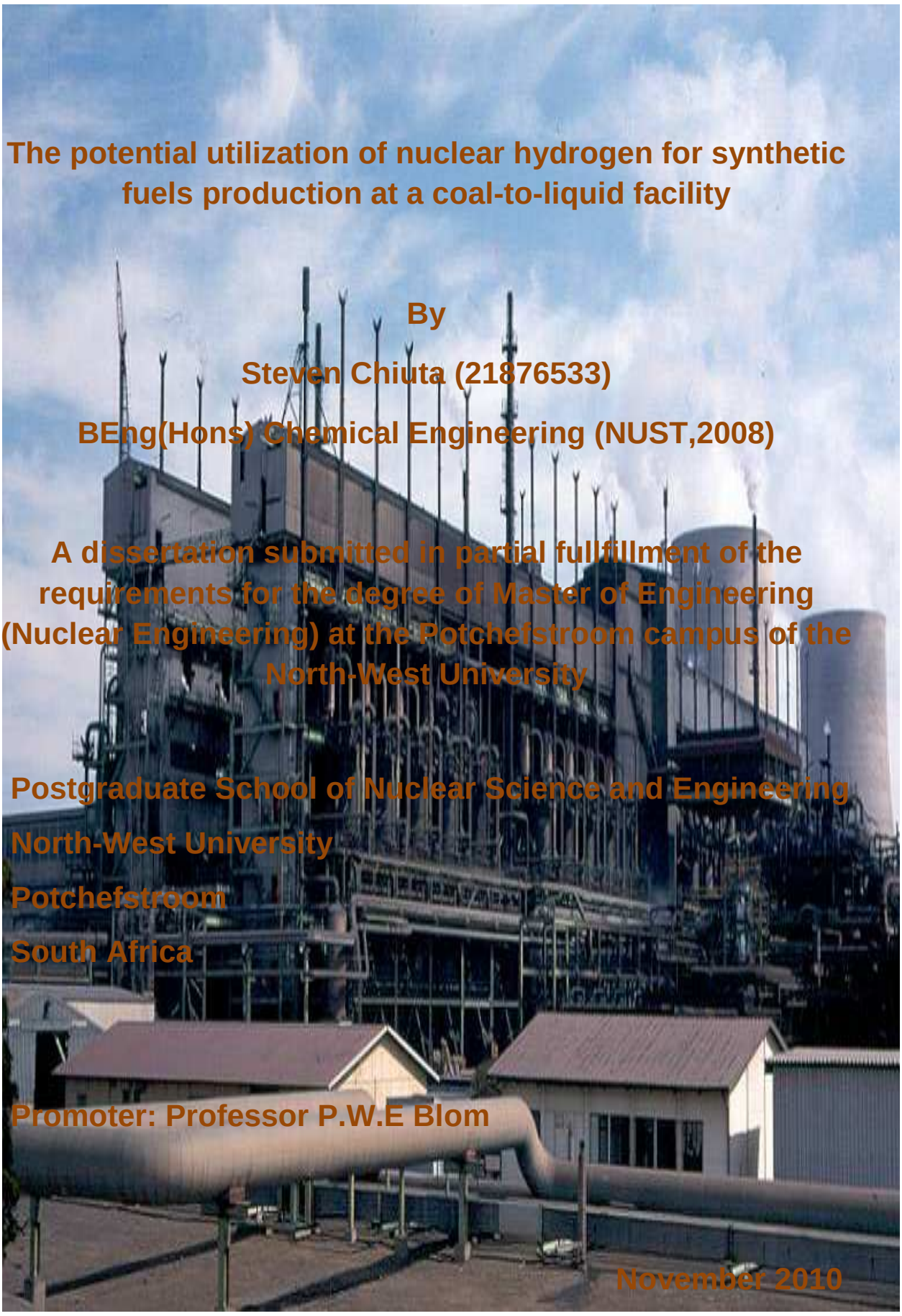


The potential utilization of nuclear hydrogen for synthetic fuels production at a coal-to-liquid facility

By

Steven Chiuta (21876533)

BEng(Hons) Chemical Engineering (NUST,2008)

A dissertation submitted in partial fullfillment of the requirements for the degree of Master of Engineering (Nuclear Engineering) at the Potchefstroom campus of the North-West University

Postgraduate School of Nuclear Science and Engineering

North-West University

Potchefstroom

South Africa

Promoter: Professor P.W.E Blom

November 2010

Acknowledgements

My most sincere gratitude goes to my principal supervisor, Professor P.W.E Blom, for his general impartation of ideas, guidance, advice, time and unwavering support. I salute you.

I am most indebted to my wife, Patience, and my son, Danian Anashe, for the splendid encouragement and support. I salute you.

Many thanks go to Mr. K. Kander and Mr. M. Francis for organizing my visit to the Sasol Secunda Synfuels factory. I salute you.

Special thanks go to Dr. M.J Keyser for shedding light on some of the complicated aspects of gasification. I salute you.

My utmost salutation and heartfelt thanks go to Hydrogen South Africa (HySA) for providing financial assistance to my entire studies. I salute you.

And, to God, the almighty, who deserves all honour. I salute you.

Solemn Declaration

I, Steven Chiuta, declare herewith that the dissertation entitled;

The potential utilization of nuclear hydrogen for synthetic fuels production at a coal-to-liquid facility

Which I herewith submit to the North-West University Potchefstroom Campus, in partial compliance with the requirements set for the **MEng Nuclear Engineering (Option B)** degree, is my own work, has been text edited and has not already been submitted to any other university.

I understand and accept that the copies that are submitted for examination are the property of the University.

Signature of student _____ University number: **21876533**

Signed at _____this _____day of _____2010.

Declared before me on this _____day of_____2010.

Commissioner of Oaths: _____

Table of Contents

Acknowledgements ii
Solemn Declaration iii
Table of Contents iv
Abstract vi
List of Abbreviations vii
List of Figures x
List of Tables xi
Chapter 1 1
Introduction 1
1.1 Thesis overview 1
1.2 Thesis motivation 4
1.3 Thesis objectives 4
1.4 Thesis outline 5
Chapter 2 6
Literature review 6
2.1 Development of the CTL process 6
2.2 Basic CTL process description 6
2.2.1 Syngas production unit 7
2.2.2 The Fischer-Tropsch synthesis 11
2.2.3 Product upgrading unit 11
2.3 Nuclear hydrogen production 12
2.3.1 The pebble bed modular reactor 12
2.3.2 The HyS process 13
2.4 Nuclear applications to synthetic fuels production 14
2.5 Summary and conclusion of literature reviewed 23
Chapter 3 27
Technical analysis of a nuclear-assisted syngas plant 27
3.1 Syngas process development 27
3.2 Material balance for a conventional syngas plant 27
3.3 Nuclear-assisted syngas process development 34
Chapter 4 44
Economic analysis of a nuclear-assisted syngas plant 44

4.1 Cost analysis methodology 44
4.2 Economic assumptions 44
4.3 Measures of economic feasibility 44
4.4 Sensitivity analyses 49
4.4.1 Cost sensitivity to hydrogen production cost 50
4.4.2 Cost sensitivity to coal cost 51
4.4.3 Cost sensitivity to interest rate 52
Chapter 5 54
Conclusions and Recommendations 54
5.1 Conclusions 54
5.2 Recommendations 57
Bibliography 58
Appendix 1 63

