Academic Journal of Science and Technology
ISSN: 2771-3032 | Vol. 1, No. 3, 2022

Process Design of Isopropyl Alcohol Synthesis Section of 80,000 Tons/Yea

Junfei Zhou, Xiaoguang Wang*

School of Chemistry and Chemical Engineering, Zhoukou Normal University, Zhoukou Henan, 466001, China.

Abstract: Isopropanol is a chemical product with great application value and can be used as a chemical raw material and organic solvent. This design is a synthesis section of 80,000 tons/year isopropanol, using acetone hydrogenation synthesis process. At a temperature of 180 °C, a pressure of 0.8 MPa, n (hydrogen)/n (acetone) = 1.5 : 1, performed in a column tubular fixed bed reactor. This design uses a 4-stage tubular fixed-bed reactor with an effective length of 8.5 m, a total length of 15.705 m, and a housing diameter of 2.9 m. The total number of 4-segment column tubes is 10,444, and the column tubes are made of seamless stainless steel pipes with a diameter of 38 mm and a thickness of 4 mm. The design improves production safety and reduces energy losses. The design results have certain guiding significance for actual production and application.

Keywords: Synthesis of isopropanol, Acetone hydrogenation, Process planning.

1. Introduction

Isopropanol has many applications. As chemical raw materials, acetone, hydrogen peroxide, isopropyl chloride, fatty acid isopropyl ester, and chlorinated fatty acid isopropyl ester can be produced [1].

Before 2010, the production of isopropanol in China was far from meeting the demand and needed to be imported to make up for it. However, since 2020, due to the serious impact of the epidemic, the demand for isopropyl alcohol has been increasing, so it is the general trend to build factories producing isopropyl alcohol and optimize the production process [2].

At present, there are three main production routes of isopropyl alcohol, namely propylene water method, acetone hydrogenation method and transesterification method [3]. However, due to the limitation of the existing technological level and product value, this project plans to build a new isopropanol production project for a factory. With acetone from a factory as the main raw material, isopropanol is prepared through synthesis, separation and other processes, and data are simulated by Aspen software.

2. Determination of Design Scheme

Hydrogenation of acetone to produce isopropanol mainly includes three sections, namely, synthesis section of isopropanol, separation section, extraction of by-products and recovery of azeotrope section [4]. Among these three sections, only synthesis section involves chemical reactions.

At present, isopropyl alcohol has achieved industrial production in the world in two categories: acetone hydrogenation and propylene hydration, and propylene hydration can be divided into liquid phase direct hydration, gas phase direct hydration and gas liquid miscible hydration [5]. The gas phase direct water method has a high utilization rate for propylene. Most of propylene can be converted into target products, and only a small part can be converted into by-products. But at the same time, the disadvantages should not be ignored: in order to prevent the dissolution of phosphoric acid, water must be converted from liquid to gas, resulting in low propylene conversion rate [6]. The liquid phase direct water catalyst has high activity. Compared with the gas phase direct water catalyst, the reaction speed is several times higher under the same concentration of hydrogen ion, and the product selectivity is good, the service life is long, and there is no pollution. However, the heat ratio of hydroene is large, the heat consumption of distillation is large, the reaction pressure is too high, and the equipment investment is high [7].

The application of acetone hydrogenation method in isopropanol production process is not as wide as that of direct water method, because the method has high requirements for raw materials and large demand, which is not conducive to its economic benefits. However, this method still has advantages, low energy consumption is more important, and acetone hydrogenation has less corrosion to production equipment [8].

From the perspective of catalyst, nickel catalyst is expensive, but long life, and waste catalyst can be recycled, environmental protection pressure is low; The price of acidic catalyst is relatively low, but the service life is short and loss occurs in the reaction process. The catalyst needs to be continuously supplemented during the reaction, which also corrodes the reactor [9]. Acetone hydrogenation reaction conditions are mild, and the one-way conversion rate is high, and the reaction process is not complicated. Therefore, this project adopts the acetone hydrogenation process with nickel-based catalyst.

