SIMULATION OF CARBOHYDRATE PRODUCTION USING CO_2 CAPTURED FROM FLUE GASES WITH ASPEN PLUS SIMULATION TOOL

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AUGUST, 2024

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A DISSERTATION SUBMITTED TO THE SCHOOL OF POSTGRADUATE STUDIES IN PARTIAL FULFILMENT OF THE REQUIREMENTS FOR THE AWARD OF THE MASTER OF ENGINEERING DEGREE IN CHEMICAL ENGINEERING IN THE DEPARTMENT OF CHEMICAL ENGINEERING, COLLEGE OF ENGINEERING, COVENANT UNIVERSITY, OTA, NIGERIA

AUGUST, 2024

ACCEPTANCE

This is to attest that this dissertation is accepted in partial fulfilment of the requirement for the award of the degree of Master of Engineering (M.Eng) in Chemical Engineering in the Department of Chemical Engineering, College of Engineering, Covenant University, Ota, Nigeria.

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(Secretary, School of Postgraduate Studies) **Signature and Date**

Prof. Akan B. Williams
(Dean, School of Postgraduate Studies) **Signature and Date**

DECLARATION

I, **AONDOAKAA, EPHRAIM AHILE (22PCF02409),** declare that this research, **"SIMULATION OF CARBOHYDRATE PRODUCTION USING CO_2 CAPTURED FROM FLUE GASES WITH ASPEN PLUS SIMULATION TOOL"**, was conducted by me under the supervision of Dr. Francis B. Elehinafe and Dr. Temitayo E. Oladimeji of the Department of Chemical Engineering, College of Engineering, Ota, Nigeria. I attest that the dissertation has not been presented either wholly or partially for another degree at this or any other institution. All sources of data and scholarly information used in this dissertation has been duly acknowledged in the text, and a list of references has been provided.

AONDOAKAA, EPHRAIM AHILE

Signature and Date

CERTIFICATION

We certify that this dissertation titled "**SIMULATION OF CARBOHYDRATE PRODUCTION USING CO_2 CAPTURED FROM FLUE GASES WITH ASPEN PLUS SIMULATION TOOL**" is an original research work conducted by **AONDOAKAA, EPHRAIM AHILE (22PCF02409)** in the Department of Chemical Engineering, College of Engineering, Covenant University, Ota, Ogun State, Nigeria under the supervision of Dr. Francis B. Elehinafe and Dr. Temitayo E. Oladimeji. We have examined and found this work acceptable as part of the requirements for the award of the degree of Master of Engineering (M.Eng) in Chemical Engineering.

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DEDICATION

This research project is dedicated to God Almighty, who helped me to the point of completion, my sponsor Mr. Sunil Mahbubani, Mr. Mahesh Punjabi, and Major General Chris Jemitola for their financial support, and my entire family and friends for their encouragement during my course of study. I also dedicate it my lecturers in the department of Chemical Engineering, Covenant University. May God bless them all with paradise.

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LIST OF ABBREVIATIONS

CO_2	-	Carbon dioxide
CO	-	Carbon monoxide
CH_4	-	Methane
NO_X	-	Oxides of Nitrogen
SO_2	-	Sulfur dioxide
SO_X	-	Oxides of Sulfur
Hg	-	Mercury
HCl	-	Hydrogen Chloride
HF	-	Hydrogen Fluoride
NH_3	-	Ammonia
H_2S	-	Hydrogen Sulfide
N_2O	-	Nitrous Oxides
N_2	-	Nitrogen
H_2O	-	Water
O_2	-	Oxygen
H_2	-	Hydrogen
PM	-	Particulate Matter
AP	-	Artificial Photosynthesis
PS I	-	Photosystem I
PS II	-	Photosystem II
GHG	-	Greenhouse Gases
ESP	-	Electrostatic Precipitator
PD	-	Potential Difference
FF	-	Fabric Filters
VOCs	-	Volatile Organic Compounds
ACs	-	Activated Carbon

