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Mathematical Modeling and Process Simulation of Packed Bed Reactor for Methanol Synthesis from Carbon Dioxide Hydrogenation

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Abstract: *Due to increase in carbon footprint, and demands for effective sequestration of carbon dioxide for clean environment, this work focused on the kinetic and thermodynamic modeling of a packed bed reactor (PBR), for methanol production from CO_2 hydrogenation. The system kinetics and thermodynamics are being modelled via application of the fundamental principles of mass, energy and momentum at steady state with negligible catalytic effects, such that the space time, reactor's length, volume, and heat transfer are structured as function of the concentration gradient of the system feed (CO_2 and H_2), such that depletion of the feed concentration into methanol act at proportionate bases to changes at the reactor performance parameters. Sensitivity of the mathematical models over the studied system were was achieved using MATLAB, and results depicts that increase in the fractional conversion of methanol production system promotes the depletion rate of CO_2 concentration from 87.3452 mol/m^3 to 39.2105 mol/m^3 with a change in the packed bed reactor (PBR) volume to 13.5155m^3 at 99% fractional conversion of the system with a 1.4452m reactor's length attained over 1.6413 min space time, yielding 94.29% methanol (MeOH) of 103.0486 mol/m^3 concentration at exothermic (heat loss) bases. Results achieved from the sensitivity assessment of the developed kinetic and thermodynamic models were in agreement with most presented by other researchers on similar system though using different modeling techniques, which proves the accuracy of the developed models achieved in this work for methanol synthesis from CO_2 hydration in a PBR system.*

Keywords: reactor performance, kinetics, MATLAB, greenhouse gases (GHGs), methanol additive, environmental pollution, space time, rate law, Daltons law of partial pressures, material balance

INTRODUCTION

Globally, this current era of life suffers greatly from effects of environmental and atmospheric pollution, and this has created diverse methods, ideas and concepts towards the remediation of industrialized and populated regions, which have been identified to have been suffering the most form factors or effects

generated from contaminants present in the environment. Environmental pollution can be rooted to different paths, but one of the greatest roots is the production, processing and utilization of fossil. Solid waste gasification, incineration, wrongful deposition of wastes, and bush burning though contributes impurities such as CO_2 into the atmosphere but not comparable with the amount generated from daily gasoline incomplete combustion, industrial gas flaring, crude oil processing and treatments, coal burning, etc. All the above-mentioned process are the promoters or roots of greenhouse gas (GHGs) in the atmosphere which CO_2 is rated among the highest in their pollutants group (Tsitsi and David, 2021; Ugi *et al.,* 2023; Perry's and Green, 2007) that can promotes materials deterioration du to corrosion (Ugi *et al.,* 2023; Benedict and Fredrick, 2023, Benedict *et al.,* 2022; Ugi *et al.,* 2023; Ugi *et al.,* 2026; Ugi *et al.,* 2021). Environmental contamination and atmospheric pollution facilitated by the continual growth in greenhouse gases (GHGs), which is generated from industrialization and technological elopements as earlier said, as well as from man's dependency on fossil fuels consumption and solid waste incineration, has become a point of great concern to the world as large, such that the world mission 2050 seeks to eradicate GHGs presence, for clean and healthy environments (Ugi *et al*., 2023). Advancement in industrialization, increase in population, and high dependency of man's towards benefits of crude oil / fossil fuels tends to make this mission a hard goal to be achieved perfectly and functional. Highly industrious areas like the USA, Russia, as well as populated regions such as China faces lots of negative effects of GHGs in the atmosphere, which promotes the formation of acidic rain, promotes cancerous cells formation, destroys one's vision or eyes.

Honestly, the environment is not the only path affected by pollutants contributed from fossil fuel and GHGs promotive activities, human's health as well that of microorganisms are exposed to same effects which systematically impact social and economic status of the region. In 2019, over nine (9) millions of people in the world were killed as a result of environmental pollution and from the mortality rate air pollution was rated as the lead of over three-quarters of the overall 9 million (Fuller *et al.,* 2022). Researchers depicts that anthropogenic chemical pollution has outgrown the planetary boundaries hence threaten the entire ecosystems (Persson, 2022; Pandey *et al.,* 2020). According to Manisalidis *et al.,* (2020), air pollution is currently classified among the world greatest scourges with higher effects in this present era, such which render high degree of life threats to human as well as to climatic change which accounts daily increase in public and individual morbidity as well as mortality. There are different types of contaminants that affects human health in different ways, among them is Particulate Matter (PM), which are tiny particulates of dust with abilities of penetrating into the lungs via inhalation, leading to serious cardiovascular and respiratory diseases and others as seen at Figure 1.

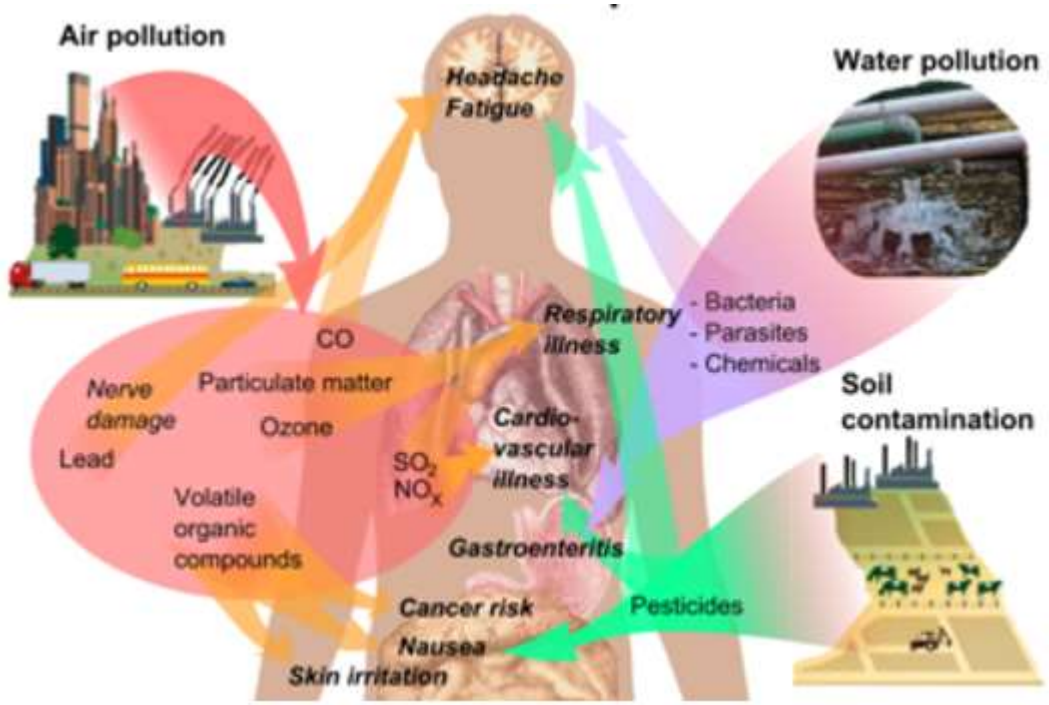

Fig.1: Health effects of environmnetal pollution on life

According to Shetty *et al.* (2023), continual increase in diseases faced by humans on daily bases is attributed to **n**umerous contaminants significantly found in the environments, which purses the abilities of promoting climatic change which all results to increase in morbidity and mortality. Continues exposure to contaminants from fossil as well as those from poor wastes management is a key reason to promote wastes management, for appropriate wastes manages promotes good health, safe environment as well as increase wealth. Most times humans wait until they are been affected before the provide suitable solutions, same is in the case of environmental pollution which presently has been presented with multiple solutions to remediates the contaminated regions and restore good and healthy living A better understanding connecting environmental toxins and human health is a great deal that will resolve the continual increase in mortality that the world is currently recording factored to environmental pollution.

Fossil fuels are organic composites energy source that are used in different sectors of the world as fuel, and their usage promotes massive release of carbonated compounds such as carbon dioxide (CO_2) and methane (CH_4) which are the primates of environmental thermal pollution, air contaminations as well as reduction in quality agricultural cultivation. They are in common term referred to as the greenhouse gases (GHGs), and their presence is faced in all corners of the worlds that depends on fossil fuel as energy source. Greenhouse gases promotes massive climate change and global warming, of which effects are

destructive to mankind and other organisms (Ugi *et al.*, 2023). According to Khozema *et al.*, **(**2020) climate change as a factor has gain a considerable stand of concern in the world especially during this anthropocentric era. Researchers and Scientists strongly believe that global warming rate and the rate of climatic change varies proportionally (directly) with increase in GHGs concentration (Ugi *et al.,* 2023), especially that of the carbon dioxide. Though the global warming effects due to GHGs has a tendency to be reduced starting from the applications of minor measures such as algae cultivation, to the major or classical measures, which assist in CO_2 capturing. According to John (1997), microalgae are microscopic plants capable of being cultivated in a large open pond, such that among other technologies known for capture and utilization of CO_2, when cultivated holds a great deal of reducing the CO_2 amount from the atmosphere. But the requirements for its large-scale cultivations, starting from the land size to favorable climate, and the ample of required water supplies, greatly restrict the effectiveness of the technology.