3. Technological Process

Acetone mixed with hydrogen, heated and pressurized into the reactor for reaction, reaction mixture through condensate 30℃, and then into the air and liquid separator for separation, the main component of the gas is hydrogen, so we cycle hydrogen and hydrogenation, liquid phase of the liquid separator contains a small amount of water, acetone, pressure to atmospheric pressure, flow into the next section. According to the general situation of the annual operation time of the chemical plant continuous production unit, the operation time of this project is determined to be 8000 h/a. Simulated by Aspen Plus, the flow chart is as follows:

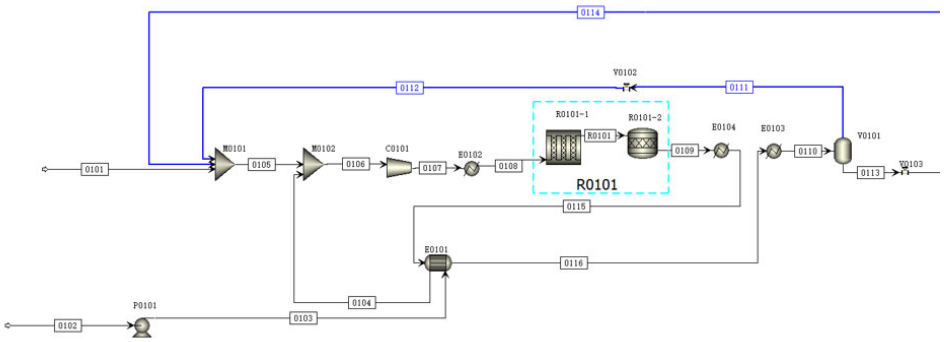

Figure 1. Schematic diagram of isopropyl alcohol synthesis section

4. Material Balance

Process simulation was carried out through Aspen Plus Dynamics V11 and material balance was calculated in the following table:

Table 1. Total material balance of isopropanol synthesis section

Project	Unit	Imported material			Export material
		Acetone feed	Hydrogen feed	Backflow of acetone	Component after flash
Phase		Liquid phase	Vapor phase	Vapor phase	Liquid phase
Temperature	℃	20.000	20.000	55.729	29.993
Pressure	Mpa	0.101325	0.101325	0.101325	0.12159
Volume flow	m3/hr	12.8033	4210.733	654.571	25.051
Mass flow rate	kg/hr	10168.1	352.876	1382.190	11903.196
C_3H_6O-1	kg/hr	10168.1	0.000	1368.707	1370.044
H_2	kg/hr	0.000	352.876	0.9544	0.9543
C_3H_8O-2	kg/hr	0.000	0.000	12.174	10256.317
$C_6H_{14}O$-3	kg/hr	0.000	0.000	0.1324	234.360
H_2O	kg/hr	0.000	0.000	0.2224	41.520
$C_2H_6O_2$	kg/hr	0.000	0.000	0.000	0.000
$C_3H_6O_2$-2	kg/hr	0.000	0.000	0.000	0.000
Total	kg/hr		11903.166		11903.196

5. Material Balance

The heat balance of reactor calculated by Aspen in the following table:

Table 2. Flow enthalpy change calculation table

	Unit	Input	Output
Moore flow	kmoL/hr	501.084	326.036
Mass flow rate	kg/hr	12306.835	12306.835
Volume flow	m3/hr	2359.921	1535.482
Temperature	℃	180.008	180.000
Pressure	Mpa	0.800	0.800
Gas fraction	/	1.000	1.000
Liquid fraction	/	0.000	0.000
Solid fraction	/	0.000	0.000
Molar enthalpy	J/kmoL	-78476790.721	-152138712.345
Quality enthalpy	J/kg	-3195253.822	-4030499.677
Moore entropy	J/kmoL-K	-76127.696	-170464.818
Quality entropy	J/kg-K	-3099.608	-4516.000
Flow enthalpy	Watt	-10923183.735	-13778526.202

6. Material Balance

6.1. Kinetics of Acetone Hydrogenation

Through the reaction of the established kinetic model data determination, the final measured parameters. The reaction rate constant of acetone hydrogenation [10] is $K_a = 2.98 \times 10^{12}\exp(-70.7/RT)$ mol/$(m^3 \cdot h)$. The catalyst density we used is 800 kg/m3, so the reaction rate constant based on catalyst mass can be obtained:

$$k_a = 2.98\times10^{12}\exp(-70.7/RT)\div800$$

$= 3.725\times10^{9}\exp(-70.7/RT)$ mol/(kg·h)

$= 1.03\times10^{3}\exp(-70.7/RT)$ kmol/(kg·s)

