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DESIGN OF REACTOR FOR THE PRODUCTION ETHYL ACETATE

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Abstract

The aim of this research is to design a simple Continous Stirred Tank Reactor (CSTR) type reactor and analyze the reactor through computational analysis by calculating the reactor, the stirrer used and the mass balance using Microsoft Excel. Based on the calculation results of the CSTR reactor dimensions, the design pressure was obtained at 4.3040 psig, the thickness and height of the cylinder tube were 0.1242 in and 233.8306 in respectively, the thickness of the top and bottom caps of the cylinder tube was 0.1859 in and 0.1859 in and so on. the height of the top and bottom covers of the cylinder tube is 72.6587 in and 124.2581 in and the height of the reactor is 16.7542 in. Not only that, the reactor is also equipped with 1 stirrer with impeller diameter, height, length, width respectively 3.8125 ft, 25.875 ft, 9.7031 ft, 7.7625 ft. with stirring power, stirring shaft diameter, stirring shaft length respectively 1662 HP, 9.1889 ft, and 2.1929 ft. It is hoped that writing this article will be a useful reference as a learning method for designing reactors to produce ethyl acetate CH2COOC2H5 products which are several thousand times larger than laboratory scale.

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Abstrak

Tujuan dari penelitian ini adalah untuk merancang reaktor sederhana tipe Continous Stirred Tank Reactor (CSTR) dan menganalisis reaktor melalui analisis komputasi dengan menghitung reaktor, pengaduk yang digunakan dan neraca massa menggunakan Microsoft Excel. Berdasarkan hasil perhitungan dimensi reaktor CSTR, diperoleh tekanan design sebesar 4.3040 psig, tebal dan tinggi tabung silinder masing-masing 0,1242 in dan 233.8306 in, ketebalan tutup atas dan bawah tabung silinder adalah 0,1859 in dan 0,1859 in begitu pun ketinggian tutup atas dan bawah tabung silinder sebesar 72.6587 in dan 124.2581 in serta tinggi reaktor sebesar 16.7542 in. Tidak hanya itu, reaktor juga dilengkapi 1 pengaduk dengan impeller diameter, height, length, width masing – masing 3.8125 ft, 25.875 ft, 9.7031 ft, 7.7625 ft. dengan stirring power, diameter poros pengaduk, Panjang poros pengaduk masing masing 1662 HP, 9.1889 ft, dan 2.1929 ft. Penulisan artikel ini diharapkan menjadi referensi yang bermanfaat sebagai metode pembelajaran perancangan reaktor untuk

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menghasilkan produk etil asetat $CH_2COOC_2H_5$ yang beberapa ribu kali lebih besar dari skala laboratorium.

Introduction

Ethyl acetate (CH3COOCH2CH3) is an organic compound which is an ester of ethanol and acetic acid. Ethyl acetate is a volatile, non-toxic, and non-hygroscopic medium polar solvent. Ethyl acetate is often used as a solvent because ethyl acetate can extract compounds that can provide antibacterial activity, including pilohydroxy flavonoids and other phenols.

Ethyl acetate is commonly used as an industrial solvent used for paints, coatings, wood stains, oil-based varnishes and enamels, adhesives, cellulose, inks, plastics, or fats. In addition, ethyl acetate can be used in making photographic films and plates, as a drug intermediate or nail polish remover (Johnston, V. J., et al. 2011).

Esterification is an ionic reaction between a carboxylic acid and an alcohol where addition reactions and elimination rearrangements occur which produce esters. Ester is a hydrocarbon derived from carboxylic acid. Efforts to speed up the glycerol esterification reaction which increases the conversion to Triacetin can be reviewed based on factors that influence the reaction, namely temperature, catalyst, stirring and ratio of reactants.

Method

1. Synthesis of Ethyl Acetate

Sintesis etil asetat dari etanol dan asam asetat dilakukan dengan menggunakan katalis asam sulfat (H2SO4) dan asam para toluen sulfonat (PTSA). Selain itu katalis untuk sintesis etil asetat ada berupa Dimethylsulfoxide (DMSO) Penggunaan katalis PTSA bertujuan untuk mengetahui efektivitas esterifikasi etil asetat dibandingkan dengan katalis H2SO4.

