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Design of Batch Reactor for the Production of MgO Nanoparticles

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Abstract (English)
The objective of this project is to develop batch reactor designs for the production of MgO particles. The computational analysis and calculation of the reactor and its stirrer were used in this study, including calculations of the volume, height, thickness, number of stirrers, impeller length and diameter, and mass balance. The Microsoft Excel application was used to perform the reactor design calculations. According to the calculated values of the batch reactor design in the MgO process of production, the reactor has a volume of 14,507 ft^3 and a height of 1,3471 ft. The reactor has one stirrer with four blades and a power of one horsepower. The results of this computation and analysis could be used to improve and compare reactor performance in a manufacturing process as a learning medium and producing mechanism.

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Abstrak (Indonesia)
Tujuan dari proyek ini adalah untuk mengembangkan desain reaktor batch untuk produksi partikel MgO. Analisis komputasi dan perhitungan reaktor dan pengaduknya digunakan dalam penelitian ini, termasuk perhitungan volume, tinggi, ketebalan, jumlah pengaduk, panjang dan diameter impeler, dan keseimbangan massa. Aplikasi Microsoft Excel digunakan untuk melakukan perhitungan desain reaktor. Berdasarkan hasil perhitungan desain reaktor batch pada proses produksi MgO, reaktor memiliki volume 14.507 ft3 dan tinggi 1.3471 ft. Reaktor ini memiliki satu buah pengaduk dengan empat buah sudu dan daya sebesar satu tenaga kuda. Hasil dari perhitungan dan analisis ini dapat digunakan untuk meningkatkan dan membandingkan kinerja reaktor dalam suatu proses manufaktur sebagai media pembelajaran dan mekanisme produksi.

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Background

MgO is one of the interesting metal oxides that are commonly used when it comes to industrial applications i.e heating apparatus, refractory materials and infrared optics etc. [1-2]. Its band gap is attractive because of its wide like insulator [3]. It is crystallized in cubic Fm3m space group. Currently, many studies have been done on the synthesis and applications of MgO. Examples of these studies are hydrothermal, sol-gel, flame spray pyrolisis, combustion and aqueous wet chemical, chemical gas phase deposition, and solid-soild reaction [4-9]. ZnO is one of the most popular materials widely used in medical and industrial applications. Sometimes, it is referred to as a bewitched material due to it's wide applications range and elasticity of preparation in various morphologies with particular properties [10]. As mention before, ZnO and MgO nanoparticle's were used for different applications, but in radiation shielding they have less used in this form, there, these types of pure nanoparticle have an attractive for the scientists in the field of radiation shielding. This branch is considered as an issue that needs to be addressed. It is well-known that nuclear research laboratories, number of nuclear power plants, medical radiation facilities for diagnostic and treatment applications in the medical field are increasing in global World.

There are many metal oxides in nature, but a few of the metal oxides are the most useful in terms of their uses in science and technology. Some transition metal oxides, such as ZnO, Fe_3O_4, and TiO_2 have proven to be suitable options for a wide range of applications. CuO is another useful metal oxide that has numerous applications in a variety of areas. CuO nanoparticles are special in that, while metallic in bulk, they behave like semiconductors when reduced to nanoscale [11].

Magnesium oxide (MgO) is one of the most useful ceramic materials because it has a high melting temperature (around 2800^{o}C) [12]. Magnesium oxide is commonly used for catalysis and remediation of toxic wastes or as an additive in paints [13]. Magnesium oxide also has good additive properties, which can be applied to high fuel oils [14]. Magnesium oxide is needed in industrial, environmental, and health products. Magnesium oxide is used industrially as a catalyst in many applications includes organic carbonate synthesis catalysts [15]. Another application of magnesium oxide is in steel manufacture because it is highly corrosion-resistant [16].

Magnesium oxide nanoparticles can be produced through several synthesis methods. Synthetic methods that can be used in the synthesis of magnesium oxide nanoparticles include combustion [17], synthesis of plant extracts [18], sonochemical synthesis [19], solid-state synthesis [20], sol-gel synthesis [21], and precipitation [22]. Of the several methods, the precipitation method is one of the most preferred methods for the synthesis of magnesium oxide nanoparticles because it allows control over the particle size so that the time required is relatively short and can be carried out at low temperatures [22].

To produce MgO on an industrial scale, a batch reactor is needed. Batch reactors are vessels that hold substances and allow them to dissolve and react properly to achieve the desired results. In an ideal batch reactor, the quantity, efficiency, pressure, and temperature are all supposed to be exactly the same at any given time [23].

