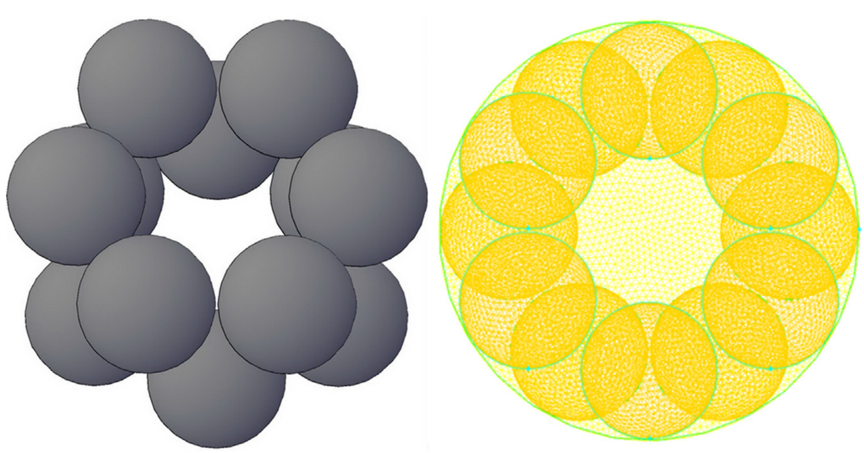
## 2. Physical model

Fig. 1 shows the physical model of the cross-sectional view of the randomly packed-bed reactor, which is a cylinder with a diameter of 25.4 mm. This model directly invokes the porous module in Fluent, thus the catalyst does not need to be considered here.

To solve the problem of the monolithic reactor mentioned earlier, large catalyst particles with a diameter of 1 mm were adopted in the structured packed-bed reactor. The tube-to-particle diameter ratio ($N$) was 3, and two different particle arrangements (denoted Model A and Model B) in the tubes of the structured packed-bed reactor were investigated, as demonstrated in Fig. 2. The packing can be realized by making a gap of an appropriate size between the tube wall and a net, which allows the catalyst particles to fill the gap; the net does not affect the fluid flow in the reactor. The left side of Fig. 2 shows schematic representations of the particle arrangement and the right side shows the model meshes from the top view. The structured packed beds have lower specific area than randomly packed beds, thus the structured packed reactors should be extended so that the reaction can achieve the same conversion as in the randomly packed reactor. The length of



Model A



Model B

**Fig. 2.** Catalyst particle packing in the tube of the structured packed-bed reactor.

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