Abstract

The production of synthetic fuels (synfuels) in coal-to-liquids (CTL) facilities has contributed to global warming due to the huge CO_2 emissions of the process. This corresponds to inefficient carbon conversion, a problem growing in importance particularly given the limited lifespan of coal reserves. These simultaneous challenges of environmental sustainability and energy security associated with CTL facilities have been defined in earlier studies. To reduce the environmental impact and improve the carbon conversion of existing CTL facilities, this paper proposes the concept of a nuclear-assisted CTL plant where a hybrid sulphur (HyS) plant powered by 10 modules of the high temperature nuclear reactor (HTR) splits water to produce hydrogen (nuclear hydrogen) and oxygen, which are in turn utilised in the CTL plant. A synthesis gas (syngas) plant mass-analysis model described in this paper demonstrates that the water-gas shift (WGS) and combustion reactions occurring in hypothetical gasifiers contribute 67% and 33% to the CO_2 emissions, respectively. The nuclear-assisted CTL plant concept that we have developed is entirely based on the elimination of the WGS reaction, and the consequent benefits are investigated. In this kind of plant, the nuclear hydrogen is mixed with the outlet stream of the Rectisol unit and the oxygen forms part of the feed to the gasifier. The significant potential benefits include a 75% reduction in CO_2 emissions, a 40% reduction in the coal requirement for the gasification plant and a 50% reduction in installed syngas plant costs, all to achieve the same syngas output. In addition, we have developed a financial model for use as a strategic decision analysis (SDA) tool that compares the relative syngas manufacturing costs for conventional and nuclear-assisted syngas plants. Our model predicts that syngas manufactured in the nuclear-assisted CTL plant would cost 21% more than that produced in the conventional CTL plant when the average cost of producing nuclear hydrogen is US$3/kg H_2. The model also evaluates the cost of CO_2 avoided as $58/t CO_2. Sensitivity analyses performed on the costing model reveal, however, that the cost of CO_2 avoided is zero at a hydrogen production cost of US$2/kg H_2 or at a delivered coal cost of US$128/t coal. The economic advantages of the nuclear-assisted plant are lost above the threshold cost of $100/t CO_2. However, the cost of CO_2 avoided in our model works out to below this threshold for the range of critical assumptions considered in the sensitivity analyses. Consequently, this paper demonstrates the practicality, feasibility and economic attractiveness of the nuclear-assisted CTL plant.

Keywords: Synthesis gas, nuclear hydrogen, HTR, coal gasification, carbon dioxide, economics

List of Abbreviations

ABB – Asea-Brown-Boveri (Pty) Ltd

AFT – Ash Fusion Temperature

AR – As Received

ASF – Anderson-Schulz-Flory

ASPEN – Advanced System for Process Engineering

ASU – Air Separation Unit

Bbl – barrel

BPD – barrel per day

BTL – Biomass-to-Liquids

CCS – Carbon Capture and Storage

CEA – Chemical Equilibrium with Applications

CEPCI – Chemical Engineering Plant Cost Index

CO – Carbon monoxide

CO_2 – Carbon dioxide

COS –Carbonyl Sulphide

CPI – Chemical Process Industry

CTL – Coal-to-Liquid

DOD – Department of Defense

EO – Equation-Oriented

ETS – Emissions Trading Scheme

EU – European Union

FBDB – Fixed Bed Dry Bottom

Fe – Iron

FOB – Free On Board

F-T – Fischer-Tropsch

GO – General Overhaul

GHG – Greenhouse Gas

GHV – Gross Heating Value

GW – Global Warming

H_2 – Hydrogen

H_2O -Water

HTE – High Temperature Electrolysis

HTFT – High Temperature Fischer-Tropsch

HTR –High Temperature Reactor

HyS – Hybrid Sulphur

Kpa –Kilo-Pascal

Kmol – Kilo-mole

LPG – Liquefied Petroleum Gas

MAF – Moisture and Ash Free

MATLAB^{TM} – MATrix LABoratory

MM – million million

MPa – Mega-Pascal

MTG – Methanol-to-Gasoline

MW – Megawatt

MW_{avg} – Average molecular weight

O_2 – Oxygen

PBMR^{TM} – Pebble Bed Modular Reactor

ppm – parts per million

rtp – room temperature and pressure

RWGS – Reverse Water Gas Shift

SAS^{TM} –Sasol Advanced Synthol

SDA – Strategic Decision Analysis

SI – Sulphur Iodine

S-L – Sasol-Lurgi

Syncrude – Synthetic crude

Synfuels – Synthetic fuels

Syngas – Synthesis gas

TGA – Thermo-gravimetric analyzer

TPD – Tons per day (tpd)

TRISO – Triple-coated Isometric

US – United States

WGS – Water-gas shift

List of Figures

Figure 2.1 Basic CTL process diagram 7
Figure 2.2 The Lurgi moving-bed gasifier 9
Figure 2.3 Single module hybrid sulphur diagram 13
Figure 2.4 A coupling of the PBMR to the CTL process 16
Figure 2.5 An integrated solar-assisted coal gasification plant 17
Figure 2.6 A conventional CTL plant 19
Figure 2.7 A hybrid nuclear-CTL plant 19
Figure 2.8 The utilisation of nuclear hydrogen in CTL 200 20
Figure 2.9 Nuclear-assisted syngas production 22
Figure 3.1 Material balance schematic..... 27
Figure 3.2 Conventional syngas process flow scheme 28
Figure 3.3 Comparison of the actual and EO model mole fractions.....37
Figure 4.1 Syngas cost sensitivity to hydrogen cost 50
Figure 4.2 Sensitivity of the cost of CO_2 avoided to hydrogen cost.....50
Figure 4.3 Syngas cost sensitivity to delivered coal cost.....50
Figure 4.4 Sensitivity of the cost of CO_2 avoided to delivered coal cost 51
Figure 4.5 Syngas cost sensitivity to capital charge rate.....51

List of Tables

Table 2.1 Industrial development of CTL technology 6
Table 2.2 CTL process stream identification 7
Table 2.3 Carbon dioxide emissions from Sasol synfuels plants 10
Table 2.4 Hybrid methanol plant stream identification 17
Table 2.5 A comparison of CTL plant figures-of-merit 21
Table 3.1 Coal proximate analysis 29
Table 3.2 Volatile matter composition 29
Table 3.3 Raw gas composition (dry basis) 30
Table 3.4 Gasifier steady-state operating parameters 30
Table 3.5 Estimated miscellaneous parameters 30
Table 3.6 Process basis and specifications 30
Table 3.7 Material balance summary at 100 TPD(MAF) gasifier coal feed 31
Table 3.8 Material balance summary at nominal gasifier coal feed 32
Table3. 9 Syngas plant material balance summary 33
Table 3.10 Wet raw gas composition 34
Table 3.11 Comparison for dry raw gas composition ..... .42
Table 4.1 Main investment parameters for costing model 44
Table 4.2 Capital cost data for system modules and components 45
Table 4.3 Annual manufacturing cost for conventional syngas plant 46
Table 4.4 Nuclear-assisted syngas plant capital cost data 47
Table 4.5 Annual manufacturing cost for nuclear-assisted syngas plant 47

Chapter 1

Introduction

Chapter 1 presents an overview of the thesis through a concise background description and motivation. The objectives of the study are also presented in this chapter.

1.1 Thesis overview

A number of studies show that the world population is expected to reach between 9 and 9.5 billion by the end of the 21st century. The studies moreover indicate that oil and natural gas production will reach a peak and start to decline to half of todays level by 2050 (EIA, 2006). Coal is the most abundant and reliable primary energy source in the world. Despite its relative abundance, coal continues to be a limited resource under enormous demand. In a future scenario, defined by the mismatch between energy consumption and production, synthetic fuels (synfuels) will have to be derived from other lower grade natural resources or at the least, the coal consumption per barrel (bbl) of synfuel produced must be reduced.

The production of synfuels via the coal-to-liquid (CTL) technology has been an area of intense development for several decades. The most notable technology has been the Sasol technology developed and operated in South Africa since 1955.The continued rise of oil prices has ensured economic viability and subsequent growth of CTL facilities worldwide. For instance, eight (8) synfuel plants are expected to open in China with seventeen (17) more planned for the future. In the USA, three (3) states namely Montana, Illinois and Kentucky, contributing 56% of US coal deposits are promoting CTL technology and offering tax incentives for new-built plants. Furthermore, four-hundred (400) million gallons of synfuel are required for the US Department of Defence (DOD) alternative fuels program to fuel half the North American fleet with a petroleum-synfuel blend (McCormick, 2008). Such is the hype of activity worldwide in a bid to attain energy security.