Many research on batch reactor analysis and design have been conducted, including reactors for lignocellulosic ethanol [24], sugar [25], biodiesel [26], Fe_3O_4/ZnO nanocomposite [27], ZnO-Mn [28], grapesseed oil [29], copper extraction [30], short-chain fructooligosaccharides [31], meat production [32], nanomaterial adsorbent [33], carbonization of biomass [34], and anionic polymerization of isoprene [35].

Batch reactors have the number of advantages compared with other kinds of reactor designs, which is they are easily built, operated, and controlled, can be shaped to meet specific needs, batch reactors require fewer pipe networks and channels than other techniques, a single basin can be used for homogenization, and they are generally cheaper [35].

This article utilizes the Microsoft Excel software to accomplish a computational analysis and calculation of the reactor, its stirrer, and the mass balance in order to improve the production of MgO on an industrial level.

Methode

1. Synthesis of MgO particles

Magnesium chloride dihydrate [$MgCl_2 \cdot H_2O$] and sodium hydroxide [NaOH] were used as precursors in the experiment for producing MgO nanoparticles. Magnesium chloride dihydrate (0.2 M) in deionized [DI] water and NaOH (0,5 M) in DI water were prepared as separate solutions

[36]. When magnesium chloride dihydrate reacts with sodium hydroxide in an aqueous medium to form $Mg(OH)_2$ nanowires, the following reaction occurs, as shown in equation 1 and 2.

$MgCl_2 \cdot 2H_2O + NaOH + H_2O \rightarrow Mg(OH)_2 + 2NaCl$ (1) Conversion : 98%

$Mg(OH)_2 \longrightarrow MgO + H_2O$ (2)

2. Mathematical model for reactor design

The reactor is constructed of stainless-steel SA 240 Grade M Type 316 and has a vertically cylinder type with a concave standard top lid and a cone bottom wrap and a peak angle of 120 °, while the stirrers are made of High Alloy Steel SA 240 Grade M type 316 and have an angular turbine type 4 blade angle of 45°. The assumptions for the requirements are shown in **Table 1.**

Table 1. Assumptions of specifications design of reactor and stirrer

Specification	Value
Reactor type	An upright cylinder with dished standard top cover and conical bottom cover with apex angle of 120°
Stirrer type	Axial turbine 4 blade angle 45
Stirrer impeller material	High Alloy Steel SA 240 Grade M type 316
Stirrer shaft material	Hot Roller Steel SAE 1020
Temperature	25°C
Pressure	1 atm
Operation time	1 h
Construction material	Stainless steel SA 240 Grade M Type 316
Allowable Stress (*f*)	18750
Welding	Double welded butt joint
Corrosion factor	0,0625
Amount of incoming substance	1.058,22 lb/h
Volumetric rate	328,64 ft^3/h

With a one-hour operation, the reactor's working temperature and pressure are set to 25°C and 1 atm, respectively. The total amount of material entering the reactor is 1.058,22 lb/h. When data is collected, mass balance analysis is done manually using the Microsoft Excel software (equation 1-18). The calculated reactor and stirrer specifications are shown in Table 2.

Table 2. Calculation of reactor and stirrer parameters

Section	Parameters	Equation	Eq.
Dimension of reactor	Total volume of reactor (V_r)	$V_r = precursor\ vol. + 20\% \times blank\ space\ vol.$ Where, V_r = total vol. of reactor (ft^3)	(1)
	Vessel dimension (d_i)	$V_r = V_{bottom\ lid} + V_{cylinder} + V_{top\ lid}$ $V_r = \left(\frac{\pi {d_i}^3}{24\tan\left(\frac{1}{2}\alpha\right)}\right) + \left(\frac{\pi {d_i}^2}{4} \times H_c\right) + 0.0847{d_i}^3$ Where, V_r = total vol. of reactor (ft^3) d_i = Vessel dimension (in) $\alpha = 120^o$ H_c = height of cylinder assumption = $1.5d_i$	(2)
	Volume of liquid in the cylinder (V_{lc})	$V_{lc} = V_{liquid} - V_{bottom\ lid}$ Where, V_{lc} = Volume of liquid in the cylinder (ft^3)	(3)
	Height of liquid in the cylinder (H_{lc})	$H_{lc} = \frac{V_{lc}}{\left(\frac{\pi {d_i}^2}{4}\right)}$ Where, H_{lc} = Height of liquid in the cylinder (in) V_{lc} = Volume of liquid in the cylinder (in^3) d_i = Vessel dimension (in)	(4)
	Pressure of design (P_i)	$P_i = P_{atm} + P_{hydrostatic}$ $P_i = 14.7\ psia + \left(\frac{\rho(H_{lc} - 1)}{144}\right) psia$ Where,	(5)

