

Design of Biodiesel Reactor Using Nanocatalyst ZnO From Castor Oil

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Abstract. Mass transfer during the reaction process is limited in industrial biodiesel manufacture. Therefore, to overcome this problem, a reactor from castor oil transesterified using ZnO nanocatalyst was designed. ZnO can be used as a catalyst for biodiesel production due to the nature of ZnO which has high catalytic activity, low material costs and is environmentally friendly. This study aims to design a design for the manufacture of zinc oxide (ZnO) nanocrystals using a continuous stirred tank reactor (CSTR) reactor. By giving data on incoming feedstock and product flow produced by the reactor, mass balance calculations were used in this study as a benchmark to determine whether the reactor was operating appropriately. Additionally, using Microsoft Excel, manual calculations were done for the reactor design and agitator design employed in the reactor. According to calculations used in reactor design, the reactor has a volume of 1967.78 liters, a vessel diameter of 44.77 inches, a height of 19.25 inches, and a thickness of 44.98 inches. The reactor is equipped in one stirrer with a power on a typical 10 hp agitator motor, turbulent agitator flow conditions exist.

Keywords: ZnO nanocrystal, biodiesel production, Continuous Stirred Tank Reactor, catalyst, stirrer reactor

Abstrak. Perpindahan massa selama proses reaksi dibatasi dalam pembuatan biodiesel industri. oleh karena itu, untuk mengatasi masalah tersebut dirancang sebuah reaktor dari minyak jarak yang ditransesterifikasi menggunakan reaktor dengan nanokatalis ZnO. ZnO dapat digunakan sebagai katalis untuk produksi biodiesel karena sifat ZnO yang memiliki aktivitas katalitik yang tinggi, biaya material rendah dan bersifat ramah lingkungan. Penelitian ini bertujuan untuk membuat rancangan desain pembuatan nanokristal seng oksida (ZnO) dengan menggunakan reaktor *continuous stirred tank reactor* (CSTR). Dengan memberikan data feedstock yang masuk dan aliran produk yang dihasilkan oleh reaktor, perhitungan neraca massa digunakan dalam penelitian ini sebagai tolok ukur untuk menentukan apakah reaktor beroperasi dengan baik. Selain itu, dengan menggunakan Microsoft Excel, perhitungan manual dilakukan untuk desain reaktor dan desain agitator yang digunakan dalam reaktor. Menurut perhitungan yang digunakan dalam desain reaktor, reaktor tersebut memiliki volume 1967,78 liter, diameter bejana 44,77 inci, tinggi 19,25 inci, dan tebal 44,98 inci. Reaktor dilengkapi dalam satu pengaduk dengan daya pada motor agitator 10 hp tipikal dengan kondisi aliran agitator turbulen.

Kata Kunci: ZnO nanocrystal, produksi biodiesel, Continuous Stirred Tank Reactor, katalis, reaktor pengaduk

I. INTRODUCTION

The use of biodiesel has increased in popularity across many nations, driven by concerns about the environment, energy security, and economics. Transesterification of vegetable or animal fats with short-chain alcohols like methanol or ethanol produces fatty acid alkyl esters, or biodiesel, and is the most popular method for producing it [1]. The restriction of mass transfer under reaction circumstances is the fundamental issue in the manufacture of biodiesel. The solution to this issue is to employ a continuous stirred tank reactor and a ZnO nanocatalyst in a transesterification process from castor oil (CSTR) [2].

A reactor is a tool used in the chemical industry to create chemical substances and serve as a space for reactions to occur. Whether it's a chemical reaction where a substance can transform from one form to another, a reactor is a device that acts as a location for a reaction to occur. Some of the alterations may occur naturally or with the aid of energy like heat. To reduce operational costs and maximize production, reactor makers must ensure that reactions will produce the desired end product with the highest level of efficiency. generally found in the reactor [3].

Biodiesel is a type of fuel derived from long-chain fatty acid mono-alkyl esters produced from renewable resources like vegetable and animal oils. Due to its renewable status and lower emissions of greenhouse gases and particulate matter than conventional diesel fuel, biodiesel is a potential replacement [4]. An acid or alkaline solution is frequently used as a catalyst in the transesterification process to produce biodiesel from biomass sources like plant oils and animal fats. However, the main drawbacks of biodiesel include its reduced energy content, lessening of power, higher nitrogen oxide emissions, higher cost of production, and increased engine wear. [5].

