Design of a CSTR to produce 2,000,000 tons per year of Magnesium Chloride from Neutralization Reaction of Magnesium Oxide and Hydrochloric Acid

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Abstract

The research considered the design of a continuous stirred tank reactor (CSTR) for the production of 2 million tons per year of magnesium chloride from the neutralization reaction between magnesium oxide and hydrochloric acid. The design and temperature effect models were developed from the conservation principle of mass and energy at steady state process condition. The design models were simulated using MATLAB at fractional conversion range of $X_A \geq O \leq 0.95$ and operating temperature of 291.36k to give the reactor design or specifications. At fractional conversion of 0.95, the reactor functional parameters such as volume, height, diameter, space time, space velocity, quantity of heat generated and the quantity of heat generated per unit volume of the reactor were 77.760m^3, 7.344m, 3.672m, 15.247sec., 0.066sec^{-1}, 3560.125j/s and 45.783j/sm^3 respectively. The height and diameter of CSTR stirrer or agitator dependent on acceptable clearance of 0.5m and 1m respectively are 6.888m and 2.672m. The cost for yearly production of the commercial product dependent on the reactor volume and production rate at maximum fractional conversion in Dollars and Naira are $6,879.360 and N9.608,402.112 respectively using the relationship of $1 = N1,396.7 as published online in March 27, 2024. The effect of operating temperature and fractional conversion on the reactor functional parameters are displayed in profile 3 to 9. The research showed that magnesium chloride is produced in a continuous stirred tank reactor at steady state operation which is the key to sustainability and availability of the economic product.

1. Introduction

Magnesium is ranked second to sodium chloride due to its relative abundance in sea water. It is a mineral salt with a wide range of industrial application such as dust controlling agent in road construction, road die-sing, drying agent (hygroscopic) etc.(Akpa *et al*.,2019). However, there is a renewed interest in magnesium chloride because of its commercial or economic viability as a catalyst support for Ziegler Natta catalysts and its application in petrochemical and plastic industries for production of polyethylene, Grignard reagents, borates, oarnallites and pharmaceuticals as a cofactor in most enzymatic reactions involving protein synthesis and carbohydrate metabolism, body detoxifying and health care agent to the brain, nervous system, teeth and bones (Kipcak *et al*.,2013).

The magnesium itself in the past and recent past have been described as a miracle mineral because of its ability to heal diseases, rejuvenate aging body, play a huge role in most enzymes catalyzed reactions like cellular energy production and antibiotic effect for health care (Akpa *et al*.,2019).

Based on the economic importance of magnesium chloride, the goal of this research is to ensure its availability and sustainability by considering the design of a continuous stirred tank reactor (CSTR) for the production of magnesium chloride from neutralization reaction involving magnesium oxide and hydrochloric acid. The CSTR is used since magnesium oxide can also exist as a conductive liquid and the hydrochloric acid is in aqueous solution which makes the neutralization process a liquid phase reaction. The CSTR design for the production of 2,000,000 tons per year of magnesium chloride from neutralization reaction between magnesium oxide and hydrochloric acid requires a good knowledge and experience from chemical engineering process and equipment design, reaction kinetics, mass and heat transfer, economics, etc. The principle of conservation of mass and energy balance is utilized as the basis for the reactor design.

Several researches have been carried out to ensure the availability and sustainability of magnesium or its derivatives as well as continuous stirred tank reactor design and its applicability in process industries and thus; Khaled *et al* (2013) researched on separation of magnesium chloride from sea water by applying preferential salt-separation (PSS) approach andstated that Na^+, K^+, Mg^+, Cl^- and $SO4^-$ are the major components that characterize the solubilityproperties of natural sea water with constant relative proportions. The PSS technology model was tested experimentally on a semi pilot scale and the result showed that the end product of any evaporative method (continuous or batch process) would be a dense magnesium chloride solution. The experimental set up of the dynamic (continuous) model integrates a constant head tank, infra red heaters, evaporator (PSS) and a feed tank while the proposed, PSS model also called the static (batch) model is an evaporation process that occurs in a tank using solar-heated water jacket. The results obtained from both model showed that concentrated magnesium chloride was recovered from both process but more yield of the magnesium chloride was obtained from the dynamic or continuous model as a result of continuous operation of the evaporation process. Chemical engineering equipment design involves sizing and is governed by the principle of mass and energy balance conservation which is essential in the production of petrochemicals and other economical viable products (Wosu & Ezeh, 2024; Ojong *et al*, 2024; Wosu *et al*, 2024a; Wosu *et al*, 2023; Wosu *et al*, 2024b)

Corey *et al* (2022) researched on the purification of magnesium chloride from mixed brines using hydrogen chloride absorption with temperature and pressure regeneration of super azeotropic hydrochloric acid and emphasized on the negative impact of discharging brines to seawater which affects aquatic lives and land body as a result of climatic change which causes ocean surge or flooding which affects lives and properties. The researchers designed a pilot scale continuous process for high purity magnesium chloride recovery from desalination of brines as well as CO_2 treatment to overcome the water-energy-climate nexus by providing clean water, mitigate environmental issues and effect of atmospheric CO_2.

