Journal of Newviews in Engineering and Technology (JNET)
Vol 4, Issue 3, December 2022
Available online at http://www.rsujnet.org/index.php/publications/2022-edition
e- ISSN: 2795-2215

Modeling and Simulation of a Non-Isothermal Continuous Stirred Tank Reactor for Methanol Synthesis Using Different Catalyst

Odogwu, J. O., Akpa, J. G. and Wordu, A. A.

Department of Chemical/Petrochemical Engineering,
Rivers State University, Port Harcourt, Rivers State, Nigeria
E-mail: odogwu_janet@yahoo.com, akpa.jackson@ust.edu.ng, wordu.animia@ust.edu.ng

ABSTRACT

An unsteady state models for a continuous stirred tank reactor was developed applying principles of conservation of mass and energy to predict feed (reactants) depletion and product formation using three different catalysts namely alumina (Al_2O_3), Zinc oxide (ZnO) and Copper (Cu). The results obtained from the developed model showed the concentration of product formation using three different catalysts. As the reaction progresses in the reactor the temperature increases which shows a corresponding conversion of the feeds in the reactor. The temperature increased to a maximum of 592K. The developed models were validated with literature values. The simulation was done by MATLAB R2020 and numerically solved using Runge-Kutta method. A sensitivity analysis was carried out on the fractional conversion on Methanol formation. The optimal values from the simulation were obtained using the calculus second differential method to be 0.7426mol/l, 0.6094mol/l, 1.3712mol/l and 1.4054mol/l, respectively.

KEYWORDS: CSTR, Langmuir Hinshelwood, Modeling, Sensitivity Analysis, Simulation.

Cite This Paper: Odogwu, J. O., Akpa, J. G. & Wordu, A. A. (2022). Modeling and Simulation of a Non-Isothermal Continuous Stirred Tank Reactor for Methanol Synthesis Using Different Catalyst. *Journal of Newviews in Engineering and Technology*. 4(3), 39 – 49.

1. INTRODUCTION

Synthesis of Methanol has increased over the years. Methanol consumption in the energy sector is larger than 40% and is used as either direct or indirect energy source. In addition, methanol is a basic chemical feed stock and plays a significant role in the chemical industry (Vincenzo *et al*., 2018). Over the past years, modeling has shown its importance in chemical synthesis process. The study of modeling helps in reactor design, and it is an important way of knowing the entire process for better yield and process modification. These models when adjusted and confirmed will provide understanding as to how the process functions, changes in operation measures and how it is controlled (Kuozynski, *et al.,* 1987). A comprehensive knowledge of the reaction system can pave the way for a better production process resulting in substantial revenues. One of such industrial importance of modeling is in the synthesis of Methanol (Daaniya, 2012).

Methanol synthesis can take place through three main reactions:

i. Hydrogenation of Carbon Monoxide

The production of methanol produces three moles of Hydrogen for every mole of Carbon Monoxide, however the reaction for Methanol synthesis only needs two moles of hydrogen.

$$CO + 2H_2 \rightarrow CH_3OH \quad (1)$$

ii. Hydrogenation of Carbon dioxide

Carbon dioxide is introduced into the reactor which would react to give this reaction:

$$CO_2 + 3H_2 \rightarrow CH_3OH + H_2O \quad (2)$$

iii. Water-gas Shift reaction

This describes the reaction of carbon Monoxide and water vapour to form carbon dioxide and hydrogen.

$$CO + H_2O \rightarrow CO_2 + H_2 \quad (3)$$

Journal of Newviews in Engineering and Technology (JNET)
Vol 4, Issue 3, December 2022
Available online at http://www.rsujnet.org/index.php/publications/2022-edition
e- ISSN: 2795-2215

Methanol can be used to produce chemical compounds like paraffins, olefins, biodiesel, transportation fuel and as fuel additives. It can be used also as an industrial solvent to produce dyes, resins, adhesives, inks, refrigerant, chemical intermediates, and paints. For an industrialist, the focus is to get maximum yield for the desired production process. Chemical process modeling involves a system of interrelated components which are then solved to get the dynamic or steady state behaviour (Alan, 1999). Simulation of the process shows how experimenting with different values would vary the reaction (Taylor, 2021). The reaction is highly exothermic, reversible and equilibrium controlled. More lately, the Cu/ZnO catalyst is favoured due to its ability to lower the pressure (Issa, 2015).

