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Design of Reactor for The Production of Ethanol from Hydration of Ethene

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Abstract (English)

The objective of this research is to formulate the design of a Continuous Stirred Tank Reactor (CSTR) employed in ethanol production. The study incorporates mass balance calculations as a reference to assess the reactor's performance by understanding the influx of raw materials and the resultant product output. Additionally, both the reactor and stirrer designs are manually computed using Microsoft Excel in this study. The calculated design for the reactor indicates a volume of 103.09 ft3, featuring a vessel dimension of 51.06 in, a cylinder height of 3.18 in, and a cylinder thickness of 1.74 in. The top cap measures 8.63 in with a thickness of 1.52 in, while the bottom lid measures 14.75 inches with a thickness of 3,49 inches. Consequently, the overall height of the reactor amounts to 2.28 feet. The reactor is furnished with a single stirrer, boasting a shaft diameter of stirrer 6,93 in, and shaft length of stirrer measuring 1,64 feet. Turbulent stirring flow conditions are maintained, and the standard motor power for the stirrer is 713 HP.

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Tujuan dari penelitian ini adalah merumuskan desain Continuous Stirred Tank Reactor (CSTR) yang digunakan dalam produksi etanol. Studi ini mencakup perhitungan neraca massa sebagai referensi untuk menilai kinerja reaktor dengan memahami aliran bahan baku dan hasil keluaran produk. Selain itu, desain reaktor dan pengaduk keduanya dihitung secara manual menggunakan Microsoft Excel dalam penelitian ini. Desain yang dihitung untuk reaktor menunjukkan volume sebesar 103,09 ft3, dengan dimensi wadah sebesar 51,06 inci, tinggi silinder 3,18 inci, dan ketebalan silinder 1,74 inci. Tutup atas memiliki ukuran 8,63 inci dengan ketebalan 1,52 inci, sedangkan tutup bawah memiliki ukuran 14,75 inci dengan ketebalan 3,49 inci. Akibatnya, tinggi keseluruhan reaktor mencapai 2,28 kaki. Reaktor dilengkapi dengan satu pengaduk, dengan diameter poros pengaduk sebesar 6,93 inci, dan panjang poros pengaduk sebesar 1,64 kaki. Kondisi aliran pengadukan turbulen dipertahankan, dan daya motor standar untuk pengaduk adalah 713 HP.

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Introduction

The production of ethanol from the hydration of ethene is a significant process within the realm of chemical engineering, playing a crucial role in the biofuel and chemical industries. This paper aims to explore the design considerations for reactors employed in the production of ethanol through the hydration of ethene, a process central to the synthesis of this valuable alcohol. Ethanol finds numerous uses in the industrial and pharmaceutical domains as a solvent for materials intended for human consumption, such as fragrances, flavorings, dyes, and pharmaceuticals (Spivey, 2010).

Ethanol, a versatile compound with applications ranging from fuel to pharmaceuticals, is conventionally produced by reacting ethene (C_2H_4) with water (H_2O) in the presence of a catalyst. This reaction, known as the hydration of ethene, yields ethanol (C_2H_5OH) as a key product. The design of the reactor system for this process involves careful consideration of various factors to optimize efficiency and yield. Numerous methods exist for ethanol production, including ethanol fermentation, the indirect process involving esterification-hydrolysis, and the direct hydration of ethylene (Logsdon, 2000). Petrochemical methods, encompassing both direct and indirect hydration, along with biological processes involving yeast fermentation, are employed for ethanol production. While the majority of industrial processes have traditionally relied on fermentation, the outcomes have been inconsistent (Weissermel, 2003).

In this paper, we will delve into the critical aspects of reactor design, including the selection of reactor type, operating conditions, and the influence of catalysts. The impact of temperature and pressure on reaction kinetics, as well as the integration of control systems for optimal performance, will be explored. Additionally, we will discuss the importance of reactor capacity in the context of ethanol production. Understanding and optimizing the reactor design for the production of ethanol from ethene hydration is pivotal for ensuring a sustainable and economically viable process. By addressing these key design considerations, this paper aims to contribute valuable insights to the field of chemical engineering and enhance our understanding of the ethanol production process.

A reactor functions as a site where diverse reactions occur, encompassing chemical changes that cause a substance to shift from one state to another. These modifications can happen spontaneously or with the assistance of external energy, such as heat. Ensuring that the reaction attains maximum efficiency in producing the intended final product is imperative when manufacturing reactors. This is vital for industries engaged in reactor production to reduce operational costs while optimizing product output. The frequently encountered reactor type in industrial environments is the stirred reactor, commonly known as a Continuous Stirred Tank Reactor (CSTR) (Mata & Smith, 1981).