In 2022, Fontance *et al* presented a technical review of magnesium recovery from seawater desalination brines. Some of the reviews cited by the researchers include; Ahmad *et al* (2019) a review on the extraction of minerals from saltwater reverse osmosis brine for recovery of magnesium. Bardi in 2010 performed an energy analysis during the recovery of magnesium mineral from saltwater. Casas *et al* (2014) performed an analysis of by-products such as calcium and magnesium obtained from saltwater desalination brines and mining operation as well as its application in water treatment while Cipollina *et al* in 2015 stated that magnesium oxide (MgO) can be recovered from brine using additives techniques to enhance the production of magnesium chloride and the researchers emphasized on the effect of the process on the environment and the need to propose other techniques with less impact on the environment.

Herrero-Gonzalez *et al* (2020) stated that the environmental effect and sustainability challenges encountered during magnesium chloride production from brine (Saltwater) can be evaluated using electrodialysis and bipolar membranes. The salt removal or desalination technology can be classified into membrane-based or evaporation based processes (Zarzo & Prat, 2018), where the membrane-based technology involves generating electrical energy which is usually energy intensive while the evaporation-based technology is powered by either mechanical compression or heat supply which is more practicable in the industry. Ahmad & Baddour (2014) included that brine disposal results to detrimental effect on the environment which posses substantial financial burdens. The application of reverse osmosis of brine is equivalent to twice the concentration of salt in sea water and usually contains chemicals that were introduced during the pretreatment and membrane cleaning processes which also affect aquatic lives (Portillo *etal*., 2014).

Panagopoulos *et al* (2019) researched on comparative analysis of zero liquid discharge (ZLD) and minimal liquid discharge (MLD) technologies in a bid to mitigate the adverse environmental impact associated with brine discharge. The waste management strategies ensured that the salt produced or water can be discharged to land which will minimize its environmental impact. These technologies are capable of recovering up to 99% fresh water which can be reused or applied in agricultural sector, industrial processes like cooling systems and domestic purposes like cooking, drinking and cleaning etc. the solid waste can be recycled, processed and reused or disposed (COM, 2020). The comparison of the techniques showed that in terms energy efficiency, the MLD is more economically viable but in terms of total fresh water recovery rate, it is about 10% less than the ZLD system. The researchers included that the MLD is characterized with the potential for maximum water recovery, low operating cost and less energy requirement. Davis in 2006 researched on waste brines valorization through resource recovery and posited that the recovery of fresh water and salt can be seen as a waste to wealth program for resource management and economic advancement.

Konne *et al* (2016). Researched on extraction and characterization of magnesium chloride from different blackish water sources in

Rivers State and stated that the exploitation of seawater for mineral recovery have not really gained much attention compared to the effort made on exploitation of crude oil for petrochemical production. The seawater also known as brines contain minerals like Na, Mg, Ca, Ba, Li, Al, S, Si, Fe, Sn, Mn, Mo, Zn, Ni, Co, Cr, Cu, V, Ti, Cd, Pb, Au, Th, U, etc (Al-mutaz & Wagialia, 1990). These minerals can be used as feed materials for the production of commercial or economic value products in petrochemical, pharmaceutical and plastic industries (Podder *et al*., 2013). The researchers extracted samples of blackish water from Kaa, Eagle Island, Opobo and Iwofe water fronts in Rivers State using conventional techniques. The samples were characterized using x-ray diffraction (XRD) and x-ray fluorescence (XRF) to obtain physiochemical properties like pH, conductivity and total salinity of salts. The results obtained showed that Kaa sample displayed more performance characteristics followed by Eagle Island, Opobo and Iwofe. The XRD showed high reflections of hydrated magnesium chloride salt while the XRF reflected more of the elemental compositions with high concentration of magnesium, sulfur content and significant presence of Sn, Sb, Al, Si, P, Fe, Cu, Zn, W and Mo were also observed on the XRF charts of the samples.

Erdogan *et al* (2013). Stated that high quality magnesium chloride can be produced from recycled waste magnetsite powder and described magnesite ($MgCO_3$) as a primary source for theproduction of magnesium and magnesium compounds. The magnesite constitute 47.6% MgO and SiO_2, Fe and Ca as impurities which makes it a raw material for the production of alkaline refractory products and applied in glass, paper, pharmaceutical, cement, sugar, iron-steel, paint and ink industries (Abali *et al*., 2006). The research carried out by Erdogan *et al* showed that waste magnesite powder can be optimized using leaching in hydrochloric acid solutions to produce high quality magnesium chloride and magnesite powder as waste which can be recycled for further processing.