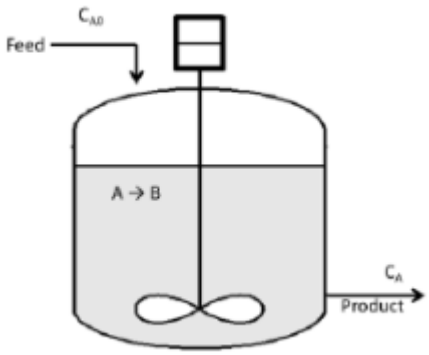

Figure 1: Schematic of a CSTR

Carsten *et al*. (2021) wrote an article on optimization of methanol synthesis under forced periodic operation. The work showed other means of methanol synthesis by forced periodic operation modes using numerical optimization. A well-mixed isothermal reactor with two periodic inputs for CO concentration in the feed and total feed flow rate. A kinetic model was used to describe the dynamics of the catalyst- $CuO/ZnO/Al_2O_3$. Nonlinear programming NLP was used to compare optimal steady state solutions. The essence of the NLP was to get the methanol outlet flow rate and the methanol yield based on the total carbon in the feed. The results showed that significant improvement for both the objective function was possible through periodic forcing of the two inputs.

Amenaghawon and Okeimien (2011) researched on the dynamic modeling, simulation, and optimization of an isothermal CSTR for methanol synthesis. The study showed the operation of an isothermal CSTR to investigate and process methanol synthesis. A dynamic model was developed, and simulation carried out using an advanced equation-oriented modeling software. The formulated model was a system of Differential and Algebraic Equation (DAEs) which was simulated at the initial state to obtain time paths of all variables considered at steady state. The model process formulated gives understanding on how the process responds to changes in operating procedure and the process control. A regulator was introduced to operate the outlet valve to control the pressure in the reactor. The model developed was validated against experimental data by estimating the kinetic parameters (rate constant and K- values). Plots were made to show how well the results predicted by the model fit the experimental data. Simulation results was gotten and compared with the experimental data which showed that the model results corelates with that of the experimental data. The results gotten when the reactor operates isothermally compared with the simulated results showed that it took the process 120hours to reach its new steady state.

Wordu *et al*. (2019) worked on design and optimization of system of CSTR for methanol production. The work showed the mathematical modeling of a CSTR in series maintaining isothermal process at steady state. A methanol chemical production using Carbon monoxide and Hydrogen in liquid form in a CSTR in series of three reactors was exposed to an economic study for the best reactor. The kinetic balance and the reactor's power of utilization rate was considered. MATLAB V 7.7 software was used for the simulation and profile plots of reaction rate, reactor volume, reactor diameter, mixer revolution, and cost of reactor. Space time and

Journal of Newviews in Engineering and Technology (JNET)
Vol 4, Issue 3, December 2022
Available online at http://www.rsujnet.org/index.php/publications/2022-edition
e- ISSN: 2795-2215

space velocity against molar conversion rate figures.

The research work also showed the sizing and the design of a CSTR. The results showed that molar conversion rate was higher for a single CSTR than a CSTR in series and its more economical with respect to cost.

Issa (2015) carried out a study on a model and simulation of methanol synthesis system. The study showed a novel approach to synthesize methanol using modeling and simulation techniques to come up with a possible plant design and operating conditions. The study used modeling and simulation techniques. The main raw materials were CO_2, H_2, H_2O and CH_3OH as a seed product, Aspen Hysys V. 7.3 software was used to complete environment platform for developing a complete system to mimic real life steps. The basic conditions set up were CO_2/H_2 ratio as feed with 40^0C, 4000kpa and SRK (Soave Redlich Kwong) equation for ideal gases as fluid package for vapour phase reactions to yield liquid. Two case studies were performed (a) Pressure versus actual conversion (b) Temperature versus mole fraction for CO_2/ H_2 respectively. Results showed 0.98 conversion for methanol at a pressure of 2000kpa and temperature of 40^0C. The CO_2/ H_2 ratio was 0.5. More comprehensive research using modeling and simulation techniques was recommended.

The study of methanol synthesis from past years and from literature put into consideration a few chemical reactors such as slurry reactors, packed bed, and trickle bed reactors. These reactors, although efficient, showed some irregularities within the system such as wetting efficiency, flow irregularities and heat + temperature profiles (Hamad, 1992). Research from literature has not taken into consideration the use of the CSTR model as a preferred model for methanol synthesis. The use of CSTR models would eliminate the irregularities posed by the other reactors models from literature. The consideration of different catalyst effectiveness helps deduce the reactor performance and the fact that the CSTR model can be applied in a Methanol Synthesis reactor.