The existence of these GHGs in the environment is a key driver of climatic change as well as global warming, which is known to affects both agricultural, economic, social and health status of life**.** Exposure to heat especially that resulted from global warming which is factored by climate change can lead to high dehydration and heat stroke, as well global warming facilities cardiovascular, cerebrovascular and respiratory disease. (Crimmins *et al.*, 2016; Luber *et al.*, 2014) Protections from PM as well as from heat effects is a thing which looks easier to be applied by everyone but despite how it seems it requires capital, and that makes it not applicable by low-income enders or households (Luber *et al.*, 2014)**.**

With the rising state of anthropogenic global warming most research bodies and scientific communities has held conviction and research about the reality of anthropogenic heat effects as global warming. The warnings have prompted the United Nations Environment Program (UNEP) and the World Meteorological Organization (WMO) to form the Intergovernmental Panel on Climate Change (IPCC) board in 1988, to help address and control industrial activities as well as those of domestic actions that promotes or generates greenhouse gas emissions. The IPCC report of 2018 was able to depict that since preindustrial times human activities have been majorly responsible for 1.4 and 2.2 °F (0.8 and 1.2 °C) increase in the worldwide average temperature increase, and that even the global warmings effects that will experienced within the most of the 20th century could be due to increase in human activities, especially that which involves the burning and processing of fossil fuels. (Gaur *et al.*, 2024)

Fossil fuels are products of organic matters that has undergoes composition and molecular restructuring at suitable chemical reactive environments. In general form, it is fossil fuels which could either be solid, liquid and gases in form (coal, crude oil and natural gas) are products of hydrocarbons that are generated over a long period decomposition of organic matters at suitable operating temperature and pressure. Crude oil consist majorly of paraffins, aromatics and naphthenes, and all of them are made up of hydrocarbons chains which when decomposed generates lots of pollutants, of which CO and CO_2 are listed as the most

dominating generated contaminants achieved from the combustion of either of the crude oils fuel types; solid Contaminants generated from crude oil varies between the type, composition, nature of formation and degree of microbial deformation rate of organic matters, and these contaminants in most cases are been reduced during the processing of crude oil before its refining.

Generally, after the recovery of oil and gas from the reservoir, the oil is been sent to the refinery where different process come to play vital roles that enables crude oil processing, yielding energy base products such as gasoline, and some essential petrochemicals (Ugi *et al.*, 2023; Ugi *et al.*, 2025; Sammy *et al.*, 2023; Benedict and Fredrick, 2023, Igwe *et al.*, 2026; Ogolo *et al.*, 2026). Some of the processes that takes place in the refinery includes crude oil preprocessing, down streaming, reforming, cracking, products quality enhancement, etc. Above all mentioned, one of the most interesting and complicated process is that which involves the down streaming of the recovered crude oil in a distillation column into light and heavy chain hydrocarbons called distillates, which includes gasoline, kerosene, diesel and other heavier distillates such as asphalt and lubricants. Products of the distillation column are precursors to so many other daily consumable products and utilities such as detergent, dissolvers, plastics; cosmetics, insecticides, lube base oil, solvents, textiles, refrigerants, paint, synthetic rubber, fertilizers, additives, pharmaceuticals, etc. Crude oil processing focuses on removal of impurities such as Sulphur from oil stream (Ugi *et al.*, 2023; Perry's and Green, 2007; Wordu *et al.*, 2023), and as demands for cleaner environments keeps increasing, the cost for effective treatment of crude oil as well as qualitative refining of the oil stream to reduce the degree of contaminants and reduction in the CO_2 emission of crude oil distillates used as combustible engine fuels , increases.

Crude oil contaminants are in mostly exposed to the environment during the production, processing and utilization of crude oil products as well as other fossil fuels. Carbon dioxide (CO_2) among all other possible impurities, is mostly released into the atmosphere due to incomplete combustion of fossil fuel. As human activities on earth increase, so as well their consumption rate of fossil fuels proportionally increases (Ugi *et al.*, 2023), so keeping the concentration of CO_2 in the environment at a continual increasing rate. This combustion effects of crude oil as well as other fossil fuel types is always assesses based on the CO_2 concentration of an environment, of which industrialized zones (Figure 2), and over populated regions are always rated to suffers most of the contamination effects generated from CO_2 concentration increase promoted by continual exploration, processing and utilization of crude oil products as fuel / energy source, petrochemicals, etc. Crude oil among all others is listed as the most abundantly utilized section or group of fossils (Sammy *et al.*, 2023; Igwe *et al.*, 2026) that generates more than 75% of the active GHGs in today's atmosphere (Ugi *et al*., 2023). Crude oil products are used as fuels in automobile engines as well as all other heavy load engines. Also, fossil products are used and discarded always by man, and the hydrocarbon composites when fed by microorganisms promote the concentration of GHGs in the environments.

Greenhouse Gases (GHGs) are mainly acidic gases of carbon, nitrogen and chlorofluorocarbons (CFCs and HCFCs). That purses the abilities of promoting greenhouse effects, which contributes to environmental heating (Karl and Trenberth, 2003). These gases actively reduce the available environmental oxygen as well as affects the environmental durability especially in thermal environments, due to their promotive abilities to environmental thermal pollution. The five most abundant greenhouse gases, listed in decreasing order of average global mole fraction, are water vapor, carbon dioxide, methane, nitrous oxide, and chlorofluorocarbons (CFCs and HCFCs). Water vapor causes about half of the greenhouse effect, acting in response to other gases as a climate change feedback. The presence of GHGs and other contaminants in the environment promotes the Global Warming Potential (GWP) of an environment. GWP is a measure of how much energy a greenhouse gas (GHG) traps in the atmosphere over a specific time period, compared to carbon dioxide (CO_2). Different GHGs have different GWPs, so those with greater values such as the Sulfur hexafluoride (SF_6) will raise more effects on the environment over time than compared. Gases with higher GWP absorbs more energy per pound, and thus contribute more environmental thermal pollution. The removal of greenhouse gases from the atmosphere is also among the world's quest to creation of suitable environment for human. According to Ou *et al.* (2021) a stabilized climate change that will have to be well below the temperature range of 2 °C to 1.5 °C, requires the world to be of a comprehensive GHGs mitigation state, such that will mitigate both the CO_2 gases as well as the non-CO_2 gases emissions. They postulated in their research that when non-CO_2 mitigation contributions are incompletely implemented, the timing for a net-zero CO_2 environment will be achieved within two decades.

Fig. 2: Atmospheric pollution contributions by crude oil refining processes

Though Sulphur is one of the contaminants of crude oil streams that also promotes global warming, but its effects and concentration in the environment is quite lesser when compared to the carbonic gases (such as CO_2), and this is because some of the sulphur in crude oil such as the mercaptans, are first desulphurized before the crude oil is been refined, leaving a very small and insignificant amount in the useable fuel oils though still dangerous to health over a long period of gasoline usage. Sulfur dioxide (SO_2) which is a colorless but toxic smelling gas that irritates the eyes especially when concentrated, is a nonflammable gas that is essential for production of multiple products but as well keyed as a well-known thermal pollutant**.** Sulfur has been identified to be very effective in the wearing out or degradation of industrial materials especially those made from metals, and supportive works have been done relating to sulfur and its corrosion contributions to oil and gas industrial loses, as well as the methods of remediating sulfur corrosion effects via use of inhibition, electricity, etc. Multiple researchers have identified the effects of Sulphur and its oxides on corrosion of metals and industrial utilities (Benedict and Fredrick, 2023, Benedict *et al.,* 2022; Ugi *et al.,* 2023; Ugi *et al.,* 2026; Ugi *et al.,* 2021). Benedict and Fredrick *et al.* (2023) identified the performance of sulfur in the presents of water to be catastrophically corrosive. In their experiment\ in which they assess the corrosive effects of Sulphur via elemental sulfur hydrolysis in sulfur-mild, sulfur was highly identified to be effectively reactive in water at elevated temperature above ambient as well as that greater than 80°C of which significant acidification corrosion was noticed.

Sulfur dioxide continual emissions as well as its presence in the environment is the greatest precursor of acid rain formation, and global warming; though cannot absorb infrared radiations, but when oxidized it will. Due to these effects, countries such as the United States generate a means whereby the SO_2 will be burnt into some useful chemical compounds in some of the industrial processing such as the desulphurization and processing of crude oil, leaven CO_2 as one of the greatest environmental effects arising from the continual utilization of crude oil. Carbon dioxide (CO_2) among others is one of the basic primary GHGs with about 100 years global warming ability, generated from human daily activities. CO_2 is an odorless and colorless gas that consist 0.04% of the atmosphere as a one of the mixtures of environmental air. Carbon dioxide as a gas is 53% denser than normal dry air, but when assessed on the bases of gas mixability, CO_2 has a longer existence and mixability in the atmosphere.