Most of the reviews have shown that extensive research have been carried out on magnesium chloride production from naturally occurring magnesium as a mineral deposited in seawater or brines and its effect on aquatic lives and environment. This research considered the design of CSTR for production of magnesium chloride from neutralization reaction of magnesium oxide and hydrochloric acid to ensure continues production and sustainability of the commercial product in the world.

2 Materials and Methods

2.1 Materials

The materials used in this research are a computer set, data obtained from journals, textbooks and the simulation tool used is MATLAB.

2.2 Methods

The methodology adopted in this research is quantitative and the data used are obtained from thermodynamic properties of the reactant species and products, literature data and calculated/derived data. The procedures adopted in this research are;

i. Development of the reaction kinetic models

ii. Development of design or sizing models for reactor volume, height, diameter, space time, space velocity, quantity of heat generated as well as quantity of heat generated per unit volume of the reactor.

iii. Energy balance model development

iv. Development of the stirrer design models

v. Costing of the reactor.

2.2.1 Development of the Reaction Kinetic Models.

The kinetic models of this research can be developed from the reaction kinetic scheme of the process. The chemistry of the process involves neutralization reaction as shown in equation (1)

$$MgO + 2HCl \xrightarrow{k_1} MgCl_2 + H_2O \tag{1}$$

The 3rd order irreversible neutralization reaction can be expressed symbolically as;

$$A + 2B \xrightarrow{k_1} C + D \tag{2}$$

The rate law of the neutralization reaction can be expressed as a function of feed rate depletion and kinetic parameters as follows;

$$-r_A = k_1 C_{Ao}{}^3 (1 - x_A)(m - 2x_A)^2 \tag{3}$$

2.2.2 Development of CSTR Design/Sizing Models

Consider the schematic representation of a continuous stirred tank reactor with feed and product streams

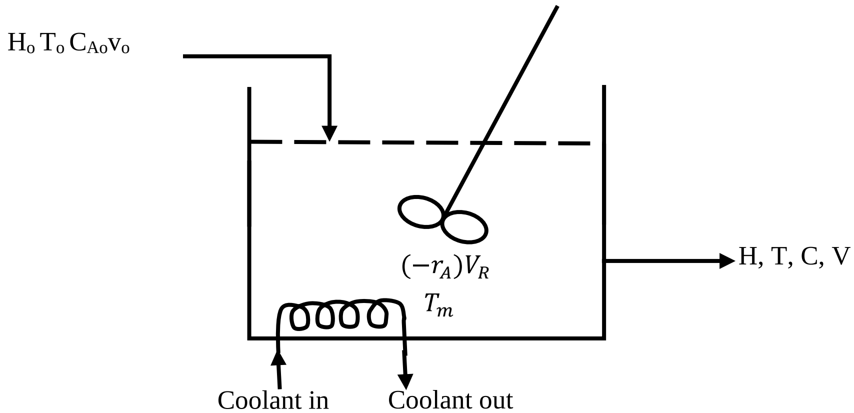

Figure1: CSTR with Mass and Heat Effect

For the neutralization reaction in 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 conservation principle of mass can be performed over the reactor for the development of the CSTR design model as follows;

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

The terms in equation (4) is defined, substituted and simplified at steady state operation to give the design model of the CSTR volume, height, diameter, space time and space velocity thus;

$$V_R = \frac{F_{Ao}x_A}{K_o e^{-E/RT} C_{Ao}^{3}(1-x_A)(m-2x_A)^2} \tag{5}$$

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

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

$$\tau_{CSTR} = \frac{x_A}{K_o e^{-E/RT} C_{Ao}^{3}(1-x_A)(m-2x_A)^2} \tag{8}$$

$$S_V = \frac{K_o e^{-E/RT} C_{Ao}^{3}(1-x_A)(m-2x_A)^2}{x_A} \tag{9}$$

The quantity of heat generated during the process and the quantity of heat generated per unit volume of the reactor are mathematically given as;

$$Q = \Delta H_R F_{Ao} x_A \tag{10}$$

$$q = \frac{\Delta H_R F_{Ao} x_A}{V_R} \tag{11}$$

The energy balance model of the CSTR for the neutralization reaction is given in equation (12)

