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Preliminary reactor design for the gold nanoparticles production by the Turkevich method on an industrial scale

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Abstract

This study aims to design and analyze the design of a batch-type reactor to optimize the production of gold nanoparticles on an industrial scale. The method used in the design of this reactor is the computational analysis of the reactor calculations, including stirring and mass balance as initial calculations using the Microsoft Excel application manually. The calculation results show that the designed reactor specifications have a reactor volume of 21.7335 ft3, cylinder height of 13.4612 in, a height of solution in the cylinder of 8.9046 in, vessel diameter of 73.2984 in, design pressure of 9.9978 psig, impeller length of 9.1840 in, shaft length of 10.5418 in, with stirring power 62.5228 Hp. Reactor design analysis is an important stage in the design of production processes on an industrial scale, where the specification results from the designed reactor can be used not only to adjust the reactor to the product but also to be used as a reference for production costs. The results of computational analysis and calculations performed on the reactor design in this study can be used as a reference and can be applied in the design of reactor performance analysis as a learning media, including operating mechanisms in the production process

Keywords: Gold nanoparticles, Reactor design, Batch Reactor, Industrial Scale

1. Introduction

Gold nanoparticles are known to have many uses because of their uniqueness, namely as catalysts [1-3], biosensors [4-5], X-ray imaging [6], drug delivery [7], and bioelectric devices [8]. Thus, various methods have been carried out by researchers to produce gold nanoparticles whose uses are very broad. These methods include biosynthesis using various plant extracts [2, 9–17], the Turkevich method [18-21], chemical reduction [22-23], laser ablation [24-25], sputter deposition [26], sonochemical [27], irradiation-y [28].

The Turkevich method using citric acid is a way to produce gold nanoparticles using a designed reactor. The Turkevich method is a form of synthesis of gold nanoparticles by reduction of HAuCl4 citrate, where this synthesis produces mono dispersion particles from growth mediated by seed particles. The advantage of this method is its high reproducibility [29]. In gold nanoparticle synthesis, the Turkevich method is relatively simple and reproducible for the particles synthesized between 10-30 nm. However, the particles become less spherical, the size distribution becomes wider, and the results are less reproducible for the synthesis of AuNPs above 30 nm in size [30].

Besides that, the type of batch reactor was chosen in the design of this reactor. Batch reactor design has been studied from various perspectives in system optimization tools developed to improve performance. Batch reactor design is not only about equipment design but also operation design. Traditionally, batch reactor designs that consider the effects of mixing have been handled using correlations of all parameters, including mixing time, power draw, and impeller pumping capacity [31].

Several studies have reported the design of batch reactors, namely for the production of vanillin [32], production of volatile fatty acids [33], biohydrogen production [34], biodiesel [35–37], and synthesis of nanoparticles [38-40]. Batch reactor's use shows advantages in cost savings for materials, maintenance, fabrication, and certification. The batch reactor used in this study is also equipped with aids such as stirrers, thermocouples (inserted into the thermowell), nozzles (for various purposes), and pressure gauges [41].

Therefore, this study was conducted to design and analyze the batch reactor design for gold nanoparticle production with the Turkevich method using computational analysis methods for reactor calculations, including stirring and mass balances as initial calculations with the Microsoft Excel application.

2. Research method

2.1. Synthesis of gold nanoparticles with the Turkevich method

The procedure for synthesizing gold nanoparticles on a laboratory scale using the turkevich method has previously been carried out by Dong et al. (2020), where a flow chart of the process is shown in "Figure 1". The gold nanoparticle synthesis was initiated by preparing 50 ml of a 0.25 mM gold chloride ($HAuCl_4$) solution in a flask. Likewise, a 34.0 mM (1.0 wt.%) solution of trisodium citrate (NaCt) was prepared. The flask containing the $HAuCl_4$ solution is heated using a hotplate with constant and robust stirring. Disposable Petri dishes are used to cover the flasks to avoid contamination and solvent evaporation during synthesis. After the HAuCl4 solution reached the boiling point under ambient pressure, a specific volume of NaCt solution was quickly injected into the $HAuCl_4$ solution (1:4). Synthesis is complete when the colour of the suspension no longer changes. Usually, the reaction takes 2-5 minutes. The sample is cooled naturally to room temperature [30].

