Applied Thermal Engineering 71 (2014) 445–449

Contents lists available at ScienceDirect

Applied Thermal Engineering

journal homepage: www.elsevier.com/locate/apthermeng

Design of an isopropanol–acetone–hydrogen chemical heat pump with exothermic reactors in series

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HIGHLIGHTS

- We propose the IAH-CHP system with exothermic reactors in series.
- The COP and exergy efficiency of the system increase by 7.6% and 10.3% respectively.
- The work input of the system is reduced notably at the same quantity of heat released.

ARTICLE INFO

Article history:
Received 4 May 2014
Accepted 20 June 2014
Available online 27 June 2014

Keywords:
Chemical heat pump
Acetone hydrogenation
Exothermic reactor
Energy performance

ABSTRACT

The isopropanol–acetone–hydrogen chemical heat pump system with a series of exothermic reactors in which the reaction temperatures decrease successively is proposed. This system shows the better energy performances as compared with the traditional system with a single exothermic reactor, especially when the higher upgraded temperature is need. At the same amounts of the heat released, the work input of the compressor and the heater are both reduced notably. The results indicate that the advantages of the IAH-CHP system with exothermic reactors in series are obvious.

1. Introduction

It is important for saving energy to reuse the low-temperature waste heat which is usually released to the environment in industrial processes. The waste heat can be utilized more easily by upgrading its quality. Mechanical heat pumps have been widely used in various process industries, but many shortcomings of mechanical heat pump such as high operation cost, low efficiency and low upgrading temperature are still present [1,2]. In recent years, Many researchers [3–9] are putting more focus on chemical heat pump, which converts the low-level heat to high-quality thermal energy through a reversible chemical reaction, because of its advantages such as high upgrading temperature, possibility of energy storage, and low hazard. The schematic diagram of an isopropanol–acetone–hydrogen (IAH-CHP) system is shown in Fig. 1. In this system, the dehydrogenation of isopropanol takes place at the temperature T_L in the endothermic reactor (reboiler in Fig. 1) to yield acetone and hydrogen. The low-level heat Q_L is introduced to drive the reaction and subsequently to separate of acetone and isopropanol in the distillation column. The acetone and hydrogen as the distillate are compressed by the compressor, and then are heated in the recuperator. Subsequently, the acetone and hydrogen are introduced to the exothermic reactor after being heated up to the reaction temperature in the heater. Acetone hydrogenation occurs at the temperature T_H in the exothermic reactor and the high-temperature heat Q_H is produced and released. The effluent is cooled in the recuperator and subsequently gets back to the distillation column to close a cycle.

In recent decades, many researchers put focus on catalyst design [10–12] and performance evaluation [7–9] for the IAH-CHP system. But little literature investigated this system from the view of chemical reactor engineering. Our previous works [13,14] proposed an IAH-CHP system with a reactive distillation column to couple the endothermic reactor and distillation column, and experimentally verified its superiority. The optimal design of the exothermic fixed-bed reactor for high-temperature acetone hydrogenation was also carried out [15,16]. However, a contradiction is present for exothermic reaction of the IAH-CHP system. From the view of waste heat recovery, the higher upgraded temperature is more interesting. Accordingly, when the upgraded thermal energy with a

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http://dx.doi.org/10.1016/j.applthermaleng.2014.06.041
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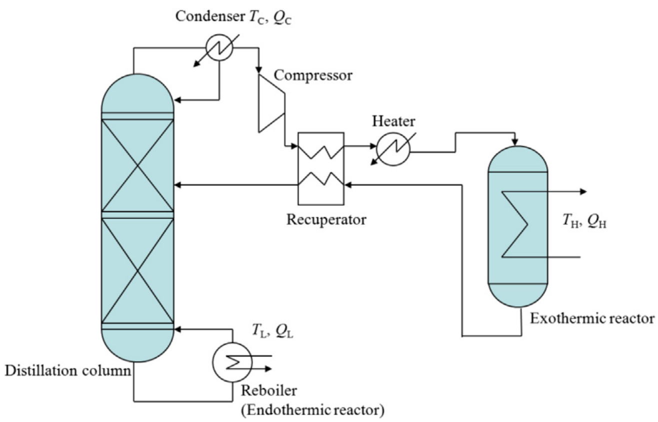

Fig. 1. Schematic diagram of the isopropanol–acetone–hydrogen chemical heat pump with a single exothermic reactor.

higher temperature is need, we must increase the reaction temperature in the exothermic reactor. Nevertheless, the higher temperature in the exothermic reactor reduces the equilibrium conversion of acetone from the view of the thermodynamic aspect and ends the reaction when the equilibrium composition is reached (18% at 483 K [17]). Thus the amounts of the heat released from the system are also decreased. Moreover, the lower conversion results in the invalid cycle of hydrogen and acetone in the system and hence increases the power consumption of the compressor and the energy cost during the separation process. Unfortunately, to our best knowledge, how high-temperature heat recovery and chemical equilibrium limitation can be balanced is still not clear in the literature.