For the biodiesel production process, castor oil were used which was catalyzed by Zinc Oxide (ZnO). A multipurpose amphoteric transition metal oxide with exceptional physical, chemical, electrical, mechanical, and optical characteristics is zinc oxide. ZnO has been utilized as a catalyst, photocatalyst, energy producer, gas sensor, chemical or biosensor, catalyst, and material of choice for biomedical purposes [5]. ZnO with varying physical and chemical properties that are advantageous for a particular application can be generated by utilizing a variety of synthetic techniques. Numerous techniques have been investigated in the literature to date for the synthesis of nanometric or micrometric ZnO, including vapor deposition, electrochemical deposition, coprecipitation, sol-gel, solvothermal technique, hydrothermal, microwave assisted hydrothermal, thermal decomposition, combustion synthesis, and sonochemical synthesis. These processes resulted to the creation of ZnO, which has been carefully compiled in a review with all the necessary details (synthesis conditions, precursors, characteristics, and applications of created oxide) [6].

In this study, it is essential to create an efficient and precise reactor design in order to predict the mechanism based on the experimental data. This can be done by analyzing how changes in reaction rate relate to changes in each reactant and formulating the final equation for reaction rate. This is due to the requirement for optimizing the generation of biodiesel from used castor oil catalyzed by ZnO.

II. METHODOLOGY

A. *Synthesis of ZnO nanocrystal*

The hydrothermal method's schematic and PFD for creating ZnO nanocrystals are depicted in Figures 1 and 2.

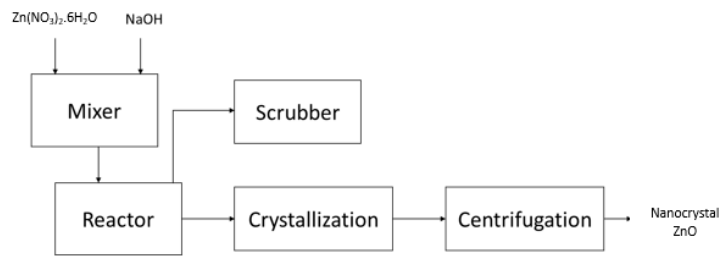


Figure 1. Nanocrystal ZnO manufacturing process

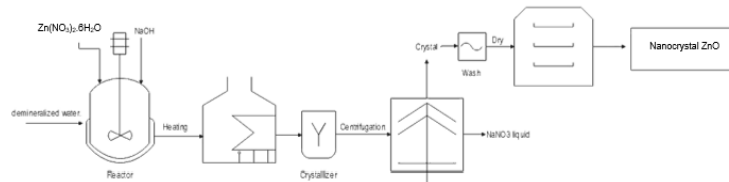


Figure 2. PFD on the manufacture of nanocrystal ZnO

ZnO nanocrystal production is based on research done by Lamba et al. in 2019 [7]. The castor tree's seeds were pressed to obtain castor oil, which was subsequently used in the trials. Hexahydrate of zinc nitrate ($\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$), dihydrate of zinc acetate ($\text{Zn}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$), pluronic F127, diethylene glycol, ethylene glycol, hexamethylene tetramine (HMTA), and 100% analytical-grade ethanol were purchased from Sigma Aldrich. We obtained butyl laurate, sodium and potassium hydroxides, methanol (HPLC quality), oxalic acid, and n-heptane (HPLC grade) from the Merck compounds. The hydrothermal process can be used to create ZnO nanorods. The synthesis of ZnO-NR was carried out hydrothermally. An analogous procedure that has been previously described was employed to produce ZnONR. [8]. 14.75 g of zinc acetate dihydrate were dissolved in methanol to create a solution. The solution was completely stirred with a magnetic stirrer while being kept on a heating plate that was

kept at 65 °C. The solution on the heating plate was then gradually mixed with KOH methanolic solution. The resulting combination was heated for two hours in order to evaporate half of the alcohol from it and increase its concentration.`

After 2 hours, the mixture was transferred to a hydrothermal reactor with a Teflon liner and heated for 10 hours at 120 °C in a muffle furnace to produce the necessary material. The ZnO-NR was obtained by collecting the precipitate after the reaction, washing it three to four times with deionized water, and drying it for eight hours at 120 °C [7].

