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Research Article

Design and Mechanical Analysis of a Continuous Stirred Tank Reactor (CSTR) for the Optimum Operation and Production of Propylene Glycol from Propylene Oxide Hydrolysis

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Abstract: This study aimed to optimize the production of propylene glycol by designing a continuous stirred tank reactor (CSTR) and analyzing its wall thickness. The research involved developing a reaction kinetic scheme and mass and energy balance models to determine key reactor functional parameters and account for temperature effects. Simulation results for a yearly production of 400,000 tons of propylene glycol showed that the reactor volume, height, diameter, space-time, space velocity, and heat generation per unit volume at maximum conversion and operating temperature were 62.08 m^3, 6.81 m, 3.41 m, 2,608.70 s, 0.00038 s^{-1}, and -1.30 $J/m^3 \cdot s$, respectively. The relationship between fractional conversion, operating temperature, and reactor functional parameters was presented, while the mechanical design of both the CSTR column and stirrer was considered. The study recommended a thickness specification of 23 mm for an ellipsoidal-shaped column head made from 304-type stainless steel due to its ability to withstand operating conditions. CSTR design and its thickness analysis are crucial for the optimum production of propylene glycol because they ensure the proper mixing of reactants and prevent heat loss during the exothermic reaction. This leads to increased reaction efficiency, higher yields, and improved product quality. Results showed that proper CSTR design and thickness analysis are essential for optimal propylene glycol production for domestic and industrial applications.

***Keywords*:** natural gas, CSTR, propylene glycol, simulation, propylene oxide

1. Introduction

Propylene glycol (PG) is a versatile chemical compound that is widely used in domestic and industrial applications for its unique physical properties.[1] It is a colourless, odourless, and non-toxic liquid that is soluble in water and has a sweet taste, making it a popular ingredient in many consumer products. Here are some of the current domestic and industrial applications of propylene glycol. Domestic Applications of propylene glycol include the Food and Beverage Industry: Propylene glycol is used as a food additive in the manufacture of many products, including soft drinks, baked goods, and salad dressings. It acts as a thickener, stabilizer, and preservative.[2] Cosmetics and Personal Care: Propylene glycol is a common ingredient in many skincare and personal care products such as moisturizers, shampoos, and toothpaste. It is used as a humectant that helps to retain moisture in the skin and hair. Electronic Cigarettes: Propylene

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glycol is a key ingredient in e-cigarettes or vape devices. It is used as a carrier for the nicotine and flavourings that are vaporized and inhaled.[3]

Industrial Application Chemical Industry: Propylene glycol is used as a solvent in the production of various chemicals, including unsaturated polyester resins, paints, and coatings. It is also used as a reactant or intermediate in the synthesis of other chemicals. Pharmaceutical Industry: Propylene glycol is used as a solvent and excipient in the formulation of medicines, vaccines, and cosmetics.[4] It is also used as a carrier for sterile injectable drugs. Heat Transfer Fluids: Propylene glycol is a common heat transfer fluid that is used in refrigeration and air conditioning systems, as well as in industrial heating and cooling applications.

Propylene glycol is a versatile chemical compound that is widely used in domestic and industrial applications. Its unique physical properties make it an attractive ingredient in many consumer products, and its usefulness as a solvent and heat transfer fluid has established it as an essential component of many industrial processes.[5,6]

Every industrial chemical process is designed to produce a desired product with economics and safety in mind.[7,8] In the design of a continuous stirred tank reactor for the production of economically viable petrochemical products like propylene glycol, both uncontrollable cost (*C*ost of raw materials) and controllable cost (*C*ost of production) must be considered extensively because of market competition.[9,10] For efficiency and optimum production process that is, providing the lowest production cost, analysis of alternative flowsheets and consideration of material types and thickness for reactor fabrication becomes highly imperative. The continuous stirred tank reactor design (size specification of the reactor in terms of its volume, diameter, height, space-time and space velocity) can be achieved from the application of the mass and energy balance conservation principle.[11,12] The production of propylene glycol in a CSTR is very important in petrochemical industries because of its wide range of applications and usage in the production of moisturizers in medicines, cosmetics like toothpaste, shampoos, hair-wash, sanitisers, antibacterial lotions for personal care and skin care. They are obtained and accessible as highly purified products.[13]

Several researches have shown that propylene glycol can be produced industrially in a CSTR and thus; Propylene glycol can be produced in an adiabatic CSTR where hydrolysis of propylene oxide occurs in the presence of sulfuric acid as a catalyst. According to the researcher, methanol was introduced during the reaction process to prevent phase-splitting and the reaction rate was described as first-order concerning propylene oxide which means that the reaction is independent of other reactant species. This research considered the development of the reaction kinetic scheme of the process as well as the mass and energy balance model of the process.[14]

Propylene glycol can be produced in a CSTR using a non-isothermal process condition and utilized the principles of mass and energy balance in the development of the transient or dynamic model of the process which was controlled using different controller strategies and highlighted the need for configuration of controllers in the plant for effective and safe operation during the process.[15] Batch manufacture of propylene glycol by excess water hydrolysis of propylene oxide in the presence of a minute concentration of sulfuric acid as catalyst. According to the researchers, the reaction occurs at near ambient temperature but for a batch process, an appreciable rise in temperature is required to overcome the heat of the reaction during the process. Since propylene oxide is more volatile than water, temperature control is required to maintain or keep the reaction process in the liquid phase. The resulting non-ideal reactant mixture was modeled adequately with the NRTL equation and they developed propositions for the manufacture of one batch of propylene oxide.[16,17]

