Numerical Study of a Metal Foam Reactor for Acetone Hydrogenation in Chemical Heat Pumps: Postprint

Authors: Peng Wenping, Xu Min, Huai Xiulan

Date: 2017-10-17T00:00:00+00:00

Abstract

The isopropanol-acetone-hydrogen chemical heat pump (IAH-CHP) is a system capable of simultaneously upgrading energy grade and achieving energy storage. The acetone hydrogenation reactor constitutes a crucial component of the IAH-CHP system, exerting significant influence on its overall performance. This paper employs a metal foam reactor to implement acetone hydrogenation, thereby enhancing both reaction efficiency and energy utilization. First, a model of the acetone hydrogenation metal foam reactor is established, followed by a comparative performance investigation between metal foam and packed-bed reactors through simulation. The results demonstrate that for slow reactions such as acetone hydrogenation, the metal foam reactor outperforms the packed-bed reactor when wall heat transfer is considered, primarily attributable to its excellent wall heat transfer characteristics and low pressure drop.

Full Text

Preamble

Numerical Study on Metal Foam Reactors for Acetone Hydrogenation in Chemical Heat Pumps

Peng Wen-ping[1,2], Xu Min[1], Huai Xiu-lan[1,*] [1] Institute of Engineering Thermophysics, Chinese Academy of Sciences, Beijing 100190, China [2] University of Chinese Academy of Sciences, Beijing 100049, China

Abstract

The isopropanol–acetone–hydrogen chemical heat pump (IAH-CHP) is a system capable of simultaneously upgrading energy grade and storing energy. The

acetone hydrogenation reactor constitutes a critical component of the IAH-CHP system and exerts a decisive influence on overall system performance. This study introduces metal foam reactors for acetone hydrogenation to enhance both reaction efficiency and energy utilization. A detailed reactor model for metal foam reactors is developed using acetone hydrogenation as a representative slow reaction. The performance advantages of metal foam reactors over conventional particle-packed reactors are investigated numerically. The results demonstrate that superior wall heat transfer characteristics and low pressure drop make metal foam reactors for acetone hydrogenation over amorphous Raney nickel catalyst significantly outperform particle-packed reactors.

Keywords: Metal foam reactors; Acetone hydrogenation; Chemical heat pump

1. Introduction

In industrial processes, substantial amounts of low-temperature waste heat (e.g., boiler flue gas) and low-grade thermal energy (e.g., solar, geothermal) remain insufficiently recovered and utilized. The key challenge in harnessing such thermal energy lies in elevating its temperature and enabling storage. Among various approaches, the isopropanol–acetone–hydrogen chemical heat pump (IAH-CHP) represents a particularly suitable system for this purpose [Figure 1: see original paper]. This system offers numerous advantages, including excellent temperature adaptability, significant temperature lift capability, and energy storage capacity, making it especially appropriate for the deep utilization of intermittent and fluctuating low-temperature heat sources [2]. The IAH-CHP system comprises two primary reactions: an endothermic isopropanol dehydrogenation reaction that absorbs low-temperature heat, and an exothermic acetone hydrogenation reaction that releases high-temperature heat. The acetone hydrogenation reaction is a gas-phase catalytic process that, due to its slow kinetics, is typically implemented in particle-packed reactors. Although such reactors provide high catalyst loading per unit volume, their performance is constrained by poor wall heat transfer and high pressure drop.

Metal foam reactors utilizing high-porosity metal foams as catalyst supports have found extensive applications in strongly exothermic/endothermic reactions, including hydrocarbon reforming [3], hydrocarbon partial oxidation and combustion [4], and carbon monoxide preferential oxidation [5]. The high porosity, large specific surface area, high gas-solid heat transfer coefficient, and favorable mechanical properties of metal foams render these reactors particularly suitable for intense heat-generating or heat-absorbing processes [6]. However, no attempts have yet been made to apply metal foam reactors to slow reactions such as acetone hydrogenation.

The objective of this study is to establish a mathematical model for metal foam reactors applied to the slow acetone hydrogenation reaction and subsequently

compare the acetone hydrogenation performance of metal foam reactors against that of particle-packed reactors.

2. Reactor Structure

Designing an acetone hydrogenation reactor with high conversion, high selectivity, high exothermic temperature, and low pressure drop represents a significant engineering challenge. This study employs a metal foam reactor to implement acetone hydrogenation. The reactor structure is illustrated in [Figure 2: see original paper]. Copper foam is selected due to copper' s excellent thermal conductivity. The washcoat support material is -Al2O3, with Raney nickel serving as the active catalyst. The specifications of the Raney nickel catalyst [7] are presented in , while the reactor structural parameters and operating conditions are summarized in .

3. Reactor Model

One-dimensional heterogeneous energy conservation equations and species transport equations are employed to describe the physical phenomena within the reactor. The governing equations and boundary conditions are listed in . The solid phase comprises both the metal struts and the catalyst washcoat. Heat transfer occurs throughout the metal strut region, while mass transfer and chemical reactions take place within the washcoat region. Given that the thermal conductivity of the metal struts and washcoat far exceeds the species transport capability within the micro/nanoscale porous washcoat, the temperatures in the metal struts and washcoat are assumed equal. Consequently, for heat transfer calculations, the metal struts and washcoat are treated as a single phase.