$$\begin{bmatrix} \text{Rate of} \\ \text{accumulation} \\ \text{of heat} \\ \text{within the} \\ \text{volume} \end{bmatrix} = \begin{bmatrix} \text{Rate of} \\ \text{Input of} \\ \text{heat to} \\ \text{the volume} \end{bmatrix} - \begin{bmatrix} \text{Rate of} \\ \text{Output of} \\ \text{heat from} \\ \text{the volume} \end{bmatrix} - \begin{bmatrix} \text{Rate of} \\ \text{depletion} \\ \text{of heat due} \\ \text{to chemical} \\ \text{reaction} \end{bmatrix} - \begin{bmatrix} \text{Rate of} \\ \text{heat} \\ \text{removal} \\ \text{to the} \\ \text{surrounding} \end{bmatrix} + \begin{bmatrix} \text{Shaft} \\ \text{work} \\ \text{done by} \\ \text{the shirrer} \end{bmatrix} \tag{12}$$

The terms in equation (12) can be defined, substituted and simplified at steady state operation to give the temperature effect model of the reactor thus;

$$T = \frac{\tau \Delta H_R r_i v_o + UA_c T_c + \rho v_o c_p T_o}{\rho v_o C_p + UA_c} \quad (3.45) \tag{13}$$

The capital cost of a continuous flow stirred tank reactor is given by (John, 2007)

$$\text{Cost} = \$200{,}000 \left(\frac{V_{CSTR}}{1000}\right)^{0.6} \tag{14}$$

Where V_{CSTR} is the volume of CSTR in m^3. The above model is for a life of 20years with no salvage values.

2.2.3 Data for Evaluation

The data for evaluation in this research are the properties/thermodynamic data, calculated/derived data and data obtained from literatures as presented in table 1 and 2.

Table 1: Properties/Thermodynamic Data

Data/Parameter	Values	Description
ρ_A	3580kg/m^3	Density of magnesium oxide
ρ_B	1048kg/m^3	Density of hydrochloric acid
ρ_C	2320kg/m^3	Density of magnesium chloride
ρ_D	997kg/m^3	Density of water
R	8314Nmmol^{-1}K^{-1}	Gas constant

Table 2: Data Obtained from Literatures

Data	Values	Description	References
T_o	291.15K	Initial temperature of feed	Akpa *et al*, 2019
T	301.15K	Operating temperature of the reactor	Akpa *et al*, 2019
T_c	296.15K	Coolant temperature	Akpa *et al*, 2019
k_i	0.0683s^{-1}	Rate constant	Akpa *et al*, 2019
$-r_A$	6.1×10^{-5}mol/m^3	Reaction rate	Akpa *et al*, 2019
ΔH_R	56722.99kJ	Change in enthalpy of reactants	Akpa *et al*, 2019

3 Results and Discussion

The CSTR design results for the production of magnesium chloride from neutralization reaction of magnesium oxide and hydrochloric acid are presented in table 3 and profiles below.

Table 3: Design Results Showing Fractional Conversion, Temperature, Reactor Volume, Height, Diameter, Space Time, Space Velocity, Quantity of Heat Generated and Quantity of Heat Generated per unit Volume of the Reactor is Presented.

X_A	T(K)	$V_R(m^3)$	H_R(m)	D_R(m)	τ(s)	$S_V(s^{-1})$	Q(J/s)	$q(J/m^3s)$
0.05	291.36	0.011	0.387	0.193	0.002	449.856	187.375	16527.810
0.15	291.36	0.043	0.600	0.300	0.008	120.045	562.125	13231.410
0.25	291.36	0.091	0.774	0.387	0.018	56.076	936.875	10301.270
0.35	291.36	0.170	0.952	0.476	0.033	30.085	1311.625	7737.398
0.45	291.36	0.304	1.157	0.579	0.060	16.754	1686.375	5539.794
0.55	291.36	0.556	1.415	0.707	0.109	9.176	2061.125	3708.457
0.65	291.36	1.086	1.768	0.884	0.213	4.697	2435.875	2243.388
0.75	291.36	2.456	2.321	1.161	0.482	2.077	2810.625	1144.583
0.85	291.36	7.731	3.402	1.701	1.510	0.650	3185.375	412.051
0.95	291.36	77.760	7.344	3.672	15.247	0.066	3560.125	45.783

Table 3 shows the result of design or size specification of a CSTR for the production of 2,000,000 tons of magnesium chloride from neutralization reaction of magnesium oxide and hydrochloric acid obtained from the MATLAB simulation at initial feed and operating temperature of 291.36k and 301.36k with fractional conversion changes within the range of $x_A \geq 0 \leq 0.95$ at 0.05 interval, the reactors functional parameter such as volume, height, diameter, space time and the quantity of heat generated increases during the process while the space velocity and the quantity of heat generated per unit volume of the reactor decreases during the process.