However, the production of synfuels in a CTL plant produces enormous volumes of CO_2.The Sasol CTL plant in Secunda, South Africa, producing 150 000 bpd synfuels is one of the planet's single biggest point source of CO_2 emissions, emitting 50 million tonnes of CO_2 per year (Winkler, 2007). CO_2 is the most important greenhouse gas (GHG) which has resulted in global warming (GW), a phenomenon debatably accepted worldwide as the gravest threat to humanity. Thus, the environmental impact of coal-based synfuels production could have

far-reaching and deleterious consequences unless cost-effective and reliable technical solutions are drafted and implemented.

South Africa's economic growth, and indeed that of many nations, is based on a fossil fuel energy-intensive industry. This has resulted in the country being the highest emitter of CO_2 per capita in the world (Earthlife, 2009).The Secunda CTL plant has significantly contributed to this position, emitting about 21% of South Africa's total GHG emissions per year .The twenty-three (23) coal-fired power stations around the country contribute to the remainder. Against this background, it is inevitable that governments of nations, which are under immense pressure as signatories to the Kyoto Protocol and follow-up conventions, invoke paradigm shifts in their energy policies.

A more attractive futuristic option for the governments would be the imposition of heavy taxes or penalties levied on the release of CO_2 to the atmosphere. The consequential effects of this mode of CO_2 emission monetization on the CTL plant is the internalization of the associated costs, culminating in a significant increase in operating costs. Despite the predicted change in energy policies, the governments will continue to demand CTL facilities to produce synfuels at the present or increased capacity. At the very least, it becomes prudent that technology be developed that primarily reduces or eliminates the large environmental footprint of CTL plants.

Carbon sequestration (CCS) has been widely suggested as a solution to this quagmire. CCS involves capturing CO_2 and storing it in deep geological aquifers. However, the economic and ecological challenges facing this technology are a long way from being resolved. Furthermore, CCS has not yet reached technical maturity and cannot be an ultimate solution to the GW phenomenon. Muradov & Veziroglu (2008) perceive CCS as a technology that presents delays in finding a permanent solution to GW and also as a technology that creates a false impression of a solution. Furthermore, even though CCS was an option, South Africa, for instance has no in-land sequestration options and very little possibility for sequestration at sea (Van Heerden, 2005; Mwakasonda & Winkler, 2005). It is on this basis that this study discredits CCS and endeavours to look for a sustainable solution to the CTL predicament.

Nuclear energy has been accepted by and large as an essential option towards the establishment of sustainable development. In particular, the chemical process industry (CPI) has found much needed relief in the extensive development of nuclear process heat applications. Of major significance has been the on-going research and development of clean hydrogen production through a combination of thermo-chemical water splitting and Generation IV high-temperature reactor (HTR) nuclear technologies.

South Africa has designed and developed its own first-of-a-kind HTR, the PBMR. The PBMR (Pty) Limited has chosen the HyS process for the large scale production of nuclear hydrogen and oxygen. Greyvenstein (2008) proposed possible strategies of utilizing HTR technology integration in a possible hydrogen economy in South Africa. One of the strategies conceives the possible emergence of an environmentally friendly CTL solution through the utilisation of nuclear hydrogen and oxygen as feedstock to a CTL facility.

The potential benefits arising from the use of hydrogen in coal conversion have been trivially mentioned by various researchers. These include an increase in carbon utilization resulting in a higher product yield per unit coal input (Boardman, 2008; Forsberg, 2008; Greyvenstein, Correia, & Kriel, 2008). An increase in carbon utilization imply reduced CO_2 emissions hence the integration of the nuclear-based hydrogen production and CTL technologies would stand to benefit CTL facilities immensely. One of the immediate benefits of interest would be the revenue accumulating from carbon credits in a CO_2 emissions trading scheme (ETS).

However, the benefits of using nuclear hydrogen and oxygen as feedstock to a CTL facility have only been proposed and no extensive study has been performed showing the feasibility and economic viability of these concepts. Most of the studies have focused on hydrogen production systems than on niche' markets and downstream end-user technologies. The possibility of obtaining clean hydrogen via the HyS process creates a new wave of innovation to the fossil fuel facet. Thus, the main focus of this study is to develop a nuclear-assisted CTL plant in which nuclear hydrogen and oxygen form a significant part of the feedstock. As important as determining how and where in the process the nuclear hydrogen is to be fed, are the costs involved in implementing the drafted technical solutions. A hypothetical CTL plant such as the Sasol Synfuels factory is taken as the base case in this

study and the technological solutions drawn up are predicted to be suitable for implementation at any CTL facility in a retrofit or new-design strategy.

1.2 Thesis motivation

This study explores the integration between nuclear and thermo-chemical water splitting technologies to enable the reduction of the huge carbon footprint inherent in current CTL plants. In addition, technological solutions derived herein, are also aimed at increasing the lifespan of available coal deposits which at the present consumption rate, are limited to no more than 200 years (Gibson, 2007). This study explores the concepts of using nuclear hydrogen to solve the simultaneous sustainability challenges of CO_2 emissions and dwindling coal supplies in perspective of an inevitable population explosion.

In addition, most research and development has focused on several HTR concepts, water splitting technologies and advanced heat transfer loops prevalent in the hydrogen production systems. Other researchers have managed to couple nuclear and CTL technologies using nuclear heat directly in the coal gasification process of the CTL plant (Kosky, 1981; Yoshitomo, Motoo, Makoto, & Yutaka, 2000; Forsberg, 2008). The total integration of the nuclear-derived hydrogen and CTL technologies to achieve energy and environmental security has not been done before and a base case is thus established for this study. This study endeavours to find and outline a practical method of utilizing nuclear hydrogen and oxygen in CTL production facilities.

1.3 Thesis objectives

The main focus of this study is to establish how nuclear hydrogen and oxygen, derived from a thermo-chemical water splitting HyS process, could be incorporated into the CTL plant in order to reduce the CO_2 footprint while simultaneously reducing the coal feed per barrel of synfuels produced.

The objectives of this study are to:

I. Develop an understanding of the basic processes of a CTL plant and identify CO_2 point sources.
II. Develop a technical solution based on the utilization of nuclear hydrogen and oxygen to reduce the large environmental footprint and coal inventory inherent in a conventional CTL plant.
III. Establish a strategic decision analysis (SDA) tool through comparison of the economics of the conventional and nuclear-assisted CTL facilities.

IV. Win government confidence through demonstrating that CO_2 emissions per capita can be reduced and Kyoto protocol targets sufficiently met without hindering economic growth and policy objectives.

1.4 Thesis outline

Chapter 1 presents an overview of the thesis through a concise background description and motivation. The objectives of the study are also presented in this chapter.

Chapter 2 presents a literature review which gives an assessment of nuclear technology and thermo-chemical processes that have been used to produce clean hydrogen as well as the past endeavours on utilizing nuclear hydrogen and nuclear process heat in synfuels production facilities. A base case for the study is motivated.

Chapter 3 presents the technical analysis where a first-order mass analysis model is established and subsequently used to develop the nuclear-assisted syngas plant on the basis of the operational parameters of a reference hypothetical CTL plant.

Chapter 4 presents an economic analysis where the conventional and nuclear-assisted CTL plants are compared on the basis of the manufacturing cost of syngas. The comparison forms the backbone of a strategic decision analysis model where a decision to invest or not to invest into the turnkey nuclear-assisted CTL plant is made.

Chapter 5 concludes with a summary and recommendations based on the techno-economic assessment performed in Chapters 3 and 4.

Chapter 2

Literature review

Chapter 2 presents a literature review that primarily gives an assessment of nuclear technology and thermo-chemical processes that have been used to produce clean hydrogen as well as the efforts by numerous research entities to utilize nuclear hydrogen and nuclear process heat in synfuels production facilities. A base case for the study is motivated.

2.1 Development of the CTL process

Liquid hydrocarbons can be obtained from coal by indirect hydrogenation in a process known as the Fischer-Tropsch (F-T) process, invented by Franz Fischer and Hans Tropsch (1920) in Germany. Coal is first converted into syngas, a mixture of CO and $H_{2,}$ which is subsequently purified and passed through a solid catalyst to produce liquid hydrocarbons.

