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Application of Mechanistic Design Model for Sustainable and Effective CSTR Operation during Titanium Dioxide Production

Wosu Chimene Omeke
Department of Chemical Engineering,
Federal University Otuoke, Bayelsa State, Nigeria
Correspondence: wosuco@fuotuoke.edu.ng

Abstract

This study optimizes the production of titanium dioxide, a crucial material in various industries, through hydrolysis of titanium tetrachloride in a continuous stirred tank reactor (CSTR). Using mathematical modelling and MATLAB simulation, the research determines the ideal CSTR design specifications and reactor thickness to ensure efficient, sustainable, and corrosion-resistant operation which improves the lifespan of the reaction media. The CSTR design models were developed from the first principle of mass and energy balance and simulated using MATLAB R2023a version to obtain the CSTR design specification and the relationship between the fractional conversion of the feed materials and the functional parameters of the reactor. At a maximum fractional conversion of 0.9, the CSTR volume, height, diameter, space-time, space velocity, the quantity of heat generated as well as the quantity of heat generated per unit volume of the reactor were obtained as 26.6884m^3, 5.1416m, 2.5708m, 4.1021sec., 0.2438sec^{-1}., 806.7600J/s, and 30.2288J/m^{3}s respectively. The mechanistic design model showed that a thickness of 6.500mm for the reactor body (cylindrical) and head (standard ellipsoidal) is specifically recommended for stainless steel type (304) for construction. Also, the design of the CSTR agitator height and diameter were obtained as 4.6416m and 1.5708m respectively. This article showed that the design and thickness specification of the CSTR is crucial for optimum, continuous and sustainability of titanium dioxide production.

Keywords: ***CSTR, Thickness Design, Titanium Dioxide, Hydrolysis Reaction, MATLAB.***

Introduction:

The production of Titanium dioxide is of high significant interest in process industries because of its distinguishing feature as an economically viable or cheap product and its capability of withstanding strong chemical corrosion as well as its utilization in the production of optical materials (Khan *et al*, 2015; Fares *et al*., 2022). Research in the past and recent past showed that Titanium dioxide also plays a vital role in industries such as Metallurgical industries, polymer industries, paint industries, plastic industries, ceramic pharmaceutical industries and cosmetics industries in the production of economic and valuable products for both domestic and industrial applications (Zhang et al, 2011; Agustina *et al*., 2024; Agustina *et al*., 2021; Prasetya *et al*., 2022).

Based on the economic versatility of titanium dioxide, this article is focused on the application of the mechanistic design models of the continuous stirred tank reactor (CSTR) specially designed for the production of titanium dioxide from the hydrolysis of titanium tetrachloride. Here, titanium tetrachloride reacts with water in the CSTR to produce titanium dioxide (target product) and hydrochloride acid. The reaction rate is said to be first-order concerning titanium tetrachloride and zero-order concerning water.
The selection or preference of the CSTR over other reactor types is because of its configuration and ability to perfectly handle liquid phase (hydrolysis) reactions with a high level of conversion or yield of the target or product of interest (Wordu & Wosu, 2019; Rudnick & Gao, 2003).

Significant research has been carried out on the production and extraction of titanium dioxide using various methods such as lactobacillus Bulgaricus (Agustina *et al*., 2024), application of titanium ore as a field material for titanium dioxide pigment and titanium metal production (Gazquez *et al*.,2014). Barksdale in 1966 stated that titanium dioxide can be extracted naturally from ilmenite which constitutes FeO. $T_i\,O_2$ or T_i

Fe O_3 with $T_i O_2$ composition of 40% - 65% as well as the ferrous and ferric iron oxides with impurities such as silicon, calcium, aluminium, magnesium, vanadium, manganese, chromium all of which depend on their geological structure. In 2011, Gambogi stated that ilmenite is mostly produced in countries such as South Africa, Australia, Canada, China, India, Vietnam, Norway and Ukraine with a Production rate within the range of 0.20 metric tons to 1.05 metric tons. Research forecasts have shown that both ilmonite and rutile are major titanium dioxide reserves with a prognosis of 650,000,000 metric tons and 42,000,000 metric tons respectively (Gamboji, 2010; Gamboji, 2009). This titanium dioxide also occurs naturally from plant, animal and water sources (Knittle, 1983).

Based on past research on titanium dioxide production, it is obvious that much effort has not been made into the design of reactors where titanium tetrachloride hydrolysis occurs for titanium dioxide production as well as the thickness consideration of the reaction media for equipment lifespan improvement and sustainability. It is on this fact that the intrinsic urge for this research becomes highly imperative for effective, efficient and optimum production of titanium dioxide.