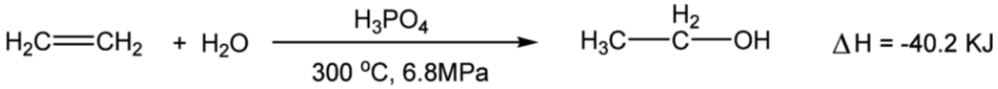
The Continuous Stirred Tank Reactor (CSTR) operates by introducing reactants and raw materials into a stirred tank, where a stirring device facilitates the production of the desired product. The design of the stirrer is tailored to the specific material being stirred, ensuring thorough mixing for optimal reaction outcomes. In large-scale industries, CSTR reactors are commonly preferred due to their adjustable reactor capacity. Furthermore, CSTR offers advantages such as superior temperature control compared to alternative reactor types, cost-effectiveness in operation, suitability for two-phase reactions, ease of maintenance, and cleanliness (Nauman, 2002).

This study involved the design and examination of a batch reactor for ethanol production through the hydration of ethene. Computational analysis and calculations pertaining to the reactor, stirrer, and mass balance were conducted using the Microsoft Excel application. The aim is to potentially upscale ethanol production to an industrial level, necessitating a dedicated facility for reacting the raw materials used in ethanol manufacturing.

Method

1. Synthesis of Ethanol

Shell introduced the catalytic direct hydration of ethylene for the first time in 1947 (Weissermel, 2003). Ethanol is produced through the hydration of ethene ($CH_2{=}CH_2$), representing the most straightforward and cost-efficient method for ethanol manufacturing.. It is preferred that the ethene and water reagents utilized in the process be of high purity (Mars, 1972). Ethene, derived from the petroleum industry, serves as an easily accessible raw material. The reaction occurs in the presence of phosphoric acid (H_3PO_4) acting as a catalyst, coated over silicone dioxide (Fougret, 1999). Ethene is combined with steam in a fixed molar ratio of ethene to water (1:0.60). The mixture undergoes heating to 300°C, 6.8 MPa (67 atm), causing the gases to react over the catalyst, resulting in the formation of ethanol (Chauvel, 1989). The reaction is exothermic. The gaseous mixture, comprising unreacted ethene and product ethanol, is cooled to liquefy ethanol. The separated product entails the recycling of unreacted ethene back into the reaction chamber. Productivity per cycle (or pass) ranges from 5.0% to 25.0%, contingent upon the catalyst's activity. The efficient recycling of ethene and the removal of ethanol from the reaction system contribute to achieving a high yield. In addition to the manufacturing process, the synthesis of ethanol is depicted in the following reaction (Llano-Restrepo, 2011).



$$H_2C{=}CH_2 + H_2O \xrightarrow[300\ ^oC,\ 6.8MPa]{H_3PO_4} H_3C{-}\overset{H_2}{C}{-}OH \qquad \Delta H = -40.2\ KJ$$

Figure 1 The mechanism of alcohol production from the hydration of ethene.

2. Mathematical Model for Design a Reactor

The chosen material for the reactor is stainless steel of SA 240 Grade M Type 316, featuring an upright cylinder design, a standard dished top cover, and a conical bottom cover with an apex angle of 120˚. The agitator is constructed from high-alloy steel of SA 240 Grade M Type 316, designed with an axial turbine comprising four blades set at a 45˚ angle. The specifications are detailed 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	300˚C
Pressure	67 atm
Operation time	1 hour
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	2221.4549 lb/h
Volumetric rate	82.4770 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 operates under room temperature and pressure (RTP) conditions for a duration of 1 hour, with a cumulative incoming substance of 2221.4549 lb/hour. Data collection for mass balance analysis was manually conducted using the Microsoft Excel application based on equations 1-18. Calculated parameters for the reactor and stirrer are presented in Table 3. (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})	$H_{lc} = \frac{V_{lc}}{\left(\frac{\pi}{4}\right) d_i^2}$ Where H_{lc} (in)	(4)
	Pressure of design (P_i)	$P_i = P_{atm} + P_{hydrostatic}$ $P_i = 14{,}7\ psia + \left(\frac{\rho(HL-1)}{144}\right) psia$ Where $HL = 5.1463$ P_i (psig)	(5)
	Cylinder thickness (t_c) and d_o standardization	$t_c = \left(\frac{p_i \times d_i}{2(f \times E - 0.6P_i)}\right) + C$ Where $f = 18750$ $E = 0.8$ $C = 1/16$ $d_o = d_i + 2t_c$ Where d_o (ft)	(6)
	Height of cylinder (L_c)	$Total\ Vol. = V_{bottom\ lid} + V_{cylinder} + V_{top\ lid}$ $Total\ Vol. = \left(\frac{\pi d_i^3}{24\tan\left(\frac{1}{2}\alpha\right)}\right) + \left(\frac{\pi d_i^3}{4} \times Lc\right) + 0.0847 d_i^3$ L_c (in)	(7)