The research aim is to model and simulate a non-isothermal CSTR for Methanol Synthesis using different catalysts. The process objectives are:

i. To develop an unsteady state model for a Continuous Stirred Tank Reactor that can predict reactants depletion and product formation using three different catalysts (Al_2O_3/ZnO/Cu) based on the principle of conservation of mass.
ii. To develop a dynamic state model for a Continuous Stirred Tank Reactor that can predict the temperature progression in the reactor using three different catalysts (Al_2O_3/ZnO/Cu) based on the principle of conservation of energy.
iii. To write a MATLAB program to solve the developed models using plant data.
iv. To perform sensitivity study and process optimization on the overall performance of the reactor.

2. Materials and Methods

2.1 Reaction Kinetics

This research work focuses on methanol synthesis from CO and H_2 over $Cu/ZnO/Al_2O_3$ catalyst. The equation of reaction considers the various equilibrium reaction. The equation is written as:

$$CO + 2H_2 \leftrightarrow CH_3OH \quad (4)$$

Then, the reaction kinetic can be written as: $A + B \leftrightarrow C$

$$A + B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} C$$

Where:
A = CO
B = H_2
C = CH_3OH

$$K_{eq} = \frac{k_1}{k_2}$$

Journal of Newviews in Engineering and Technology (JNET)
Vol 4, Issue 3, December 2022
Available online at http://www.rsujnet.org/index.php/publications/2022-edition
e- ISSN: 2795-2215

2.2 Model Development for a CSTR

The model equations developed can predict the performance: concentrations of the reactant and products with time and temperature variation/ progression within the reactor with time. The principle of conservation of mass and energy were applied on the reactor to obtain the model equations.

2.2.1 Model to Predict the Concentration of Reactants and Product

The law of conservation of mass states that in a chemical reaction, mass can neither be created nor destroyed (Okun, 2009). Applying the law of conservation of mass into the development of the model to predict the concentration of reactants and product in equation 5.

The following Model Assumptions are considered:

i. The reactor mixture is well stirred, and the composition of the reacting mixture is uniform at any time. Thus, the composition of the exit stream is the same as that within the reactor
ii. Balance can be made about the entire volume of reactor.
iii. The shaft work done by impeller of the stirred tank is negligible.
iv. The process is non-isothermal.
v. The modelling is based on the Langmuir Hinshelwood rate expression (Amenaghawon & Okiemen,2011)

Journal of Newviews in Engineering and Technology (JNET)
Vol 4, Issue 3, December 2022
Available online at http://www.rsujnet.org/index.php/publications/2022-edition
e- ISSN: 2795-2215

$$\begin{pmatrix}\text{Rate of accumulation}\\ \text{of feed as product}\\ \text{wihtin the CSTR}\end{pmatrix} = \begin{pmatrix}\text{Rate of feed/reactant}\\ \textit{into}\\ \text{the CSTR}\end{pmatrix} - \begin{pmatrix}\text{Rate of feed/reactant}\\ \textit{out of}\\ \text{the CSTR}\end{pmatrix} \mp \begin{pmatrix}\text{Rate of feed/reactant}\\ \text{deplection/product formation due to}\\ \text{chemical}\\ \textit{reaction within the}\\ \text{CSTR}\end{pmatrix} \quad (5)$$

$$\frac{dC_j}{dt} = \frac{1}{\tau}(C_{jO} - C_j) - (-r_j)\rho_{catalyst} \quad (6)$$

Equation 6 is the model equation that predicts the Concentration of Reactants and product.