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This implies that the more the reactant or feed are converted during the process (increase in fractional conversion), the more the desired or target product (magnesium chloride) is produced. At maximum fractional conversion of 0.95, the reactor volume, height, diameter, space time, space velocity, quantity of heat generated and the quantity of heat generated per unit volume of the reactor was $77.760m^3$, 7.3344m, 3.672m, 15.247seconds, $0.066sec^{-1}$, 3560.12j/sand45.783j/sm^3 respectively.

3.1 Profile of the Reactor Volume (V_R) and Fractional Conversion (X_A)

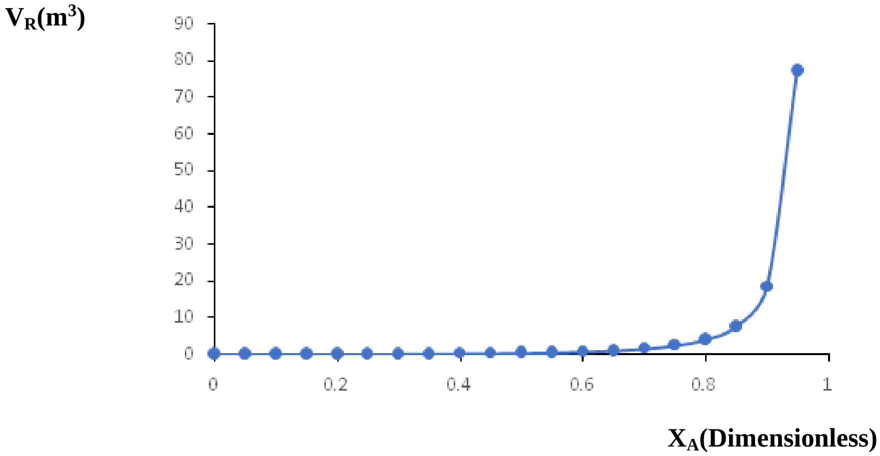
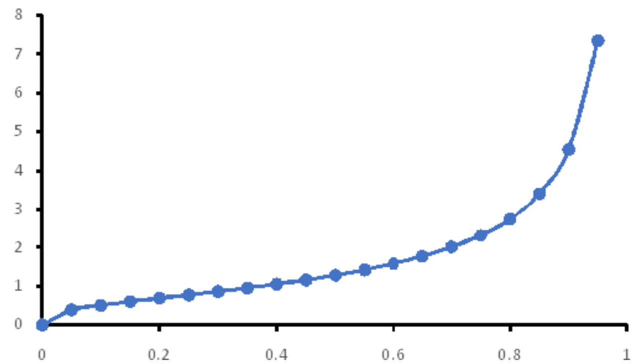


Figure 2: Plot of CSTR Volume (V_R) and Fractional Conversion (X_A)

Figure 2 is a profile or relationship between the volume of CSTR and fractional conversion during the production of magnesium chloride from neutralization reaction of magnesium oxide and hydrochloric acid. This plot was developed from the MATLAB simulation of the steady state performance model of the CSTR volume at initial feed and operating temperature of 291.36k and 301.36k with fractional conversion variation from 0 to 0.95 at an interval of 0.05. According to the plot, the reactor volume increases exponentially as the fractional conversion increases during the process. This showed that the conversion or transformation of reactants or feed materials has a great influence on the magnesium chloride yield. At a maximum fractional conversion of 0.95, the CSTR volume was 77.760m^3.

3.2 Profile of the CSTR Height (H_R) and Fractional Conversion (X_A)

H_R(m)



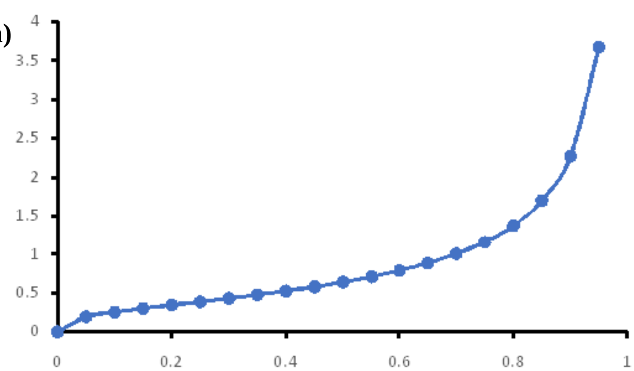
X_A(Dimensionless)

Figure 3: Plot of the CSTR Height (H_R) and Fractional Conversion (X_A)

Figure 3 is a graphical relationship between the CSTR height and fractional conversion obtained from MATLAB simulation of the steady state performance model of the reactor during magnesium chloride production from neutralization reaction between magnesium oxide and hydrochloric acid. According to the profile, there is a slight linear increase in the reactor height at fractional conversion below 0.05. At higher fractional above 0.05, an exponential increase in the reactor height was observed till the end of the process. This showed that an increase in feed or liquid content of the CSTR will increases the height of the reactor. At a maximum fractional conversion of 0.95, the reactor height was 7.344m.