The structural characteristics and transport properties for flow, heat transfer, and mass transfer in both particle-packed and metal foam reactors are detailed in . The reaction mechanism for acetone hydrogenation over Raney nickel catalyst has been investigated in relevant literature [8]. Reaction products can be categorized into three types: hydrogenation products (main reaction), namely isopropanol; cracking products (first side reaction), namely carbon monoxide and light alkanes; and condensation products (second side reaction), such as methyl isobutyl ketone (MIBK). Since the second side reaction accounts for only 0.1% of total products, it is neglected in this study. The rate equations for the main and first side reactions are presented in and the reaction network is shown in [Figure 3: see original paper].

4. Simulation Method

To reduce computational time, steady-state processes are simulated directly. The species transport equations in the washcoat and bulk regions are solved separately. First, mass transfer and chemical reactions within the washcoat are solved to obtain the effectiveness factor, which is then substituted into the governing equations for the bulk region to solve for momentum, heat, and mass transfer. The same solution strategy is applied to particle-packed reactors. For washcoat geometry, the metal strut cross-section is assumed circular, resulting in an annular washcoat structure as shown in [Figure 4: see original paper]. The structural parameters of the coated metal foam are listed in , and the physical property parameters of the metal struts and washcoat are given in .

The calculated effectiveness factors for acetone hydrogenation under different washcoat thicknesses are presented in . For both main and side reactions, the effectiveness factors are substantial, exceeding 98.8%.

---

5. Results and Discussion

5.1 Metal Foam Reactor Performance

The calculated acetone conversion and pressure drop in metal foam reactors with different washcoat thicknesses at constant catalyst loading are shown in Figure 6: see original paper. Acetone conversion increases with decreasing washcoat thickness because enhanced wall heat transfer at lower thicknesses results in lower reactor temperatures Figure 6: see original paper. Lower temperatures promote the main reaction while suppressing side reactions. Pressure drop increases with decreasing washcoat thickness because reactor length must increase to maintain constant catalyst loading. The isopropanol selectivity in metal foam reactors at constant catalyst loading is depicted in Figure 6: see original paper. Clearly, isopropanol selectivity increases with decreasing washcoat thickness due to improved wall heat transfer. These results demonstrate that enhancing wall heat transfer to maintain lower reactor temperatures is key to improving acetone conversion and increasing high-temperature heat output.

5.2 Comparison with Particle-Packed Reactors

The calculated acetone conversion and pressure drop in particle-packed reactors with different particle diameters at constant catalyst loading are shown in Figure 7: see original paper. Acetone conversion increases with decreasing particle diameter due to improved wall heat transfer and consequently lower reactor temperatures Figure 7: see original paper. However, higher conversion comes at the cost of dramatically increased pressure drop. Even with particle diameters as small as 20 μm, the acetone conversion in particle-packed reactors remains lower than that in metal foam reactors, while the pressure drop is far greater. Furthermore, isopropanol selectivity in particle-packed reactors is lower than in

metal foam reactors. These findings underscore that the advantages of metal foam reactors over particle-packed reactors lie in their superior wall heat transfer characteristics and low pressure drop.

---

6. Conclusions

This study establishes a model for metal foam reactors applied to acetone hydrogenation and conducts a comparative performance analysis against particle-packed reactors. The results demonstrate that for the slow acetone hydrogenation reaction, metal foam reactors outperform particle-packed reactors, primarily due to their excellent wall heat transfer characteristics and low pressure drop.

References

[1] Peng W.P., Xu M., Huai X.L., Liu Z.G.. 3D CFD simulations of acetone hydrogenation in randomly packed beds for an isopropanol–acetone–hydrogen chemical pump[J]. Applied Thermal Engineering, 2016, 94:238-248.

[2] Wongsuwan W., Kumar S., Neveu P., Meunier F.. A review of chemical heat pump technology and applications[J]. Applied Thermal Engineering, 2001, 21:1489-1519.

[3] Richardson J.T., Hung J.K.. Carbon dioxide reforming with Rh and Pt–Re catalysts dispersed on ceramic foam supports[J]. Applied Catalysis A: General, 2003a, 255:69-82.

[4] Williams K.A., Schmidt L.D.. Catalytic autoignition of higher alkane partial oxidation on Rh-coated foams[J]. Applied Catalysis A: General, 2006, 299:30-45.

[5] Chin P., Sun X., Roberts G.W., Spivey J.J.. Preferential oxidation of carbon monoxide with iron-promoted platinum catalysts supported on metal foams[J]. Applied Catalysis A: General, 2006, 302:22-31.

[6] Zhao C.Y.. Review on thermal transport in high porosity cellular metal foams with open cells[J]. International Journal of Heat and Mass Transfer, 2012, 55:3618-3632.

[7] Xu M., Fang X., Li X.F., Huai X.L., Guo J.F., Liu H.. Equilibrium model and performances of an Isopropanol—acetone—hydrogen pump with a reactive distillation column[J]. Industrial & Engineering Chemistry Research, 2013, 52:4040-4048.

[8] Duan Y.J., Xu M., Huai X.L.. High temperature catalytic hydrogenation of acetone over Raney Ni for chemical heat pump[J]. Journal of Thermal Science, 2014, 23:85-90.