Materials and Methods

This study utilized or employed a quantitative and analytical approach, leveraging derived data and literature sources. The research methodology consists of:

i. Rate law development
ii. The CSTR design model development
iii. Design of the CSTR agitator
iv. Application of the CSTR mechanistic models

Rate Law Development

The reaction chemistry or stoichiometry for the liquid phase hydrolysis of titanium tetrachloride is given as;

$$TiCl_4 + 2H_2O \xrightarrow{k_1} TiO_2 + 4HCl \quad (1)$$

Equation (1) can be expressed symbolically as:

$$A + 2B \xrightarrow{k_1} C + 4D \quad (2)$$

The reaction rate is 1st-order concerning titanium tetrachloride and zero-order concerning water and thus, the depleting rate of the reaction kinetics is given as;

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

CSTR Design Model Development

Consider the schematic representation of a continuous stirred tank reactor with feed stream, product stream and heat effects.

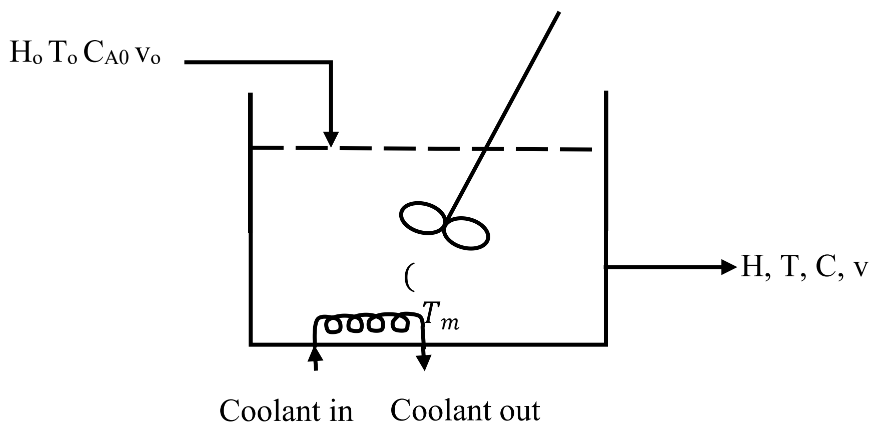

Figure 1: CSTR with Mass and Heat Effects for Titanium Dioxide Production

For the CSTR, the following assumptions can be made.

i. The feed assumes a uniform composition throughout the reactor
ii. The reacting mixture is well-stirred
iii. The composition of the exit stream is the same as that within the reactor
iv. Shaft work by the impeller or stirrer is negligible
v. The temperature within the reactor is kept at a constant value by the heat exchange medium

The CSTR design parameters can be obtained by applying the principle of material balance stated as follows

$$\begin{bmatrix}\text{Rate of}\\ \text{accumulation}\\ \text{of material}\\ \text{within the}\\ \text{volume}\end{bmatrix} = \begin{bmatrix}\text{Rate of}\\ \text{input of}\\ \text{feed into}\\ \text{the volume}\end{bmatrix} - \begin{bmatrix}\text{Rate of}\\ \text{outflow of}\\ \text{feed from}\\ \text{the volume}\end{bmatrix} - \begin{bmatrix}\text{Rate of}\\ \text{depletion of}\\ \text{feed due to}\\ \text{chemical}\\ \text{reaction}\end{bmatrix} \quad (4)$$

The terms in equation (4) can be defined, substituted, and simplified at steady state to give the CSTR functional parameters thus;

$$V_R = \frac{F_{Ao}x_A}{k_o e^{-E/RT} C_{Ao}(1-x_A)} \quad (5)$$

$$H_R = \left[\frac{16F_{Ao}x_A}{\pi K_o e^{-E/RT} C_{Ao}{}^3 (1-x_A)(m-2x_A)^2}\right]^{\frac{1}{3}} \quad (6)$$

$$D_R = \frac{\left[\frac{16F_{Ao}x_A}{\pi k_o e^{-E/RT} C_{Ao}(1-x_A)}\right]^{\frac{1}{3}}}{2} \quad (7)$$

But; $F_{Ao} = C_{Ao}v_o$

$$\tau_{CSTR} = \frac{x_A}{k_o e^{-E/RT} C_{Ao}(1-x_A)} \quad (8)$$

$$S_V = \frac{k_o e^{-E/RT} C_{Ao}(1-x_A)}{x_A} \quad (9)$$

$$Q = \Delta H_R F_{Ao} x_A \quad (10)$$

$$q = \frac{\Delta H_R F_{Ao} x_A}{V_R} \quad (11)$$

The energy balance of the CSTR in Figure 1 can be obtained by applying the principles of conservation of energy and the resultant model is the temperature effect model of the alkylation process.