The adsorption equilibrium constant of gas phase acetone on Ni-Cu/SiO_2 catalyst is:

$$K_a=3.30\times10^{-8}\exp(58.7/RT)\ kPa^{-1}$$

$$\ln(K_a) = -17.227 + 7060.4/T$$

The adsorption equilibrium constant of hydrogen on Ni-Cu/SiO_2 catalyst is:

$$K_b = 1.83\times10^{-11}\exp(82.2/RT)\ kPa^{-1}$$

$$\ln(K_b) = -24.724 + 9886.9/T$$

Therefore, the kinetic factor of the reaction is:

$$K = k_a \cdot K_a \cdot K_b = 6.249\times10^{-16}\exp(70.2/RT)\ kmol/(kg\cdot s)$$

6.2. Reaction Condition Selection

6.2.1. Determination of Catalyst

Referring to Yang Qingquan's study on acetone constant pressure gas phase hydrogenation reaction and catalyst [11], we selected the following properties of catalyst: shape: spherical, particle size: 3 mm, bulk density: 800 kg/m3, life: 5 years.

6.2.2. Reaction Temperature Selection

According to the suitable range of active temperature of catalyst and Yang Qingquan's Study on Gas Phase Hydrogenation of Acetone under normal Pressure and Catalyst [13], the inlet temperature of reaction gas was selected as 180 ℃.

6.2.3. Reaction Pressure Selection

Referring to Yang Qingquan's study on acetone normal-pressure gas phase hydrogenation reaction and catalyst [11] and based on Aspen simulation, the inlet pressure of reaction gas was selected as 0.8mpa.

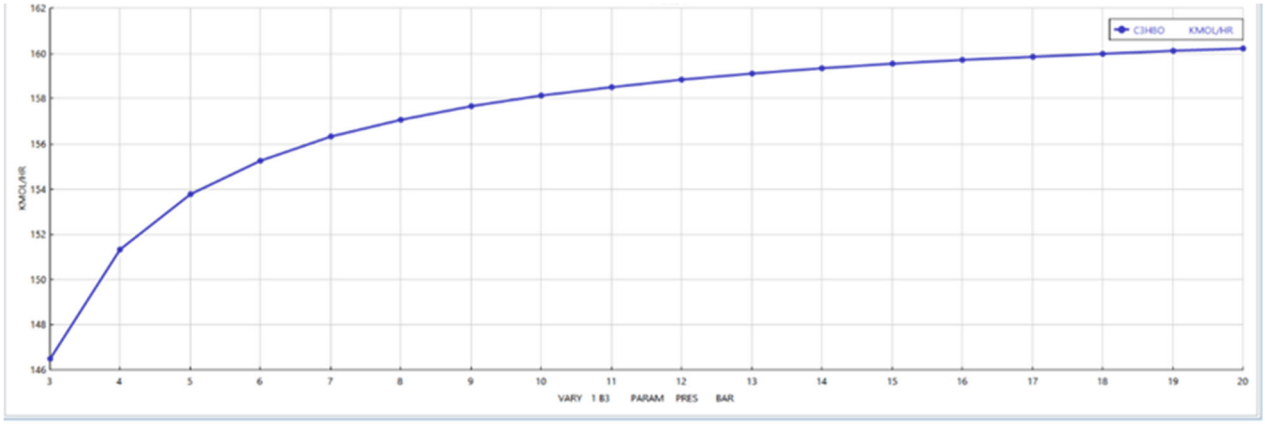

Figure 2. Simulation results of Aspen pressure

6.2.4. Hydrogen Acetone Feed Ratio

Referring to Yang Qingquan's study on acetone normally pressurization gas phase hydrogenation reaction and catalyst [11] and based on Aspen simulation, acetone hydrogenation reactor of this project was selected: $n_{(氢气)}/n_{(丙酮)} = 1.5 : 1$.