CO_2 is contributed daily into the atmosphere in a very large amounts, of which some of it is been adsorbed into water bodies via ocean carbon sinking process, and this takes place effectively hence CO_2 is partially soluble in water, and some amounts are been consume by plants and others are been adsorbed by the soil microbes. Although this compound (CO_2) is naturally and actively present in atmosphere as air composites, due to carbon cycle (circulation of the gas among atmosphere, plants, animals as well as oceans). But human activities based on usage of fossil fuels (coal, natural gas, and crude oil), solid waste, trees and other biological materials, CO_2 yielding reactions, promotes the CO_2 amount at the atmosphere, making it a pollutant with a great effect to the environment. Despite the multiple attempts made by

researchers, the sequestration (removal) of CO_2 from the atmosphere tends to be an impossible remedy to the developed and industrialized communities. The emission of CO_2 is as a result of the following activities of man and many more;

i. Use of fossil fuels by automobile engines.
ii. Fossil utilization for Electricity**.**
iii. Industry chimneys and gas flaring processes**.**

The presence of CO_2 in the environment do not only promote thermal pollution, but as well contributes to acidic rain formation which when in contact with the skin promotes the formation of cancerous cells which are very hazardous to life. Also, CO_2 promotes the increase of corrosion on metallic materials which are exposed to acidic rain, leading to machine and equipment's failure. Reducing the rate of emission of carbon for oxidation is a quest of almost all the crude oil producing zones of the world, but the truth remands that the most effective approach is by reducing or stop (if possible) the use of fossil fuels, and to do this, a new form of energy source needs to be discovered; such that will be more efficient than fossil energies. The Carbon Capture and Sequestration (CCS) method is a vital area in environmental sciences which assist in remediation of environments from carbon oxides effects. CCS method involves the capturing and sequestration of Carbon dioxide using modern technologies that can possibly and potentially mitigate CO_2 or reduce its emissions from the environment and atmosphere. The processes that are applied as technologies of CCS methods are all focused on the carbon capture, utilization, and storage of environments (Sekera & Lichtenberger., 2020). Some of these techniques includes industrial stacks control, calcium looping (CaL) technology, geological carbon sequestration, CO_2 pipeline transportation, biotechnological approach which uses green plants cultivation or algae culturing, calcium looping process, etc. (Kazlou *et al.,* 2024; Hepburn *et al.,* 2019; Martin-Roberts *et al.*, 2021). According to Tahreem *et al.* (2022), one of the most promising solution to carbon dioxide concentrated environment remediation is the application of microalgae. They are identified to be very active in carbon capture and utilization (CCU) system with a highly proven facts over is CO_2 reducing abilities in real life systems. Tahreem *et al.* focused their research on disclosing CO_2 fixation process through green approach as measure of CO_2 removal from contaminated environment, using Dictyosphaerium sp. of *DHM1* & *DHM2* strain (as a novel microalgal species).

According to Cordoba-Perez & de-Lasa (2021), photosynthesis which is a system of plants utilizing CO_2 from an environment in the presence of sunlight fundamentally converts bicarbonates via *Chlorella vulgaris* photosynthesis, to effective energy used by the plants as their fundamentals of surviving. In such one can effectively obtain biofuel from the system which can be used as a carbon dioxide emission free energy source.

According to Abraham *et al.* (2023), the introduction and application of microalgae cultivation in environmental pollution control, is considered as an attractive and effective measure of negative emission technology (NET) due to algae abilities of removing or consuming environmental CO_2 from contaminated atmosphere as well as from flue gases. Some of the microalgae consume CO_2 from the environment in the form of bicarbonate (HCO_3^-) for survival. Conventional carbon mineralization approach is another NET concept of carbon capturing, such that deals with the fixing of carbon oxide into carbonate minerals generating compounds such as calcite ($CaCO_3$), nesquehonite ($MgCO_3$-$3H_2O$), magnesite ($MgCO_3$), nahcolite ($NaHCO_3$), etc., which serves as precursors to production other essential products such as cosmetics.

Among all the CCS methods identified in this work, the calcium looping (CaL) process or technology which is also known as the Regenerative Carbon Cycle (RCC), is one of the most effective measures to carbon dioxide sequestration. The process is mostly applied in cement production industries, power plants, and hydrogen production system. The CaL process which requires a lot or series reversable chemical reactions is a two-way chemical process (Blamey, *et al.* 2010);

i. **Carbonation process**: which takes place at a temperature of 650-950 °C and requires the use of calcium oxide (CaO) as sorbent which reacts with CO_2 composite in gas stream to form calcium carbonate ($CaCO_3$)
ii. **Calcination process**: this is the second phase of the system in which the calcium carbonate ($CaCO_3$) formed is heated and decomposed into CaO and a nearly pure CO_2 gas stream which separately can be perfectly used for their perspective purposes.

In most cases the CaO separated from the Calcination process is been reused to capture more of the CO_2 from the environment, as a cost and time conservative measure. While the CO_2 captured via carbonation and separated via calcination is been effectively used as a precursor to essential chemicals such as methanol, ethanol as well as other fuel oils. The carbonator's is a special reactor type that operates at a temperature of 650-950 °C suitable for exothermic processes that are of low reaction rate, such as that of carbonation step in CaL system. Similarly, the calcinator is also an autoclave reactor but operates at reactor temperature >850 °C The reactor balances the increased rate of reaction which comes from the calcination process at higher temperatures.

CaO-based sorbent used in CaL process is a typically product mostly derived from limestone, is a fundamental composite that favors CO_2 capturing. It reacts with the carbon dioxide composite of gas stream via reversible reaction, in which the forward process which is endothermic is referred to as **calcination** while the reversed process is referred to as **carbonation**, which is exothermic. For capturing of CO_2 a stream of gas consisting CO_2 is been fed into a carbonator where the exothermic process takes

place; reacting CaO with the CO_2 in the gas stream, before been passed into the calciner reactor where the CO_2 is been separated from the $CaCO_3$ formed from the carbonator, to enable the CO_2 separated and trapped or captured for either for further usage or restriction from the environment (sequestration), while the separated CaO is been recycled into the carbonator to improve its initial concentration to be used as a fresh (reactive) Ca-sorbent for effective capturing. The final unreactive Ca-sorbent will be passed to cement production unit.

According to Ugi *et al.* (2023) in his work where environmental wastes were converted efficiently into petrochemicals and gasoline-based fuel using special catalyst, he stated clearly that "***Waste is wealth when effectively and efficiently managed, hence wastes shouldn't be wasted***". Methanol is wealth and is achievable from wastes when not wasted. Methanol among the others generatable from CaL process is essentially used as additive as well as fuel in substitute to gasoline in some developed countries in the world. Methanol (also called methyl alcohol and wood spirit, amongst other names) is an organic chemical and the simplest aliphatic alcohol, with the formula CH_3OH (a methyl group linked to a hydroxyl group, often abbreviated as MeOH). It is a light, volatile, colorless, flammable liquid with a distinctive alcoholic odor similar to that of methanol (potable alcohol). (*National Institute for Occupational Safety and Health, 2008*) A polar solvent, methanol acquired the name wood alcohol because it was once produced chiefly by the destructive distillation of wood. Today, methanol is mainly produced industrially by hydrogenation of carbon monoxide. (*Fiedler et al, 2005*), methanol is an organic compound with the following properties; Molar mass: 32.04 g/mol, Boiling point: 64.7°C. Density: 792 kg/m³. Vapor pressure: 13.02 kPa, Melting point: -97.6 °C, Classification: Alcohol. Methanol is the precursor to most simple methylamines, methyl halides, and methyl-ether. (*Fiedler et al, 2005*) Methyl esters are produced from methanol, including the transesterification of fats and production of biodiesel via transesterification.

Methanol can as well be used as additive to gasoline, to produce an efficient fuel known as methyl tertiary butyl ether (MTBE) which can have lower emissions than conventional gasoline. Methanol properties makes is a perfect antifreezer especially in windshield washer fluid, it presents the fluid from freezing by influencing its boiling points. In natural gas transportation methanol is been injected into the pipeline to lower the gas freezing point for save and speedily transport.

Fig 3: Methanol as additive and fuel for internal combusion engines

Methanol is of a higher octane rating (114) compared to gasoline (90 – 97) hence serves as fuel in some automobile vehicles (Figure 3). Methanolof lower volatility and burns even at temperature lower than that capable of combusting gasoline, hence methanol is of higher thermal efficiency and power output in engines, but consumes faster, but when added to gasoline as additives it improves the quality and octane number of the gasoline, given it a high calorific value (Gassoumi *et al.*, 2023). Methanol is also a good fuel additive, not just with its good abilities of increasing the octane number of gasoline stream, but also reduces the CO_2 generative abilities of fuel, which is a good combustion property for perfect environmental and atmospheric health.

Few researchers have made attempts in producing methanol from carbon dioxide and very few effectively model a suitable reactor for high performance of the system. According to Sreetama *et al.*, (2021) Catalytic hydrogenation of CO_2 to methanol has gained considerable interest for its significant role in CO_2 utilization using heterogeneous catalysts. Their study proposes a kinetic model based on Langmuir-Hinshelwood-Hougen-Watson (LHHW) mechanism for CO_2 hydrogenation to methanol over a highly effective indium oxide (In_2O_3) catalyst. Their work focuses on different reaction conditions mainly revolving around the variation of operating temperature, total reactor pressure, H_2/CO_2 molar feed ratio and weight hourly space velocity (WHSV) of the system. The experimental data were modeled using a

competitive single-site kinetic model based on LHHW rate equations. A parameter optimization procedure was undertaken to determine the kinetic parameters of the developed rate equations. The model predicts that when the methanol synthesis reaction becomes equilibrium limited, the progress of the RWGS reaction forces the methanol yield to decrease due to the reversal of the methanol synthesis reaction. A mixture of CO_2 and H_2 has been used as the reactor feed in all the cases. Significantly with respect to the CO_2 partial pressure, the reaction rate for methanol synthesis initially increased and then slightly decreased indicating a varying order. The single-site model accurately predicted the trends in the experimental data which would enable the development of reliable reactor and process designs.