Propylene glycol can be produced from glycol using the method of catalytic hydrogenolysis and a designed pathway involving the reactant feed, pre-treatment step, synthesis and separation process. Here, the feed refers to biodiesel which is a biofuel alternative to petroleum diesel. The biodiesel can be produced through transesterification.[18,19] The pre-treatment step involves treatment of the feed (glycol) to produce technical grade glycol with high purity of (90% to 100%) before it is fed into the reactor where glycol, hydrogen and methanol are mixed and heated between 150 °C to 240 °C at pressure range between 20 atm to 80 atm. The synthesis step is a process technology that is based on the hydrogenolysis of glycol in a packed bed reactor using a copper-based catalyst. The final stage involves the separation of the target product (*P*ropylene glycol) from other by-products such as methanol, acetol, water and other minor alcohol solutions.[20,21] For high-purity propylene glycol production, some procedures allow for additional separation steps. In 1942, Dow Chemical Company stated that commercial production of propylene glycol is by high pressure. High-temperature non-catalytic hydrolysis of propylene oxide. This propylene oxide is manufactured by the chlorohydrin process which involves combining chlorine, propylene and water to form propylene chlorohydrin which then reacts with

an inorganic base yield oxide to form propylene oxide. A large excess of water is used in the conversion of mono-, di-, and tri-propylene glycols of 90% target product and 10% co-products.

Mechanical design of an industrial absorber and regenerator of a Triethylene glycol (TEG) dehydration plant and stated that for effective natural gas dehydration to meet the pipeline specification for processing and transmission of gas, the mechanical design of the basic unit operation such as absorber and regenerator is essential for optimum or safe operation of the plant as it considers the best material type suitable for equipment design, minimum thickness of equipment, corrosion allowance, allowable internal pressure and temperature of the unit, design stress factor and welded joint efficiency.[22,23] The dehydration plant was designed using HYSYS and the mechanical design models of the unit operation (absorber and regenerator) were solved using MATLAB for minimum thickness, determination of the column body (cylindrical shape) and head (torispherical, ellipsoidal and flat-head). The researchers concluded by stating that for economics and optimization, the column body (cylindrical) and head (standard ellipsoidal) are recommended for the safe operation of the plant.

Proactively, in every production and manufacturing process in industries, one major guiding principle is the overall cost of material (cost/kg or cost/m^3) and its properties such as compatibility (resistance to corrosion, rust or stains during the reaction), oxidative resistance, conductivity (ability to allow the passage of heat), thickness, weldability and complexity, fabrication cost, operating cost, etc. all of which constitute the overall cost of production. An expensive material could be feasible if it will reduce the fabrication costs. Mechanical strength is considered the most common requirement.[24]

Generally, metallic materials are considered suitable for reactor fabrication and could be classified as ferrous (wrought iron, plain carbon steels, alloy steels, stainless steels and cast irons), or non-ferrous (aluminum, copper, lead, aluminum bronze and copper-nickel).[25]

For this research, stainless steel will be considered as the material for the mechanical design of the reactor but certain design factors such as design pressure, membrane stresses, design temperature, design stress, welded joint efficiency, corrosion allowance, design loads and minimum practical wall thickness must be considered.

2. Materials and method

To optimize the production of propylene glycol, a continuous stirred tank reactor (CSTR) was designed using MATLAB software. The CSTR was based on a standard cylindrical shape with a flat bottom and ellipsoidal-shaped column head. The CSTR column was made from stainless steel material type 304 and had a capacity of 62.08 m^3. The kinetics of the reaction were studied using a reaction kinetic scheme. The scheme was developed based on previous research. Reaction rate constants and activation energies for each reaction were determined using the arrhenius equation. Mass and energy balance models were developed to determine key reactor functional parameters and account for temperature effects. These models were used to calculate the volume, height, diameter, space-time, space velocity, and heat generation per unit volume for the CSTR. Simulation of the CSTR was carried out using ASPEN Plus software. The simulation was carried out for a yearly production of 400,000 tons of propylene glycol. The mechanical design of the CSTR was considered in this research. The thickness of the ellipsoidal-shaped column head was analyzed using SolidWorks software. The thickness specification was determined based on the operating temperature and pressure of the CSTR.

The procedures adopted in this research are:

i: Development of the reaction kinetic model or rate law of the process.

ii: Development of the mass and energy balance models of the reactor for determination of the reactor functional parameters and temperature effect model of the process.

iii: Mechanical design of the reactor.

iv: Design of the CSTR stirrer.

2.1 *Development of the reaction kinetic model*

Propylene glycol can be produced from the hydrolysis of propylene oxide in the presence of sulfuric acid as a catalyst. The non-isothermal process is shown below.[26,27]

$$C_3H_6O + H_2O \xrightarrow{k_1} C_3H_8O_2 \quad (1)$$

Symbolically, equation (1) can be represented as

$$A + B \xrightarrow{k_1} C \quad (2)$$

where A represents propylene oxide, B is process water, C is propylene glycol and k_1 is the reaction rate constant. It is important to note that in the hydrolysis reaction, sulfuric acid is used as a catalyst and methanol was fed into the reactor to prevent phase-splitting. The rate of reaction is first order concerning the limiting reactant (propylene oxide) and can be expressed as:

$$-r_A = k_o e^{-E/RT} C_{Ao}(1 - x_A) \quad (3)$$

where $-r_A$ is the rate of depletion of propylene oxide in mol/m^3/s, k_o is the pre-exponential or frequency factor in s^{-1} and E is the activation energy in kJ/mol, T is the operating temperature in Kelvin, R is the gas constant in N·m·mol^{-1}·K^{-1}, C_{Ao} is the initial concentration of the limiting reactant in mol/m^3 and x_A is called the fractional conversion ($x_A > 0 < 1$).