Performance Equation

$$CO + 2H_2 \leftrightarrow CH_3OH \quad (7)$$

For Carbon Monoxide, CO:

$$\frac{dC_{co}}{dt} = \frac{1}{\tau}(C_{co,O} - C_{co}) - (-r_{co}) \quad (8)$$

For Hydrogen, H_2:

$$\frac{dC_{H_2}}{dt} = \frac{1}{\tau}(C_{H_2,O} - C_{H_2}) - (-r_{H_2}) \quad (9)$$

For Methanol, CH_3OH:

$$\frac{dC_{CH_3OH}}{dt} = \frac{1}{\tau}(C_{CH_3OH,O} - C_{CH_3OH}) - (-r_{CH_3OH}) \quad (10)$$

2.2.2 Model to Predict the Temperature Variation in the Reactor

The law of conservation of energy states that energy can neither be destroyed nor created but can be converted from one form to another (Donev *et al.*, 2020). Appling the principle of energy balance to the development of the model to predict the heat effect on the non-isothermal reactor is given in equation below:

$$\begin{pmatrix}\text{Rate of accumulation}\\ \text{of energy}\\ \text{within the CSTR}\end{pmatrix} = \begin{pmatrix}\text{Rate of inflow}\\ \text{of energy}\\ \text{into the CSTR}\end{pmatrix} - \begin{pmatrix}\text{Rate of outflow}\\ \text{of energy}\\ \text{out of the CSTR}\end{pmatrix} \mp \begin{pmatrix}\text{Rate of energy released/absorbed}\\ \text{due to}\\ \text{chemical reaction within the CSTR}\end{pmatrix} \quad (11)$$

$$\frac{dT}{dt} + \frac{1}{\tau}T = \frac{1}{\tau}T_o - \left(\frac{\Delta H_R}{\rho C_{pj}}\right)(-r_j) \quad (12)$$

Equation 12 is the model equation that predicts the temperature variation in the reactor.

2.2.3 Rate of Reaction

The rate determining step reaction for methanol synthesis used was:

$$CO + 2H_2 \leftrightarrow CH_3OH \quad (13)$$

The catalyst considered is Al_2O_3/ZnO/Cu and the Langmuir Hinshelwood type rate expression was used. The rate expression for methanol synthesis using the Langmuir Hinshelwood rate expression (Amenaghawon & Okieimen, 2011) is given as:

$$r_j = \frac{K_r\left(P_{CO}P_{H_2}^2 - \frac{1}{K_{eq}P_{CH_3OH}}\right)}{\left(1 + K_{CO}P_{CO} + K_{H_2}P_{H_2} + K_{CH_3OH}P_{CH_3OH}\right)^3} \quad (14)$$

The rate expression was expressed in terms of concentration.

$$r_j = \frac{K_r\left(P_T\frac{C_{CO}}{C}P_T^2\frac{C_{H_2}}{C} - \frac{1}{K_{eq}P_T\frac{C_{CH_3OH}}{C}}\right)}{\left(1 + K_{CO}P_T\frac{C_{CO}}{C} + K_{H_2}P_T\frac{C_{H_2}}{C} + K_{CH_3OH}P_T\frac{C_{CH_3OH}}{C}\right)^3} \quad (15)$$

2.2.4 Non – Isothermal Models

The developed models with the rate expression incorporated in it:

Journal of Newviews in Engineering and Technology (JNET)
Vol 4, Issue 3, December 2022
Available online at http://www.rsujnet.org/index.php/publications/2022-edition
e- ISSN: 2795-2215

$$\frac{dC_j}{dt} = \frac{1}{\tau}(C_{jo} - C_j) - \frac{K_r\left(P_T\frac{C_{CO}}{C}P_T^2\frac{C_{H_2}}{C} - \frac{1}{K_{eq}P_T\frac{C_{CH_3OH}}{C}}\right)}{\left(1+K_{CO}P_T\frac{C_{CO}}{C}+K_{H_2}P_T\frac{C_{H_2}}{C}+K_{CH_3OH}\,P_T\frac{C_{CH_3OH}}{C}\right)^3} \quad (16)$$

$$\frac{dT}{dt} + \frac{1}{\tau}T = \frac{1}{\tau}T_o - \left(\frac{\Delta H_R}{\rho C_{pj}}\right) - \frac{K_r\left(P_T\frac{C_{CO}}{C}P_T^2\frac{C_{H_2}}{C} - \frac{1}{K_{eq}P_T\frac{C_{CH_3OH}}{C}}\right)}{\left(1+K_{CO}P_T\frac{C_{CO}}{C}+K_{H_2}P_T\frac{C_{H_2}}{C}+K_{CH_3OH}\,P_T\frac{C_{CH_3OH}}{C}\right)^3} \quad (17)$$

2.3 Determination of Model Parameters

The Model parameter used to perform the simulation and further evaluation of the reactor functional parameters are gotten from Amenaghawon and Okieimen (2011). MATLAB software program (Ode 45 Runge Kutta method) was used for the actual calculation of the non-isothermal CSTR Model with the rate kinetics incorporated in it. This would help to simplify the processing output data for the reactor.