Table 2.1 Industrial development of CTL technology

Year	Inventor	Invention
1902	Sabatier.P et al	Hydrogenation of CO over Ni catalyst to produce methane
1913	Badishe.A et al	Preperation of hydrocarbons and oxygenates by hydrogenation of CO on oxide catalyst
1923	Fischer.F & Tropsch.H	Obtained Synthol from hydrogenation of CO over Fe catalyst
1925	Fischer.F & Tropsch.H	Synthesis of high hydrocarbons at atmospheric pressure on Co & Ni Catalysts
1932	Fischer.F & Meyers.K	Development of new Co & Ni catalysts to improve yield of liquid hydrocarbons
1933	Ruhrchemie A.G	Pilot plant test using newly developed Ni catalyst
1937	Fischer.F & Pichler	Greatly improved synthesis of hydrocarbons on Fe catalyst at 5 to 20 atm
1950	Hydrocarbon Research	Fluidised bed process developed in Texas(Brownsville) using reformed natural gas
1955	SASOL	SASOL 1 plant opened at Sasolburg, South Africa.Plant uses Fe catalyst in fixed bed and entrained bed reactors
1975	SASOL	SASOL 2 plant opened at Secunda, South Africa.Plant uses Fe catalyst in entrained bed reactors.
1979	SASOL	SASOL 3 plant opened at Secunda, South Africa.Plant uses Fe catalyst in SAS reactor.

Table 2.1 above summarizes the development of CTL technology. From 1935 to 1945, several commercial plants were built in Ruhr, Germany. The alkalized Fe catalyst became the catalyst of choice in these commercial plants (Kotanigawa, Chakrabartty, & Berkowitz, 1981; Rao, Stiegel, Cinquegrane, & Srivastava, 1992).

2.2 Basic CTL process description

The production of synfuels from coal via the CTL technology has been an area of intense development for several decades as shown in Table 2.1. The CTL plant is basically divided into three processing stages;

I. Syngas production

II. Fischer-Tropsch synthesis

III. Product upgrading

Figure 2.1 below shows a simplified block diagram of a CTL plant and a brief description of the processes is given.

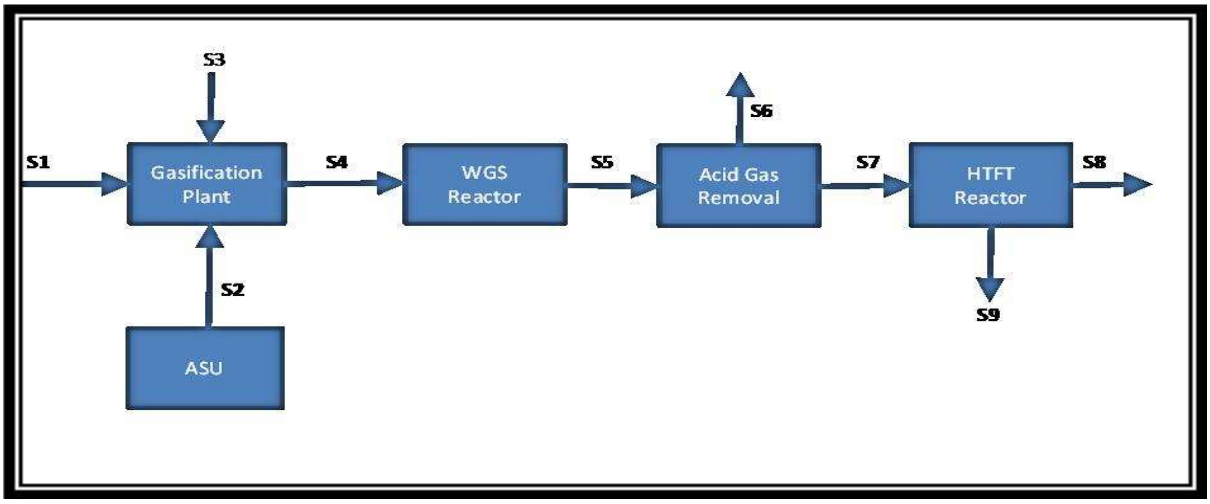


Figure 2.1 Basic CTL process diagram (Steynberg & Nel, 2004)

The streams S1 to S9 in Fig. 2.1 are defined below in Table 2.2

Table 2.2 CTL process stream identification

Stream	Component
S1	Steam
S2	Oxygen
S3	Coal
S4	Raw Syngas
S5	Shift Gas
S6	Carbon Dioxide
S7	Syngas
S8	Tailgas
S9	Syncrude

2.2.1 Syngas production unit

The objective of this stage is to produce syngas that meets the feed specifications and requirements of the F-T synthesis section. The syngas production unit consists of the following major sub-sections;

I. Coal handling plant

II. Gasification plant

III. Syngas cooling and purification plant

2.2.1.1 Coal handling plant

The coal handling plant is an essential part of the CTL plant. Its main purpose is to receive and prepare the raw coal for gasification thus ensuring a high plant availability factor and high plant efficiency (Johnson & Conger, 1981). Coal preparation consists of a series of screening, crushing and de-dusting (washing) and blending unit operations (Meyers, 1981). There is a particle size distribution required for each gasification process. For instance, the feed to a Sasol-Lurgi fixed-bed dry bottom (S-L FBDB^{TM}) gasification plant is sized between 6-75mm. The coal handling plant is capital intensive and demands high energy due to the high capacity and robust operations involved (Detman, 1977).

2.2.1.2 Gasification plant

The gasification plant converts coal feed to raw gas in a battery of gasifiers in parallel operation. A mixture of oxygen and steam is used as the blast or gasifier agent. The oxygen is prepared in the air separation unit (ASU) where air is compressed to 5 bars, water and carbon dioxide condensed and removed, and air is separated in a cryogenic distillation unit (Hersh & Abrardo, 1977; Wolff, Eyre, & Grenier, 1979). Nitrogen is the main by-product of the ASU and may be used for pneumatic conveying of coal, inerting or as a chemical feedstock to an ammonia plant.

Coal gasification processes vary depending on the type of coal feed and desired syngas heating characteristics.The methods of gas-solid contact for gasification processes are moving-bed, fluidised-bed, and entrained-bed (Smoot & Smith, 1985). The moving-bed coal gasifiers produce 89% of world's syngas and has been extensively used particularly for low rank, non-caking coal. For instance, the South African coal is low rank and Sasol use the S-L FBDB^{TM} gasifier. The entrained-bed gasifiers such as those used in the Shell gasification process are capable of handling any type of coal and tend to yield higher CO in the raw gas.

2.2.1.2.1 S-L FBDB^{TM} gasifier operation

A batch of coal fed at the top of the S-L FBDB^{TM} gasifier moves down towards the bottom at a velocity of 3mm/s countercurrent to a stream of the blast.The average upward gas velocity through the gasifier is 0.3m/s (Mahalingham, 1985).The gasification of coal takes place at 0.1-2.7MPa. Devolatilisation of the coal occurs initially, and is then followed by gasification within the temperature range 1150K to 1400K. The residence time of gas in the gasifier is 8 to 10 seconds and that for coal is about 1 hour.