Equation (3) is called the rate law or reaction kinetic scheme for propylene glycol production. It is important to note that the rate constant k_1 is related to the pre-exponential or frequency factor by the Arrhenius model given by.

$$k_1 = k_o e^{-E/RT} \quad (4)$$

2.2 *Development of the mass and energy balance models*

The mass and energy balance models can be developed from the first principle of conservation of mass and energy. The mass balance is utilized in the development of the reactor performance or design models while the energy balance model helps to analyze the effect of temperature during the process. The input and output streams of the reactant species and product are shown in the hypothetical CSTR diagram in Figure 1.

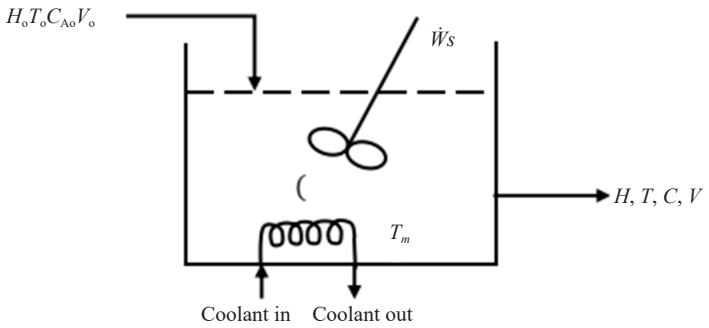

Figure 1. CSTR in steady state operation with heat effect

For the continuous stirred tank reactor above, the following assumptions can be made.
i: The composition of the feed is uniform.
ii: The reactant species is well stirred in the reactor.
iii: The input and output streams have the same composition as the content in the reactor.
iv: The shaft work done by the agitator is negligible.
v: Constant temperature is maintained in the reactor by the heat exchange medium.
The mass balance principle of the reactor can be stated mathematically as[4]

$$\begin{bmatrix}\text{Rate of}\\ \text{accumulation}\\ \text{of mass}\\ \text{within the}\\ \text{reactor}\end{bmatrix}=\begin{bmatrix}\text{Rate of}\\ \text{inflow}\\ \text{of mass}\\ \text{to the}\\ \text{reactor}\end{bmatrix}-\begin{bmatrix}\text{Rate of}\\ \text{outflow}\\ \text{of mass}\\ \text{from the}\\ \text{reactor}\end{bmatrix}-\begin{bmatrix}\text{Rate of}\\ \text{depletion}\\ \text{of mass due}\\ \text{to chemical}\\ \text{reactor}\end{bmatrix} \tag{5}$$

The terms in equation (5) can be defined, substituted and simplified to obtain the reactor functional parameters such as the reactor volume (V_R), height (H_R), diameter (D_R), space-time (τ) and space velocity (S_v) as:

$$V_R = \frac{F_{Ao}x_A}{k_o e^{-E/RT}C_{Ao}(1-x_A)} \tag{6}$$

$$H_R = \left[\frac{16F_{Ao}x_A}{\pi k_o e^{-E/RT}C_{Ao}(1-x_A)}\right]^{\frac{1}{3}} \tag{7}$$

$$D_R = \frac{\left[\frac{16F_{Ao}x_A}{\pi k_o e^{-E/RT}C_{Ao}(1-x_A)}\right]^{\frac{1}{3}}}{2} \tag{8}$$

$$\tau = \frac{x_A}{k_o e^{-E/RT}(1-x_A)} \tag{9}$$

$$S_v = \frac{k_o e^{-E/RT}(1-x_A)}{x_A} \tag{10}$$

The energy balance principle of the reactor can also be stated just like the mass balance.[1]

$$\begin{bmatrix}\text{Rate of}\\ \text{accumulation}\\ \text{of energy}\\ \text{within the}\\ \text{reactor}\end{bmatrix}=\begin{bmatrix}\text{Rate of}\\ \text{input of}\\ \text{energy}\\ \text{to the}\\ \text{reactor}\end{bmatrix}-\begin{bmatrix}\text{Rate of}\\ \text{output of}\\ \text{energy}\\ \text{from the}\\ \text{reactor}\end{bmatrix}-\begin{bmatrix}\text{Rate of}\\ \text{energy}\\ \text{removal}\\ \text{to the}\\ \text{surrounding}\end{bmatrix}+\begin{bmatrix}\text{Shaft}\\ \text{work}\\ \text{done}\\ \text{by the}\\ \text{stirrer}\end{bmatrix} \tag{11}$$

Assuming that the system operates at a steady state with constant density and neglecting the shaft work done by the stirrer. The terms in equation (11) can be defined, substituted and simplified into equation (12), where *UA*c is the Heat transfer Coefficient (Kg/m^{2}S0C).

$$T = \frac{\tau_{CSTR}\Delta H_R r_A v_o + UA_C T_C + \rho v_o c_p T_o}{\rho v_o c_p + UA_C} \tag{12}$$

The quantity of heat generated per unit volume of the reactor is given as:

$$\frac{Q}{V_R} = \frac{\Delta H_R F_{Ao}x_A}{V_R} \tag{13}$$

$$q = \frac{\Delta H_R F_{Ao} x_A}{V_R} \tag{14}$$

2.3 *Mechanical design of the reactor*

In the mechanical design of process equipment (CSTR), certain properties such as material for construction, design pressure, membrane stresses, design temperature, design stress, welded joint efficiency, corrosion allowance, design loads and minimum practical wall thickness must be considered.[28]

2.4 *Material for construction*

For this research, the stainless steel grade (304) is considered as the material for the CSTR construction and fabrication. This is because the reactant species such as sulfuric acid, methanol, water and propylene oxide are capable of corroding the reaction media (reactor) during the reaction process. The material grade (304) is recommended specifically because it contains the minimum amount of chromium, Cr (18%) and Nickel Ni (8%) that gives a stable austenitic structure and good welding characteristics that do not require post-weld annealing when welding thin sections. Table 1 and 2 shows the chemical and mechanical composition of the stainless-steel grade (304) type.[29]

Table 1. Chemical composition of stainless-steel grade (304)[29]