3.3 Profile of the CSTR Diameter (D_R) and Fractional Conversion (X_A)

D_R(m)



X_A(Dimensionless)

Figure 4: Plot of the CSTR Diameter (D_R) and Fractional Conversion (X_A)

Figure 4 is a profile showing the relationship between CSTR diameter and fractional conversion obtained from the MATLAB simulation of the reactor steady state performance model for neutralization reaction between magnesium oxide and hydrochloric acid for magnesium chloride production. During the process, a linear increase of reactor diameter was observed at fractional conversion below 0.05. At higher fractional conversion above 0.05, an exponential increase in the reactor diameter was observed till the end of the process. The significance of this is that higher conversion of the feed in the reactor will result to high yield of the target product (magnesium chloride) and increase in the reactor size even in terms of its diameter. At maximum fractional conversion of 0.95, the reactor diameter was 3.672m.

3.4 Profile of the CSTR Space Time (τ) and Fractional Conversion (X_A)

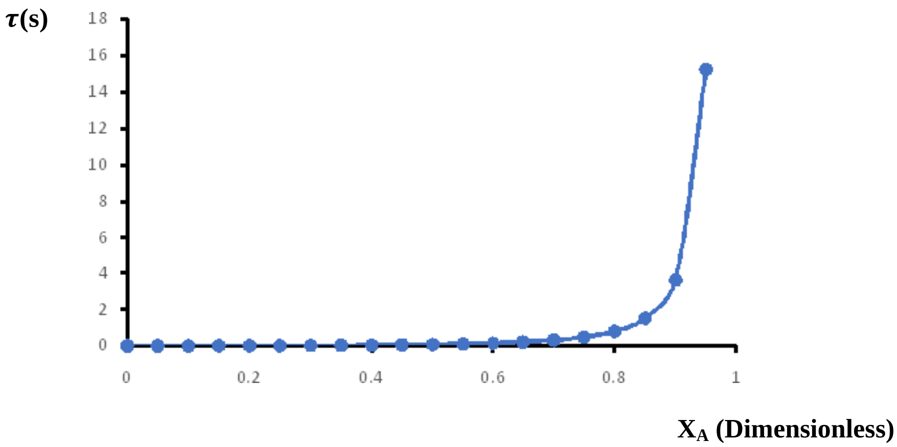


Figure 5: Plot of the CSTR Space Time (τ) and Fractional Conversion (X_A)

Figure 5 is a relationship between space time and fractional conversion obtained from the MATLAB simulation of the CSTR steady state model for space time during the production of magnesium chloride from the neutralization reaction between magnesium oxide and hydrochloric acid. From the plot, there was a slow exponential increase in the space time between the initial fractional conversion to 0.6 and this exponential increase became rapid at higher fractional conversion. This increase in space time showed that more time is required to process the reactant or feed in the reactor during the neutralization process. At a maximum fractional conversion of 0.95, the space time required taken for processing the feed or reactant species was 15.247seconds

3.5 Profile of the CSTR Space Velocity (S_V) and Fractional Conversion (X_A)

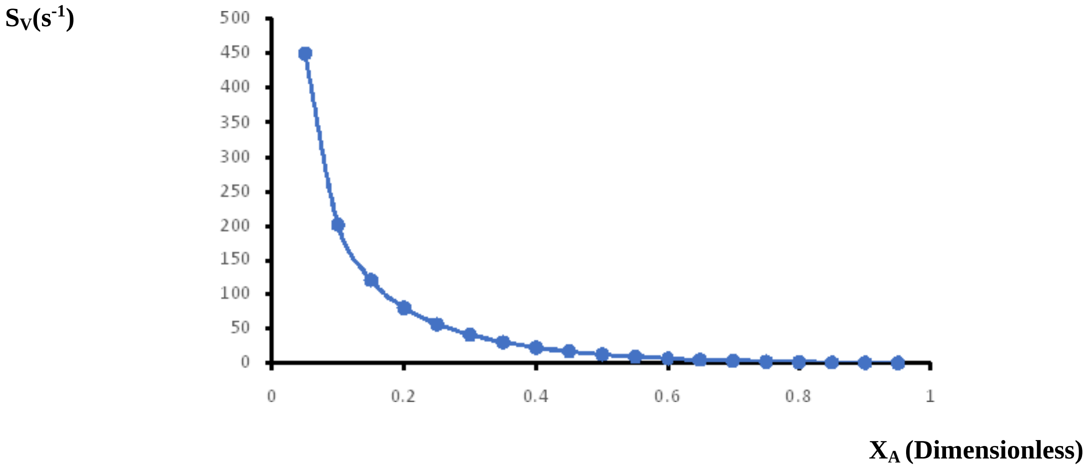


Figure 6: Plot of CSTR Space Velocity (S_V) and Fractional Conversion (X_A)