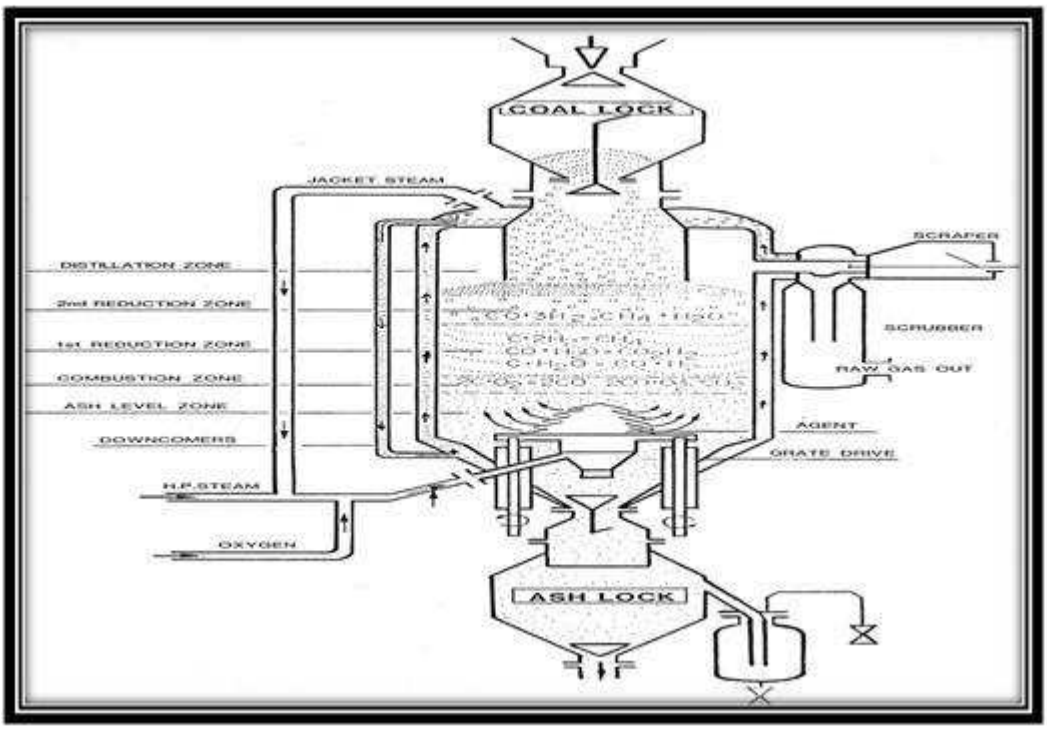


Figure 2.2 The Sasol-Lurgi FBDB^{TM} gasifier (Hebden & Stroud, 1981)

Steam is the source of hydrogen and maintains the gasifier operating temperature below the ash fusion temperature (AFT) of the coal. The combustion of a portion of the devolatized coal (char) with oxygen supplies the heat required by the endothermic gasification reactions (Lee, 1982). A revolving grate at the bottom of the gasifier reactor suppports the coal bed, removes the ash, and introduces the blast into the gasifier. The gasifier produces gas continuously although the coal lock and ash lock are operated batchwise. The crude syngas leaving the gasifier at temperatures between 450^{o}Cand 550^{o}C contains tar oils, phenols, and ammonia (Ricketts, 1963). The latter are called volatiles.

The coal bed in the gasifier moves through four poorly-defined, overlapping reaction zones namely drying and pyrolysis, devolatilisation, gasification and combustion.The coal is subjected to increasingly high temperatures on traversing the gasifier height until it reaches the oxidation zone where it is combusted to leave behind ash. The composition of the gas is also continuosly changing with gasifier height. The drying and pyrolysis zone is situated at the top of the gasifier bed. In this zone, the temperature is not too severe and the volatiles evolve from the coal to yield char. The reactivity of the char depends on the coal type and the pyrolysis conditions encountered in the devolatisation zone. The pyrolysis zone is therefore an important sub-section of the gasifier (Morgan, 1991).

Most of the chemical reactions prevalent in the gasifier occur in the reduction (gasification) and oxidation (combustion) zones. The devolatized char enters the reduction zone where the following equilibrium reactions take place:

$$C + H_2O \Leftrightarrow CO + H_2 \quad (R1)$$

$$C + CO_2 \Leftrightarrow 2CO \quad (R2)$$

$$C + 2H_2 \Leftrightarrow CH_4 \quad (R3)$$

$$\alpha C + O_2 \Leftrightarrow 2(\alpha - 1)CO + (2 - \alpha)CO_2 \quad (R4)$$

$$CO + H_2O \Leftrightarrow CO_2 + H_2 \quad (R5)$$

R1 to R3 are the reduction reactions whilst R4 is the oxidation reaction. The water-gas shift (WGS) reaction (R5) is the most significant of the numerous side reactions and determines the thermodynamic equilibrium of the gas phase. The factor α is dependant on the type of coal used and can vary between one and two. The α factor for South-African low-rank, high-ash coal has been found to be unity (Morgan, 1991).

2.2.1.3 The syngas cooling and purification plant

This sub-section is considered part of the gasification plant depending on the CTL plant set-up. The raw gas exiting the gasifier is steam-saturated in the wash cooler and subsequently cooled down in successive stages using the waste-heat boiler, the pre-coolers, air coolers, trim coolers and the final coolers. The raw gas is cooled down to about 35^{o}C and the volatiles are condensed to yield gas liquor. Depending on the type of gasification plant, the syngas is fed to the WGS reactor to increase its hydrogen concentration to the feed specifications of the F-T reactor. The WGS reaction is the primary cause of the carbon dioxide which has to be removed in the acid gas removal (Rectisol) unit before F-T synthesis.

Table 2.3 Carbon dioxide emissions from Sasol synfuels plants

Plant	Carbon dioxide Source	Amount (MMTPY)	Concentration (%)
Sasol 1(Sasolburg)	Boilers & Heaters	7	10 to 15
	Downstream Gasifiers	4	90 -98
Sasol 2 (Secunda)	Boilers & Heaters	9	10 to 15
	Downstream Gasifiers	14	90 to 98
Sasol 3 (Secunda)	Boilers & Heaters	9	10 to 15
	Downstream Gasifiers	14	90 to 98
TOTAL		57	

Adapted from (Engelbrecht, Golding, Hietkamp, & Scholes, 2004)

Table 2.3 shows the point sources and distribution of CO_2 emissions from the Sasol Synfuels plants. The WGS reaction in the Sasol gasification process occurs inside the gasifiers, contrary to the other plants that have an external WGS reactor. Thus, from a process perspective, the gasifier and WGS reactor are identified as some of the emissive point sources of carbon dioxide in a CTL plant. According to Table 2.3, the gasifiers at the Secunda CTL plants produced a total of 28 million tons of carbon dioxide for the year 2004.

2.2.2 The Fischer-Tropsch synthesis

The pure syngas is converted to hydrocarbon liquid (syncrude) in the F-T reactor. For instance, Sasol operates ten (10) Sasol Advanced Synthol (SAS^{TM}) reactors at its Secunda Synfuels plant. The liquid hydrocarbon product slate is quite complex and depends on the reactor operating conditions. The F-T reaction is presented as:

$$2n\,\mathrm{CO} + n\mathrm{H}_2 \rightarrow n(\text{-}\,\mathrm{CH}_2\,\text{-}) + nH_2\mathrm{O}$$

CH_2 is the basic building olefin monomer. The exact mechanism for the F-T reaction is still a centre of controversy but most researchers have agreed on the Anderson-Schulz-Flory (ASF) model representing the polymerization equation. The ASF model assumes a stepwise addition of carbon on the hydrocarbon chains attached to the catalyst surface. The high-temperature F-T (HTFT) reactor contains only gas and catalyst (iron-based) with no liquid phase outside the catalyst pores. The HTFT operating temperature is between 320^{o}C and 350^{o}C and the reactor is typically operated at a pressure of about 25 bars to yield a highly olefinic hydrocarbon product. Furthermore, the HTFT reactor requires syngas with high hydrogen concentration to avoid rapid catalyst deactivation due to carbon formation. The minimum H_2/CO ratio required to avoid carbon formation on catalyst during the F-T synthesis is 1.8 (Steynberg, Espinoza, Jager, & Vosloo, 1999). The iron-based F-T catalyst in the HTFT reactor is WGS active hence the F-T reactor becomes another point source of the carbon dioxide emissions. However, this emission point source is not of relevance in this study and will not be treated further.