$$\begin{bmatrix}\text{Rate of}\\ \text{accumulation}\\ \text{of heat}\\ \text{within the}\\ \text{volume}\end{bmatrix} = \begin{bmatrix}\text{Rate of}\\ \text{Input of}\\ \text{heat to}\\ \text{the volume}\end{bmatrix} - \begin{bmatrix}\text{Rate of}\\ \text{Output of}\\ \text{heat from}\\ \text{the volume}\end{bmatrix} - \begin{bmatrix}\text{Rate of}\\ \text{depletion}\\ \text{of heat due}\\ \text{to chemical}\\ \text{reaction}\end{bmatrix} - \begin{bmatrix}\text{Rate of}\\ \text{heat}\\ \text{removal}\\ \text{to the}\\ \text{surrounding}\end{bmatrix} + \begin{bmatrix}\text{Shaft}\\ \text{work}\\ \text{done by}\\ \text{the stirrer}\end{bmatrix} \quad (11)$$

The terms in equation (11) can be defined, substituted, and simplified at steady state to give the temperature effect model thus;

$$T = \frac{\tau \Delta H_R r_i v_o + UA_c T_c + \rho v_o c_p T_o}{\rho v_o C_p + UA_c} \quad (12)$$

Design of CSTR Agitator

The CSTR stirrer design is done by allowing a clearance C between the stirrer height (H_{ST}) and diameter (D_{ST}) (Perry *et al*., 2008)

$$H_{st} = H_R - C \quad (13)$$

$$D_{st} = D_R - 2C \quad (14)$$

CSTR Mechanistic Model

The mechanistic model of the CSTR is applied for the determination of the reactor or column body and head thickness. The thickness design consideration of equipment most importantly reaction medium is of great importance in engineering practice since the lifespan of process equipment solely depends on it. In process industries, the major problem facing process equipment is the effect of corrosion and the impact of external or internal stresses equipment experiences during operation or shutdown. (Sinnott & Towler, 2009; Wosu *et al*., 2024a; Wosu *et al*., 2024b). To improve the continuous production of titanium dioxide ensure sustainability and improve the lifespan of the reaction media (CSTR), certain factors such as material for construction, the effect of pressure, the effect of temperature, membrane and design stresses, efficiency of welded join, corrosion, load and minimum practical wall thickness are crucial and must be taken into serious consideration.

CSTR Fabrication Material

For this research, the stainless steel (304) grade is utilized as the fabrication material of the CSTR for effective operation and optimum product on titanium dioxide. This material grade ideally constitutes 8% nickel (Ni) and 18% Chromium (Cr) which is capable of withstanding corrosion-related issues, providing austenite structure and making welding stress-free under specified conditions without requiring heating when welding narrow sections. The chemical and mechanical constituent of the stainless steel fabrication material type (304) is presented in Tables 1 and 2 (Wosu *et al*.,2024b)

Table 1: Chemical Composition of Stainless-Steel Grade (304)

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)

	Mechanical Properties		**Elongation after Fracture (A%)**	
	Yield Stress (MPa)	**Tensile Strength (MPa)**	**A_5 (%)**	**50mm(%)**
Minimum	230	450	45	40
Maximum	330	580	NA	NA

Design Pressure

The consideration of design pressure for any equipment design is essential for the equipment (CSTR) to surmount the maximum acceptable pressure that will be applied to it during operation. Conventionally, the design pressure specification is about 5 to 10% above the operating pressure (Wosu *et al*., 2024b). This specification will ensure that the equipment can withstand any unforeseen or additional disturbance such as fluid pressure or any stress that may arise during operation.

Design Temperature

Just like the design pressure, the design temperature should be specified in such a way that it is well above the operating temperature of the CSTR during the process. This will help in mitigating the effect of heat on the reaction media (CSTR) as well as preventing thermal runaway or any uncertainty during the process.

Membrane and Design Stresses

Several factors such as loading effect, nature of the material, uncertainties, design procedures, configuration and operation-ability can be controlled using standard design stress factors. The maximum allowable stress (membrane) that will act on the CSTR also called the normal design strength is an important factor for consideration during the mechanical design of equipment to ensure safe operation and improve the lifespan of equipment. The various material types and their standard stress factors are presented in Table 3.