Element	C	Si	Mn	P	Cr	Ni	Nb	Cu	Co	N
% Composition	0.020	0.32	1.57	0.38	18.30	8.1	0.008	0.38	0.20	0.016

Table 2. Mechanical properties of stainless-steel grade (304)[29]

	Mechanical properties		Elongation after fracture (A%)	
	Yield stress (MPa)	Tensile strength (MPa)	A_5 (%)	50 mm (%)
Minimum	230	450	45	40
Maximum	330	580	NA	NA

2.5 *Design pressure*

The continuous stirred tank reactor must be designed to withstand the maximum pressure it will be subjected to during operation. The design pressure of the reactor must be 5 to 10% greater than the operating pressure to prevent spurious actions during minor process upsets. The hydrostatic pressure of the reactor base should be added to the operating pressure to constitute the design pressure.[30]

2.6 *Membrane stresses*

The membrane stresses in shells of revolution which constitute the thickness of reactor walls (cylindrical and conical) and heads (hemispherical, ellipsoidal and torispherical) must be considered to mitigate the effect of external and internal loads during operation.

2.7 *Design temperature*

The increase in temperature (heat) during a process decreases the strength of metallic reactor media. Based on this fact, the maximum allowable design stress is usually a function of the material temperature. This implies that the

temperature of the material (stainless steel) should be taken as the maximum operating temperature of the process with due allowance to curb or mitigate any uncertainties.

2.8 *Design stress*

The design stress is also called the normal design strength and it refers to the maximum allowable stress the reactor will be subjected to. The application of a suitable design stress factor under standard operation conditions is a tool for the determination of the design stress. The effect of loading, quality of materials, uncertainty of design methods and workmanship are controlled by the design stress factor some common materials and their typical stress values are shown in Table 3.

Table 3. Design stress factors at different temperatures[1]

Material	Tensile strength (N/mm^2)	Design stress at temperature °C (N/mm^2)									
		0 to 50	100	150	200	250	300	350	400	450	500
Carbon Steel (Semi-killed or silicon killed)	360	135	125	115	105	95	85	80	70	-	-
Carbon-Manganese Steel (Semi-killed or silicon killed)	460	180	170	150	140	130	115	105	100	-	-
Carbon-molybdenum Steel 0.5% Mo	450	180	170	145	140	130	120	110	110	-	-
Low alloy steel (Ni, Cr, Mo, V)	550	240	240	240	240	240	235	230	220	190	170
Stainless Steel 18Cr/8Ni Unstabilised (304)	510	165	145	130	115	110	105	100	100	95	90
Stainless Steel 18Cr/18Ni Ti Stabilized (321)	540	165	150	140	135	130	130	125	120	120	115
Stainless Steel 18Cr/8Ni Mo $2\frac{1}{2}$% (316)	520	175	150	135	120	115	110	105	105	100	95

2.9 *Welded joint efficiency*

Different types of joints abound and the strength of welded joint is a function of the type of joint used as well as the quality of welding. The quality of welds can be checked by visual inspection and radiography. The butt joint is usually recommended. The welded joint efficiencies are allowed under ASME BPV code Sec. VIII D1 is shown in Table 4.

Table 4. Welded joint efficiencies allowed under ASME BPV Code Sec. VIII D.1[6]

Joint description	Joint category	Degree of radiographic examination		
		Full	Spot	None
Double-welded butt joint or equivalent	A, B, C, D	1.00	0.85	0.70
Single-welded butt joint with backing strip	A, B, C, D	0.90	0.80	0.65
Single-welded butt joint without backing strip	A, B, C	NA	NA	0.60
Double full fillet lap joint	A, B, C	NA	NA	0.55
Single full fillet lap joint with plug welds	B, C	NA	NA	0.50
Single full fillet lap joint with plug welds	A, B	NA	NA	0.45

2.10 *Corrosion allowance*

The determination of corrosion allowance is very difficult but an accurate corrosion allowance can be obtained by judging from experiences of the same or similar process operation or condition. For the CSTR fabrication with stainless steel material type (304), a corrosion allowance of 4.0 mm is recommended.[6]

2.11 *Load design*

The continuous stirred tank reactor must be designed strong enough to withstand or resist deformation from both internal and external loads. Design loads could be classified as major or subsidiary loads. The major loads are design pressures (including any significant static load), maximum vessel weight and reactant species in it, wind loads, seismic (earthquake) loads, etc. While the subsidiary loads include the local stresses caused by supports, connecting pipes and internal structures, shock loads, bending moments due to eccentricity of the centre of the working pressure relative to the neutral axis of the reactor, stresses due to temperature variations and changes in materials coefficient of expansion and loads resulting from pressure and temperature swings or fluctuations.

2.12 *Minimum practical wall thickness*

For the continuous stirred tank reactor, a minimum thickness is recommended to enhance its rigidity to withstand its weight and any external loads associated with it. Generally, the thickness of reacting vessels is a function of its diameter and must include a corrosion allowance of 2 mm.[8]

The standard for reactor wall thickness is presented in Table 5 below.

Table 5. Minimum practical wall thickness

Reactor diameter (m)	Minimum thickness (mm)
1	5
1 to 2	7
2 to 2.5	9
2.5 to 3.0	10
3.0 to 3.5	12

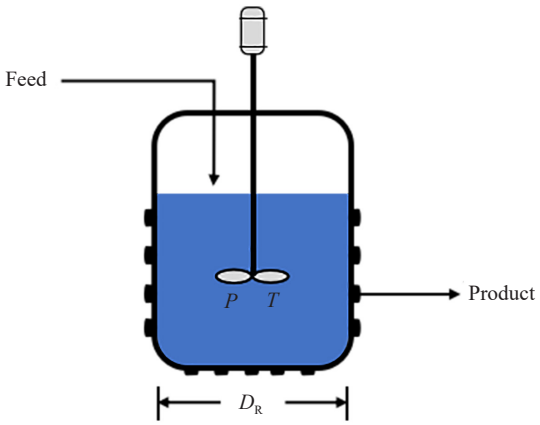

Figure 2. Mechanical design of the CSTR

Consider the mechanical design schematics of the continuous stirred tank reactor in Figure 2.