2.2.3 Product upgrading unit

The product upgrade unit comprises of the hydrocarbon product recovery plant that separates the syncrude into various products. It consists of the following operations: Olefin oligomerization, naphtha hydrocracking and product fractionation. Hydrogen is an essential feed for the hydrocracking operations and is used to saturate the heavy hydrocarbon fraction from the F-T synthesis. Some of the final products from the product upgrade section are premium-quality petro-chemical naphtha, gasoline, liquefied petroleum gas (LPG) and a diesel blend. Diesel or gasoline production is maximized by design. The processes are

purely petro-chemical operations prevalent at any petroleum refinery. The product upgrade section is another source of CO_2 emissions due to the extensive heat exchange network consisting of gas turbines, furnaces and boilers that characterise the distillation units. However, the use of nuclear process heat can alleviate the environmental problem arising, but this is outside the scope defined for the present study.

2.3 Nuclear hydrogen production

Nuclear energy has generally been accepted as an essential option towards the establishment of the principle of sustainable development. South Africa is involved in the research and development of the production of clean hydrogen through a combination of thermo-chemical water splitting and Gen IV HTR nuclear technologies. The integration of these two technologies has yielded strategic hybrid technology advancement for hydrogen production. This section gives a brief discussion of the hydrogen production technology developed.

2.3.1 The pebble bed modular reactor

South Africa has designed and developed its own first-of-a-kind HTR, the pebble bed modular reactor (PBMR). The PBMR is a graphite-moderated HTR that operates on a closed helium cycle. The reference design is a $500MW_{th}$ vertical steel pressure vessel that uses TRISO pebble reactor fuel. Helium is used as a coolant and energy transfer medium to drive a closed cycle gas turbine and generator system. The helium coolant enters the reactor vessel at a temperature of 500^oC and a pressure of 9MPa. The coolant moves down between the hot fuel pebbles and attains a reactor outlet temperature of 900^oC. The high reactor outlet temperature of the helium coolant gives the HTR significant opportunities to provide CO_2 -free process heat for a variety of applications. This heat can be used directly in various energy-intensive industrial processes, further extending the lifespan of coal reserves.

However, hydrogen production would need a heat-to-electricity conversion system of the PBMR. In this module, the hot helium then enters the gas turbines which drive the compressors and electrical generator. The coolant exits the last turbine at 500^oC and 2.6MPa after which it is cooled, recompressed and returned to the reactor vessel. It is the electricity-producing module of the PBMR that is integrated to the HyS thermo-chemical water-splitting process to yield nuclear hydrogen and oxygen. The construction of the PBMR demonstration power plant in South Africa has been delayed and the government has recently decided to postpone the project. However, the USA, China and Korea are at advanced stages of HTR development and are most likely to be the first to unveil the design.

2.3.2 The HyS process

Major international players in HTR process heat applications have chosen thermo-chemical water splitting as the technology of choice in hydrogen production because they have potential for higher efficiencies than water electrolysis and more favourable scale-up characteristics (Kuhr, 2008). The PBMR (Pty) Limited has chosen the HyS process for the large scale production of nuclear hydrogen and oxygen. Although the HyS or SI (Sulphur Iodine) processes have not yet been commercialised, they have been demonstrated at a laboratory scale to confirm performance characteristics (Gorensek & Summers, 2009).

Figure 2.3 below shows the HyS process. Sulphuric acid is fed to the decomposition reactor where it is thermally reduced using the HTR process heat. The products of the reduction process are sulphur dioxide, oxygen and water. The oxygen is separated from the SO_x stream and make-up water is added. The water-sulphur dioxide mixture is then electrolysed to generate hydrogen gas. In the electrolysis process, sulphuric acid is regenerated and is recycled back to the decomposition reactor. The HyS process produces eight times more oxygen than hydrogen, on a mass basis (Gorensek & Summers, 2009). This has the implication that the expensive to operate ASU at a CTL plant could be eliminated resulting in significant savings in operating costs. The electrical power for electrolysis is provided by the same HTR module that supplies the thermal energy to the decomposition reactor.

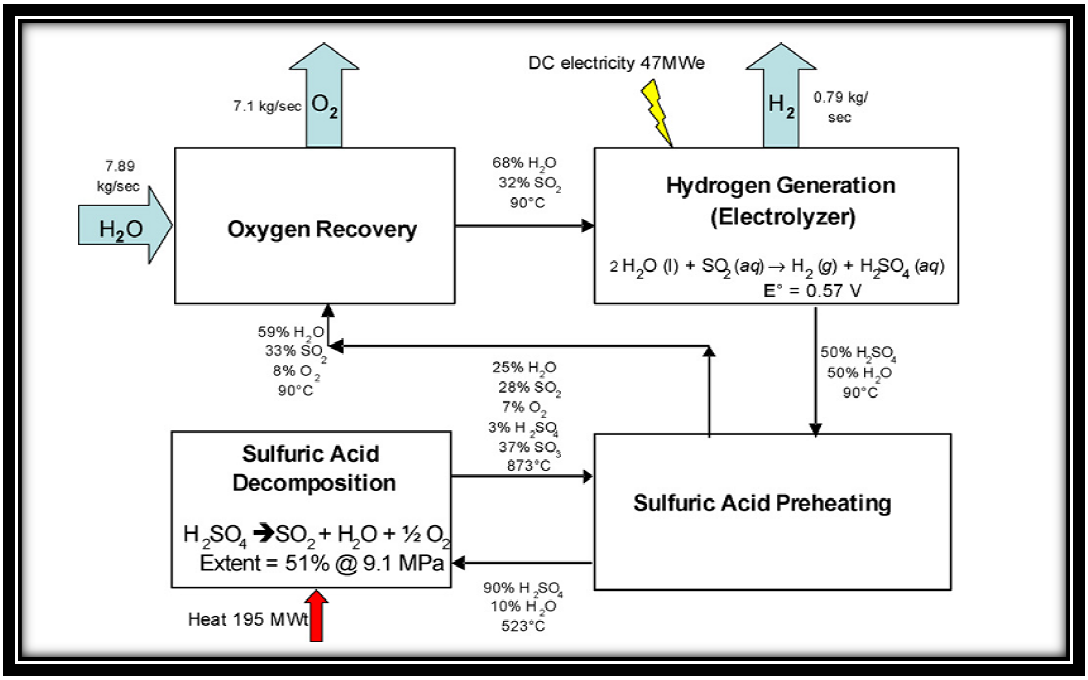


Figure 2.3 Single module hybrid sulphur diagram (Lahoda, et al., 2006)

However, the HyS process is still under development with the decomposition reactor being the critical path and currently under various stages of optimization at a number of institutions worldwide. Furthermore, operating and capital costs need to be lowered to make the HyS process a success (Gorensek & Summers, 2009). The cost of hydrogen produced from the HyS is estimated at $3 to $5/kg with potential to decrease with HyS development and technology maturation.

2.4 Nuclear applications to synthetic fuels production

This section reviews and analyzes the efforts made by numerous research entities in attempting to find sustainable solutions to the environmental and energy security problems identified herein through the utilization of HTR technology in synfuels production facilities.

Yoshitomo et al (2000) illustrated a method of utilizing nuclear heat in a two-stage fluidized-bed gasifier. The result was an effective reduction in CO_2 emissions compared to a conventional gasification process. The nuclear heat provided the heat of reaction to the endothermic gasification reactions which would otherwise be supplied by coal combustion in the gasifier. However, direct utilization of nuclear heat in a hypothetical moving-bed gasifier presents enormous technical challenges due to the difficulty associated with placing bayonet heat transfer tubes in a fixed-bed configuration without upsetting gasifier operational parameters.

Forsberg (2008) provided a limited scope focusing specifically on the direct use of HTR in liquid fuels production systems using natural gas feedstock. In circumstances where CTL was used to produce synfuels, he proposed using HTR process heat at the product recovery section including the utilities, both of which are energy intensive sections. The result was the reduced coal consumption and subsequent reduction in GHG emissions.

Song & Guo (2007) performed the co-gasification of coal and natural gas in a fixed-bed reactor to yield reduced CO_2 emissions and subsequently an increase in the H_2/CO ratio of the resultant syngas. This is a significant result which Sasol are pursuing at their Secunda Synfuels complex but is not of much relevance to the current study.