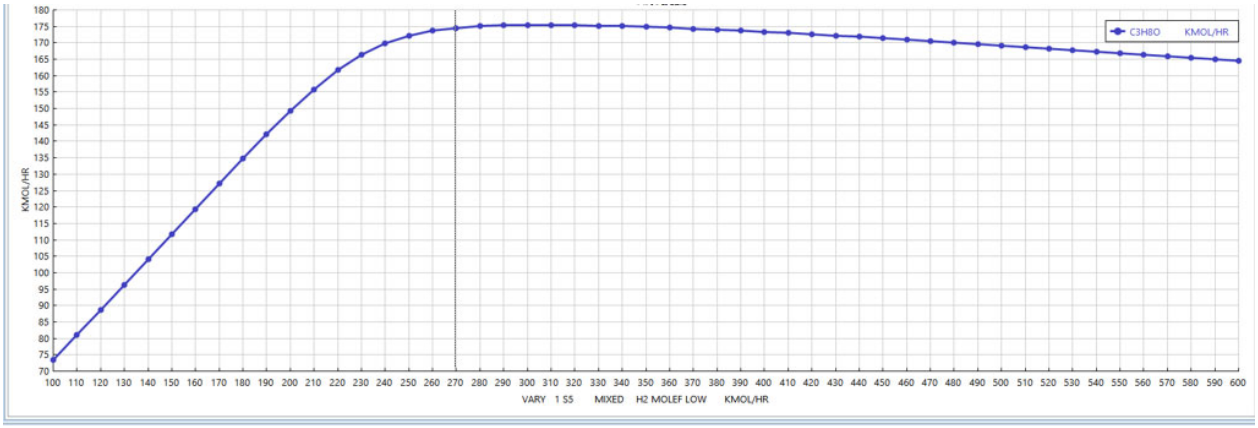

Figure 3. The simulation results (N (hydrogen)/ N (acetone) = 1.5:1)

6.3. Reactor Structure Design

6.3.1. Design Conditions

The pressure in the reactor can be obtained from the Aspen flow simulation information Pw = 0.8 Mpa. The design pressure is generally selected as P = (1 ~ 1.1)Pw, because the design temperature is generally higher than the maximum temperature.

$$P = P_w \times 1.1 = 0.8 \times 1.1 = 0.88\ Mpa$$

$$T = 180 + 20 = 200\ ℃$$

6.3.2. Determination of Catalyst Bed Diameter

Firstly, the diameter of the catalyst bed was calculated in an ideal tubular reactor. For the operating pressure of 0.8 Mpa, under the premise of ensuring the conversion rate and pressure drop, the empty bed flow rate of the compressed gas was 0.095 m/s, so the bed diameter was calculated as follows:

$$D_b=\sqrt{\frac{4V_0}{3600\pi u}}=\sqrt{\frac{4\times2354.77415}{3600\times\pi\times0.095}}\approx2.96m$$

After rounded, 3.0m bed diameter is taken.

6.3.3. Design of Tube Size and Number of Roots

In order to ensure adequate heat dissipation, the inner diameter of the reaction tube should be minimum, so the inner diameter of the reaction tube should be 30 mm. Refer to GBT17395-2008 Dimensions, Shape, Weight and Allowable Deviation of Seamless Steel Tube [12]. The specifications of the seamless stainless steel tube selected are ϕ38×4mm, and the material used is 12Cr2Mo1.

The number of tubes in the reactor should conform to the diameter of the catalyst bed, so the number of tubes needed is as follows. The number of tube roots was 10444 after rounding.

$$n=\frac{D_b^2}{d_i^2}=\frac{3.0^2}{0.03^2}\approx10000$$

6.3.4. Determination of Inner Diameter of Shell

The inner diameter of the shell is calculated by the following formula:

$$D=2e+(b-1)\times t$$

In the formula, t is the distance between the tubes , $t=1.25d_0$, $d_0$is the outer diameter of the tubes.

The reactor was designed to be composed of four reactors, arranged in staggered equilateral triangle, with 10,444 tubes in total.

Shell inner diameter : D = =0.045×2+(59-1)×0.0475=2.845m

After being rounded, it is 2.9m.

The appropriate reactor volume was selected based on the simulation and improvement data of Aspen Plus acetone hydrogenation reactor and various factors (see figure). At the same time, when the catalyst bed porosity of 0.4 and density of 800 kg/m3 are filled, the one-way yield of isopropanol is 85.3% and the selectivity is 97.4%[13], so it can be calculated that the conversion rate of acetone under such conditions is 87.6%. When the length of the reactor was 0.85m, the corresponding conversion rate was 87.56%. Therefore, the length of the reactor was 8.5 m.