In Figure 2 above, P represents the operating pressure of the reactor in bar, T is the operating temperature of the reactor in ℃ and D_R is the diameter of the reactor in meters. The thickness (e) of the reactor body (cylindrical) and head (tori spherical, ellipsoidal and flat head) is given as.

2.13 *Reactor column body (cylindrical)*

$$e = \frac{P_i D_i}{2JF - P_i} \tag{15}$$

where e is the minimum thickness of the reactor in (mm), P_i is the design pressure in N/mm^2, D_i is the diameter of the reactor in meters, J is the welded joint efficiency and F is the design stress.

2.14 *Reactor column head (tori spherical)*

$$e = \frac{P_i R_i C_s}{2JF - P_i\left(C_s - 2\right)} \tag{16}$$

where R_i is equivalent to the diameter of the reactor, C_s is called the stress concentration factor, R_K is Knuckle radius (m) and R_x is Crown radius it is expressed mathematically as

$$C_s = \frac{1}{4}\left[3 + \sqrt{\frac{R_i}{R_k}}\right] \tag{17}$$

2.15 *Reactor column head (standard ellipsoidal)*

$$e = \frac{P_i D_i}{2JF - 0.2P_i} \tag{18}$$

2.16 *Reactor column head (flat)*

$$e = C_p D_c \sqrt{\frac{P_i}{F}} \tag{19}$$

where C_p is usually given as 0.4 for full face gasket and D_c is the bolt circle diameter in (mm).

The total thickness of the reactor's body and heads as shown in equation (15), (16), (18) and (19) is given as

$$\text{Thickness } (t) = e + \text{corrosion allowance.} \tag{20}$$

2.17 *CSTR stirrer design*

Usually, a clearance is allowed between the stirrer blade and the reactor side. The length and diameter of the stirrer are given mathematically as:

$$L_{st} = H_R - C \tag{21}$$

where L_{st} is the length of the stirrer in meters, H_R is the reactor height in meters and C is called the clearance.

$$D_{st} = D_R - 2C \quad (21)$$

where D_{st} is the diameter of the stirrer, and D_R is the diameter of the reactor.

2.18 *Data for evaluation*

The data for simulating the design models are given in Table 6. The data above was used in the MATLAB simulation of the developed performance or design models of the CSTR.

Table 6. Data for evaluation

Data	Values	Description	References
V_o	0.0238 m^3/s	Initial volumetric flow rate of reactants	3
C_{Ao}	0.0424 mol/m^3	The initial concentration of the limiting reactant	3
F_{Ao}	0.001009 mol/s	The initial flow rate of limiting reactants	3
x_A	0.9 (Dimensionless)	Fractional conversion	3
ΔH_R	-84,666 J/mol	Change in enthalpy of reaction	3
ΔC_p	-29 J/molK	Change in specific heat capacity	3
T_o	287.44 K	The initial temperature of the feed	4
K_o	4.71109 s^{-1}	Frequency factor	4
E	75.362 kJ/mol	Activation energy	4
T	324.7 K	Reactor operating temperature	4
T_D	51.67 °C	Reactor design temperature	8
P	21.67 bar	Reactor design pressure	8
C_s	1.77 (dimensionless)	Stress concentration	1
F	165 N/mm^2	Stress Factor	1
J	1 (dimensionless)	Welded Joint-efficiency	1

3. Results and discussion

The results of the continuous stirred tank reactor size specification and mechanical design are presented in the profiles and tables below.

Figure 3 shows a profile of reactor volume, height and diameter versus fractional conversion. According to the plot, the reactor functional parameters or size specification in terms of volume, height and diameter increases exponentially as the fractional conversion increases. This implies that the reactor design (size specification) is dependent on the ratio of the amount of feed reactant (propylene oxide and water) introduced into the reactor and the amount of feed reacted. At the fractional conversion of 0.9, the reactor volume, height and diameter for optimum production of propylene glycol are 62.08 m^3, 6.81 m and 3.41 m respectively.

The reactor volume, height, and diameter all have an impact on the fractional conversion of a chemical reaction. The reactor volume determines the number of reactants that can be processed at once. A larger reactor volume provides more space for the reactants to react, allowing for a higher conversion rate as there are more opportunities for the reactants to react with each other. However, this can also lead to longer reaction times and decreased selectivity, as there may be more side reactions occurring. The reactor height impacts the concentration gradients within the reactor. A taller reactor can maintain a more even concentration gradient by allowing more time for the reactants to mix and react as they

move through the reactor. As a result, a greater conversion rate can be achieved. However, taller reactors can also result in longer reaction times, increased pressure drop, and greater heat and mass transfer limitations. The reactor diameter influences the balance between the surface area and the volume of the reactor. A wider reactor allows for greater surface area and more efficient heat and mass transfer, which can lead to higher conversion rates. However, wider reactors can also lead to larger gradients in concentration and temperature, as well as a higher pressure drop. The selection of reactor volume, height, and diameter should be based on a careful evaluation of the desired reaction conditions and the specific characteristics of the reaction.