Figure 6 shows the graphical relationship between the space velocity (reciprocal of space time)and fractional conversion of reactant or feed (magnesium oxide and hydrochloric acid) during magnesium chloride production from the neutralization reaction in a CSTR. This profile was obtained from the MATLAB simulation of the steady state performance model of the reactor space velocity. According to the plot, the space velocity decreases exponentially as the fractional conversion increases. At higher fractional conversion above 0.95, the value of the space velocity tends towards negative infinity ($-\infty$) but at a maximum fractional conversion of 0.95, the space velocity decreased value was $0.066s^{-1}$. This clearly justifies the mathematical relationship between the space time and space velocity.

3.6 Profile of the CSTR Quantity of Heat Generated (Q) and Fractional Conversion (XA)

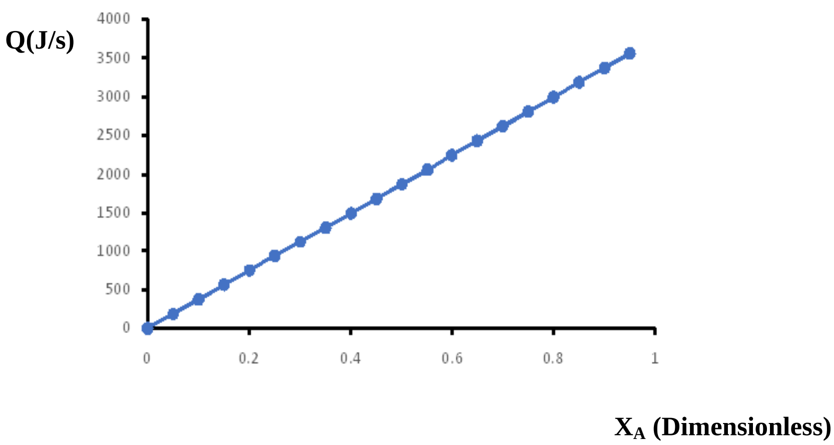


Figure 7: Plot of the CSTR Quantity of Heat Generated (Q) and Fractional Conversion (X_A)

Figure 7 shows there is a linear increase in the quantity of heat generated as the fractional conversion increases during the production of magnesium chloride from neutralization reaction between magnesium oxide and hydrochloric acid in the CSTR. What this signifies is that the more heat is generated during the process, the more the conversion of the reactant species occurs. At a maximum fractional conversion of 0.95, the quantity of heat generated was 3560.12j/s.

3.7 Profile of the CSTR Quantity of Heat Generated per unit Volume of the Reactor (q) and Fractional Conversion (X_A)

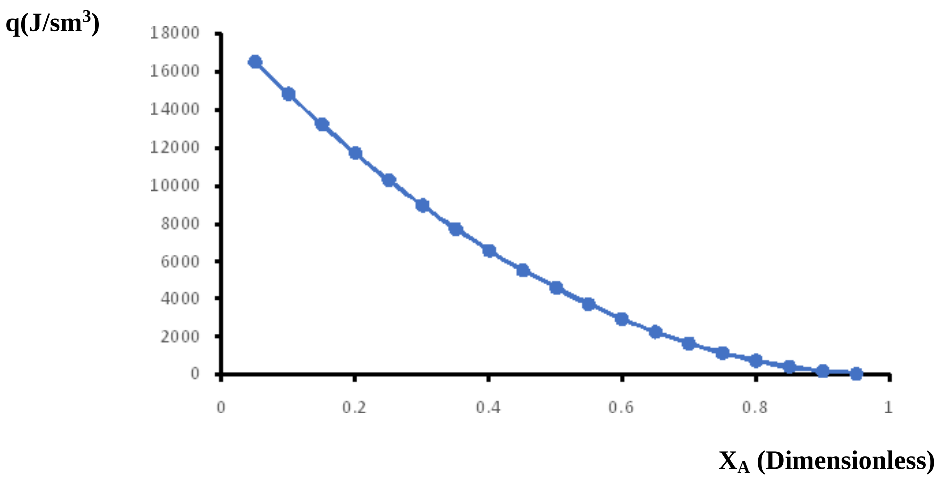


Figure 8: Plot of the CSTR Quantity of Heat Generated per unit Volume of the Reactor (q) and Fractional Conversion (X_A)

Figure 8 shows that the quantity of heat generated per unit volume of the CSTR decreases exponentially as the fractional conversion increases. This simply means that since an increase in fractional conversion increases the reactor volume, the quantity of heat generated per unit volume of the reactor will therefore decrease at higher fractional conversion. At a maximum fractional conversion of 0.95, the quantity of heat generated per unit volume of the CSTR was decreased to 45.783j/sm^3. This result showed that less quantity of heat will be generated for high yield of magnesium chloride.