Table 1 Shows Input Parameter

Parameter	Literature Value
k_{Co}	0.03186
k_{H2}	0.01932
k_{CH_3OH}	0.04668
k_r	0.00017
k_{eq}	0.67960
P_T	1300kpa

Source: (Amenaghawon & Okieimen, 2011)

The methods used to simulate the developed ODE using fourth order Runge-Kutta methods which is also known as classical fourth Runge-kutta whose algorithm are written as follows:

$$y_{i+1} = y_i + {}^1/_6(K_1 + 2K_2 + 2K_3 + K_4)h \quad (18)$$

In general form equation 14 may be written as:

$$y_{i+1} = y_i + \emptyset h \quad (19)$$

Where:

$$\emptyset = {}^1/_6(K_1 + 2K_2 + 2K_3 + K_4) \quad (20)$$

2.3.1 Sensitivity Analysis

The concentration of the inputs which is Carbon monoxide and Hydrogen (Independent variable) shall be altered to see the effect it has on the output concentration which is Methanol (Independent variable). Also, the concentration of the feeds can be expressed in terms of fractional conversion by using the relation:

Fractional conversion =

$$\frac{(Number\ of\ Moles\ in\ Feed - Number\ of\ Moles\ in\ Product)}{(Number\ of\ Moles\ in\ Feed)} \quad (21)$$

3. Results and Discussion

3.1 Components Concentration with Different Catalyst

The developed dynamic model equation in terms of reactants depletion and product formation with time were simulated using three different catalyst and presented thus:

Figure 2 below shows the profile plot of product (CH_3OH) formation with time using different catalyst. After 50 hrs, CH_3OH with an initial Conc. of 0mol/l using Al_2O_3 Catalyst increased to 0.5745mol/L, with ZnO catalyst it increased to 0.5824mol/L and that of Cu

Journal of Newviews in Engineering and Technology (JNET)
Vol 4, Issue 3, December 2022
Available online at http://www.rsujnet.org/index.php/publications/2022-edition
e- ISSN: 2795-2215

catalyst increased to 0.5919mol/L showing copper catalyst as the catalyst with the higest rate of reaction. The graph also shows that concentration was increasing with time for all three catalyst.

Product formation with Time using different Catalyst.

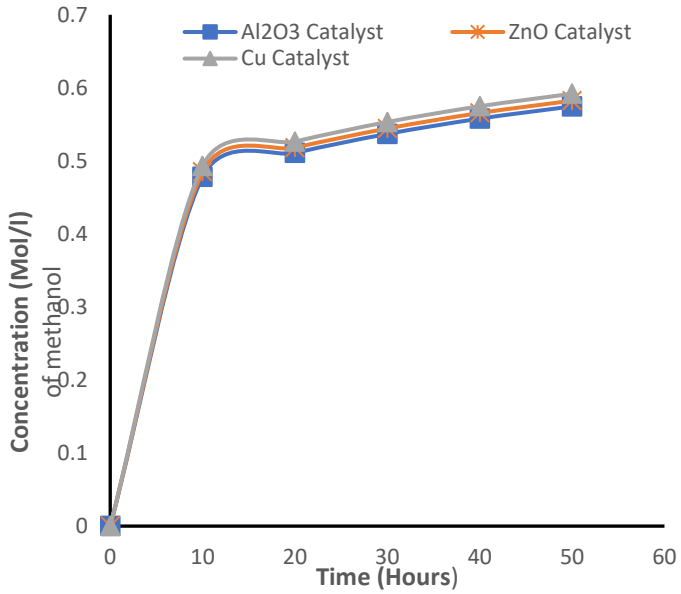

Figure 2: Product formation with Time using different Catalyst

Figure 3 below shows the profile plot of Temperature variation with Time using different catalyst. After 50 hrs, using Al_2O_3 Catalyst with a starting temp. of 488k, the temperature increased 534.41k, with ZnO catalyst the temp. was 552.97k and that of Cu catalyst was 592.42k. All three catalysts showed a variation in temperature but all variations are within the stipulated temperature for methanol synthesis.