Hishida et al (1997) acknowledged the need to reduce the CO_2 emissions from coal combustion activities. They identified a process for reforming coal to synfuels that was to significantly reduce the CO_2 emissions. Integral to the coal reforming process proposed were two nuclear heat applications. They proposed a fixation process based on the re-use of CO_2 to produce synfuel and other chemical products with the aid of nuclear heat. In this scheme, the HTR supplied thermal energy directly to the steam-gasification process. Part of the thermal energy was utilized for the production of hydrogen in a steam electrolysis process. The nuclear hydrogen so produced was mixed with CO_2 rich syngas from the gasifier prior to a methanol synthesis reactor.

The supplemental nuclear hydrogen was critical to achieving the desired H_2/CO ratio of 2 for the methanol synthesis reaction. The methanol produced was supplied to a methanol-to-gasoline subsystem (MTG). This sub-system has a huge potential of reducing CO_2 emissions and is a possible technical solution to the sustainability challenges being addressed by the current study. It must be noted that the MTG is an off-the-shelf technology and that the study under review was a paper study emphasizing possible nuclear heat applications to reduce GHG emissions. No commercial set-up is available.

Kuhr (2008) specified the role of HTR in CTL plants as that of providing electricity to the water-splitting technology thus avoiding the cost of conversion of coal to CO_2. In addition, he mentioned the elimination of a significant fraction of the coal handling and gasification facilities. However, there is no elaboration or hint as to how this is to be achieved in practice.

Greyvenstein et al (2008) outlined the strategies that South Africa need to adopt in order to benefit from the PBMR. The PBMR was used to provide electricity to the hydrogen production system and the nuclear hydrogen so produced used as feedstock to the CTL plant. According to Figure 2.4 below, the supplemental hydrogen was introduced to the raw gas just prior to the HTFT reactor. This eliminated the WGS reaction or step which in the conventional CTL plant produces additional hydrogen to tailor the H_2/CO ratio to a minimum of 1.8. In addition, the oxygen from the HyS process was introduced as feed to the gasification plant rendering the traditional ASU obsolete.

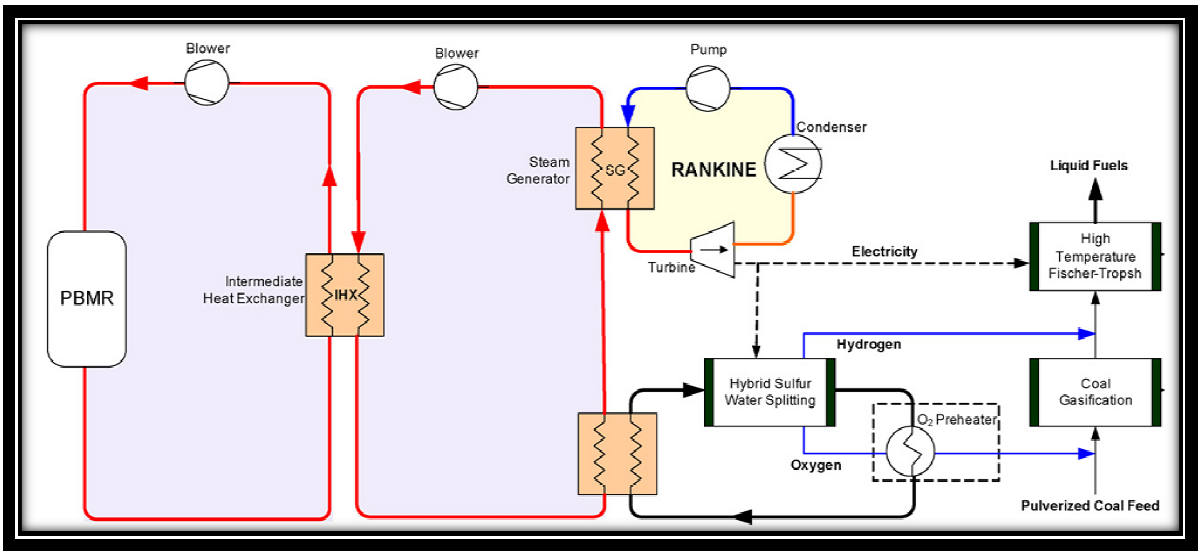


Figure 2.4 A coupling of the PBMR to the CTL process (Greyvenstein, Correia, & Kriel, 2008)

The utilization of nuclear hydrogen and oxygen is thus driven by economic factors which include major offsets in capital and operating costs. The study addressed in part, the central statement of this thesis but is essentially an informative study providing a baseline for future research.

Forsberg (2005) evaluated the potential of nuclear hydrogen in a future era where nuclear energy becomes the primary technology for initiating the hydrogen economy. Of interest is the mention of the possible use of nuclear hydrogen in liquid fuels production although this is not elaborated upon. The review however motivates the current study.

Koump (1982) attempted to achieve clean coal gasification by reducing the concentration of polycyclic aromatic hydrocarbons released during coal devolatilization. In the embodiment of the invention, he recycled a split stream of raw syngas to the gasifier to maintain a high partial pressure of hydrogen (20-40 atm). The result was the prevention of polymerization of the free radicals formed. The work carried out indirectly addressed the current study in that it presented an insight into the feasibility of a hydrogen feed into the gasifier although the primary aim was different from that to be achieved by this thesis. Given a similar set-up, the current study would have further evaluated the effects of a gasifier hydrogen feed on the raw gas CO_2 concentration.

Katayama & Tamaura (2005) acknowledged the huge extent of environmental challenges in both coal gasification and natural gas steam-reforming in a methanol production system. The study proposed a zero CO_2 emission system that essentially was a combination of a fossil fuel and renewable solar energy as shown in Figure 2.5 below.

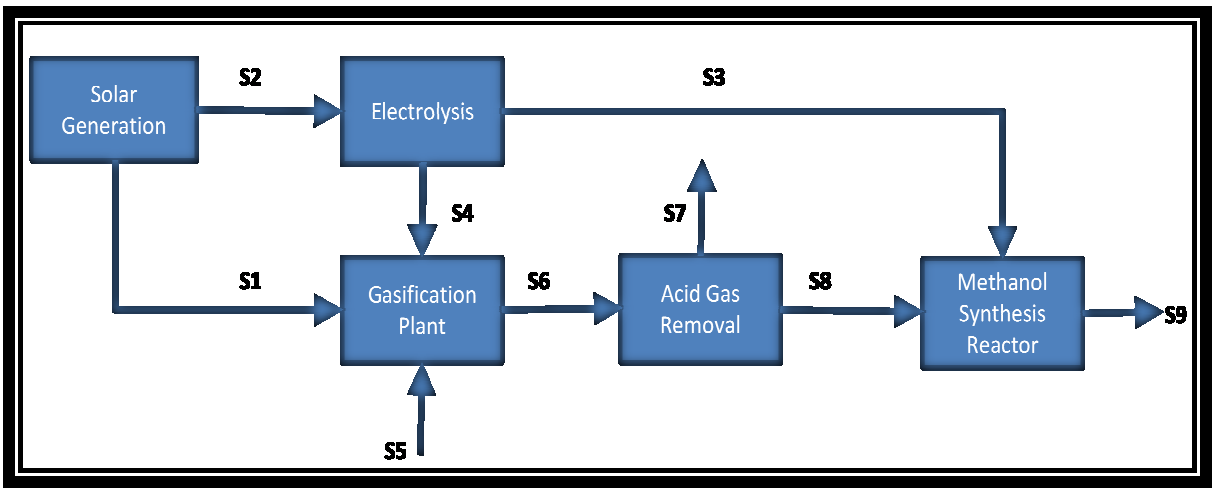


Figure 2.5 An integrated solar-assisted coal gasification plant

The respective streams of Figure 2.5 are shown below in Table 2.4 below. The methanol could be an intermediate to synfuel production hence the proposal is relevant to the current study. The solar heat utilization in the gasifier implies that all the coal feed is solely consumed by the gasification reduction reactions for syngas production rather than by the oxidation reaction hence reduced CO_2 emissions. The supplemental hydrogen corrects the H_2/CO ratio for the methanol synthesis reaction.