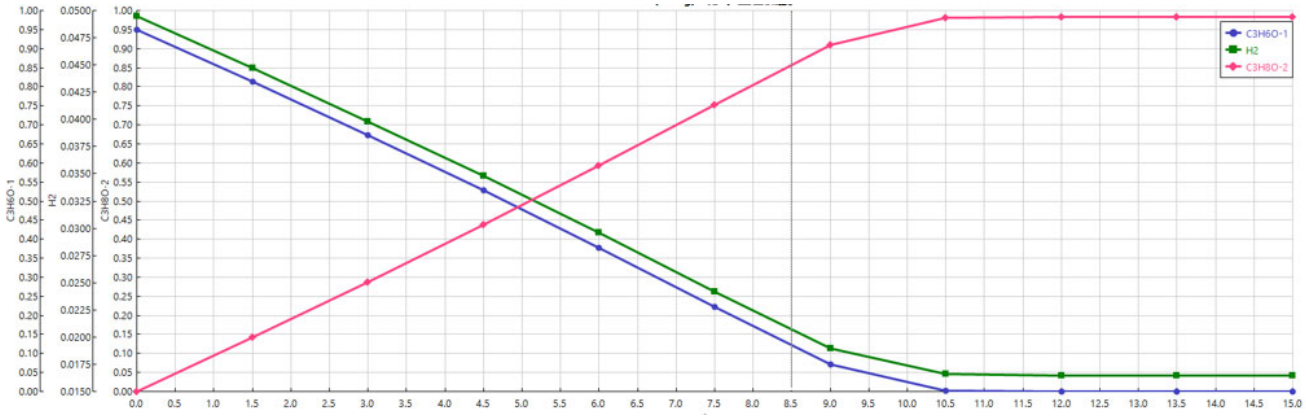

Figure 4. Sensitivity analysis results of reactor length

Volume of catalyst bed:

$$V_R=\frac{n\pi d_i^2}{4}\times H_1=10444\times\frac{\pi0.03^2}{4}\times8.5=62.75\ m^3$$

Taking 800 kg/m3 as the filling density of catalyst, the amount of catalyst can be obtained:

$$m=\rho V=800\times62.75=50200\ kg$$

Ratio of catalyst diameter to reactor tube diameter :D/d = 6~12

6.4. Reactor Heat Transfer Calculation

6.4.1. Overall Profile

Aspen Plus is used to simulate the reaction of the mixture system, and it can be obtained that when the reaction reaches the set goal, the heat transfer load is Q = 2846.61 ÷ 4 = 711.65 kW, the heat transfer area is:

$$A_{Real}=n\pi d_oL=10444\div4\times\pi\times0.038\times8.5=2649.472\ m^2$$

6.4.2. Estimation of Reactor Heat Transfer Coefficient

1)Design and calculation of heat transfer coefficient between cooling medium and wall surface.

$$\alpha_0=0.36\frac{\lambda_0}{d_e}\left(\frac{d_eu_0\rho_0}{\mu_0}\right)^{0.55}\left(\frac{C_p\mu_0}{\lambda_0}\right)^{\frac{1}{3}}\left(\frac{\mu}{\mu_w}\right)^{0.14}$$

μ_0= 0.219cP, λ_o= 0.6845W/(m·K), C_p= 4788.78J/(kg·K);

$\left(\frac{\mu}{\mu_w}\right)^{0.14}$=1.05

ρ_0 = 891.30kg/m³ , $d_e=\frac{4\left(\frac{\sqrt{3}}{2}t^2-\frac{\pi}{4}d_0^2\right)}{\pi d_o}$,

$$d_e=\frac{4(\frac{\sqrt{3}}{2}\times0.0475^2-\frac{\pi}{4}\times0.038^2)}{\pi\times0.038}=0.02750\ m$$

$$\alpha_o=0.36\times\frac{0.219}{0.02750}\times\left(\frac{0.02750\times1.25\times891.3}{0.219\times10^{-3}}\right)^{0.55}\times\left(\frac{4788.78\times0.219\times10^{-3}}{0.6845}\right)^{\frac{1}{3}}\times1.05=2347.31W/(m\cdot K)$$

2)Design and calculation of heat transfer coefficient between bed and wall surface

$$\frac{\alpha_td_t}{\lambda}=3.5\left(\frac{d_pG}{\mu}\right)^{0.7}\exp\left(-4.6\frac{d_p}{d_t}\right)$$

d_t = 0.03m, λ = 0.0894 W/(m·K), μ = 0.01433 cP, G = 0.4598 kg/(m²·s); $\alpha_i=3.5\times\left(\frac{0.003\times0.4598}{0.01433\times10^{-3}}\right)^{0.7}\times\exp\left(-4.6\times\frac{0.003}{0.03}\right)\times\frac{0.0894}{0.03}=161.035$ W/(m·K)

As the fouling thermal resistance is related to heat transfer medium and cleaning cycle, it is impossible to calculate the precise value, 0.00072 m²·K/W[14].

3)Design and calculation of the total heat transfer coefficient

$$K=\frac{1}{\frac{1}{\alpha_0}+\frac{b}{\lambda}\cdot\frac{d_o}{d_m}+\frac{1}{\alpha_i}\cdot\frac{d_0}{d_i}+R_{so}+R_{si}\cdot\frac{d_o}{d_i}}$$

Plug in and calculate the total heat transfer coefficient, K = 97.4926 W/(m·K).