Temperature Variation with Time using Different Catalyst

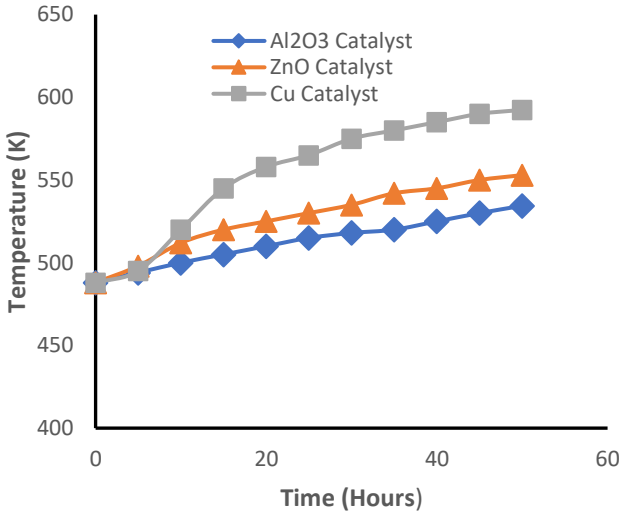

Figure 3: Temperature Variation with Time using Different Catalyst

3.2 Model validation

Model validation helps determine the model accuracy under the condition of its intended use.

Table 2 below shows the results of the simulated CSTR models with three different catalyst which is compared with literature data.

Table 2 Model Validation with Al_2O_3 catalyst

Components	Model result	Literature Data (Abdelghamy & Nassar 2011,)	Deviation
CO	0.1078	0.0512	1.11
H_2	0.0025	0.3097	0.99
CH_3OH	0.5746	0.3670	0.56
Temp(K)	534.41	530	

Source: Abdelghamy & Nassar, 2011

Journal of Newviews in Engineering and Technology (JNET)
Vol 4, Issue 3, December 2022
Available online at http://www.rsujnet.org/index.php/publications/2022-edition
e- ISSN: 2795-2215

Table 3: Model Validation with ZnO Catalyst

Components	Model result	Literature Data (Abdelghamy & Nassar 2011,)	Deviation
CO	0.1025	0.0512	1.00
H_2	0.0222	0.3097	0.93
CH_3OH	0.5823	0.3670	0.59
Temp(K)	552.97	530	

Source: Abdelghamy & Nassar, 2011

Table 4: Model Validation with Cu Catalyst

Components	Model result	Literature Data (Abdelghamy & Nassar 2011,)	Deviation
CO	0.0960	0.0512	0.87
H_2	0.0182	0.3097	0.94
CH_3OH	0.5919	0.3670	0.61
Temp(K)	592.42	530	

Source: Abdelghamy & Nassar, 2011

3.3 Effect of Varying reactants Concentration

The effect of increasing the concentration of Carbon monoxide while keeping the concentration of Hydrogen constant to produce methanol was investigated and presented Figure 4 to 6 below.

As seen from Figure 4 below, concentration of Carbon monoxide and Methanol is increasing, and fractional conversion of Carbon monoxide and Hydrogen are 86% and 93% respectively.

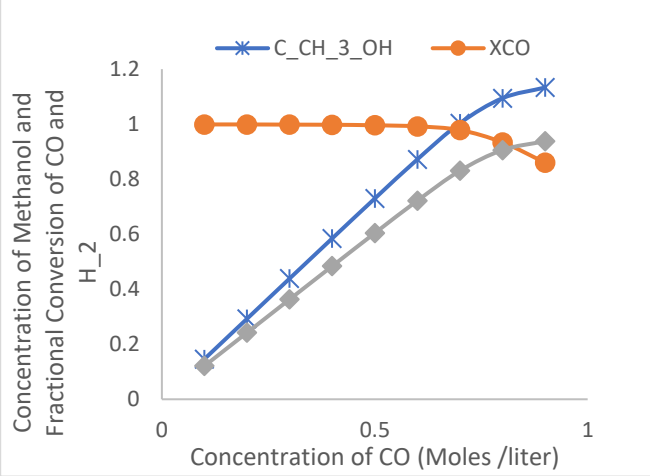

Figure 4: Concentration Profile of methanol with carbon monoxide

The effect of keeping the concentration of Carbon monoxide constant which increases the concentration of Hydrogen to see the effect on the output product methanol was shown on Figure 5.

As seen from Figure 5 below, Concentration of Hydrogen and Methanol is increasing, and fractional conversion of Carbon monoxide and Hydrogen are 99.99% and 33.68% respectively.