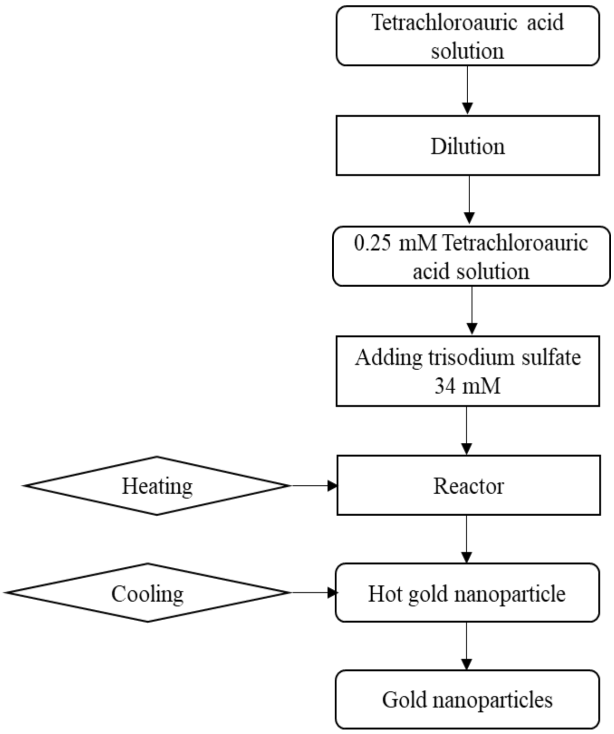

Figure 1. Schematic of the synthesis of gold nanoparticles by the turkevich method.

2.2. Assumptions of reactor and stirrer design specifications

The design specifications for the reactor and stirrer are assumed to be by choosing the material for the reactor, namely, stainless steel SA 240 Grade M Type 316 with an upright cylinder type and a standard dish top cover and a conical bottom cover with a peak angle of 120o, while for the stirrer the material is selected high alloy steel SA 240 Grade M type 316 with four angles 45oC axial turbine type. The complete specification assumptions are shown in "Table 1".

Table 1. Assumptions of reactor and stirrer design specifications

	Specifications	Assumption
Reactor	Type	Upright cylinder with standard dished top cover and conical bottom cover with apex angle of 120°
	Temperature	90°C
	Pressure	1 atm
	Operational time	24 hours
	Material	Stainless steel SA 240 Grade M Type 316
	Allowable voltage	18750
	Corrosion factor	0.0625
	Amount of incoming material	20.585 kg/hour
	Volumetric level	23.3844 ft^3/hour
Stirrer	Type	Axial turbine four corners 45°C
	Impeller material	Material high alloy steel SA 240 Grade M type 316
	Shaft material	Hot Rolled Steel SAE 1020

2.3. Mathematical models in reactor design

Various mathematical models are needed to design a reactor to produce gold nanoparticles, including material volume and reactor design, to determine the dimensions of the reactor and stirrer parameters which are manually calculated using Microsoft Excel. The data processing process is presented in "Table 2".