6.4.3. Calculation of Heat Exchange Area

The heat transfer driving force can be calculated as 55℃ through the temperature calculation of import and export

materials.

The heat exchange area is:

$$A_{calculate}=\frac{Q}{\Delta t_m \cdot K}$$

Plug in and calculate the heat transfer area, $A_{calculate}$=132.714 m^2.

The actual heat exchange area is 1870.215 m^2, which meets the heat exchange requirements.

6.4.4. Total Reactor Height

The total height is divided into five parts, namely, the height of the cylinder,H_1= 8.5 m; Skirt is highH_2 = 4 m: For the head high, H_3 = 650 + 40 +15= 705 mm = 0.705 m. At the same time, the height of the reactor also includes the top and bottom of the cylinder. According to literature [15], the top space is 1m and the bottom space is 1.5m.

The total reactor height:

$H = H_1+H_2+H_3+H_4+H_5$= 8.5+4+0.705+1+1.5 =15.705 m

7. Conclusion

Isopropanol is a chemical product with great application value, which can be used as chemical raw materials and organic solvents. The design of 80,000 tons/year isopropanol synthesis section, using acetone hydrogenation synthesis process. Under the conditions of temperature 180 ℃, pressure 0.8 MPa, N (hydrogen)/ N (acetone) = 1.5:1, the experiment was carried out in a tubular fixed-bed reactor. In this design, a four-section tubular fixed-bed reactor was adopted, with an effective length of 8.5m, a total length of 15.705m and a shell diameter of 2.9m. There are 10,444 tubes in 4 sections, and the tubes are seamless stainless steel tubes with a diameter of 38 mm and a thickness of 4 mm. The design improves production safety and reduces energy loss. The design result has certain guiding significance for practical production and application.

References

[1] H. Ma. Research progress of isopropanol production technology [J]. Yunnan Chemical Industry, Vol. 48(2021) No.7, p.18-20.

[2] F. Yan. Production technology of isopropanl alcohol and domestic and foreign market prospects[J]. Pharmaceutical and Chemical Industry. Vol.10(2007) , p.12-15.

[3] J. X. Liu, H. J. Wang. Heilongjiang Science and Technology Information, Vol.30(2008) No.30, p.42. (in Chinese)

[4] Q.Q. Tang, L.H. Xu, B.L. Tian, et al. Production technology and application of isopropanol [J]. Petrochemical Industry, Vol.50(2021) No.3, p.285-288.

[5] J.W. Yan, Y.Yang. Analysis of isopropyl alcohol and its production technology comparison [J]. China Petroleum and Chemical Standards and Quality, Vol.11(2014), p.25-25.

[6] Q. W. Zhou. Preparation of isopropanol by direct hydration of propylene. (MS., Dalian University of Technology, 2015).

[7] M.G. Sun. Study on catalyst of propylene hydration to isopropanol. (MS., Dalian University of Technology, 2016).

[8] Y. W. Xu, L. Xiang. Analysis and selection of isopropanol production technology[J]. Silicon Valley, Vol.17(2011) , p.193-193.

[9] W. J. Bai. Study on hydrogenation of Acetone to isopropanol over Ni based catalyst. (MS.,Shanxi: Taiyuan University of Technology, 2016).

[10] P. Liu, F.M. Jiang, J.W. Cen. Thermodynamic study of isopropanol/acetone/hydrogen chemical heat pump [J]. Acta Energiae Solaris Sinica, Vol.35(2014) No.5, p.809-813.

[11] Q.Q.Yang. Study on hydrogenation of acetone under normal pressure and catalyst. (MS.,Tianjin: Tianjin University, 2000).

[12] General Administration of Quality Supervision, Inspection and Quarantine of the People's Republic of China, Standardization Administration of China. Seamless steel tube dimensions, shape, weight and allowable deviation: GB/T 17395-2008.

[13] Y. Zhong, J.T. Liu. Catalytic performance of acetone hydrogenation to isopropanol [J]. Industrial Catalysis, Vol.29(2021) No.11, p.63-66.

[14] Z.F. Li, J.P. Wu, X.B. Wang. Integrity management of heat exchanger tube harness[J]. China Equipment Engineering, Vol. 01(2022), p.153-155.

[15] L.M. Sun. Discussion on The Design of Pressure Vessel [J]. Science and Technology Wind, Vol. 03(2010), p.276.