B. Mathematical Models for Designing Reactors

Table 1 shows the reactor parameters to be calculated. Data analysis is in the form of manual calculations using basic Microsoft Office applications based on equations 1-20.

Table 1. Calculation of reactor parameters

No	Section	Parameter	Equation	Eq
1.	Reactor planning	Volume Reaktor (V_{total})	$V_{total} = V_{material} + V_{free\ space}$	(1)
		Vessel Diameter (Di)	$V_{total} = V_{top\ lid} + V_{cylind} + V_{top\ cov}$ $V_{total} = \frac{\pi di^3}{24 \tan 1/2\alpha} + \frac{\pi di^2}{4} \times Ls + 0,0847 di^3$ $Di = \text{vessel diameter}$ $\pi = \text{the value of 3.14}$ $Ls = \text{cylinder height}$	(2)
		Volume of Liquid in The Cylinder (V_{ls})	$V_{ls} = V_{liq} + V_{top\ lid}$ $V_{ls} = V_{liq} + \frac{\pi di^3}{24 \tan 1/2\alpha}$ $V_{ls} = \text{the volume of liquid in the cylinder}$ $Di = \text{vessel diameter}$ $\pi = \text{the value of 3.14}$	(3)
		High Liquid in The Cylinder (L_{ls})	$L_{ls} = \frac{V_{ls}}{\left(\frac{\pi}{4}\right) \times di^2}$ $L_{ls} = \text{high liquid in the cylinder}$ $V_{ls} = \text{the volume of liquid in the cylinder}$ $\pi = \text{the value of 3.14}$ $Di = \text{vessel diameter}$	(4)
		Design Pressure (Pi)	$Pi = P_{atm} + P_{hydrostatic}$ $P_{hydrostatic} = \frac{\rho (HL - 1)}{144}$	(5)
		Cylinder Thickness (Ts)	$Ts = \frac{Pi \cdot di}{2(f.E - 0,6Pi)} + C$ $Ts = \text{cylinder thickness}$ $Pi = \text{design pressure}$ $Di = \text{vessel diameter}$	(6)
		Cylinder Height (Ls)	$V_{total} = V_{top\ lid} + V_{cylinder} + V_{top\ cov}$ $V_{total} = \frac{\pi di^3}{24 \tan 1/2\alpha} + \frac{\pi di^2}{4} \times Ls + 0,0847 di^3$ $Di = \text{vessel diameter}$ $\pi = \text{the value of 3.14}$ $Ls = \text{cylinder height}$	(7)
		Top Cover Thickness (tha)	$tha = \frac{0,885 \times Pi \cdot di}{2(f.E - 0,1Pi)} + C$ $tha = \text{top cover thickness}$ $Pi = \text{design pressure}$	(8)

		Di = vessel diameter	
		$ha = 0,169 Di$	(9)
Top Cover Height (ha)		ha = top cover height Di = vessel diameter	
Bottom Cover Thickness (thb)		$thb = \frac{Pi.di}{2(f.E-0,6Pi) \cos 1/2\alpha} + C$	(10)
		hb = bottom cover thickness Pi = design pressure Di = vessel diameter	
Bottom Cover Height (hb)		$hb = \frac{1/2 d}{\tan 1/2\alpha}$	(11)
2.	Reactor stirrer	Impeller Diameter (Da)	$Da = Dt \times 0.5$ (12)
		Da = impeller diameter Dt = cylinder inside diameter	
Impeller Height from Tank Bottom (C)		$C = \frac{1}{3} \times Di$	(13)
		C = cylinder inside diameter Di = vessel diameter	
Impeller Length (L)		$L = \frac{1}{4} \times Da$	(14)
		L = impeller length Da = impeller diameter	
Impeller Width (W)		$W = 0.20 \times Da$	(15)
		W = impeller width Da = impeller diameter	
Number of Stirrer (n)		$n = \frac{H liquid}{2 \times Da^5}$	(16)
		n = the number of stirrer Da = impeller diameter	
Reynold Number (N _{Re})		$N_{Re} = \frac{L^2 \times n \times \rho}{\mu}$	(17)
		N_{Re} = the Reynold number L = impeller length n = stirrer rotation, set = 100 rpm = 1,67 rps ρ = density (lb/ft ³)	
Stirring Power (P)		$P = \frac{\varphi \times \rho \times n^3 \times Di^5}{gc}$	(18)
		P required = (0,1 + 0,15)P + P P = stirring power ρ = density (lb/ft ³) Di = impeller diameter gc = 32,2 lb.ft/s ² .lbf	