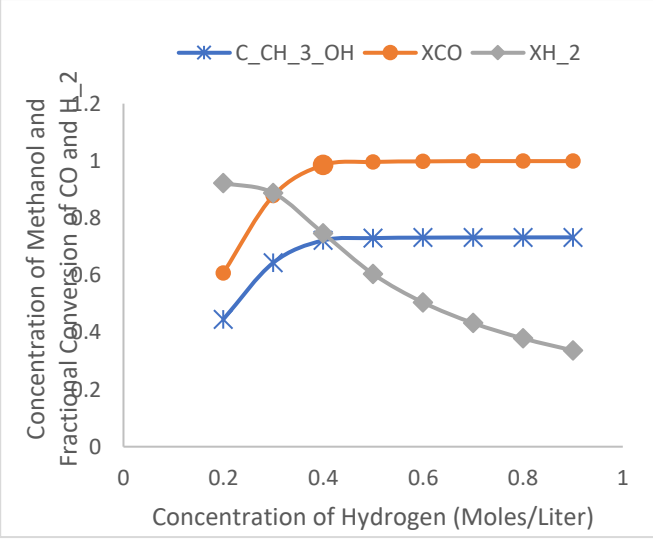

Figure 5: Concentration Profile of methanol with Hydrogen

Journal of Newviews in Engineering and Technology (JNET)
Vol 4, Issue 3, December 2022
Available online at http://www.rsujnet.org/index.php/publications/2022-edition
e- ISSN: 2795-2215

The effect increasing the concentration of Carbon monoxide and Hydrogen with equal amount was considered to see the effect on the output product methanol was shown on Figure 6.

As seen from Figure 6 below, Concentration of Hydrogen, Carbon monoxide and Methanol are increasing, and fractional conversion of Carbon monoxide and Hydrogen are 99.88% and 60.56% respectively.

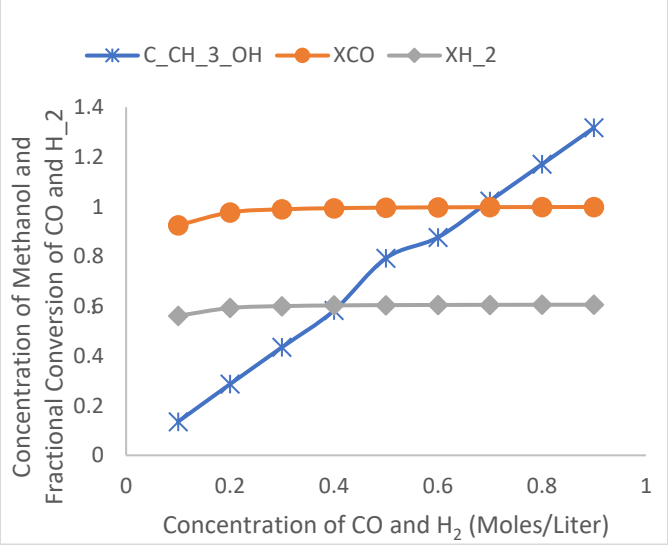

Figure 6: Concentration profile of Carbon monoxide, Hydrogen with methanol

4. CONCLUSION

A non-isothermal Continuous Stirred Tank Reactor model has been modelled and simulated for Methanol Synthesis through hydrogenation of Carbon monoxide. The use of three catalysts: Al_2O_3, ZnO, Cu was investigated to ascertain the catalyst effectiveness and the following conclusions was made:

i. For all three components, the fractional conversion using copper catalyst has the highest percentage making copper-based catalyst the best for Methanol Synthesis.
ii. The effect of the catalyst on all three components shows that Hydrogen, H_2 is the limiting reactant because it the reactant present in the least amount.
iii. All three-catalyst was used to analyse the temperature progression. The progression shows they are good and still falls within the range of temperature for methanol synthesis.
iv. The Langmuir Hinshelwood type rate expression can be expressed in terms of concentration.

Most research work uses the tubular or plug flow reactor for methanol synthesis. However, this research shows that a continuous stirred tank reactor can also be an effective alternative for methanol synthesis.

5. RECOMMENDATIONS

Based on the research done on the modeling and simulation of a non-isothermal CSTR for methanol synthesis, the following recommendations are made:

i. Experiments should be conducted to obtain kinetics data for the simulation of the developed models to evaluate the fitness of the data obtained from laboratory experiment to literature data.
ii. Other Kinetic models stated in literature can be used to evaluate Methanol Synthesis to evaluate the suitability of the models to data gotten from Laboratory experiment.
iii. Controller mechanism can be added to the reaction process to reduce the reaction time while still maintaining the same quality of production.