According to Nor *et al.* (2008), a one-dimensional mathematical model was developed to simulate the performance of catalytic fixed bed reactor for carbon dioxide reforming of methane over Rh/Al2O3 catalyst at atmospheric pressure. The reactions involved in the system are carbon dioxide reforming of methane (CORM) and reverse water gas shift reaction (RWGS). The profiles of CH_4 and CO_2 conversions, CO and H2 yields, molar flow rate and mole fraction of all species as well as reactor temperature along the axial bed of catalyst were simulated. In addition, the effects of different reactor temperature on the reactor performance were also studied. The models can also be applied to analyze the performances of lab-scale micro reactor as well as pilot-plant scale reactor with certain modifications and model verification with experimental data.

It can be summatively stated that environmental pollution due to industrialization and technological growth is a treat to humanity and the ecology as a whole that requires man to combatively address. The act and it keep calling interest of researchers towards its effective remediation. Carbon dioxide (CO_2) in the atmosphere promotes the formation of acidic rain when hydrolyzed, the rain facilities metallic corrosion and destruction of metallic equipment (Benedict & Fredrick, 2023). This same CO_2 can become useful when efficiently and effectively recycled as identified by some researchers like Mohammad *et al.*, (2015), Martínez *et al.* (2012) and some others, Different processes such as looping (CaL) process, Stack control process, and others have been introduced and assessed effectively for the sequestration of CO_2 from the environments, and researchers such as Nestler *et al.,* (2020); Fedunik-Hofman *et al.* (2019), Ramezan *et al.* (2023), Athanasios and Angeliki (2020), Sreetama *et al.,* (2021), Tsitsi and David (2021), Mohammad *et al.,* (2016) and many more made attempts of assessing catalytic effects on methanol production from CO_2, but calcium looping (CaL) process which is one of the most effective measures to carbon dioxide sequestration, lacks a well detailed chemical kinetics, simulative validations, and design profile of environmental CO_2 sequestration and reuse for methanol synthesis (incorporating both the **Carbonation** and **Calcination** processes as a single study phase), which could serve as an optimization measure for environmental remediation and methanol production. Sreetama *et al.,* (2021) experimentally studied methanol synthesis from CO_2 hydrogenation using In_2O_3 catalyst, with a supportive kinetic model but couldn't develop models following the fundamental principles of reaction rate laws at steady state, nor

present a validated process simulation supportive to **Carbonation** and **Calcination** processes for methanol system as process tool for environmental remediation from GHGs effects. This work focuses of the modelling and simulation of a catalytic packed bed reactor for methanol synthesis from carbon dioxide via application of fundamental principles of reaction rate laws at steady state for determination of the optimal performance yield of the reactor at non-catalytic state.

MATERIALS AND METHODS

Process Assumptions Applicable to Studied system

i. The CO_2 flows into the packed bed reactor at a mole flow of 1.08 Ibmol/hr
ii. The system operates at non-isothermal conditions
iii. Negligible equilibrium effects
iv. Catalytic effects is negligible
v. Feed (CO_2 and Hydrogen) are of negligible source
vi. Side reactions during the methanol formation process are neglected

Kinetic and Performance Evaluation Modelling of Methanol Production System

Considering the MeOH-Formation reaction process which is generally a second order (hydrogenation) reaction process, with reaction schematic presented as follows:

$$\boldsymbol{CO_{2(g)}} \quad + \quad \boldsymbol{3H_{2(g)}} \underset{K_2}{\overset{K_1}{\rightleftharpoons}} \quad \boldsymbol{CH_3OH_{(aq)}} \quad + \quad \boldsymbol{H_2O_{(l)}}$$

The rate law is defined as a function of the reactant and products as seen in equation (1);

$$(-r_A) = \frac{dC_A}{dt} = K_1 C_A {C_B}^3 - K_2 C_D C_E \qquad (1)$$

Where:

K_1 and K_2 = Forward and reverse equilibrium rate constants
C_A = Final concentration of CO_2
C_B = Final concentration of Hydrogen
C_D = Final concentration of Methanol
C_E = Final concentration of Water

Considering the material balance of the system determined with respect to the fundamental principle of mass balancing as;

$$\begin{bmatrix}\textbf{Rate of input of Reactant species into unit Vol. element}\end{bmatrix} - \begin{bmatrix}\textbf{Rate of output of Product from Vol. element}\end{bmatrix} + \begin{bmatrix}\textbf{Rate of depletion of species due to rnx in the Vol. element}\end{bmatrix} = \begin{bmatrix}\textbf{Rate of acc. of species in the Vol. element}\end{bmatrix} \quad (2)$$

Where;

$$\begin{bmatrix}\textbf{Rate of input of Reactant species into unit volume element}\end{bmatrix} = V_o C_{Ao}\ ;\textbf{measured in}\ (mol/sec)$$

$$\begin{bmatrix}\textbf{Rate of output of Product species from the volume element}\end{bmatrix} = V_o C_A\ ;\textbf{measured in}\ (mol/sec)$$

$$\begin{bmatrix}\textbf{Rate of depletion of species due to rnx in the volume element}\end{bmatrix} = (-r_A)V_R\ ;\textbf{measured in}\ \left(\frac{mol}{m^3 * sec} \times m^3\right)$$

$$\begin{bmatrix}\textbf{Rate of acc. of species in the volume element}\end{bmatrix} = 0\ ;\textbf{For continuous flow reactor system}$$

Taken a section of the studied packed bed reactor as a sample of the reactor performance model assessment, with inlet and outlets of the reactor defines as the function of the reactor flow rate, feed concentration, reactor space time, volume, length as well as species reactivity nature at defined process temperate as illustrated at Figure 4

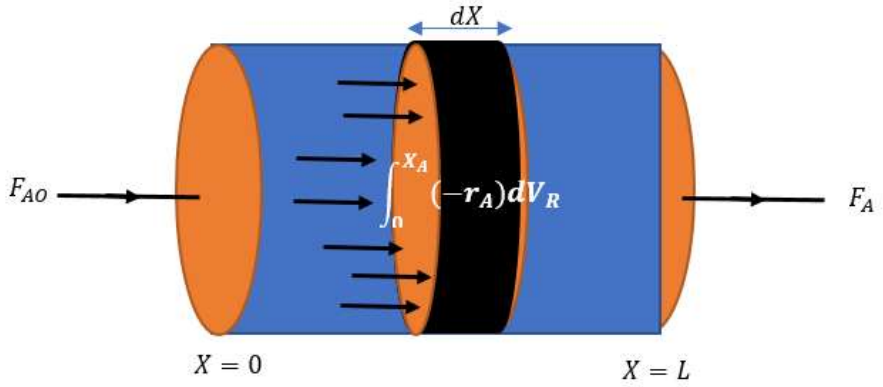

Fig. 4: Packed Bed Reactor (PBR) performance description on continues flow state

The material balance at steady state operations of the PBR is derived from equation (2) as:

$$V_o C_{Ao} - V_o C_A - (-r_A)V_R = 0 \quad (3)$$

Dividing all in equation (3.3) by the volumetric flow rate of the system (V_o);

$$C_{Ao} - C_A - (-r_A)\frac{V_R}{V_o} = 0 \quad (4)$$

Where;

$$\frac{V_R}{V_o} = Tao(\tau) \quad (5)$$

Diving all by the pulp velocity;

$$C_{A,o} - C_A - (-r_A)\tau = 0 \quad (6)$$

Relating the equation (1) with the rate laws and the fractional conversion bases;

$$C_{A,o} - C_A - \left(K_1 C_A {C_B}^3 - K_2 C_D C_E\right)\tau = 0 \quad (7)$$

$$C_{A,o} - C_A - K_1 C_A {C_B}^3 \tau + K_2 C_D C_E \tau = 0 \quad (8)$$

$$C_{A,o} - C_A\left(1 + K_1 {C_B}^3 \tau\right) = -K_2 C_D C_E \tau \quad (9)$$

So the concentration gradient model of the methanol formation system is defined as follows:

$$\therefore C_A = \frac{C_{A,o} + K_2 C_D C_E \tau}{(1 + K_1 {C_B}^3 \tau)} \quad (10)$$

Neglecting the reversibility of the system as stated in the assumptions will transform equation (10) to;

$$C_A = \frac{C_{A,o}}{(1 + K_1 {C_B}^3 \tau)} \quad (11)$$

2.1.1 PBR Space Time Deterministic Model

$$\therefore \text{If; } -\frac{dC_A}{dt} = K_1 C_A {C_B}^3 - K_2 C_D C_E \quad (12)$$

$$dt = -\frac{1}{K_1 C_A {C_B}^3 - K_2 C_D C_E} dC_A \quad (13)$$

Where change in concentration of a system is a product of the initial concentration and the reactor's fractional conversion, expressed as equation (14)

$$dC_A = C_{Ao} dX = \frac{F_A}{V_o} \quad (14)$$

$$\therefore \quad dX = \frac{F_A}{V_o} * \frac{1}{C_{Ao}} \quad (15)$$

Now substituting equation (14) into equation (13) and integrating the expression with respect to change in concentration of the feeds;

$$\tau = C_{A,o} \int_0^{X_{AF}} \frac{dX_A}{K_2 C_D C_E - K_1 C_A {C_B}^3} \quad (16)$$