	P_i = Pressure of design (psig) H_{lc} = *Height of liquid in the cylinder* (ft)	
Cylinder thickness (t_c) and d_o standardization	$t_c = \frac{P_i \times d_i}{2(f \times E - 0.6P_i)} + C$ $d_o = d_i + 2t_c$ Where, P_i = Pressure of design (psig) d_i = Vessel dimension (in) f = Allowable stress =18750 E = 0.8 C = corrosion factor = 0.0625 d_i = Vessel dimension (ft)	(6)
Height of cylinder (H_c)	$H_c = 2 \times d_i$ Where, H_c = Height of cylinder = (in) d_i = Vessel dimension (in)	(7)
Dimension of top lid	$th_t = \frac{0.885 \times P_i \times d_i}{2(f \times E - 0.1P_i)} + C$ $h_t = 0.169 \times d_i$ Where, th_t = top lid thickness (in) h_t = height of top lid (in) P_i = Pressure of design (psig) d_i = Vessel dimension (in) C = corrosion factor = 0.0625	(8)
Dimension of bottom lid	$th_b = \frac{P_i \times d_i}{2(f \times E - 0.16)\cos\left(\frac{1}{2}\alpha\right)} + C$ $h_b = \frac{\frac{1}{2}h_t}{\tan\left(\frac{1}{2}\alpha\right)}$ Where, th_b = bottom lid thickness (in) h_b = height of bottom lid (in) h_t = height of top lid (in) $\alpha = 120^o$	(9)
Height of reactor (H_r)	$H_r = h_t + H_c + h_b + S_f$	(10)

		Where, H_r = Height of reactor (ft) h_t = height of top lid (in) H_c = Height of cylinder = (in) h_b = height of bottom lid (in) S_f = 2.5	
Stirrer	Impeller diameter (D_a)	$$\frac{D_a}{D_t} = 0.5$$ Where, D_a = impeller diameter (ft) D_t = inner diameter of cylinder (ft)	(11)
	Impeller height from bottom of the tank (Z_i)	$$\frac{Z_i}{D_t} = \frac{1}{3}$$ Where, Z_i = impeller height from the bottom of the tank (ft) D_t = inner diameter of cylinder (ft)	(12)
	Impeller length (l)	$$\frac{l}{D_a} = \frac{1}{4}$$ Where, l = impeller length (ft) D_a = impeller diameter (ft)	(13)
	Impeller width (W)	$$\frac{W}{D_a} = \frac{1}{5}$$ Where, W = impeller width (ft) D_a = impeller diameter (ft)	(14)
	Number of stirrers (n)	$$n = \frac{H_{lc}}{2 \times {D_a}^2}$$ Where, n = number of stirrers H_{lc} = Height of liquid (ft) D_a = impeller diameter (ft)	(15)
	The stirring power (H)	$$P = \frac{\varphi \times \rho \times N^3 \times {D_a}^5}{g_c}$$ Where, P = stirring power (Hp) φ = power number = 0.9 ρ = density of mixture (lb/ft^3)	(16)

		g_c = 32.2 lb.ft/s^2.lbf N = stirrer rotation = 100 rpm = 100 rps $H = (0.1 + 0.15)P + P$ Where, H = Stirring power needed (Hp) 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 from input power	
	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, *D* = Shaft diameter of stirrer (in) *T* = torsion moment (lb.in) *S* = maximum allowable design shearing stress (lb/in^2) *N* = stirrer rotation = 100 rpm	(17)
	Shaft length of stirrer (*L*)	$L = h + (l - Z_i)$ $h = H_c + h_t$ Where, *L* = Shaft length (ft) *h* = cylinder height (ft) + top lid height (ft) *l* = Impeller length (ft) Z_i = impeller height from the bottom of the tank (ft)	(18)

Result and Discussion

The reactor is a manufacturing tool that can differ in size from small testing tubes to large industrial level reactors. For the efficient execution of a treatment method, effective stirring and mixing of the materials in the process is usually needed. The definitions of kneading and mixing are not synonymous. Agitation is described as a reduction motion in a given direction of a material in a vessel, with the motion typically having to follow a pattern.

In order to optimize reaction products, numerous sorts of calculations such as reactor design and size are performed. Several assumptions are made in order to optimize the reaction product, such as:

1. The raw materials used for MgO production are $MgCl_2{\cdot}2H_2O$ and NaOH
2. The MgO production process follows Figure 1.
3. MgO production is calculated based on the mass balance (Table 3).
4. Reaction process occurs in reactor tank
5. Reactor type is batch reactor
6. Construction material is stainless steel
7. Operating condition temperature is 25°C
8. Pressure is 1 atm
9. Operation time is 1 hour
10. Conversion percentage is 98%
11. The molecular weights of $MgCl_2{\cdot}2H_2O$, NaOH, MgO, $Mg(OH)_2$,NaCl and H_2O are 131, 40, 40.3044, 58, 58.5 and 18 g/mol, respectively