	Dimension of top lid	$th_t = \frac{0.885 \times P_i \times d_i}{2(f \times E - 0.1P_i)} + C$ Where th_t = top lid thickness (in) $h_t = 0.169 \times d_i$ Where h_t = height of top lid (in)	(8)
	Dimension bottom lid	$th_b = \frac{P_i \times d_i}{2(f \times E - 0.16)\cos\left(\frac{1}{2}\alpha\right)} + C$ 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 α = 120° h_b = height of bottom lid (in)	(9)
	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) $H = (0.1 + 0.15)P + P$	(16)

	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)	
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

The reactor functions as a tool for chemical processes, accommodating reactions across a spectrum of sizes—from small-scale applications like test tubes to larger industrial-scale reactors. In this specific application, the reactor serves as the environment for the reaction between ethene and water, yielding ethanol as the primary product. The reaction occurs at a temperature of 300°C under a pressure of 67 atm, facilitated by the catalyst H_3PO_4. The reactor used is the CSTR type.

The Continuous Stirred Tank Reactor (CSTR) finds application in homogeneous reactions (liquid-liquid), heterogeneous reactions (liquid-gas), and reactions involving suspended solids with the aid of stirring. Stirred tanks are predominantly utilized for continuous operations. The essential components of a CSTR include the tank and stirrer. Typically, these reactors feature inlet and outlet channels, along with additional equipment tailored to specific requirements, such as lids, thermometers, and heaters [36]. The illustrated sections of the stirred reactor are depicted in Figure 2.

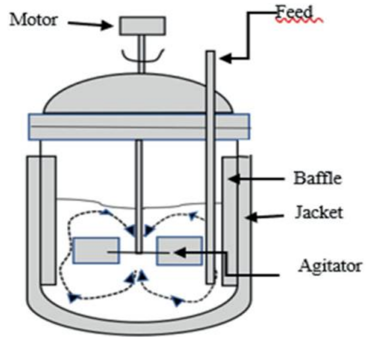


Figure 2 Continuous Stired Tank Reactor (CSTR) Design

The reactor's volume was computed as 103.09 ft^3, with a vessel diameter measuring 51.06 inches, a cylinder height of 64.70 inches, and a cylinder thickness of 1.74 inches. Once the vessel diameter was determined, calculations for the top and bottom caps' heights were performed to ascertain the overall height. The calculated height of the top cap is 8.63 inches, featuring a thickness of 1.52 inches, while the bottom cap has a calculated height of 14.75 inches with a thickness of 3.49 inches. Consequently, the reactor's overall height amounts to 2.28 feet. Table 4 presents the design parameters of the reactor based on comprehensive calculations.

Table 4 Reactor parameters designed based on calculations.

No	Parameters	Results
1	Total volume of reactor	103.09 ft^3
2	Vessel dimension (d_i)	51.06 in
3	Volume of liquid in the cylinder (V_{lc})	76.65 ft^3
4	Height of liquid in the cylinder (H_{lc})	64.70 in
5	Pressure of design (P_i)	970.30 psig
6	Cylinder thickness (t_c)	1.74 in
7	D_o standardization	54.56 in
8	Height of cylinder (L_c)	3.18 in
9	Top lid thickness (th_t)	1.52 in
10	Height of top lid (h_t)	8.63 in
11	Bottom lid thickness (th_b)	3.49 in
12	Height of bottom lid (h_b)	14.75 in
13	Height of reactor	2.28 ft

The dimensions of every element, including the agitator, also referred to as a stirrer, must be carefully evaluated. The stirrer usually incorporates a set of motors as a drive pad and an impeller or blade tailored to the specific organic material in use. The stirring action, employed in the ethanol formation process, induces a flow pattern within the reactor. The flow pattern can be modified depending on the flow velocity. For this particular design, axial flow is employed, resulting in a flow parallel to the rotation axis.

The outcomes of the stirrer calculations are detailed in table 5. A single stirrer is utilized with the stirring power 713 Hp, shaft diameter of stirrer 6,93 in, and shaft length of stirrer measuring 1,64 feet. It's worth noting that the plate employed in the stirrer corresponds to an axial turbine type featuring 4 blades set at a 45˚ angle. The turbine stirrer type is characterized by numerous blades and a relatively compact 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)	713 HP
7	Shaft diameter of stirrer (D)	6,93 in
8	Shaft lenght of stirrer (L)	1,64 ft

Conclusion

In Conclusion, the calculated design for the reactor indicates a volume of 103.09 ft^3, featuring a vessel dimension of 51.06 in, a cylinder height of 3.18 in, and a cylinder thickness of 1.74 in. The top cap measures 8.63 in with a thickness of 1.52 in, while the bottom lid measures 14.75 inches with a thickness of 3,49 inches. Consequently, the overall height of the reactor amounts to 2.28 feet. The reactor is furnished with a single stirrer, boasting a shaft diameter of stirrer 6,93 in, and shaft length of stirrer measuring 1,64 feet. Turbulent stirring flow conditions are maintained, and the standard motor power for the stirrer is 713 HP.

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