Let;

$$m = K_2 C_D C_E - K_1 C_A {C_B}^3 \quad (17)$$

$$\frac{dm}{dC_A} = -K_1 \quad (18)$$

$$\therefore \quad \tau = -\frac{1}{K_1}\int_{C_{Ao}}^{C_A} \frac{1}{m} dm \quad (19)$$

$$\tau = -\frac{1}{K_1} \ln\left(\frac{K_2 C_D C_E - K_1 C_A {C_B}^3}{K_2 C_D C_E - K_1 C_{Ao} {C_{Bo}}^3}\right) \quad (20)$$

In negligible reversibility, the space time of the system is defined;

$$\tau = -\frac{1}{K_1} \ln\left[\frac{{C_B}^3}{{C_{Bo}}^3}(1 - X_A)\right] \quad (21)$$

PBR Volume (V_R) for Packed Bed Reactor

Considering the space time (Tao) relationship with system volumetric flow rate (v_o) expressed as equation (5), cooperatively with equation (16), the volume of the packed bed reactor (PBR) in integral form is expressed as, subject to Arrhenius operations as the driver of the reactor temperature which defines the reactivity of the system, is expressed as:

$$\mathrm{V}_R = \mathrm{F}_{AO}\int_0^{X_A} \frac{dX_A}{k_0 e\left[\frac{-E_0}{RT}\right] C_A {C_B}^3 - K_2 C_D C_E} \quad (22)$$

In negligible reversibility;

$$\mathrm{V}_R = \frac{\mathrm{F}_{AO}}{k_0 e\left[\frac{-E_0}{RT}\right]}\int_0^{X_A} \frac{dX_A}{C_A {C_B}^3} \quad (23)$$

On fractional conversion bases;

$${C_B}^{n_2} = {C_{Ao}}^{n_2}\left(\frac{C_{Bo}}{C_{Ao}} - \frac{n_2}{n_1}\propto_A\right)^{n_2} \quad (24)$$

$$So, {C_B}^3 = {C_{Ao}}^3\left(\frac{C_{Bo}}{C_{Ao}} - \frac{3}{1}\propto_A\right)^3 \quad (25)$$

$$\therefore \quad \mathrm{V}_R = \frac{\mathrm{F}_{AO}}{k_0 e\left[\frac{-E_0}{RT}\right]}\int_0^{X_A} \frac{dX_A}{C_{Ao}(1-\propto_A){C_{Ao}}^3\left(\frac{C_{Bo}}{C_{Ao}} - \frac{3}{1}\propto_A\right)^3} \quad (26)$$

$$= \frac{\mathrm{F}_{AO}}{k_0 e\left[\frac{-E_0}{RT}\right] {C_{Ao}}^4}\int_0^{X_A} \frac{dX_A}{(1-\propto_A)\left(\frac{C_{Bo}}{C_{Ao}} - 3\propto_A\right)^3} \quad (28)$$

Let;

$$W = (1 - \propto_A)\left(\frac{C_{Bo}}{C_{Ao}} - 3 \propto_A\right)^3 \quad (29)$$

Therefore, redefining the variables of W as;

$$U = 1 - \propto_A \quad (30)$$

$$V = \left(\frac{C_{Bo}}{C_{Ao}} - 3 \propto_A\right)^3 \quad (31)$$

Hence in partial differential form, the W variables will now take the form;

$$\frac{dU}{d \propto_A} = -1 \quad (32)$$

$$\frac{dV}{d \propto_A} = \frac{dp}{\propto_A} \times \frac{dV}{dp} = -9\left(\frac{C_{Bo}}{C_{Ao}} - 3 \propto_A\right)^2 \quad (33)$$

$$\therefore \quad V_R = \frac{F_{AO}}{k_0 e\left[\frac{-E_0}{RT}\right] {C_{Ao}}^4} \int_0^{X_A} \frac{dW}{W} \quad (34)$$

where;

$$dW = \left(U\frac{dV}{\propto_A} + V\frac{dU}{\propto_A}\right) d \propto_A \quad (35)$$

$$= -9(1 - \propto_A)\left(\frac{C_{Bo}}{C_{Ao}} - 3 \propto_A\right)^2 - \left(\frac{C_{Bo}}{C_{Ao}} - 3 \propto_A\right)^3 \quad (36)$$

$$\therefore \; d \propto_A = \frac{1}{\left(U\frac{dV}{\propto_A} + V\frac{dU}{\propto_A}\right)} dW \quad (37)$$

$$= \frac{1}{\left\{9(\propto_A - 1)\left(\frac{C_{Bo}}{C_{Ao}} - 3 \propto_A\right)^2 - \left(\frac{C_{Bo}}{C_{Ao}} - 3 \propto_A\right)^3\right\}} dW \quad (38)$$

$$\therefore \; V_R = \frac{F_{AO}}{k_0 e\left[\frac{-E_0}{RT}\right] {C_{Ao}}^4} \frac{1}{\left\{9(\propto_A - 1)\left(\frac{C_{Bo}}{C_{Ao}} - 3 \propto_A\right)^2 - \left(\frac{C_{Bo}}{C_{Ao}} - 3 \propto_A\right)^3\right\}} \int_0^{X_A} \frac{dW}{W} \quad (39)$$

$$= \frac{F_{AO}}{k_0 e\left[\frac{-E_0}{RT}\right] {C_{Ao}}^4} \frac{1}{\left\{9(\propto_A - 1)\left(\frac{C_{Bo}}{C_{Ao}} - 3 \propto_A\right)^2 - \left(\frac{C_{Bo}}{C_{Ao}} - 3 \propto_A\right)^3\right\}} \ln[W]_{X_A=0}^{X_A} \quad (40)$$

Considering the homogeneous nature of the reaction for methanol product4ion from the CO_2, the initial concentration status of primary reactant can be restructured with respect to partial pressure as;

$$C_{Ao} = \frac{P_A}{RT} \quad (41)$$

According to Daltons law of partial pressures;

$$C_{Ao} = \frac{1}{RT}(y_A P_{T\propto}) = \frac{P_{T\propto}}{RT}\left(\frac{1-\propto_A}{1+\propto_A}\right) \quad (42)$$

Hence the volume of the packed bed reactor for methanol production at negligible catalytic effects and reversibility as a function of the fractional conversion regime of the system is modelled as;

$$V_{PBR} = \frac{F_{AO}}{k_0 e\left[\frac{-E_0}{RT}\right]\left(\frac{P_{T\propto}}{RT}\right)^4\left(\frac{1-\propto_A}{1+\propto_A}\right)^4}\frac{\ln(X_A)}{\left\{9(\propto_A-1)\left(\frac{C_{Bo}}{C_{Ao}}-3\propto_A\right)^2-\left(\frac{C_{Bo}}{C_{Ao}}-3\propto_A\right)^3\right\}} \quad (43)$$

Reactor Length (L_R) for Methanol Formation System via Hydrogenation

The length of the packed bed reactor (PBR) expressed as a function of the cross-sectional area and volume modelled as equation (40) is modelled for this system of methanol formation as:

$$LR = \frac{4F_{A0}}{\pi D^2}\int_0^{X_A}\frac{dX_A}{k_0 e\left[\frac{-E_0}{RT}\right]C_A {C_B}^3} \quad (44)$$

$$= \frac{4F_{AO}\ln(X_A)}{\pi D^2 k_0 e\left[\frac{-E_0}{RT}\right]\left(\frac{P_{T\propto}}{RT}\right)^4\left(\frac{1-\propto_A}{1+\propto_A}\right)^4\left\{9(\propto_A-1)\left(\frac{C_{Bo}}{C_{Ao}}-3\propto_A\right)^2-\left(\frac{C_{Bo}}{C_{Ao}}-3\propto_A\right)^3\right\}} \quad (45)$$

Hence, the Packed Bed Reactor (PBR) Space velocity (τ) as function of the fee initial flow rate (F_{AO}) is expressed as:

$$\text{If; } \tau = \frac{F_{A0}\int_0^{X_A}\frac{dX_A}{k_0 e\left[\frac{-E_0}{RT}\right]C_A {C_B}^3}}{V_0} \quad (46)$$

$$= \frac{4F_{AO}\ln(X_A)}{k_0 e\left[\frac{-E_0}{RT}\right]\left(\frac{P_{T\propto}}{RT}\right)^4\left(\frac{1-\propto_A}{1+\propto_A}\right)^4\left\{9(\propto_A-1)\left(\frac{C_{Bo}}{C_{Ao}}-3\propto_A\right)^2-\left(\frac{C_{Bo}}{C_{Ao}}-3\propto_A\right)^3\right\}V_0} \quad (47)$$

Space velocity of the Packed Bed Reactor (PBR) which is the number of reactors of feed treated in a unit time, is mathematically modelled as the inverse or reciprocal of apace time expressed as;

$$S_v = {}^1/_\tau \quad (48)$$

$$S_v = \frac{k_0 e\left[\frac{-E_0}{RT}\right]\left(\frac{P_{T\propto}}{RT}\right)^4\left(\frac{1-\propto_A}{1+\propto_A}\right)^4\left\{9(\propto_A-1)\left(\frac{C_{Bo}}{C_{Ao}}-3\propto_A\right)^2-\left(\frac{C_{Bo}}{C_{Ao}}-3\propto_A\right)^3\right\}V_0}{4F_{AO}\ln(X_A)} \quad (49)$$