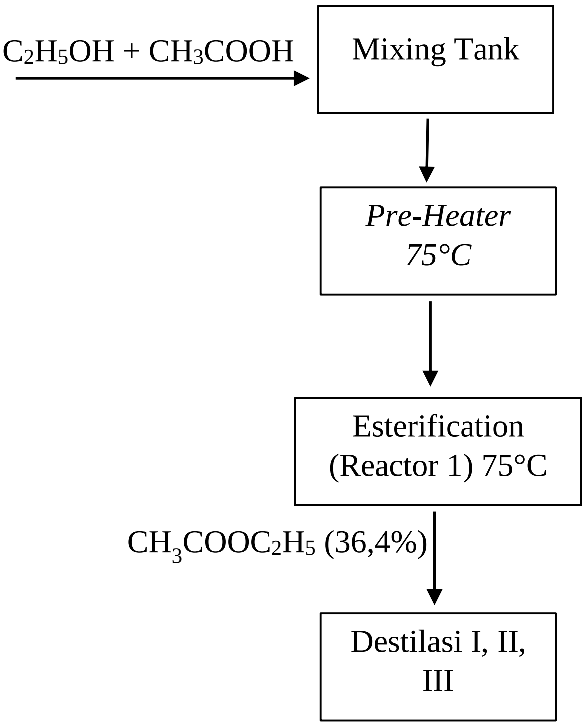

Figure 1 Diagram alir proses produksi etil asetat

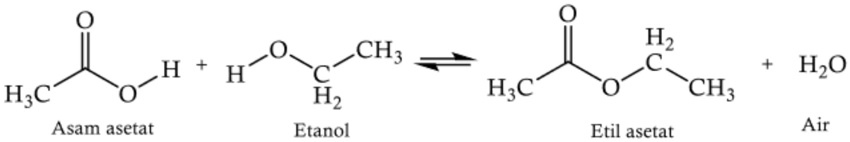

Figure 2 Mechanism Esterification Reaction (Kadarohman et al., 2022)

2. Mathematical model for designed reactor

The material selected for the reactor is SA 240 Grade M Type 316 stainless steel with an upright cylinder type with a standard dished top cover and a conical bottom cover with an apex angle of 120˚ and the agitator is SA 240 Grade M Type 316 high alloy steel with an axial turbine type 4 blade angle of 45˚. The assumptions of specification are shown in table 2.

Table 2 Assumptions of specifications design of reactor and stirrer

Specifications	Reactor
Type	Upright cylinder with standard dished top and conical bottom with 120˚ apex angle
Temperature	75˚C
Pressure	1 atm
Operation time	180 minute

Construction time	Stainless steel SA 240 Grade M Type 316
Allowable Stress (*f*)	18750
Welding	Double welded butt joint
Corrosion Factor	0.0625
Amount incoming substance	3086.472 lb/h
Volumetric rate	62,71005989 ft^3/h
	Stirrer
Type	Axial Turbine with 4 Blades at an Angle of 45˚
Impeller material	High Alloy steel SA 240 Grade M type 316
Shaft material	Hot Roller Steel SAE 1020

The reactor was operated at room temperature and pressure (RTP) for 45 minutes with a total incoming substance of 3086.472 lb/hour. Mass balance analysis was performed using Microsoft Excel application to collect data (equation 1-18). Table 3 presents the calculated parameters for the reactor and stirrer. (Anggraini, 2018).

Table 3 Calculation of reactor and stirrer parameters

Section	Parameters	Equation	Eq
Dimension of reactor	Total Volume of Reactor	$Total\ Vol.of\ reactor = precursor\ vol. + 20\% \times blank\ psace\ Vol.$ Where Total vol. of reactor (ft^3)	(1)
	Vessel dimension (d_i)	$Total\ Vol. = V_{bottom\ lid} + V_{cylinder} + V_{top\ lid}$ $Total\ Vol. = \left(\frac{\pi d_i^3}{24\tan\left(\frac{1}{2}\alpha\right)}\right) + \left(\frac{\pi d_i^3}{4} \times Lc\right) + 0.0847 d_i^3$ Where $\alpha = 60^\circ$ $L_c = 1.5$ d_i (in)	(2)
	Volume of liquid in the cylinder (V_{lc})	$V_{lc} = V_{liquid} - V_{bottom\ lid}$ Where V_{lc} (ft^3)	(3)

Height of liquid in the cylinder (H_{lc})

$$H_{lc} = \frac{V_{lc}}{\left(\frac{\pi}{4}\right) d_i^2} \tag{4}$$

Where
H_{lc} (in)

Pressure of design (P_i)

$$P_i = P_{atm} + P_{hydrostatic} \tag{5}$$

$$P_i = 14{,}7\, psia + \left(\frac{\rho(HL - 1)}{144}\right) psia$$

Where
HL = 5.1463
P_i (psig)

Cylinder thickness (t_c) and d_o standardization

$$t_c = \left(\frac{p_i \times d_i}{2(f \times E - 0.6P_i)}\right) + C \tag{6}$$

Where
f = 18750
E = 0.8
C = 1/16

$$d_o = d_i + 2t_c$$

Where
d_o (ft)