Stirrer Shaft Diameter (D)	$D = \frac{\# \times T}{\pi \times S}$	(19)
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D = stirrer shaft diameter

T = torsion number (lb.in = $\frac{63025 H}{N}$)

π = the value of 3.14

S = maximum allowable design shearing stress

Shaft Length (L)	$L = h + l - Zi$	(20)
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h = cylinder height + top cover height

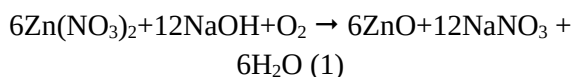
l = impeller distance from tank bottom

Zi = length of shaft above tank vessel

III. RESULT AND DISCUSSION

A. Main Reaction

NaOH and $Zn(NO_3)_2 \cdot 6H_2O$ are employed as precursors in the manufacture of ZnO nanocrystals to reduce the amount of reactants. Both times, any lingering counterions (NO_3 and OH^-) that may have been left on the surface of the spinel can be easily eliminated by calcining under mild circumstances without leaving a clumpy residue. [9]. The main reactions expected in this reaction are shown in numbers (1)



Shows that the reaction consisting of $Zn(NO_3)_2 \cdot 6H_2O$ and NaOH is reacted with the help of O_2 , it will produce ZnO as the main product in the form of a white solid and a solution of $NaNO_3$ is produced as a side product.

B. Reactor Type

In both small and big levels, such as industrial scale reactors and test tubes, the reactor is a process

tool where the reaction occurs. O_2 and $NaNO_3$ solutions were produced as byproducts of the reaction of $Zn(NO_3)_2 \cdot 6H_2O$ with NaOH in the reactor, which produced white ZnO nanocrystals as the major product at 180 °C. The reactor is of the CSTR type and is made of stainless steel type SA 240 grade M type 316. It has an upright cylindrical shape with a standard shell cover and a conical bottom lid with a 120° apex angle. This substance is acceptable for usage as a raw liquid material. The CSTR reactor has a cylindrical shape. This happens because the internal load stabilizes and is distributed uniformly when the shock wave of the liquid load inside the reactor meets the curved surface.

For homogeneous (liquid-liquid) reactions, heterogeneous (liquid-gas) reactions, and stirring-aided reactions involving suspended solids, CSTR is employed. Continuous operations represent the majority of stirred tank applications. The tank and stirrer make up the key components of CSTR. These reactors typically have an inlet port, an exit port, and, if necessary, additional equipment like shutters, thermometers, heaters, etc. [9]. Parts of a stirred reactor can be seen in Fig 3.

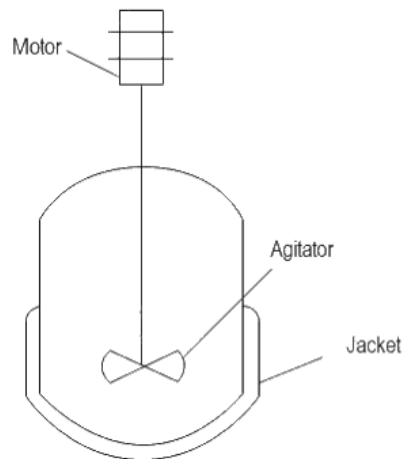


Figure 3. Desain Continuous Stirred Tank Reactor (CSTR)

The stirrer is one of the most crucial components in the construction of a CSTR type reactor. The efficiency of stirring and blending the liquids during a treatment process frequently determines its success. Agitation is the act of controlling how a substance moves within a container; the movement usually has a cyclical pattern.

Agitation is used to dissolve insoluble liquids, form emulsions or suspensions of small particles, suspend solid particles, and improve heat transmission between liquids and coatings. The agitator strives to create the best mixture with the least amount of energy.