Table 2. Reactor and stirrer design specification assumptions

	Parameters	Equation
Reactor	Diameter Vessel (Di)	$V_{total} = \frac{\pi di^3}{24 \tan 1/2\alpha} + \frac{\pi di^2}{4} \times Ls + 0{,}0847\ di^3$
	Solution volume in cylinder (Vls)	Vls = V liquid – V top lid
	Solution height in cylinder (L ls)	$L\ ls = \frac{V\ ls}{\left(\frac{\pi}{4}\right) \times di^2}$
	Design pressure (P_i)	$Pi = Patm + Phydrostatic$ $Phydrostatic = \frac{\rho\ (HL - 1)}{144}$
	Cylinder thickness (Ts)	$Ts = \frac{Pi\ di^2}{2(f.E - 0{,}6Pi)} + C$
	Cylinder height (Ls)	$V_{total} = \frac{\pi\ di^3}{24 \tan 1/2\alpha} + \frac{\pi di^2}{4} \times Ls + 0{,}0847\ di^3$
	Top cover thickness (tha)	$tha = \frac{0{,}885 \times Pi.di}{2(f.E - 0{,}1Pi)} + C$
	Top cover height (ha)	ha = 0,169 di
	Bottom cover thickness (thb)	$thb = \frac{Pi.di}{2(f.E - 0{,}6Pi)\cos 1/2\alpha} + C$
	Bottom cover height (hb)	$hb = \frac{1/2\ d}{\tan 1/2\alpha}$
Stirrer	Impeller diameter (Da)	Da = Dt × 0.5 Da = Impeller diameter Dt = Cylinder inner diameter
	Impeller height from the tank bottom (C)	$C = \frac{1}{3} \times Di$

Parameters	Equation
	C = Cylinder inner diameter Di = diameter vessel
Impeller length (L)	$L = 1/4 \times Da$ L = Impeller length Da = Impeller diameter
Impeller width (W)	$W = 0.20 \times Da$ W = Impeller width Da = Impeller diameter
Stirrer number (n)	$n = \frac{H\ liquid}{2 \times Da^5}$ n = Strirrer number Da = Impeller diameter
Reynold number (N_{Re})	$NRe = \frac{L^2 \times n \times \rho}{\mu}$ N_{Re}= Reynold number L = Impeller length n = stirrer rotation, set = 100 rpm = 1,67 rps ρ = density (lb/ft^3)
Power stirring (P)	$P = \frac{\varphi \times \rho \times n^3 \times Di^5}{gc}$ $P_{required} = (0,1 + 0,15)P + P$ P = power stirring ρ = density (lb/ft^3) Di = Impeller diameter gc = 32,2 lb.ft/s^2.lbf
Diameter shaft stirrer	$D = \frac{16 \times T}{\pi \times S}$ D = diameter shaft stirrer T = voltage number (lb.in = $\frac{63025H}{N}$) π = 3.14 S = maximum permissible shear stress
Shaft length (L)	$L = h + l - Zi$ L = Shaft length(ft) h = Cylinder height + Top cover height l = distance between the impeller and the lower tank Zi = Length of shaft above the vessel tank

3. Results and discussion

3.1. Main reaction

The batch reactor for producing gold nanoparticles functions to react hydrogen tetrachloroaurate with citric acid. This reaction is expected to occur in a batch reactor during the production process, where the reduction reaction occurs between $2HAuCl_4$ and $3C_6H_8O_7$ to form 2Au as the main product. The complete reaction that occurs during the production of gold nanoparticles is as follows [18].

$$6HAuCl_4 + Na_3C_6H_5O_7 + 5H_2O \rightarrow 6Au + 6CO_2 + 21HCl + 3NaCl$$

3.2. Reactor type

The reactor is where the reaction process can occur, both in small sizes, such as test tubes and large sizes, such as industrial-scale reactors. Computational analysis in the design of this reactor begins with mass balance calculations. Mass balance calculations are carried out to find out the volume that can enter and leave, with the calculation results shown in “Table 3”.

The results of manual calculations using the Microsoft Excel application for the complete design of the reactor and stirrer are shown in “Tables 3 and 4”, where the results show that the design specifications for the reactor have a reactor volume of 21.7335 ft3, cylinder height of 13.4612 in, the height of solution in the cylinder 8.9046 in, vessel diameter 73.2984 in, design pressure 9.9978 psig, impeller length 9.1840 in, shaft length 10.5418 in, with agitation power of 62.5228 Hp.

The synthesis of gold nanoparticles requires heating to 90°C and then cooling to 25°C. Therefore, the hot and cold fluid that can be used is water. Hot fluid enters at 90°C and leaves at 25°C. Cold liquid enters at 10°C and leaves at 30°C. After the gold nanoparticles are formed, marked with a purplish red colour, the gold nanoparticle production process has been completed and collected in the final product tank.