Table 3: Design Stress Factors at Different Temperatures (Sinott & Towler, 2009)

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 Mo2$\frac{1}{2}$% (316)	520	175	150	135	120	115	110	105	105	100	95

Efficiency of Welded Joint

The type of welds, their joints and quality are the determining factors for the life span of the CSTR fabrication. Quality welding protects equipment from corrosion attacks. Proper visual examination and radiography application improve the efficiency of welded joints. For the CSTR fabrication, the butt joint is conventionally recommended by the provision of ASME BPV code sec. VII DI as presented in Table 4.

Table 4: Welded Joint Efficiencies allowed under ASME BPV Code Sec. VIII D1 (Perry *et al*, 2008)

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

Corrosion Allowance

The negative impact of corrosion on fabricated reactors during operation is a major concern to process industries as it reduces the lifespan of process equipment. This negative impact can be reduced by adding a corrosion allowance of about 4mm to the maximum reactor thickness (Perry *et al*., 2008). The corrosion allowance for the CSTR is usually a function of the construction material type or grade, the nature of reactant species or the process occurring within the reaction media.

Design Load

The CSTR design should be done in such a way that it can overcome both internal and external loads which are sometimes referred to as major or minor leads during operation. The major leads constitute the design pressure, reactor weight, reactants species in the reactor, seismic loads, wind load or any noticeable static loads while loads due to shock, local stresses due to changes in temperature and pressure, bending moment, support and connecting pipes as well as coefficient or expansion of materials all constitute the minor loads. Both the major and minor loads are of significant importance in reactor design and must be taken into consideration to improve the lifespan and efficiency of the reactor.

Minimum Practical Wall Thickness

The minimum practical wall thickness allowance is very vital in equipment design and fabrication because of its ability to manage the equipment weight, external forces and the stresses associated. It also gives rigidity to the equipment. Conventionally, the CSTR thickness is a function of its diameter and corrosion allowance of 4mm (Wosu *et al*., 2024b). The actual standard of reactor thickness dependent on its diameter is presented in Table 5.

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

The schematic of the CSTR thickness design for titanium dioxide production showing the input and output streams with the reactor operating and functional parameters is presented in Figure 2.

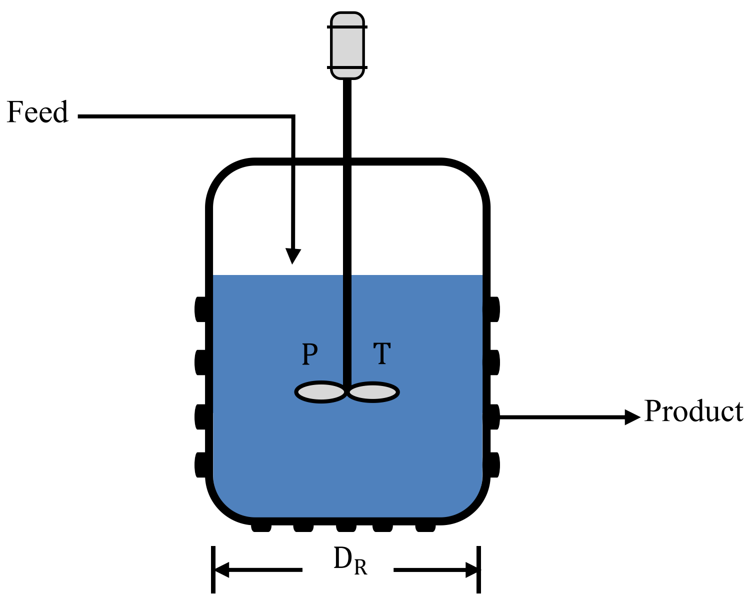

Figure 2: Mechanical Design of the CSTR

The CSTR applied models for thickness determination of the column body (cylindrical) and head (totispherical, standard ellipsoidal and flat) are presented in equations (15), (16), (18), (19) and (22) below;

Reactor Column Body (Cylindrical)

$$e = \frac{P_i D_i}{2JF - P_i} \quad (15)$$

Reactor Column Head (Torispherical)

$$e = \frac{P_i D_i C_s}{2JF - P_i(C_s - 0.2)} \quad (16)$$

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

Reactor Column Head (Standard Ellipsoidal)

$$e = \frac{P_i D_i}{2JF - 0.2P_i} \quad (18)$$

Reactor Column Head (Flat)

$$e = c_p D_c \sqrt{\frac{P_i}{F}} \quad (19)$$

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

Thickness $(t) = e +$ corrosion allowance. (20)

Data for Simulation and Evaluation

The CSTR simulation and thickness evaluation data for the titanium dioxide production is presented in Table 6.