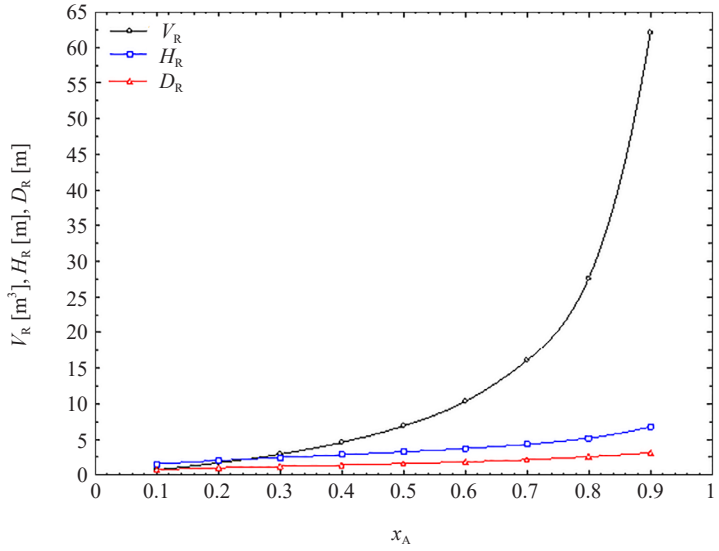

Figure 3. Profile of reactor volume, height and diameter versus fractional conversion

Figure 4 is a profile of space-time (τ) and fractional conversion (x_A). The profile shows an exponential increase in the space-time as the fractional conversion increases. This means that higher fractional conversion will require more time for the reactant or feed (propylene oxide and water) to be processed for the formation of the target product (propylene glycol). At the minimum and maximum factional conversion of 0.1 and 0.9, the space-time as indicated in the profile are 32.21 seconds and 2,608.70 seconds respectively.

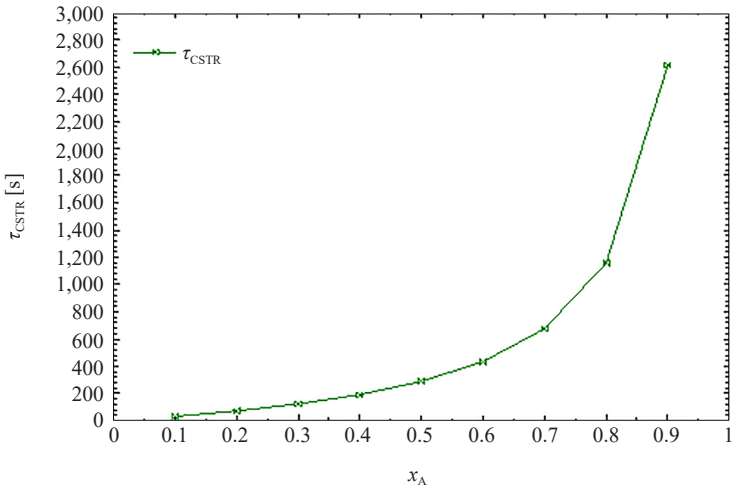

Figure 4. Profile of spacetime versus fractional conversion

Figure 5 is a plot of space velocity (reciprocal of space-time) and fractional conversion. The profile shows that there is an inverse exponential decrease in space velocity as the space-time increases. This can be justified by the mathematical relationship between space-time and space velocity. The fractional conversion of 0.1 and 0.9 corresponds to space velocities of 0.03110 sec^{-1} and 0.00038 sec^{-1} respectively.

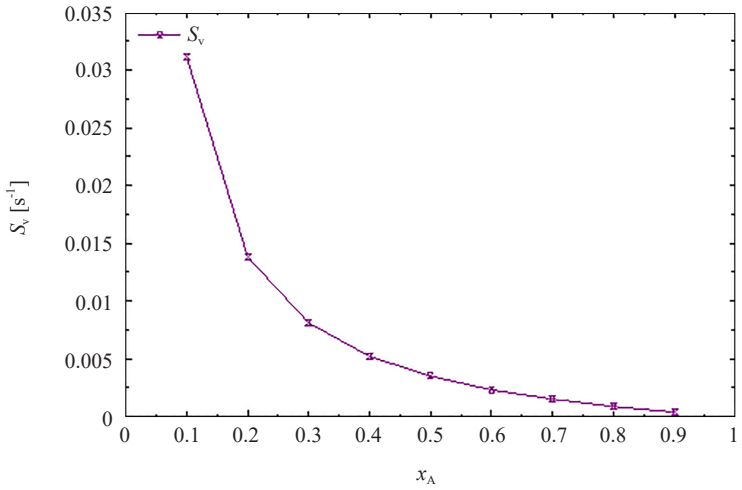

Figure 5. Profile of space velocity versus fractional conversion

Figure 6 is a relationship between the quantity of heat generated per unit volume of the reactor (q) and the fractional conversion. According to the graph, the quantity of the heat generated per unit volume of the reactor increases sinusoidally as the fractional conversion increases during propylene glycol production in a CSTR. At the fractional conversion of 0.1 and 0.9, the quantity of heat generated per unit volume of the reactor is -105.62 J/m^3 s and -1.30 J/m^3 s respectively which also indicates that the reaction occurs under non-isothermal conditions.

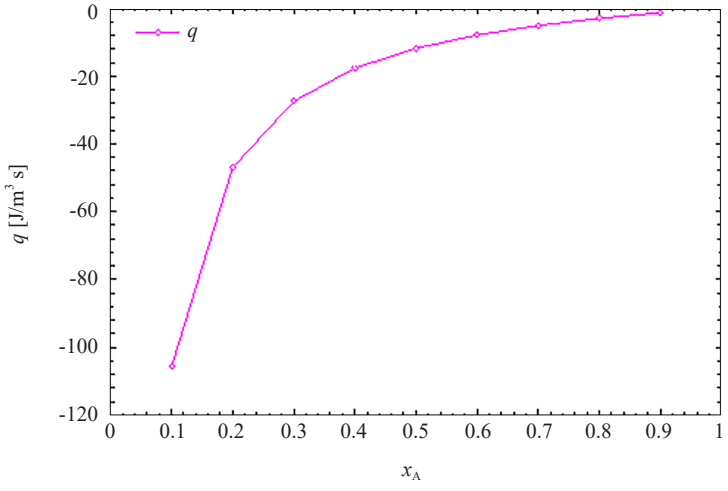

Figure 6. Profile of quantity of heat generated per unit volume of the reactor versus fractional conversion

Figure 7 shows a graphical relationship between the CSTR performance parameters such as its volume, height and diameter and the effect of its operating temperature during propylene glycol production from hydrolysis of propylene oxide. The plot clearly shows that an increase in operating temperature within the specific range for optimum production

of propylene glycol results in a corresponding increase in reactor volume, height and diameter. At an operating temperature of 287.43 K, propylene glycol can be produced optimally at CSTR specifications of 62.08 m^3, 6.81 m and 3.41 m for volume, height and diameter respectively.