Height of cylinder (L_c)

$$Total\ Vol. = V_{bottom\ lid} + V_{cylinder} + V_{top\ lid} \tag{7}$$

$$Total\ Vol. = \left(\frac{\pi d_i^3}{24 \tan\left(\frac{1}{2}\alpha\right)}\right) + \left(\frac{\pi d_i^3}{4} \times Lc\right) + 0.0847 d_i^3$$

L_c (in)

Dimension of top lid

$$th_t = \frac{0.885 \times P_i \times d_i}{2(f \times E - 0.1P_i)} + C \tag{8}$$

Where
th_t = top lid thickness (in)

$$h_t = 0.169 \times d_i$$

Where
h_t = height of top lid (in)

Dimension bottom lid

$$th_b = \frac{P_i \times d_i}{2(f \times E - 0.16) \cos\left(\frac{1}{2}\alpha\right)} + C \tag{9}$$

Where
α = 120°
th_b = bottom lid thickness (in)

$$h_b = \left(\frac{\frac{1}{2} h_t}{\tan\left(\frac{1}{2\alpha}\right)}\right)$$

Where

		$\alpha = 120^{\circ}$ h_b = height of bottom lid (in)	
	Height of reactor	$Height\ of\ reactor = h_t + L_c + +h_b + s_f$ Where s_f = 2.5 Height of rector (ft)	(10)
Stirrer	Impeller diameter (D_a)	$\frac{D_a}{D_t} = 0.5$ Where D_t = 77.6250 Impeller diameter (ft)	(11)
	Impeller height from the bottom of the tank (Z_i)	$\frac{Z_i}{D_t} = \frac{1}{3}$ Where Impeller diameter from the bottom of the tank (ft)	(12)
	Impeller length (l)	$\frac{l}{D_a} = \frac{1}{4}$ Where Impeller length (ft)	(13)
	Impeller width (W)	$\frac{W}{D_a} = \frac{1}{5}$ Where Impeller width (ft)	(14)
	Number of stirrer (n)	$n = \frac{H_{liquid}}{2 \times D_a^2}$ Where H_{liquid} = 61.7559	(15)
	The stirring power (H)	$P = \frac{\varphi \times \rho \times n^3 \times D_i^5}{g_c}$ Where φ = 0.9 g_c = 32.2 lb.ft/s^2.lbf P (Hp) $H = (0.1 + 0.15)P + P$ Where 0.1 = estimation of the amount of power leakage in the process and bearing from the input power 0.15 = estimation of the amount of belt or gear leakage form input power H (Hp)	(16)

Shaft diameter of stirrer (D)	$D^3 = \frac{16 \times T}{\pi \times S}$ $T = \frac{63025 \times H}{N}$ $S = 20\% \times 36000\ lb/in^2$ Where S = maximum allowable design shearing stress (lb/in^2) N = stirrer rotation = 100 rpm T = torsion moment (lb.in) π = 3 D (in)	(17)
Shaft length of stirrer (L)	$L = h + (l - Z_i)$ Where $h = L_c + h_t$ L (ft)	(18)

Result and Discussion

In this article, the CH2COOC2H5 ethyl acetate production process uses a Continuous Stirred Tank Reactor (CSTR). This is because CSTR's operating capabilities can be adjusted to load capacity, making it suitable for large-scale industrial production. CSTR usually operates in a steady state where the temperature is easy to control (Smith, 1981). In a production, the processing process is said to be operating successfully if the mixing and mixing of the ingredients is stable and perfectly collaborated. Stirring is a patterned movement that aims to produce a homogeneous dispersion originating from solid particles mixed with liquid using a mixer or mixing device in an emulsion system (Sudaryadi et al., 2020), so that heat transfer between the heat source and the liquid released the reactor can run quickly. Mixing is the process of collecting or blending materials randomly using mechanical force in two or more phases (Priyati et al., 2016) until a mixture is formed. Good mixing can be determined from the shape and dimensions of the stirrer used, because it can influence the effectiveness of power use and the mixing process. Apart from that, it is also necessary to pay attention to the pressure aspect in a reactor tank to avoid an explosion. The working mechanism of CSTR is that a certain volume of reactant is used for a certain volume of product produced. Therefore, to find out how much volume is coming in and going out, it is necessary to carry out a mass balance calculation.

Mass balance calculations have the general principle that the total mass of reactants is the same as the total mass of previously unknown products (Alexander, 2018). The components contained therein are produced from a substitution reaction in the synthesis of CH2COOC2H5 ethyl acetate nanoparticles. The reactant components consist of acetic acid (CH3COOH) and ethanol (C2H5OH). The product components consist of ethyl acetate CH2COOC2H5 as the main product and H2O as a side product. To obtain appropriate results based on mass balance principles, it is necessary to carry out stoichiometry calculations for each component. The mass of reactant components as starting materials can be determined according to production needs.