Reactants and products flow continuously in CSTR. The feedstock is continually fed into this process, and the reaction products are either released continuously or continuously. This is why mechanical or hydraulic agitation is necessary for CSTR to obtain uniform composition and temperature. A properly stirred reaction mixture or good mixing under ideal agitation conditions results in the CSTR ideal reactor. Complete mixing is necessary to produce a high degree of homogeneity

so that the composition and temperature are uniform at all sites since there is no change in volume and consequently no change in density (density change is overlooked).

C. Reactor Parameter Calculation Results

The quality of the product that is created depends on the reaction that occurs in the reactor. The flow of products created by a reactor and the incoming raw materials can be used to determine whether or not it is operating properly. By calculating the mass balance of the process feed from the reactor using the input and output composition, we can determine the quantity of incoming and outgoing mass to manage raw materials in the following process.

Based on the law of conservation of mass, the mass balance is used to guarantee the amount of material entering and leaving a process. In other words, the entire intake and outflow are equal. To choose the right kind and size of chisel to give the process volume, mass balance calculations can be used as a guide. [10]. Table 1 shows the results of mass balance calculations in ZnO production.

Table 2. Recapitulation of mass balance of ZnO production

Component	Mr (g/mol)	Reactants			Product		
		Massa	Mol	Fr.Mol	Mol	Fr.Mol	Massa
Zn(NO ₃) ₂	189.3898	9160	48.3658	0.137555	-227.32	0.609668	-43052
NaOH	40	6120	153	0.42032	-417.81	-1.01515	-16712.4
O ₂	32	5150	160.9375	0.442126	113.37	0.275453	3627.84
ZnO	81		0	0	95.13502	0.231148	22908.51
NaNO ₃	84.99		0	0	570.8101	1.386888	48513.15
H ₂ O	18		0	0	285.4051	0.693444	5137.291
Total		20430	362.30				20422.39

From these data it can be seen that the inlet mass of Zn(NO₃)₂ is 9160kg/hour, the inlet time for NaOH is 6120kg/hour and the O₂ gas entering is 5150kg/hour. The volume of incoming material equals the volume of material leaving the reactor, which is 20430 kg/hour.

The dimensions of the reactor are then calculated after that. The reactor is an upright cylinder with a conical bottom lid and a top lid with a conventional dish shape and a peak angle of 120 degrees. The reactor was set up to produce nanocrystals at a temperature of 180 °C, a pressure of 1 atm, and an

operating time of 1 hour. It also had a double welded butt joint with an e of 0.8 and an acceptable stress (f) of 18750. The general dimensions and dimensions of each component are included in the calculation of this reactor's dimensions. Vessel diameter, cylinder thickness, and cylinder length are examples of dimensions. While the computation of the stirrer from the reactor is included in each component's size. The reactor's top and bottom lids, as well as their thickness, must be calculated and determined. These calculations must be taken into account next.

Table 3. Reactor dimension specifications based on calculation results

No	Parameter	Result
1	Type of reactor	Upright cylinder with standard dished top cap and conical bottom cap with a peak angle of 120°
2	Volume Reaktor (V_{total})	1967.78 liter
3	Vessel Diameter (Di)	44,77 in
4	Volume of Liquid in The Cylinder (V_{ls})	1462.84 liter
5	High Liquid in The Cylinder (L_{ls})	56.73 in
6	Design Pressure (Pi)	26.60 psig
7	Cylinder Thickness (Ts)	44.98 in
8	Cylinder Height (Ls)	19.25 in
9	Top Cover Thickness (tha)	0.098 in
10	Top Cover Height (ha)	7.57 in
11	Bottom Cover Thickness (thb)	0.14 in
12	Bottom Cover Height (hb)	12.94 in
13	Reactor Height	26.33 in

Based on calculations of the reactor's dimensions, a capacity of 1967.78 liters, a vessel diameter of 44.77 inches, a cylinder height of 19.25 inches, and a cylinder thickness of 44.98 inches were determined. Calculating the height of the top

cover and the height of the bottom cover comes next after knowing the vessel's diameter. Such computations will result in a high final score. The bottom cover calculation yields a result of 12.94 inches with a thickness of 0.14 inches while the top

cover calculation yields a result of 7.57 inches with a thickness of 0.098 inches. so that the reactor's overall height is 26.33 inches.