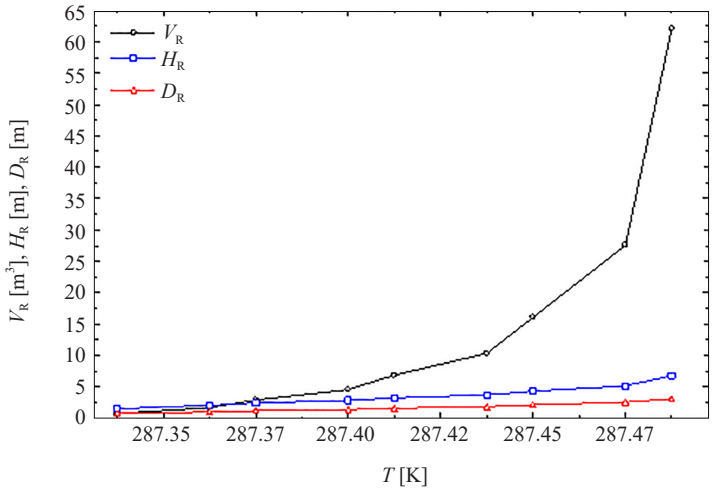

Figure 7. Profile of reactor volume, height and diameter versus temperature

Figure 8 shows an exponential increase relationship between the space-time and CSTR operating temperature. For temperature variation within the specification range of propylene glycol production from hydrolysis of propylene oxide, say 287.31 K, 287.37 K and 287.43 K, the corresponding space-time are 32.21 seconds, 289.86 seconds and 2,608.70 seconds respectively.

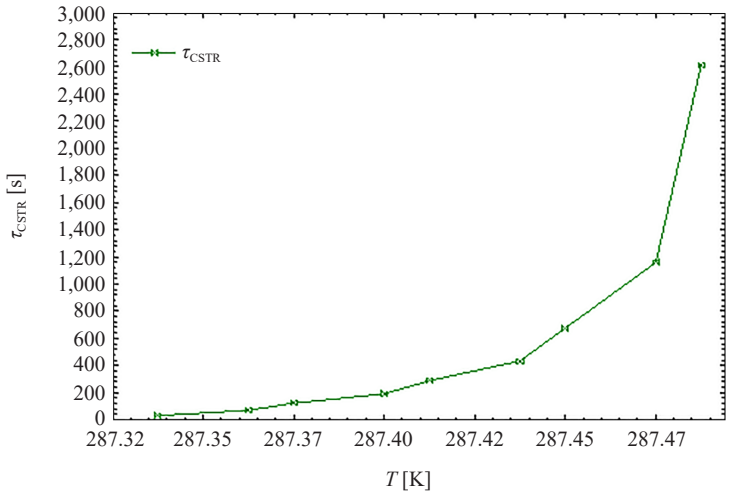

Figure 8. Profile of spacetime versus temperature

Figure 9 is a graph of space velocity and fluctuation in operating temperature within its specific range recommended for propylene glycol production from hydrolysis of propylene oxide in CSTR. From the plot, the space-time increases exponentially as the temperature increases. The minimum and maximum value of space-time, 32.21 seconds and 2,608.70 seconds occurs at operating temperatures of 287.31 K and 287.43 respectively.

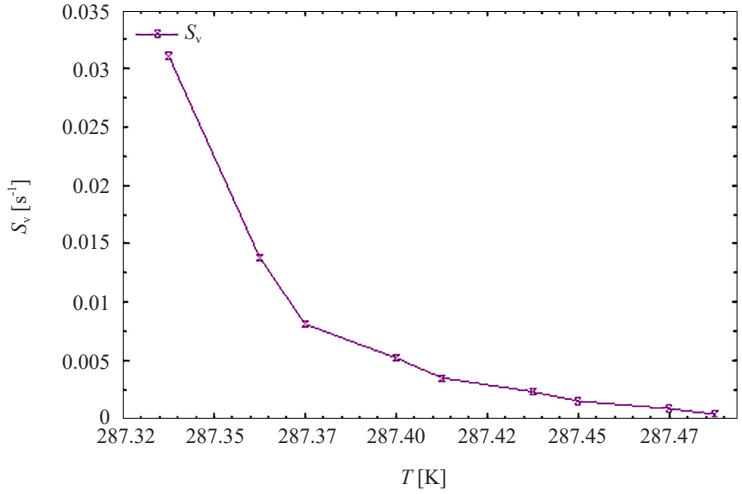

Figure 9. profile of space velocity versus temperature

Figure 10 shows that the quantity of heat generated per unit volume of the reactor during propylene glycol production from the hydrolysis of propylene oxide increases sinusoidally as the operating temperature increases within its specified recommended range. At higher temperatures above the maximum operating temperature limit, the space velocity tends towards negative infinity. However, at a minimum and maximum operating temperatures of 287.31 K and 287.43 K, the quantity of heat generated per unit volume of the reactor is -105.62 J/m^3 s and -1.30 J/m^3 s respectively.