Where;

$$R = Universal\ gas\ constant = \frac{8.314\ J/molK}{Average\ molar\ mass\ of\ reactants} \quad (50)$$

X_A = fractional conversion of methanol
V_0 = Volumetric flow rate (m^3/hr)
$\boldsymbol{T}$ = Operating temperature of the system (K)
$P_{T\propto}$ = Partial pressure of the conversion system at process temperature (Pa)
$\mathbf{F_{AO}}$ = Flow rate of the reactants (mol/hr)
$\boldsymbol{k_0}$ = Arrhenius rate constant of the system (1/mhr)
$\boldsymbol{E_0}$ = Activation energy of primary reactant in the system (kJ/mol)
$C_{Ao} and\ C_{Bo}$ = primary and secondary reactant initial concentration (mol/m^3)
D = Reactor diameter (m)

Heat Effects Assessment Model for Methanol Production in Packed Bed Reactor

The possible heat change in the Packed Bed Reactor (PBR) for methanol production via hydrogenation, at negligible catalytic effects is expressed mathematically as a function of the heat transfer through the medium via conduction as well as in consideration of the chemical reaction extent using the energy / heat balance first-principle as follows:

$$\frac{dQ}{dt} = Q_{in} - Q_{out} \pm Q + Q_r \quad (51)$$

At adiabatic conditions where it is considered that there is "No heat transfer from system to surrounding, vice-versa"; $Q_{in} - Q_{out} = 0$, therefore;

$$\frac{dQ}{dt} = Q + Q_r \quad (52)$$

$$\therefore \quad mC_p \frac{dT}{dt} = Q + (-r_A)(\pm\Delta H_r)V_R \quad (53)$$

If the heat flux in the system is a subject of the temperature difference in the system, defined by Fourier's expression as;

$$q_x = Q = -KA\frac{dT}{dr} \quad (54)$$

Considering the cylindrical nature of the kiln, the surface area will be;

$$A = 2\pi rL \quad (55)$$

Hence;

$$q_x = -K(2\pi rL)\frac{dT}{dr} \quad (56)$$

Now integrating both sides at time and temperature basis;

$$q_x \int_{r_i}^{r_o} (1/r)dr = -2\pi LK \int_{T_i}^{T_o} dT \quad (57)$$

Expressing the integral to normal place level;

$$q_x \ln(r_o/r_i) = -2\pi LK(T_i - T_o) \quad (58)$$

$$q_x = \frac{2\pi LK}{\ln(r_o/r_i)}(T_o - T_i) \quad (59)$$

$$\mathrm{mC_p}\frac{\mathrm{dT}}{\mathrm{dt}} = \frac{2\pi LK}{\ln(r_o/r_i)}(T_o - T_i) + (-r_A)(\pm\Delta H_r)V_R \quad (60)$$

$$\frac{\mathrm{dT}}{\mathrm{dt}} = \frac{2\pi LK}{\mathrm{mC_p}\ln(r_o/r_i)}(T_o - T_i) + (-r_A)(\pm\Delta H_r)\frac{V_R}{\mathrm{mC_p}} \quad (61)$$

The process temperature evaluated in terms of the production reactor's volume and negligible shaft temperature and equilibrium state of the system is expressed as;

$$\frac{\mathrm{dT}}{\mathrm{dt}} = \frac{V_R K_1 C_A {C_B}^3(\pm\Delta H_r)}{\mathrm{mC_p}} - \frac{2\pi LK}{\mathrm{mC_p}\ln(r_o/r_i)}(T_i) \quad (62)$$

RESULTS AND DISCUSSION

Results

Using the data achieved from industrial data book for methanol production process, the MATAB results of the developed kinetic models programmed with respect to the MATLAB-Simulink algorithmic logic are see resented in Table 1, with respect to their changes in fractional conversion of the system.

Table 1: Kinetic model results from MATLAB Simulation

X_A	C_A (mol/m^3)	C_D (mol/m^3)	(-rA) (mol/m^3.min)	Tao (min)	V_R (m3)	L_R (m)	Yield	dTdt (^{o}C/min)
0.0000	87.3452	**0.0000**	158.1202	0 .0000	0 .0000	0 .0000	0.0000	-79.2047
0.1000	55.2958	24.5670	100.1015	0.0751	0.6184	0.0661	0.5059	-41.5512
0.2000	39.2105	56.6164	70.9824	0.1591	1.3098	0.1401	0.6496	-22.6557
0.3000	29.4856	72.7017	53.3775	0.2542	2.0936	0.2239	0.7365	-11.2296
0.4000	22.9234	82.4266	41.4980	0.3641	2.9984	0.3206	0.7952	-3.5250
0.5000	18.1463	88.9888	32.8501	0.4941	4.0686	0.4351	0.8379	2.0783
0.6000	14.4587	93.7659	26.1745	0.6532	5.3784	0.5751	0.8708	6.3989
0.7000	11.4571	97.4535	20.7407	0.8582	7.0670	0.7557	0.8976	9.9353
0.8000	8.8636	100.4551	16.0457	1.1472	9.4470	1.0102	0.9208	13.0015
0. 9000	6.3906	103.0486	11.5688	1.6413	13.5155	1.4452	0.9429	15.8926
1.0000	inf	inf	inf	inf	inf	inf	inf	inf

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DISCUSSION OF METHANOL PRODUCTION MODELS RESULTS

PBR Sensitivity Analysis of Fractional Conversion Effects on System Concentration

The fractional conversion of the system is known to have great influence on the performance of the methanol formation system, on the basis of its abilities of controlling the depletion and formation rate which defines the yield ration of the chemical reactive system, plotted as seen in Figure 5.

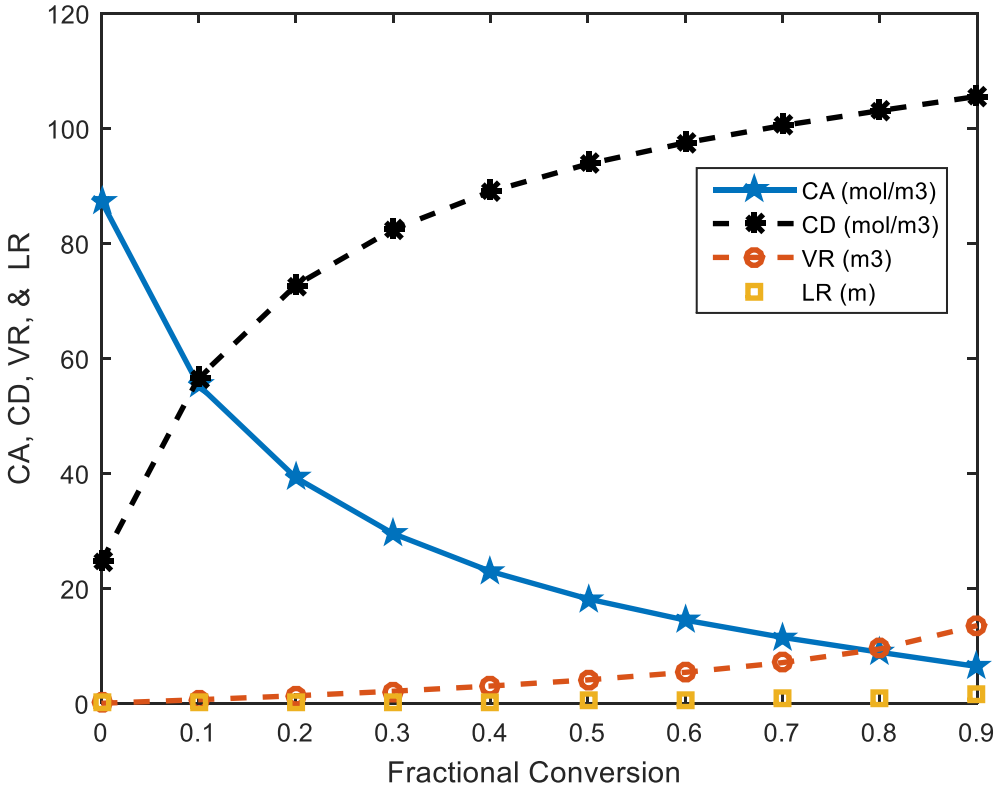

Fig. 5: Fractional conversion against PBR volume and concentration gradient performance behavior in methanol production system

As seen in Figure 5, the increase in the fractional conversion of methanol production system from carbon dioxide looping process, promotes proportionally the depletion rate of CO_2 concentration over 1.6413 min space time of the plug flow reactor (PFR). This methanol production system shows a speedy depletion of the reactants (CO_2 and H_2) concentration from 87.3452 mol/m^3 to 39.2105 mol/m^3 after 30.1% conversion rate, then the yielding rate of the system decreased to a slow but steady depletion of the CO_2 till in the system till it attains 6.3906 m^3 at 11.5688 mol/m^3s conversion rate. The depletion activity of the methanol formation process periodically promotes the Plug bed reactor (PBR) volume from 0.0m^3 to 13.5155m^3 over the 0.0% to 99% conversion of the system, with a proportional increase in the reactor length from

0.0m to 1.4452m. The result also describes the reactor volume increasing gradually within the first 20% fractional conversion of the system, which is with similar behavior of the $CO_{2(g)}$ and $H_{2(g)}$ reactants depletion form 87.3452m^3 to 39.2105m^3, then the volume rates accelerates appreciatively till the reaction termination points with a 94.29% methanol yield. The depletion and formation behavior of the homogeneous system as displayed in Figure 5 is in agreement to results presented by Nor *et al.* (2008) and in Perry's and Green (2007)

PBR Reactor's Volume and Length Relationship with Fractional Conversion

The result displayed in Figure 6 describes the behavior of the packed bed reactors volume and length with respect to change in the system fractional conversion. It depicts that the reactor's volume experiences an accelerative increase proportionate to the increase in the fractional conversion of the system, hence promoting the reactor's yield per increase in the space time.