To address the above issues, we propose the IAH-CHP system with exothermic reactors in series as shown in Figs. 2 and 3 to replace the conventional one with a single high-temperature equilibrium reactor. The first one of a series of reactors in the modified system is equal with the high-temperature equilibrium reactor of the conventional IAH-CHP, but the temperatures in the other reactors are lower than that in the first reactor. Figs. 2 and 3 show the IAH-CHP system with two and three exothermic reactors in series, respectively. Take the former for example, the acetone and hydrogen are fed into the first exothermic reactor and reach equilibrium at the highest temperature $T_{H,1}$. The heat of the effluent is released in the first recuperator, and then the equilibrium products are introduced to the second exothermic reactor and reach the other equilibrium at a lower temperature $T_{H,2}$. The effluent is cooled in the second recuperator and goes back to close the cycle. Following this method, the conversion of acetone increases and the amounts of the heat released grows while the high upgraded temperature is maintained in this system.

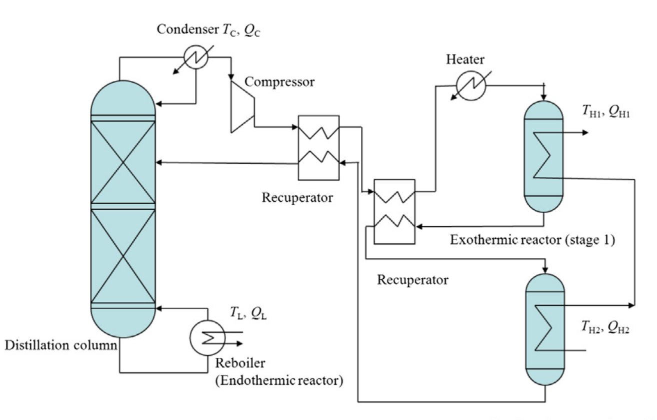

Fig. 2. Schematic diagram of the isopropanol–acetone–hydrogen chemical heat pump with two in-series exothermic reactors.

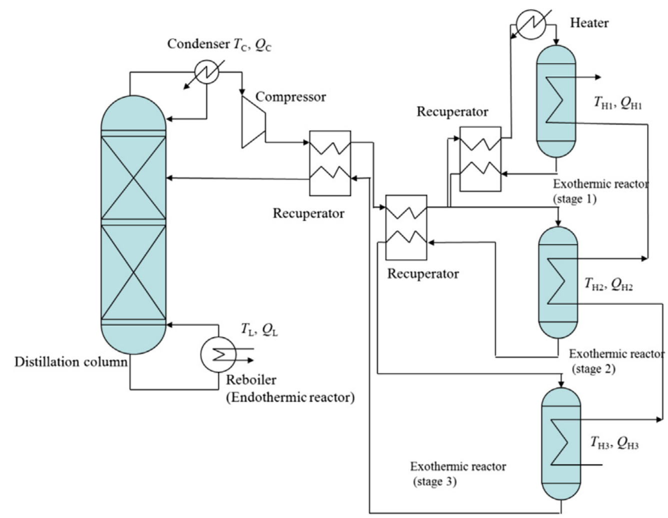

Fig. 3. Schematic diagram of the isopropanol–acetone–hydrogen chemical heat pump with three in-series exothermic reactors.

In our previous work [13,14], a rigorous mathematic model is established to simulate the IAH-CHP system with reactive distillation. In this work, we establish a mathematical model for an IAH-CHP system with a reactive distillation column and exothermic reactors in series, and the superiority of the IAH-CHP system using in-series exothermic reactors is expounded.

2. Mathematical model

In this section, the mathematical models of the IAH-CHP system with a single exothermic reactor and the system with two and three exothermic reactors in series are established. All calculations are carried out in the commercial simulation software Aspen Plus. The rigorous equilibrium stage model RadFrac is used to simulate the distillation column. The user kinetics subroutine (FORTRAN code) is used to depict the experimentally-determined reaction kinetic model in our previous work [13], and then compiled and linked with the simulation model in ASPEN PLUS by using the Aspen Plus Simulation Engine. The Compr module with isentropic type is used to model the compressor, and a simple model called HeatX is used for the recuperator. For the exothermic reactor, the RGIBBS module with specified temperatures and pressures is used. Based on our previous work, the reactive distillation column substitutes the conventional distillation column for the IAH-CHP system in this paper.

The optimized specifications and operating conditions of the IAH-CHP system with a single exothermic reactor are list in Table 1 and elaborated in details in our previous work [13]. For the IAH-CHP system with two and three in-series exothermic reactors, the optimized specifications and operating conditions are also list in Table 1. The various temperatures of the in-series exothermic reactors are specified and the temperature difference between the two adjacent reactors is set to more than 20 K. The feed stage of the distillation column is also changed to obtain the optimized energy performance. The amount of catalyst loading in the reactive distillation column increases due to the increase of acetone conversion in the in-series exothermic reactors(it is more than two-