Data	Values	Description	References
Vo	35.191m^3/s	The initial volume flow rate of the reactant	Calculated
C_{Ao}	0.0102mol/m^3	The concentration of limiting reactant	Calculated
F_{Ao}	o.359mol/s	Initial molar flow rate	Calculated
X_A	0.9 (Dimensionless)	Fractional conversion	Assumed
T_o	1190k	The initial temperature of the feed	Mark & Robert, 2003
T	1200k	Reactor operating temperature	Mark & Robert, 2003
T_c	1195k	Coolant temperature	Mark & Robert, 2003
K_o	8.0 x 10^{4}5^{-1}	Pre-exponential factor	Mark & Robert, 2003
K_1	1.182x10^{1}s^{-1}	Rate constant	Mark & Robert, 2003
E	88000J/mol	Activation energy	Mark & Robert, 2003
T_D	940.89^{0}C	Reactor design temperature	Calculated

P	3.74bar	Reactor operating pressure	Calculated
F	165N/mm^2	Stress factor	Sinnott & Towler, 2009
J	1 (Dimensionless)	Welded joint efficiency	Sinnott & Towler, 2009
Cs	1.771 (Dimensionless)	Stress concentration	Calculated
P_i	0.2981N/mm^2	Design pressure	Calculated
R_k	154.248mm	Knuckle radius	Calculated
R_c	2570.8mm	Crown radius	Calculated
C_p	0.4 (Dimensionless)	Full-face gasket	Sinnott & Towler, 2009

Results and Discussion

The CSTR design results and profiles showing the relationship between fractional conversion and the reactor functional parameters as well as the reactor stirrer and thickness specification are presented in this section.

CSTR Design Specification Results

The CSTR design specification results for the production of titanium dioxide are presented in Table 7.

Table 7: Design Results of CSTR Design Volume, Height, Diameter, Space-Time, Space Velocity and Quantity of Heat Generated Per Unit Volume of the Reactor at various Fractional Conversion and Operating Temperature.

X_A	T(K)	V_R(m^3)	H_R(m)	D_R(m)	τ_{CSTR} (s)	S_V(s^{-1})	Q(J/s)	q(J/m^{3}s)
0.10	1190.396	0.037	0.571	0.286	0.006	177.713	89.640	2448.535
0.20	1190.396	0.093	0.779	0.389	0.014	70.708	179.280	1934.645
0.30	1190.396	0.182	0.974	0.487	0.028	35.835	268.920	1481.213
0.40	1190.396	0.330	1.188	0.594	0.051	19.746	358.560	1088.238
0.50	1190.396	0.593	1.446	0.723	0.091	10.970	448.200	755.721
0.60	1190.396	1.112	1.783	0.891	0.171	5.851	537.840	483.661
0.70	1190.396	2.306	2.273	1.137	0.355	2.821	627.480	272.059
0.80	1190.396	5.931	3.114	1.557	0.912	1.097	717.120	120.915
0.90	1190.396	26.688	5.142	2.571	4.102	0.244	806.760	30.229

Table 7 presents the CSTR design results for titanium dioxide production through titanium tetrachloride hydrolysis. MATLAB R2024a simulations were conducted at a constant temperature of 1190.396K and fractional conversions ranging from 0.1 to 0.9. At the maximum conversion of 0.9, the optimum value of the CSTR functional parameters such as volume, height, diameter, space-time, space velocity, the quantity of heat generated as well as the quantity of heat generated per unit volume of the reactor was 26.688m^3, 5.142m, 2.571m, 4.102s, 0.244s^{-1}, 806.760J/s and 30.229J/m^{3}s respectively.

Profile of CSTR Volume (V_R), Height (H_R), Diameter (D_R) and Fractional Conversion (X_A)