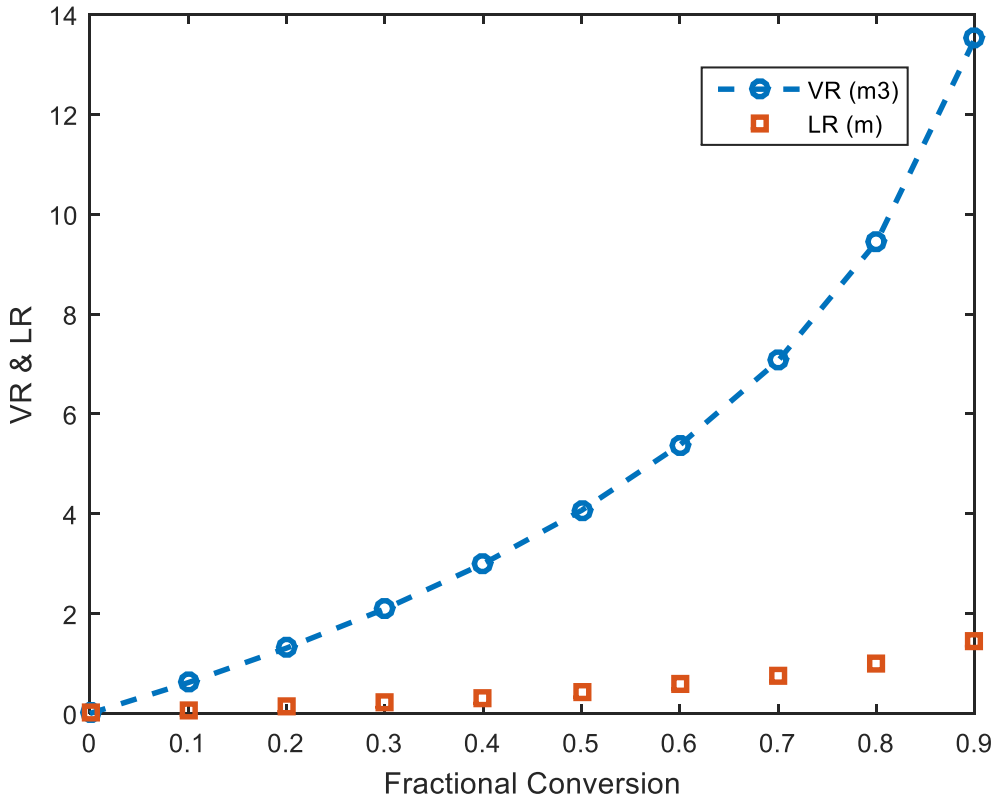

Fig. 6: Fractional Conversion relationship with PBR volume and length performance behavior in methanol production system

The reactor volume for methanol formation from CO_2 via looping process accelerates uniformly to 2.0936 m^3 within the first 40% fractional conversion of the system, the system experiences a vast increase in every 10% fractional change of the system until 13.5155 m^3 is achieved at 90% conversion of the system. This is subject to the change in temperature of the system, and increases proportionally with increase in the plug flow reactor (PFR) process temperature. As per the rector length, it increases slightly in every increase in the reactors volume such that 13.5155 m^3 attained could only yield 1.4452 m reactors length increase, which is also proportional to increase in the fractional conversion of 87.3452mol/m^3 CO_2 and H_2 in the loop system to form methanol, as studied in this work. The result is in agreement to results presented by Nor *et al.* (2008) and in Perry's and Green (2007)

Sensitivity Analysis of PBR Space Time Effects on System Concentration

In assessment of the reactor performance parametrics behaviors with respect to change in the system or reactor process space time, it was identified that the changes in the system concentration gradients, volume, length, length, and reactants status changes spontaneously with change in the reactors space time of a loop system for methanol formation. The changes experienced as studied with respect to change in space time (Tao) as seen in Figure 7 are in close resemblance to those experienced in the plug flow reactor for every change in the system fractional conversion as earlier described in Figure 5, but the rate of increase in the reactors volume which though increases with proportional increase in the system space time is very slow but spontaneous, which is resulted from the fast depleting rate of the reactants concentration to 103.0486mol/m^3 within the 1.6413min operating time of the plug flow reactor

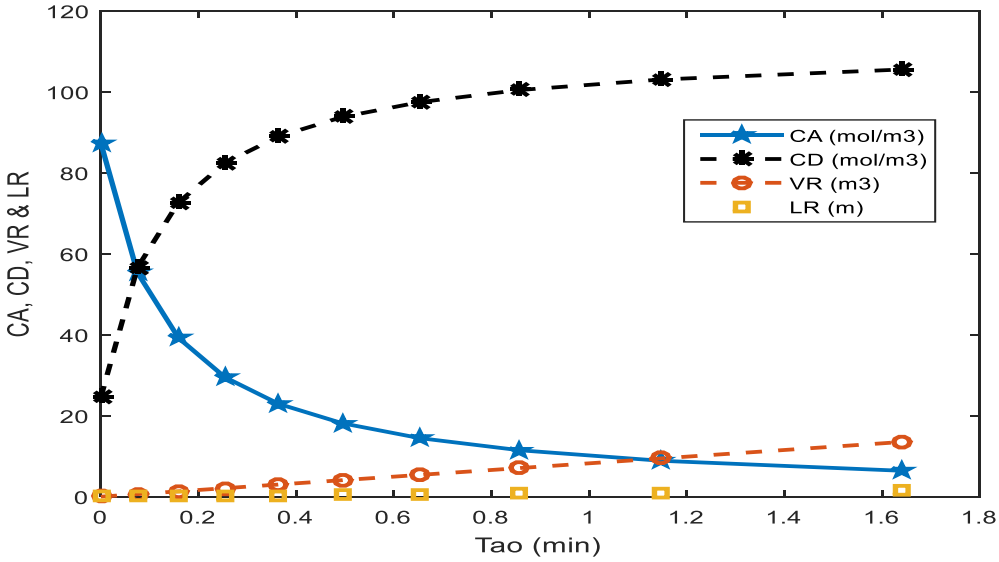

Fig. 7: Reactor Space Time, volume and reactor's length performance behavior in methanol production system

The result in Figure 7 defines a uniform yielding of methanol over the reactor time, this is due to the steady depletion of the CO_2 and H_2 as seen displayed in the depletion curve of the plot from 87.3452 mol/m^3 initial concentration bases to 6.3906 mol/m^3 at 1.2345 m^3/min volumetric flow rate of the system. The results is in agreement to results presented by Nor *et al.* (2008) and in Perry's and Green (2007)

Effects of PBR Reactor's Depletion Rate on Process Temperature and Length

The result in Figure 8 describes the methanol formation system from looping process of CO_2 as an exothermic reaction system, which is as same identified by Tsitsi and David (2021), Prry's and Green (2007), John (2005), and many others on their respective materials or diverse studies on same methanol formation system.

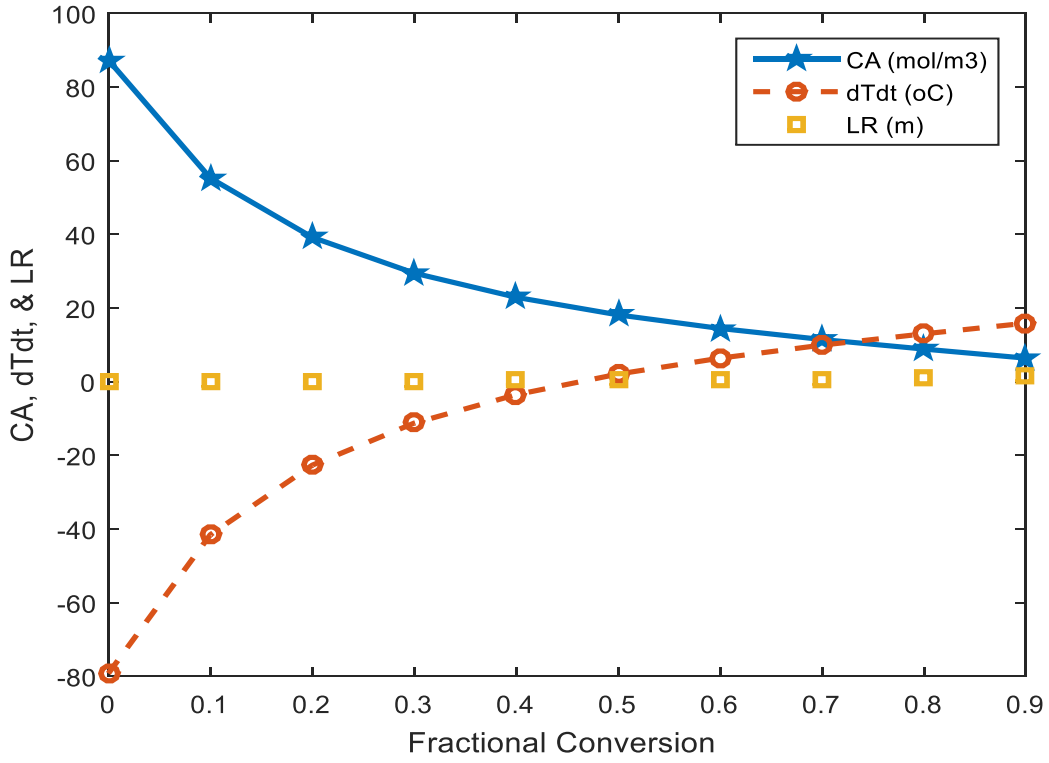

Fig. 8: Reactor's Depletion Rate effects on Process Temperature and Length

The result show that the system losses energy to the environment over time, such that as the system depletes from 87.3452 mol/m^3 to 6.3906 mol/m^3 over 1.654677 min space time of the reactor yielding 94.29% methanol yield with 103.0486 mol/m^3 concentration, the system experienced a rise in process temperature which results to increase in the heat loss to the environment from the reactor, making the system non-adiabatic in nature. This process of heat loss to environment increases proportionally to decrease in the reactant's cunctation, and increase in the methanol formation over time.