HPR	-	Hyper Crosslinked Polymeric Resins
MOFs	-	Metal-organic Frameworks
PFAS	-	Per/poly-fluoroalkyl Substances
TiO_2	-	Titanium Dioxide
IGCC	-	Integrated Gasification Combined Cycle
PCC	-	Post-combustion Carbon Capture
CaO	-	Calcium Oxides
$CaCO_3$	-	Calcium Carbonate
PSA	-	Pressure Swing Adsorption
VPSA	-	Vacuum Pressure Swing Adsorption
TSA	-	Temperature Swing Adsorption
PTSA	-	Pressure-temperature Swing Adsorption
MEA	-	Monoethanolamine
DEA	-	Diethanolamine
MDEA	-	Methyl-diethanolamine
NADPH	-	Nicotinamide Adenine Dinucleotide Phosphate
ATP	-	Adenosine Triphosphate
NP	-	Natural Photosynthesis
CO_2RR	-	Carbon Reduction Reaction
OER	-	Oxygen-evolving Reaction
Ru	-	Ruthenium
Re	-	Rhenium
Fe	-	Iron
Ir	-	Iridium
HECs	-	Hydrogen-evolution Catalysts
Rh	-	Rhodium
ASPEN	-	Advanced System for Process Engineering
PR	-	Peng-Robinson

SRK	-	Soave-Redlich-Kwong
EoS	-	Equation of State
PDF	-	Process Flow Diagram
APR	-	Artificial Photosynthesis Reaction
MJ	-	Megajoules

ABSTRACT

The Earth's global temperature requires urgent attention in order to reduce it to well below 2 °C, as stipulated by the Paris Agreement. This research models a process for capturing carbon dioxide (CO_2) from flue gases, and producing carbohydrates using post-combustion captured, adaptable to existing plants. A feed flue gas basis of 10 tons per day (300 °C, 10 bar) was considered. The capturing technique modelled achieved a CO_2 recovery of 96 % and a CO_2 purity of 93 %, meeting regulatory targets above 90 %. Based on thermodynamic equilibrium and phase equilibria calculations, the Aspen simulation of the carbon capture process via pressure swing adsorption revealed an energy requirement of 0.163 MJ per kg of CO_2, compared to 0.7 MJ per kg CO_2 reported by Nikolaidis, Kikkinides, and Georgiadis (2017). Conventional monoethanolamine (MEA) absorption processes for CO_2 capture typically require over 4 MJ per kg CO_2 (Ferrara *et al*., 2017). The process utilised a pressure swing adsorber (PSA) for CO_2 capture, followed by the direct conversion of CO_2 to saccharides (glucose, galactose, and fructose) in an artificial photosynthesis reactor. Varying the feed water flow rate from 20 kg/hr to 50 kg/hr reduced the glucose to galactose mass selectivity from 75:100 to 66:100. Varying the pressure of the artificial photosynthesis reactor (APR) from 0 to 40 bar increased the glucose to galactose mass selectivity from 72:100 to 78:100. Varying the reactor temperature from 0 °C to 320 °C decreased glucose yield from 33.1527 kg/hr to 1.6516 kg/hr, while galactose yield increased from 0.0045 kg/hr to 31.5056 kg/hr. Optimisation revealed a maximum glucose yield of 0.6824 kg per kg CO_2 (1:5.9998 molar basis), with an efficiency of 99.996 % at 0 °C, 31.741 bar, and 40 kg/hr water flow rate. The artificial photosynthesis reactor required 17,255.9375 kJ per kg of glucose (3,108.7607 kJ/mol), efficient compared to the theoretical standard enthalpy of formation, 2,802.5 kJ/mol. Optimising galactose yield demonstrated 0.6797 kg per kg CO_2 (1:6.0187 molar basis), comparable to the theoretical stoichiometry of 1:6, at 500 °C, 17.7763 bar, and 44.857 kg/hr water flow rate. The reactor required 20,454.6394 kJ per kg of galactose (3,681.8351 kJ/mol). The condensation reactor predominantly produced sucrose (31.4993 kg/hr), regardless of conditions, indicating thermodynamic favourability. Polysaccharide synthesis was infeasible due to the non-convergence of simulations, likely due to the absence of biological catalysts necessary for complex polymerisation reactions. This research highlights the potential and limitations of CO_2 conversion processes to valuable biochemicals, providing a basis for future experimental investigations.

Keywords: Carbon dioxide, Simulation, Carbohydrates, Flue Gases, Monosaccharides, disaccharides, Polysaccharides, Technologies, Aspen Plus, Optimisation, Sensitivity Analysis, Artificial Photosynthesis, Captured.