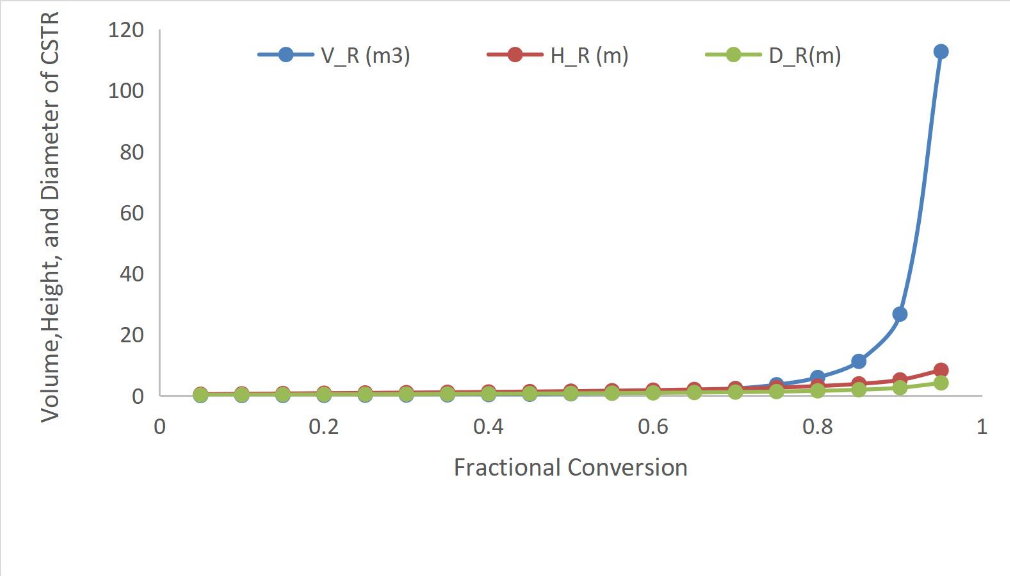

Figure 3: Graph of CSTR volume (V_R), Height (H_R), Diameter (D_R) and fractional conversion (X_A)
figure 3 illustrates the effect of increasing fractional conversion on CSTR volume, height and diameter during titanium dioxide production via titanium tetrachloride hydrolysis. The MATLAB-simulated profile reveals an exponential increase in design quantities with conversion, reaching 26.688m^3, 5.142m and 2.571m for volume, height and diameter at 90% conversion.

Profile of CSTR Residence Time (T) and Fractional Conversion

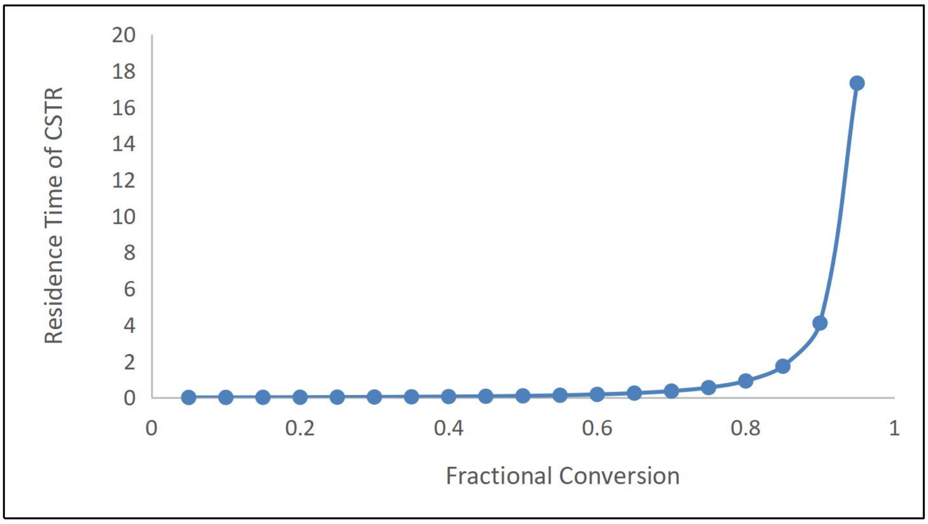

Figure 4: Graph of Residence Time (τ) and Fractional Conversion (X_A)

Figure 4 illustrates the correlation between residence time and fractional conversion, revealing an exponential relationship. Notably, increase in residence time yield higher conversions of the feed materials (reactant). The significance of this is that more yield of the target product increases as the conversion of feed increases with time (space time). At a fractional conversion of 0.1, 0.5 and 0.9, the residence time spent by fluid element in the reactor corresponds to 0.006 sec, 0.091sec and 4.102seconds respectively.