3.8 Profile of the CSTR Operating Temperature (T) and Fractional Conversion (X_A)

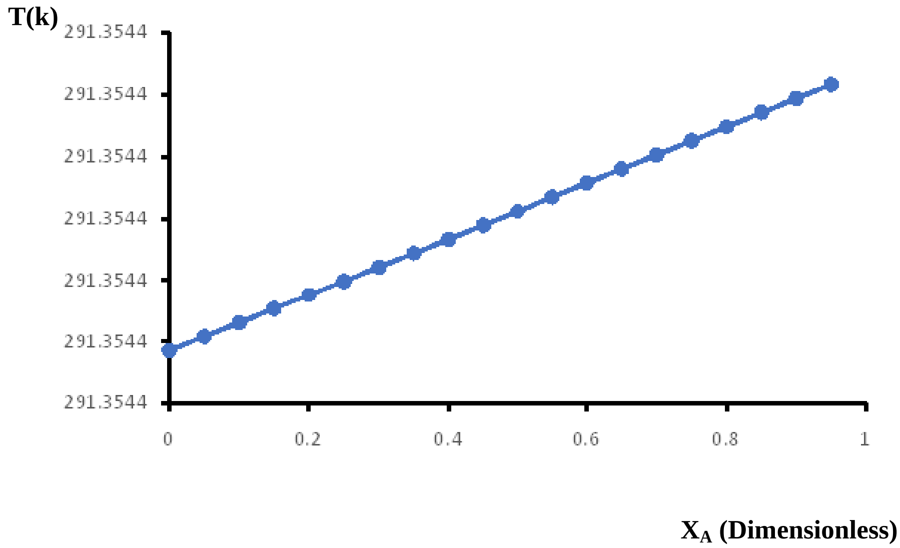


Figure 9: Profile of the CSTR Operating Temperature (T) and Fractional Conversion (X_A)

Figure 9 shows that the fractional conversion increases linearly at CSTR initial feed and operating temperature of 291.380k and 301.380k. What this result implies is that temperature within its operating range for magnesium chloride production during neutralization reaction between magnesium oxide and hydrochloric acid in a CSTR will favor or enhance the yield of the target product (magnesium chloride). This profile was obtained from the MATLAB simulation of the steady state temperature effect model of the CSTR.

Conclusion

The research focused on the design of a CSTR for the production 2,000,000 tons per year of magnesium chloride from the neutralization reaction of magnesium oxide and hydrochloric acid. The reactor design or performance model was developed from the law of conservation of mass and energy at steady state operating condition of the reactor. The simulation of the developed model was performed using MATLAB as the simulation tool. The design result from the simulation showed that the yearly production of magnesium chloride required CSTR size or design specification of 77.760m^3 volume, 7.344m height, 3.672m diameter, 15.247seconds residence time, o.o66 per seconds space velocity, 3560.125j/s quantity of heat generated and 45.783j/sm^3 quantity of heat generated per unit volume of the reactor at 0.95 maximum fractional conversion. This article has shown that for optimum production and sustainability of magnesium chloride, the CSTR design configuration is considered suitable as the reaction media for the neutralization reaction in process industries.

Nomenclature

Symbol	Definition	Unit
ΔH_R	Change in enthalpy of reactants	J/mol
A	Magnesium oxide	-
B	Hydrochloric acid	-
C	Magnesium chloride	-
C_i	Initial concentration of species	mol/m^3
C_p	Specific heat capacity	J/mol
D	Process water	-
D_R	Diameter of the reactor	M
E	Activation energy	J/mol
F_{A0}	Initial molar flow rate	mol/S
H_i	Enthalpy of species	J/mol
H_R	Height of the reactor	M

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K_o	Pre-exponential factor	S^{-1}
Q	Quantity of Heat generated	J/s
q	Quantity of heat generated per reactor volume	J/sm^3
R	Gas constant	$Nmmol^{-1}k^{-1}$
r_A	Reaction rate of species	$mol/m^3/s$
S_V	Space velocity	Sec^{-1}
T	Operating temperature	K
T_c	Temperature of coolant	K
T_o	Initial or feed temperature	K
UAc	Heat transfer coefficient	Kg/m^2sK
X_i	Fractional conversion	Dimensionless
V_o	Initial volumetric flow rate	m^3/S
V_R	Volume of the reactor	m^3
ρ_i	Density of species	Kg/m^3
τ	Space time	S

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