The sizes of each component must also be considered, and this includes figuring out how big the reactor's agitator should be. It is frequently made up of a number of motors that drive paddles, impellers, or blades depending on the type of organic material being utilized. It is also known as an agitator or stirrer. A flow pattern is produced in the reactor as a result of the agitation that occurs during the formation of ZnO nanocrystals. Based on

the flow speed, the flow pattern can be modified. Axial flow, which creates flow parallel to the axis of rotation, is used in this design.

According to the book (G.G. Brown), the stirrer plan was chosen. The stirrer to be used is an axial turbine with four blades at a 45-degree angle and an impeller made of high alloy steel SA 240 Grade M type 314. Additionally, the material used to build the stirrer shaft is hot-rolled steel SAE 1040. The calculation results are shown in Table 3 after selecting a stirrer plan and determining the stirrer's dimensions.

Table 4. Specification of stirring dimensions based on calculation results

No	Parameter	Result
1	Impeller Diameter (Da)	22.49 in
2	Impeller Height from Tank Bottom (C)	14.92 in
3	Impeller Length (L)	5.62 in
4	Impeller Width (W)	4.50 in
5	Number of Stirrer (n)	1 piece
6	Reynold Number (N_{Re})	166482.33
7	Stirring Power (P)	10 Hp
8	Stirrer Shaft Diameter (D)	1.55 in
9	Shaft Length (L)	17.52 in

Calculations show that the impeller diameter is 22.49 inches, the impeller height above the bottom of the tank is 14.92 inches, the impeller breadth is 4.50 inches, and the impeller length is 5.62 inches. The agitation number is 1 unit. It is known that the agitator's plate is an axial turbine type with four blades at a 45° angle. This particular style of short turbine agitator features a significant number of agitating blades. High speeds are employed with this type of stirrer for liquids with a wide variety of viscosities. The diameter of the turbine agitator is 30–50% of the vessel diameter. A combination of axial and radial flows are produced by turbines with blades that have a 45° pitch because they generate multiple axial flows. Because the stream travels straight down and sweeps the sediments up, this type is ideal for suspending solids.

The power of the mixer with gain losses is assessed at 10% of the input power (processing power losses, bearing/flat shaft losses), and the transmission system losses are assumed at 15% (belt or gear leaks). 9.6 hp. Therefore, a normal motor

power of 10 hp should be used for the stirrer in the stirring operation. The capacity to exploit the chemical reaction of raw components to create the desired product is known as mixing power. The magnitude of the resulting velocity gradient depends on the stirring force. The agitating system, which includes the agitator and its rotational speed, water flow, air flow, etc., produces the agitating power.

Calculate the stirrer shaft using the information that it has a diameter of 1.55 inches, a length of 17.52 inches, a shaft power of 10 hp, and a stirrer speed of 100 rpm. Typically, a force or torque follower is a shaft with a circular cross section. When making shafts, corrosion-resistant materials must be chosen. [11]. Therefore the shaft material used in this design is Hot Rolled Steel SAE 1040 which is corrosion resistant.

Apart from that, the Reynolds number is 166482.33. The link between inertia and viscosity is known as the Reynolds number. Depending on the stirrer's Reynolds number, the procedure using a

mechanical stirrer is conducted in either laminar or turbulent flow conditions. Here, there is a turbulent flow that has a value of $Re > 2100$. An unstable fluid flow with randomly moving particles is called turbulence, and it causes flow lines between the fluid particles to cross. As a result, there is a higher chance of interactions, reactions, and collisions between substances than there would be in a state of laminar flow, where the fluid moves in a static and ordered manner without traversing. [12]. A stirrer with this type of turbulent flow produces the best possible agitation.

IV. CONCLUSIONS AND RECOMMENDATIONS

Based on the calculation results of the reactor design, the reactor volume is 1967.78 liters, with a vessel diameter of 44.77 in, a cylinder height of 19.25 in and a cylinder thickness of 44.98 in. The top cover of the reactor measures 7.57 inches with a thickness of 0.098 inches while the bottom cover measures 12.94 inches with a thickness of 0.14 inches. So that the overall height of the reactor is 26.33 in. The reactor is equipped with 1 stirrer with an impeller diameter of 22.49 in, impeller height from the bottom of the tank is 14.92 in, impeller width is 4.50 in and impeller length is 5.62 in. Turbulent stirring flow conditions with a standard motor power for the stirrer is 10 HP.

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