Profile of Space Velocity (S_V) and Fractional Conversion (X_A)

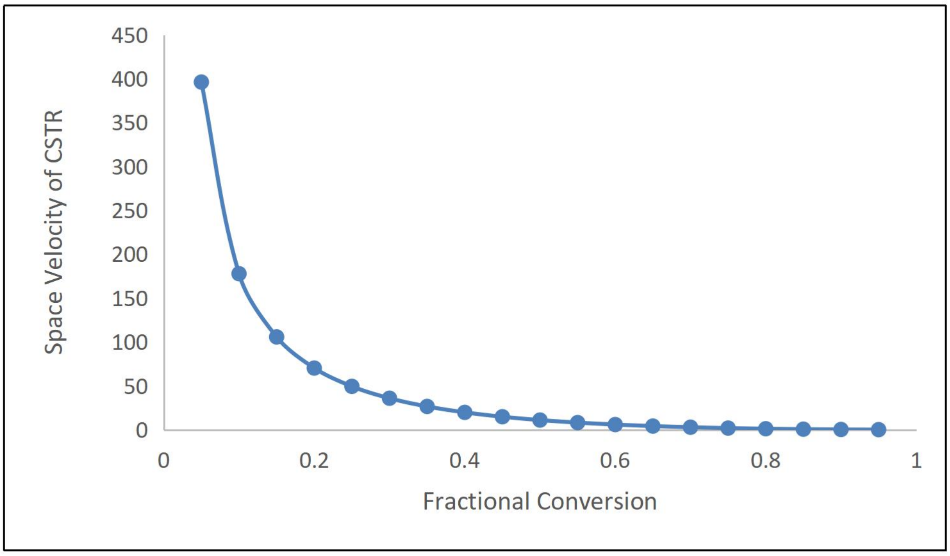

Figure 5: Graph of Space Velocity (S_V) and Fractional Conversion (X_A)

Figure 5 presents the correlation between space velocity and fractional conversion, revealing an inverse exponential relationship. This indicates that reduced space velocity corresponds to increased conversion and yield of titanium dioxide with notable reactor volume. This demonstrates the mathematical correlation between space-time (residence time) and space velocity. Space velocity is defined as the reciprocal of space-time. It is the time used to process a unit volume of the feed at inlet condition. At space velocities of 177.713sec^{-1}, 10.970sec^{-1} and 0.244sec^{-1}, the volume of the reactor which depends on the yield of the target product (titanium dioxide) were 0.037m^3, 0.593m^3 and 26.688m^3 respectively.

Profile of Quantity of Heat (Q), Quantity of Heat Generated per unit Volume (q) and Fractional Conversion (X_A)

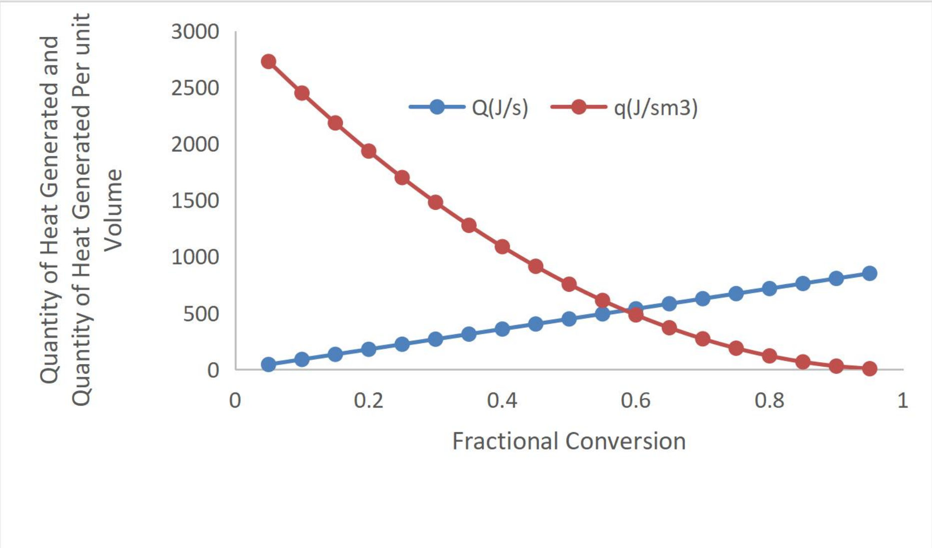

Figure 6: Graph of Quantity of Heat (Q), Quantity of Heat Generated per unit volume (q) and Fractional Conversion (X_A).

Figure 6 presents the correlation between heat generation parameters and fractional conversion in the CSTR. The results showed a linear increase in the quantity of heat generated (Q) and an exponential decrease in the quantity of heat generated per unit volume (q) as fractional conversion and reactor volume (target product yield) increased. At a maximum fractional conversion of 0.9, the values of the quantity of heat generated and the quantity of heat generated per unit volume of the reactor were 806.760J/s and 30.229J/m^3s respectively.

CSTR Agitator Design

The design or specification of the CSTR Agitator is presented in Table 8.