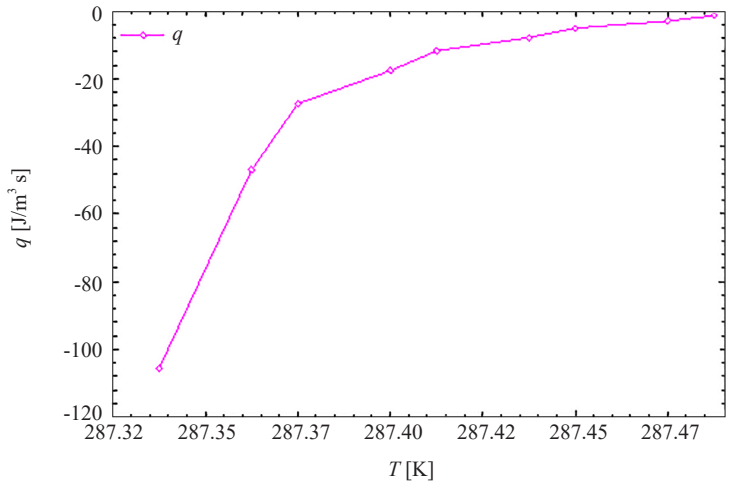

Figure 10. Profile of quantity of heat generated per unit volume of the reactor versus temperature

Table 7 shows the design results or size specification of the continuously stirred tank reactor functional parameters such as its volume, height, diameter, space-time, space velocity and the quantity of heat generated per unit volume of the reactor. Analysis of the results presented shows that an increase in fractional conversion and temperature of the reactants or feed increases the reactor volume, height, diameter, space-time and quantity of heat generated per unit volume of the reactor which is an indication of an increase in the yield of propylene glycol (product of interest). At maximum fraction, al conversion of 0.9, the reactor volume, height, diameter, space-time, space velocity and quantity of heat generated per unit volume of the reactor are 62.08 m^3, 6.81 m, 3.41 m, 2,608.70 sec., 0.00038 s^{-1} and -1.30 J/m^3 s respectively which represents the design specification for optimum production of propylene glycol (target product) yearly.

Table 7. MATLAB results of CSTR design showing fractional conversion, temperature, volume of reactor, height of reactor, diameter of reactor, space time, space velocity and quantity of heat generated per unit volume of the reactor

x_A	T (K)	V_R (m^3)	H_R (m)	D_R (m)	τ_{CSTR} (s)	S_V (s^{-1})	q (J/m^3 s)
0.10	287.31	0.77	1.57	0.79	32.21	0.03110	-105.62
0.20	287.33	1.72	2.06	1.03	72.46	0.01380	-46.95
0.30	287.34	2.96	2.47	1.24	124.22	0.00810	-27.39
0.40	287.36	4.60	2.86	1.42	193.24	0.00520	-17.61
0.50	287.37	6.90	3.28	1.64	289.86	0.00350	-11.74
0.60	287.39	10.35	3.75	1.88	434.78	0.00230	-7.83
0.70	287.40	16.09	4.34	2.17	676.33	0.00150	-5.03
0.80	287.42	27.59	5.20	2.60	1,159.42	0.00086	-2.93
0.90	287.43	62.08	6.81	3.14	2,608.70	0.00038	-1.30

Table 8 shows the mechanical design of the continuously stirred tank reactor for thickness determination of the reactor body (cylindrical shape) and head (torispherical, ellipsoidal and flat shape). The thickness of the reactor depends on the material type and column or reactor diameter. For economics, the reactor body of cylindrical shape with a thickness of 24 mm and the doomed head of ellipsoidal shape with a thickness of 23 mm is recommended for stainless steel type (304) material of construction or reactor fabrication. This is because, the material type and thickness of the reactor body and head are capable of withstanding the operating temperature, pressure, stress and any internal or external load that may occur during operation.

Table 8. Mechanical design of results of the CSTR

CSTR Design	Thickness (mm)
Colum body	-
Cylindrical	24
Column head doomed	-
Torispherical	14
Ellipsoidal	23
Flat	156

Table 9 shows the design or size specification of the continuous stirred tank reactor stirrer at the optimum value of the reactor height and diameter. The specification of the CSTR stirrer height and diameter (6.31 m and 2.41 m) respectively shows the values are less than the height and diameter of the reactor as a result of the recommended allowances as stated in the design models.

Table 9. Design of CSTR stirrer

CSTR stirrer design	Value (m)
Height of stirrer	6.31
Diameter of stirrer	2.41

4. Conclusion

This research aimed to optimize the production of propylene glycol by designing a continuous stirred tank reactor and analyzing its thickness. The study showed that the mechanical design of the CSTR was crucial for optimal propylene glycol production. The simulation results provided valuable information on the optimal reactor functional parameters required for efficient propylene glycol production. The recommended thickness specification of 23 mm for the ellipsoidal-shaped column head made from stainless steel material type 304 will ensure the CSTR can withstand the operating conditions. This research provides fundamental knowledge for the design and optimization of propylene glycol production for domestic and industrial applications. The design and mechanical analysis of a CSTR can significantly enhance the efficiency and production of propylene glycol from propylene oxide hydrolysis. The optimization of critical parameters such as temperature, pressure, and residence time can extend product yield and minimize undesirable side reactions. The successful implementation of a well-designed and optimized CSTR for the production of propylene glycol can have significant economic and environmental impacts, as it can reduce the reliance on petroleum-based products, and promote sustainability and green chemistry practices. Further research and development are still needed to improve the process efficiency and sustainability and enable the scale-up of the technology. The current achievement of designing a CSTR for the optimum production of propylene glycol from propylene oxide hydrolysis is a promising development in the field of chemical engineering.

Authors contributions

WOC, EME, and OFU: Conceptualization, methodology, original draft preparation, performed experimental work, and writing.

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Conflict of interest

The authors declare no competing financial interest.

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