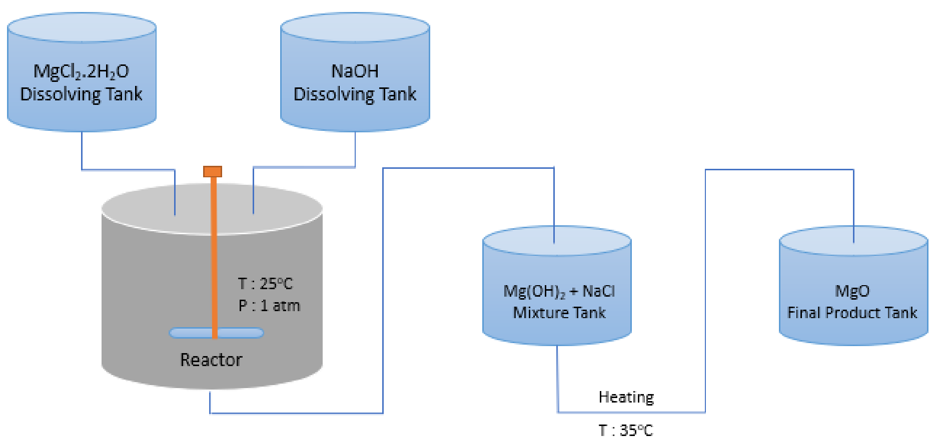

Figure 1. PFD for MgO production.

Table 3. Mass balance of MgO production.

No.	Component	Input		Output	
		Mass (kg/hour)	Mol (kmol/hour)	Mass (kg/hour)	Mol (kmol/hour)
1	$MgCl_2{\cdot}2H_2O$	300	2.290,08	6	45,802
2	H2O	100	5.555,56	59,603	3311,3
3	NaOH	80	2000	9,771	244,3
4	$Mg(OH)_2$	0	0	90,454	2244,3
5	NaCl	0	0	262,58	4488,5

Table 4. Calculated performance parameters for the reactor and stirrer.

Parameters	Result
Total volume of reactor (Vr)	14,507 ft3
Vessel dimension (di)	2,2135 ft
Volume of liquid in the cylinder (Vlc)	10,7865 ft3
Height of liquid in the cylinder (Hlc)	2,8046 ft
Pressure of design (Pi)	5,7117 psig
Cylinder thickness (tc)	0.0675 in
do standardization	2,2247 ft
Height of cylinder (Hc)	3,3201 ft
Top lid thickness (th¬t)	0,0669 in
Height of top lid (h¬t)	4,4888 in
Bottom lid thickness (th¬b)	0.0726 in
Height of bottom lid (h¬b)	7,6767 in
Height of reactor (Hr)	1,3471 ft
Impeller diameter (Da)	14.9093 in
Impeller height from bottom of the tank (Zi)	9.9395 in
Impeller length (l)	3.7273 in
Impeller width (W)	2.9819 in
Number of stirrers (n)	1
The stirring power (H)	1 Hp
Shaft diameter of stirrer (D)	0.7641 in
Shaft length of stirrer (L)	3.6296 ft

Figure 1. illustrates the designed reactor and stirrer design model. MgO is synthesized by combining $MgCl_2{\cdot}2H_2O$ and NaOH at a temperature of 25°C and a pressure of 1 atm. When NaOH is combined to $MgCl_2{\cdot}2H_2O$, a large amount of $Mg(OH)_2$ and NaCl form. Eventually, the

$Mg(OH)_2$ collected to dry at 35°C. Table 3 summarizes the results of the mass balance measurement in the production process of MgO nanoparticles based on Figure 1.

Table 4. shows the reactor specific requirements obtained from computation for MgO production based on the mass balance. One batch reactor with a volume of 14,507 ft^3, a height of 1,3471 ft, a diameter of 2,2135 ft, and a cylinder thickness of 0.0675 in is required. The number of required stirrers is one. The diameter, height, length, and width of the impeller are 14,9093 in, 9.9395 in, 3,7273 in, and 2,9819 in, respectively. The calculated impeller power is 1 Hp. This batch reactor and stirrer specification measurement can be used to research reactor design and production mechanisms in a factory.

Conclusion

The batch reactor for producing MgO nanoparticles on an industrial scale has been designed successfully. Based on the batch reactor and stirrer performance requirements, one batch reactor with a volume of 14,507 ft^3, a height of 1,3471 ft, a diameter of 2,2135 ft, and a cylinder thickness of 0.0675 in is required. Furthermore, the stirrer dimensions, stirrer diameter and stirrer distance from the tank's bottom, are 14,9093 in and 9,9395 in, respectively. The reactor has one stirrer with four blades. This research's batch reactor and stirrer specification measurement can be used to research reactor design and production mechanisms in a factory.

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