The dimensions typically consist of the diameter of the vessel, the thickness of the cylinder, and the length of the cylinder. The calculation of the stirrer from the reactor is included in the dimensions of each component. The calculation and determination of the upper and lower lids of the reactor, as well as the thickness of these lids, must be considered next.

The reactor volume was calculated to be 61522.6649 ft3, with a vessel diameter of 429.9331 in, a cylinder height of 233.8306 in, and a cylinder thickness of 0.1242 in. After obtaining the vessel diameter, the height of the top and bottom caps was calculated to determine the overall height. The top cap has a calculated height of 72.6587 inches with a thickness of 0.1171 inches, while the bottom cap has a calculated height of 124.2581 inches with a thickness of 0.1859 inches. Therefore, the overall height of the reactor is 16.7542 feet. Table 4 shows the parameters of design reactor based on complete calculation.

Table 4 Reactor parameters designed based on calculations.

No	Parameters	Results
1	Total volume of reactor	61522.6649 ft^3
2	Vessel dimension (d_i)	429.9331 in
3	Volume of liquid in the cylinder (V_{lc})	45743.465 ft^3
4	Height of liquid in the cylinder (H_{lc})	544.7550 in
5	Pressure of design (P_i)	4.3040 psig
6	Cylinder thickness (t_c)	0.1242 in
7	D_o standardization	430.1815ft
8	Height of cylinder (L_c)	233.8306 in
9	Top lid thickness (th_t)	0.1171 in
10	Height of top lid (h_t)	72.6587 in
11	Bottom lid thickness (th_b)	0.1859 in
12	Height of bottom lid (h_b)	124.2581 in
13	Height of reactor	16.7542 ft

The size of each component, including the stirrer, which is also known as an agitator, needs to be taken into consideration. The stirrer typically consists of a series of motors as a drive pad and an impeller or blade that is adjusted to the organic material being used. Stirring during the process of forming crude glycerol creates a flow pattern in the reactor. The flow pattern can be adjusted based on the flow velocity. In this design, axial flow is used, which causes flow parallel to the rotation axis.

The result of the stirrer calculation are shown in table 5. The number of stirrer is 1 piece with impeller diameter 38.8125 feet, impeller height from the bottom of the tank 25.875 feet, impeller width 7.7625 feet and impeller length 9.7031 feet. It is known that teh plate used in the stirrer is an axial turbine type 4 blades angle of 45˚. Turbine stirrer type is a type of stirrer that has many blades and is shorter in size.

Table 5 Stirrer parameters designed based on calculations.

No	Parameters	Results
1	Impeller diameter (D_a)	38,8125 ft
2	Impeller height from the bottom of the tank (Z_i)	25,875 ft
3	Impeller lenght (l)	9,7031 ft
4	Impeller width (W)	7,7625 ft
5	Number of stirrer (n)	1 piece
6	The stirring power (H)	1662 Hp
7	Shaft diameter of stirrer (D)	9,2000 in
8	Shaft lenght of stirrer (L)	2,1930 ft

Conclusion

Based on the calculations from the batch reactor and agitator specifications for ethyl acetate production at an industrial scale (60 times larger than the lab scale), a required volume specification of 61522.6649 ft^3 with a height of 16.7542 ft and one agitator with a power of 1662 Hp is determined. The calculations were performed using Microsoft Excel without considering effectiveness factors. Based on the calculation results, it can be concluded that the design and performance analysis of the reactor can be applied.

The results of the analysis of mass balance calculations in the CH2COOC2H5 ethyl acetate production process using Microsoft Excel, obtained specifications for the dimensions of the Continous Stirred Tank Reactor (CSTR) such as design pressure of 4.3040 psig, thickness and height of the cylinder tube respectively 0.1242 in and 233.8306 in, thickness of the top cover and the bottom of the cylinder tube are 0.1171 in and 0.1859 in. Likewise, the height of the top and bottom of the cylinder tube is 72.6587 in and 124.2581 in and the height of the reactor is 114.06 in. Not only that, the reactor is also equipped with 1 stirrer with impeller diameter, height, length, width respectively 3.8125 ft, 25.875 ft, 9.7031 ft, 7.7625 ft. with stirring power, stirring shaft diameter, stirring shaft length respectively 1662 HP, 9.1889 ft, and 2.1929 ft. Based on the results and analysis of these calculations, the design and analysis of reactors and production mechanisms can be used as a learning medium.

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