Reactor Space Time Relationship with Methanol Yield Over Fractional Conversion

The plug flow reactor's yield is identified in this study as aa function of the system space time and fractional conversion of the system. Their relationship is results as seen in Figure 4.10 to be proportionate to fractional changes of CO_2 in the system to yield 94.29% methanol. The result of the system as seen in Figure 4.10 depicts that the system yield increases proportionate to increase in fractional conversion of the system, as a result of increase in the system space time till it attains 1.6413 min. this change or increase in the reactor space time is at steady rate within 0% to 40% conversion of the system, which yields 79.52% methanol, then the space time accelerates vastly till it attains the reaction termination point at 90% fractional conversion. This change in the reactor's space time which is proportional to increase in the reactor fractional conversion affects the yielding rate of the system, such that the system methanol yield attains pluton after 0.3641min space time and 40% fractional conversion of the system, till it attains 94.29% methanol. The results are in agreement to results presented by Nor *et al.* (2008), Perry's and Green (2007) and by Sreetama *et al.*, (2021)

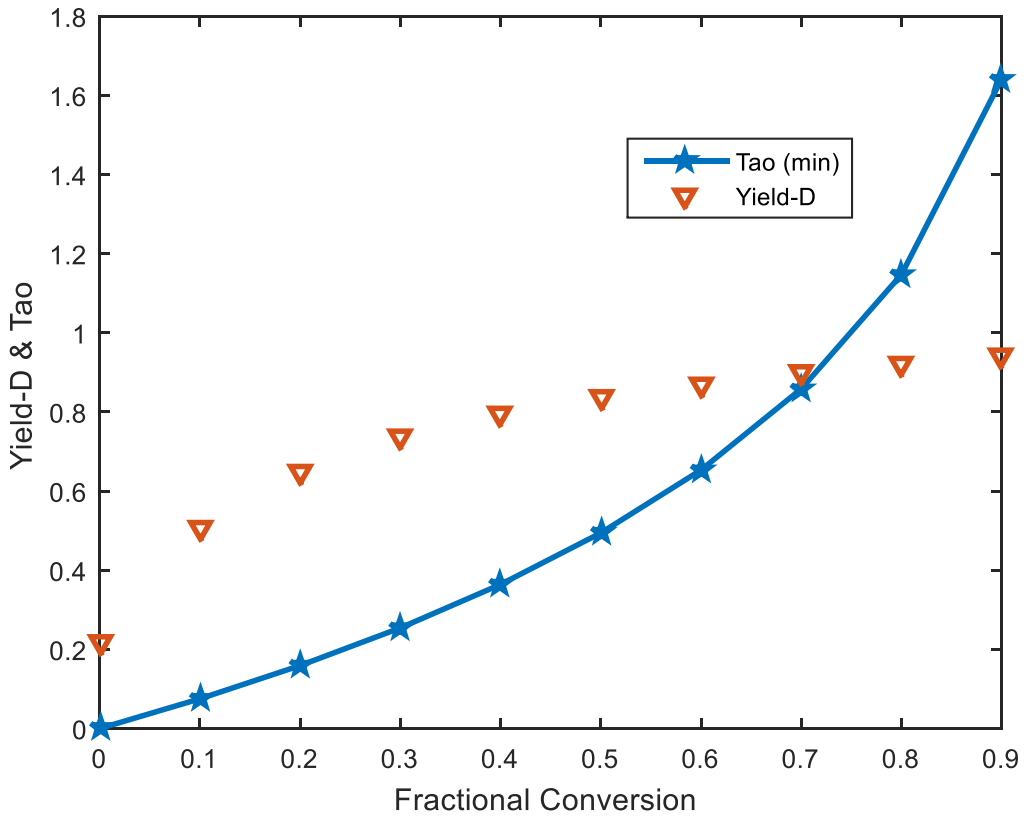

Fig. 9: Space Time Relationship with Methanol Yield Over Fractional Conversion performance behavior in methanol production system

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Reaction Rate on Packed Bed Reactor (PBR) Performance on Methanol Production

In relating the system reaction rate ($-r_A$) with the Packed bed reactor (PBR) performance of the looping process for methanol production, results as seen in Figure 10 depicts the coexisting relationship of the system, which defines the system parametrics to change with respect to the depletion of the looping process reaction rate from 158.1202 mol/m^3.min to 11.5688 mol/m^3.min, this depletion in the reaction rates promotes the formation of the reactor's yield, volume, space time and the PBR length at proportionate accelerative order. But the depletion in the reaction rate which is in favor of the VR, LR Tao and Yield as started, affects the reactants concentration in the looping system, causing the reactants concentration to depletes from 87.3452 mol/m^3 to 6.3906 mol/m^3 with heat loss to the environment proportionally.

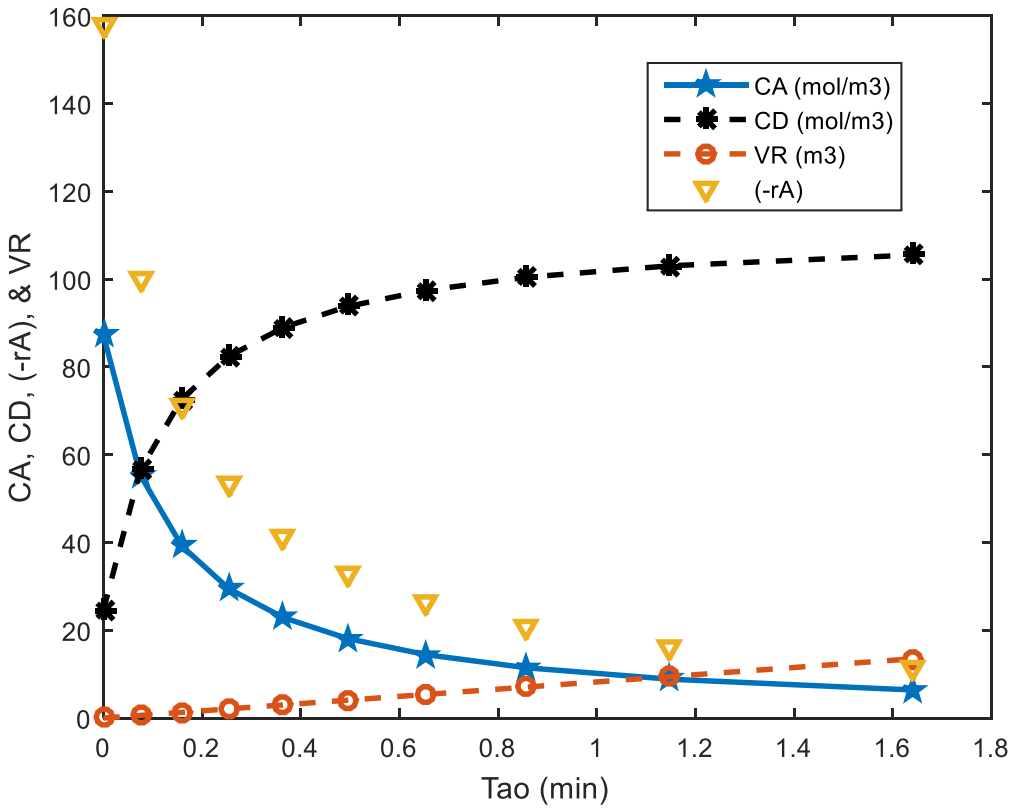

Fig. 10: Effects of reaction rate on PBR performance in methanol production system

CONCLUSION

Packed bed reactor for methanol synthesis from carbon dioxide hydrogenation has been successfully modelled mathematically in this work, and simulated for assessment of the system kinetic models' sensitivity at dynamic continuous state using MATLAB. The developed models are been achieved via application of the fundamental principles of conservation of mass, energy and momentum at steady state with negligible catalytic effects. The space time, reactor's length, volume, and heat transfer were

determined to be a function of the concentration gradient, such that depletion of the feed concentration into methanol act at proportionate bases to changes at the reactor performance parameters. The system was identified to be of 94.29% methanol yield achieved at a concentration of 103.0486 mol/m^3 as the CO_2 feed concentration depletes from 87.3452 mol/m^3 to 6.3906 mol/m^3 with heat loss to the environment proportionally

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