Journal of Newviews in Engineering and Technology (JNET)
Vol 4, Issue 3, December 2022
Available online at http://www.rsujnet.org/index.php/publications/2022-edition
e- ISSN: 2795-2215

.

REFERENCES

Abdelghany, A & Nassar, A. (2011). Optimizing the Production of Methanol from Syngas in the Fixed Bed Reactor at Lurgi Process. *Applied Catalysis*, 37(2), 54-72.

Alan, H. (1999). Chemical Modeling: from Atoms to Liquids. 1st Edition. ISBN 978-0471999034. Wiley Publishers. Online. Accessed 18/07/2021.

Amenaghawon, A. & Okieimen, C. O. (2011). Dynamic Modeling, Simulation and Optimization of an Isothermal CSTR for Methanol Synthesis. *Journal of the Nigerian Society of Chemical Engineers*, 26, 36-47.

Carsten, S., Daliborka, N., Matthias, F., Menka, P., Andreas, S. & Achim, K. (2021). Optimization of Methanol Synthesis Under Forced Periodic Operation, Processes. 9, 872. http://doi.org/10.3390/Pr 9050872.

Daaniya, R. (2012). Kinetic Modeling of Methanol Synthesis from Carbon Monoxide, Carbon Dioxide and Hydrogen over a Cu/ZnO/Cr_2O_3 catalyst. *Master's Thesis*. 4162. San Jose state University DOI: https://scholarworks.sjsu.edu/etd_theses/4162.

Donev, J., Allison, C., Hanania, J., & Jenden, J. (2020). Energy Education-law of Conservation of Energy.http://energyeducation.ca/encyclopedia/law_of_conservation_of_energy [Retrieved: Sept. 5th,2021].

Hamad, A. A. (1992). A Kinetic Study of Methanol Synthesis in a Slurry Reactor using a CuO/ZnO/Al_2O_3 catalyst. Kuwait University.

Issa, I. (2015). A Model and Simulation of Methanol Synthesis System. *Master's Thesis*. University of Gezira.

Kuozynski, M., Browne, W., Fontein, H., & Westerp, K. (1987). Reaction Kinetics for the Synthesis of Methanol from CO and H_2 on a Copper Catalyst, Chemical Engineering Process. 21, 179-191.

Okun, L. B. (2009). Energy and Mass in Relativity Theory. *World Scientific,* 20(2), 978-981.

Taylor, G. (2021). Non-Isothermal CSTR Simulation. Salt Lake City, UT 84112-9203(801) 581-6915.

Vincenzo, P., Eugenio, M., Concentta, R., Marco, M., & Antonio, R. (2018). Methanol Science and Engineering. University of Salemo, Fisciano, Italy.

Wordu, A. A., Akpa, J. G., & Elenwo, B. I. (2019). Design and optimization of system of CSTR for Methanol Production. *International Journal of Innovative Research & Development, 8*(2), 2278-2298.

NOMENCLATURE

Symbol	Definition	Unit
r_j	Rate of reaction	mol/m^3/hr
C_{jo}	Initial Concentration	mol/L
C_j	Final Concentration	mol/L
τ	Space time	hr
P_T	Total reactor pressure	kPa
C_{co}	Conc of CO	mol/L
C_{H_2}	Conc of H_2	mol/L
C_{CH_3OH}	Conc of Methanol	mol/L
C	Total Concentration	mol/L
T_0	Initial Temp	K
T	Final Temp	K
ΔH_R	Heat of Reaction	kJ/mol
C_{pj}	Specific heat or ren	kJ/kg
K_{CO}	Kinetic for CO	-
K_{H_2}	Kinetic for H_2	-

Journal of Newviews in Engineering and Technology (JNET)
Vol 4, Issue 3, December 2022
Available online at http://www.rsujnet.org/index.php/publications/2022-edition
e- ISSN: 2795-2215

K_{CH_3OH}	Kinetic for Methanol
K_{eq}	Equilibrium constant
j	CO, H_2, CH_3OH
C	Carbon Monoxide
H_2	Hydrogen
CH_3OH	Methanol
Al_2O_3	Aluminum Oxide
ZnO	Zinc Oxide
Cu	Copper