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Study on Isopropanol–Acetone–Hydrogen chemical heat pump of storage type

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Abstract

An Isopropanol–Acetone–Hydrogen (IAH) heat pump employing metal hydride for storing hydrogen to realize energy storage is investigated in the present work. The influences of some operation parameters on the performance of storage type heat pump are presented, the performance of storage type heat pump worsens with the increase of reflux ratio, endothermic reaction temperature and exothermic reaction temperature, while there exists an optimal molar ratio of hydrogen to acetone in which the storage type heat pump has the best performance. Multi-parameter optimization is employed to search the optimal design scheme, and the performance of heat pump can be improved greatly after optimization.

Keywords: Isopropanol–Acetone–Hydrogen (IAH) heat pump; Storage type; Multi-parameter optimization; Genetic algorithm; Exergy efficiency

1. Introduction

With the decline of storage capacity for fossil fuels, the utilization of solar, geothermic and waste heats has attracted considerable attentions. However, the temperature of these heats is often low; the heats should be improved to high-temperature heats before utilization. Prevost and Bugarel (1980) proposed an Isopropanol–Acetone–Hydrogen (IAH) chemical heat pump to convertlow-temperature heat into high-temperature heat with the aid of chemical reaction, which is regarded as one of the most promising chemical heat pumps (Kitikiatsophon and Piumsomboon, 2004). In this heat pump, the dehydrogenation of isopropanol takes place at Temperature T_L in the endothermic reactor, which is shown as follows:

$$(CH_3)_2CHOH_{(g)} \rightarrow (CH_3)_2CO_{(g)} + H_{2(g)} \quad \Delta H_L = 54.4\ \mathrm{kJ/mol} \tag{1}$$

Here, ΔH_L is the endothermic reaction enthalpy, and dehydrogenation reaction consumed low-temperature heat. The hydrogenation of acetone takes place in the gas phase exothermic reactor at temperature T_H, the reaction equation is shown as follows (KlinSoda and Piumsomboon, 2007):

$$(CH_3)_2CO_{(g)} + H_{2(g)} \rightarrow (CH_3)_2CHOH_{(g)} \quad \Delta H_H = -54.4\ \mathrm{kJ/mol} \tag{2}$$

Here, ΔH_H is the exothermic reaction enthalpy, and the hydrogenation reaction releases high-temperature heat. Eqs. (1) and (2) constitute a closed cycle to convert low-temperature heat to high-temperature heat, and this cycle does not consume mechanical work. Gandia and Montes (1992) numerically investigate the IAH heat pump, in which the isopropanol dehydrogenation occurs in the liquid phase. Kim et al. (1992) found that the dehydrogenation in the

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Nomenclature

m_A	molar fraction of acetone
m_H	molar fraction of hydrogen
m_P	molar fraction of isopropanol
N	number of trays
p_A	fractional pressure of acetone (atm)
p_H	fractional pressure of hydrogen (atm)
p_P	fractional pressure of isopropanol (atm)
p_T	total pressure in exothermic reactor (atm)
Q_C	heat load of condenser (kJ)
$Q_{E,H}$	heat absorbed by the effluent in the exothermic reactor (kJ)
Q_F	heat of exothermic reaction (kJ)
Q_H	heat released from the exothermic reactor (kJ)
Q_{H1}	heat recovered when the acetone and hydrogen is directly sent to the exthermic reactor (kJ)
Q_{H2}	heat recovered from the stored acetone and hydrogen (kJ)
Q_L	endothermic reaction heat (kJ)
Q_M	dehydrogenation heat of metal hydride (kJ)
Q_R	heat load of boiler (kJ)
r_H	conversion ratio of acetone in the exothermic reactor
R	reflux ratio
R_c	the ratio of the smaller heat capacity rate to the larger one in the regenerator
R_g	ideal gas constant (JK^{-1} mol^{-1})
T_a	environmental temperature (K)
T_{CC}	temperature of condenser (K)
T_H	temperature of exothermic reaction (K)
T_L	temperature of endothermic reaction (K)
T_M	dehydrogenation temperature of metal hydride (K)
T_R	temperature of boiler (K)
x_F	molar fraction of acetone in the total molar quantity of acetone and isopropanol after reaction in the exothermic reactor
x_h	molar ratio of acetone before exothermic reaction
y_o	molar fraction of acetone in the total molar quantity of acetone and isopropanol before reaction in the exothermic reactor
Greek symbols	
ΔH_H	exothermic reaction enthalpy (kJ mol^{-1})
ΔH_L	endothermic reaction enthalpy (kJ mol^{-1})
ΔG_H	standard Gibbs free energy change for the exothermic reaction (kJ mol^{-1})
η_{en}	enthalpy efficiency
η_{ex}	exergy efficiency

liquid phase can be improved by removing the gaseous acetone and the hydrogen products, and the enthalpy efficiency improves as the conversions of dehydrogenation and hydrogenation increase. Chung et al. (1997) analyzed the effects of some operation parameters on the enthalpy efficiency of IAH heat pump. Meng et al. (1997) reported that the dehydrogenation in liquid phase can be greatly improved by adopting Ru or Ru–Pt catalyst, so that the thermal efficiency of IAH heat pump increases. Chung et al. (1997) numerically investigated the optimal design of IAH heat pump employing the reactive distillation process, they found that the heat pump using a reactive distillation process is better than the heat pump using a conventional distillation. Kitikiatsophon and Piumsomboon (2004) carried out the study on the dynamic behavior of IAH heat pump under Hysys.Plant environment. The thermodynamic performance analysis of IAH heat pump was conducted in Guo et al. (2012). KlinSoda and Piumsomboon (2007) conducted a demonstration unit of IAH chemical heat pump, the major components were individually investigated and the performance of the system was evaluated. A new performance criterion for IAH heat pump was proposed in Guo and Huai (2012). Saito et al. (1987) compared the heat pump of both the conventional and storage types, they found that the conventional type has the higher enthalpy efficiency, while the storage type could obtain the higher temperature heat.

The IAH heat pump has been studied by many scholars, but the most of IAH heat pump is conventional type in literature. An important competitive advantage of chemical heat pump is energy storage; therefore, the energy storage function is very necessary for the IAH heat pump, especially when the heat source is discontinuous such as solar energy. In this work, an IAH heat pump of storage type is investigated, the effects of some parameters on the heat pump are analyzed, and the multi-parameter optimization is conducted to achieve the optimal operation scheme for the heat pump.

2. Chemical heat pump of storage type

In the IAH heat pump of storage type is demonstrated in Fig. 1, consists of endothermic reactor, distillation column, metal hydride reactor, storage tank, regenerator and exothermic reactor. The dehydrogenation of isopropanol occurs in endothermic reactor as shown by Eq. (1), the acetone and isopropanol are separated in distillation column. The separated acetone and hydrogen is fully fed into exothermic reactor to release high-temperature heat through hydrogenation reaction as shown by Eq. (2) in the conventional heat pump. In the storage type, one part of acetone and hydrogen is fed into exothermic reactor, the other part is stored as shown in Fig. 1, the acetone is stored