Therefore, the calculation of batch and stirrer specifications meets the requirements and learning standards for reactor design and operating mechanisms in the production system without calculating the effectiveness factor. The batch reactor design scheme for producing gold nanoparticles is shown in "Figure 2".

Table 3. Calculation results for reactor design specifications

Parameters	Results
Reactor type	Batch reactor
Diameter vessel (Di)	73,2984 in / 6,1082 ft
Volume larutan dalam silinder (Vls)	21,7335 ft^3
Tinggi larutan dalam silinder (L ls)	0,7420 ft / 8,9046 in
Design pressure (P_i)	9,9978 psig
Cylinder thickness (Ts)	73,4722 in
Cylinder height (Ls)	1,1217 ft / 13,4612 in
Top cover thickness (tha)	0,0841 in
Top cover height (ha)	1,0322 ft / 12,3874 in
Bottom cover thickness (thb)	0,1113 in
Botom cover height (hb)	1,7653 ft / 21,1845 in

Table 4. Calculation results for stirrer design specifications

Parameters	Results
Impeller diameter (Da)	3,0613 ft / 36,7361 in
Impeller height from the tank bottom (C)	2,0408 ft / 24,4907 in
Impeller length (L)	0,7653 ft / 9,1840 in
Impeller width (W)	0,6122 ft / 7,3472 in
Stirrer number (n)	0,0033 in / 1 buah
Reynold number (N_{Re})	17266,61
Power stirring (P)	62.5228 Hp
Diameter shaft stirrer	3,5682 in
Shaft length (L)	0,8784 ft /10,5419 in

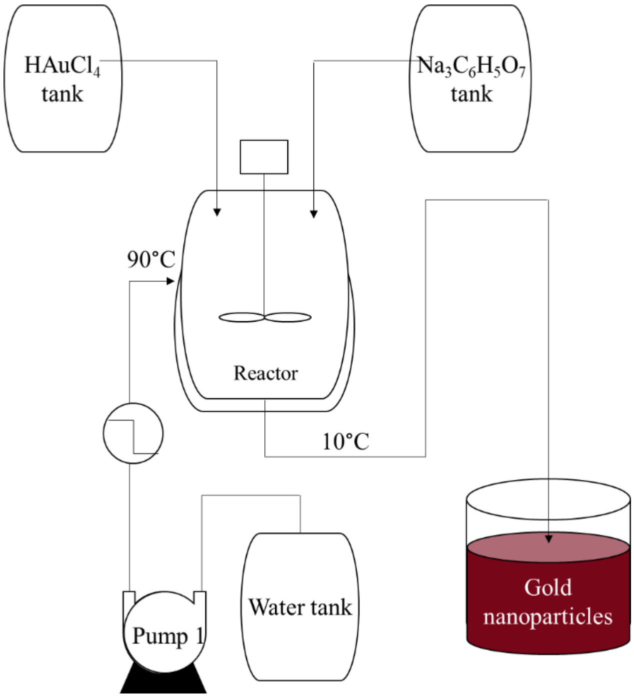

Figure 2. PFD scheme for industrial-scale production of gold nanoparticles

4. Conclusions

Based on computational analysis and reactor design results, a batch-type reactor was selected in this study to produce gold nanoparticles on an industrial scale. The results of manual calculations using the Microsoft Excel application show that the results of the reactor design produce specifications such as reactor volume 21.7335 ft3, cylinder height 13.4612 in, solution height in cylinder 8.9046 in, vessel diameter 73.2984 in, design pressure 9.9978 psig, impeller length 9.1840 in, shaft length 10.5418 in, with agitation power of 62.5228 Hp. The results of calculations and analysis of this reactor design are considered a reference for learning media for the design, calculation, and process mechanism of reactors on an industrial scale.

Declaration of competing interest

The authors declare that they have no known financial or non-financial competing interests in any material discussed in this paper.

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