Table 8: CSTR Agitator Design

CSTR Agitator Parameter	Specification (Unit)
Height of Agitator	4.642m
Diameter of Agitator	1.571m

Table 8 represents the design or size of specification of the CSTR agitator height and diameter. The CSTR agitator is responsible for ensuring a uniform mixture of the reactant species to attain a uniform composition of the content both at the inlet and outlet stream during the hydrolysis reaction. The design of the CSTR agitator in terms of height and diameter is dependent on the reactor height and diameter as well as a minimum practical allowance or clearance of 0.5. The height and diameter of the CSTR stirrer were obtained as 4.642m and 1.571m using a clearance of 0.5m and 1m respectively.

Design of the CSTR Thickness

The thickness design or specification of the CSTR is presented in Table 9.

Table 9: Design of the CSTR Thickness

Thickness Parameter	Specification (Unit)
Column Body	-
Cylindrical	6.500mm
Column Head Doomed	-
Torispherical	8.200mm
Ellipsoidal	6.500mm
Flat	47.700mm

Table 9 presents the results of the CSTR thickness design calculations, taking into account various factors such as stainless steel material type (304), operating temperature, pressure, column diameter, design loads, stresses, corrosion allowance and welded joint efficiency to ensure sustainability and optimal performance. Based on analysis of the thickness specifications obtained from the mechanistic models, a uniform thickness of 6.500mm is recommended for the CSTR cylindrical body and ellipsoidal head, utilizing stainless steel, to facilitate efficient and continuous titanium dioxide production.

Conclusion

The study successfully developed and simulated CSTR design models for titanium dioxide production via titanium tetrachloride hydrolysis, utilizing mass and energy balance principles and MATLAB R2023a version as the simulation tool as well as application of the reactor mechanistic models for its thickness specifications. Key findings showed that at a maximum conversion of 0.9, the volume, height, diameter, space-time, space velocity, the quantity of heat generated as well as the quantity of heat generated per unit volume of the reactor were 26.688m^3, 5.142m, 2.571m, 4.102sec., 0.244sec.$^{-1}$, 806.760J/s and 30.229J/m^{3}s respectively. The CSTR thickness specification was determined for stainless steel material for construction type (304) as 6.500mm for both cylindrical column body and standard ellipsoidal head. This will ensure continuous production, and sustainability and improve the lifespan of the equipment by mitigating the impact or effect of corrosion. The design specification of the CSTR agitator height and diameter was obtained as 4.642m and 1.571m respectively using a clearance of 0.5m. The research showed that titanium tetrachloride can undergo hydrolysis in a CSTR for the production of titanium oxide which is very vital for domestic and industrial applications.

Table 10: Nomenclature

Symbol	Definition	Unit
A	Titanium tetrachloride	-

B	Water	-
C	Titanium dioxide	-
D	Hydrochloric acid	-
K_1	Kinetic rate constant	s^{-1}
$-r_A$	Depletion rate of the limiting reactant	$mol/m^3/s$
C_A	The concentration of reactant specie A	mol/m^3
C_B	The concentration of reactant species B	mol/m^3
t	Reaction time	s
C_{AO}	The initial concentration of specie A	mol/m^3
C_{BO}	The initial concentration of specie B	mol/m^3
m	The mole ratio of the initial concentration of species	Dimensionless
K_o	Arrhenius or pre-exponential constant	s^{-1}
E	Activation energy	KJ/kmol
T	Operating temperature	K
R	Gas constant	j/molk
F_{AO}	The initial molar flow rate of the feed	mol/s
V_R	The volume of the reactor	m^3
H_R	Height of the reactor	m
D_R	Diameter of the reactor	m
X_A	Fractional conversion of specie A	Dimensionless
Q	Quantity of heat generated	J/s
q	Quantity of heat per unit reactor volume	J/m^3s
ΔH_R	Heat of reactor	KJ/mol
τ	Space-time	s
S_V	Space velocity	s^{-1}
v_o	Initial volumetric flow rate	m^3/s
C_p	Specific heat capacity	J/molK
A_C	Area of heat exchange	m^2
U	Heat transfer coefficient	W/m^2K
T_o	Feed initial temperature	K
T_c	Coolant temperature	K
ρ_i	Density of species	Kg/m^3

L_{st}	Length of stirrer	m
C	Clearance	m
D_{st}	The diameter of the stirrer	m
e	Minimum thickness	mm
Pi	Design pressure	N/mm^2
Di	Column diameter	m
J	Welded joint efficiency	N/mm
F	Design stress factor	Dimensionless
C_s	Stress concentration factor	Dimensionless
C_p	Full face gasket (0.4)	Dimensionless
D_c	Bolt circle diameter	mm

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