Table 2.4 Hybrid methanol plant stream identification

Stream	Component
S1	Solar Process Heat
S2	Electricity
S3	Solar Hydrogen
S4	Solar Oxygen
S5	Coal
S6	Raw Syngas
S7	Hydrogen Sulphide
S8	Carbon Dioxide laden Syngas
S9	Methanol

This strategy was suggested earlier by (Hishida, et al., 1997). The CO_2 produced in the gasifier turns up to be an essential raw material for the methanol synthesis reaction due to the availability of the carbon-free supplemental hydrogen. Such a strategy could be adopted

by the current study to eliminate the large environmental footprint of CTL plants whilst inherently extending the mineable lifespan of the limited coal reserves.

In addition, an economic analysis of the proposed system was performed and the significant result was that the methanol cost of the system was equivalent to that of a conventional methanol production system. However, the main drawback of their study was the choice of solar rather than nuclear technology to integrate the water-splitting process. Although the capital costs for the nuclear and solar technologies are comparable ,nuclear energy is intrinsically a large-scale energy production system with a much greater capacity factor compared to solar energy which is hindered by day-night and seasonal variations of the sun. If the system had been integrated with nuclear technology, the methanol so produced would be cheaper, on a neck-to-neck basis, than that produced from the conventional process.

Katayama (2006) claimed to have found a method of gasifying coal that produced high heating value syngas and very low CO_2 emission. Solar energy was used to produce electricity for the electrolysis plant whereupon in the invention, the hydrogen so produced was split into 2 streams with one stream fed to the gasifier and the other mixed with syngas downstream of the gasifier. Oxygen was introduced into the gasifier at 1 to 1.5 times the required amount of molar oxygen. Hydrogen was introduced in an amount from 2-3 times the required amount of oxygen .The steam was introduced in the gasifier at a temperature between 300-600^{o}C and in an amount 0.15 -0.6 times the weight of feed coal. As a result, the steam-gasification was carried out at a temperature from 1000-2500^{o}C and very low CO_2 emissions were attained.

However, in as much as the invention motivates the current study, the gasifier temperatures attained are far greater than the ash fusion temperatures of the inertinite-rich South African coals. The implication is that ash exits the gasifier in slag form, contrary to the gasifier operational philosophy. In addition, the choice of solar energy against nuclear energy to provide thermal heat for the water-splitting electrolysis process proves to be disadvantageous from a cost perspective given that solar energy has a lower capacity factor.

Boardman (2008) portrayed the possible role of hybrid energy systems in attaining energy and environmental security. In his analysis, he identified niche-markets for nuclear process heat in thermo-chemical hydrogen production and coal gasification systems. The idea of a nuclear-fossil hybrid energy system was conceived whereupon nuclear hydrogen and oxygen were used in a hydrocarbon conversion process. The comparison between the conventional and nuclear hybrid plant is well illustrated in Figures 2.6 & 2.7 below .The hybrid system uses 70% less coal for the same of synfuel output as a result of recycled carbon dioxide providing a carbon source in the gasifier.

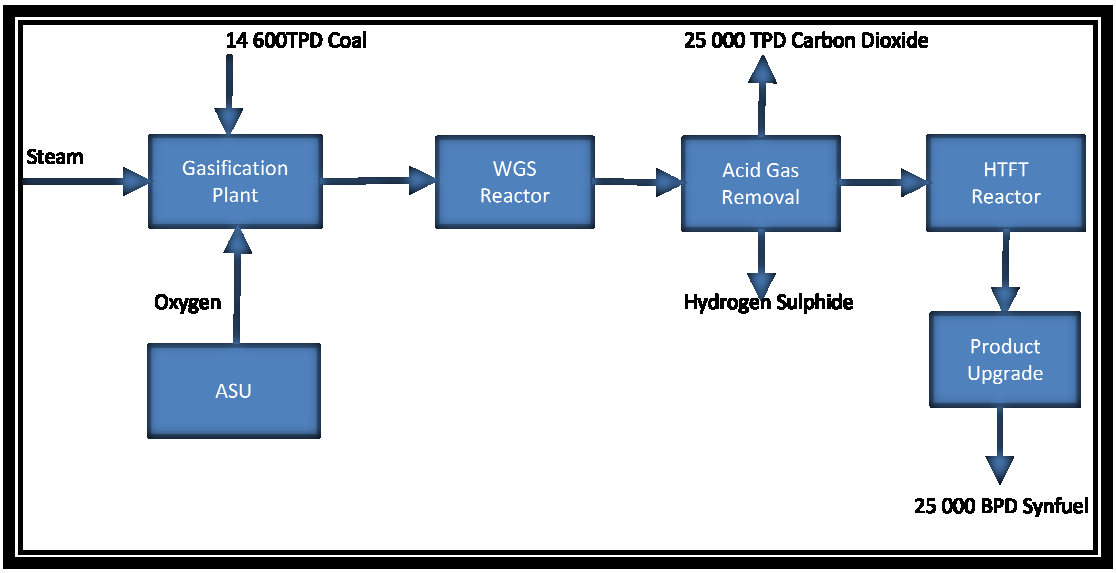


Figure 2.6 A conventional CTL plant (Boardman, 2008)

The WGS is eliminated from the hybrid system in Figure 2.7 because of the availability of a secure external hydrogen source to tailor the H_2/CO ratio of the syngas feed to the F-T reactor.

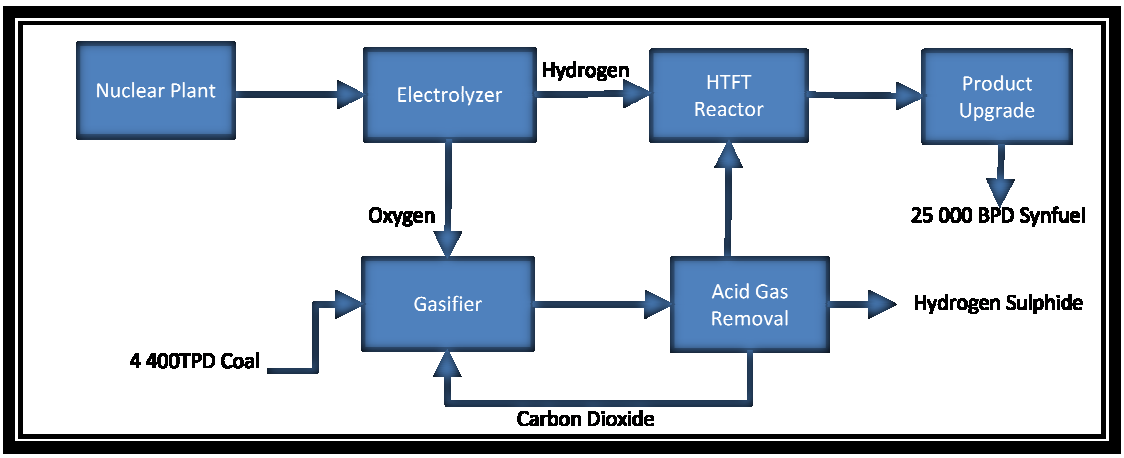


Figure 2.7 A hybrid nuclear-CTL plant (Boardman, 2008)

The elimination of external shift reaction is beneficial in that the CO_2 produced from the acid gas removal unit is sufficiently less as compared to that from the conventional CTL plant. This enables all of the CO_2 to be recycled to the gasifier. Thus, a carbon-neutral CTL plant is achieved. However, there is not yet a bench scale or demonstration test to verify this phenomenon and the economic viability of a nuclear-hybrid CTL has not been done. A base case for the current study is motivated.

Cherry & Wood (2008) proposed the recycling of CO_2 to the gasifier in an identical set-up to the Boardman scheme. They cited an increase in the carbon conversion of the gasification process and an approach to zero CO_2 emissions of the CTL plant. In another aspect of the invention, the recycling of all carbon-containing process streams including the F-T tail-gas yielded an even much higher carbon conversion. The resultant CTL module is herein identified as CTL 300 and the conventional CTL module identified as CTL 100.

In still yet another embodiment of the invention by Cherry and Wood (2008), nuclear hydrogen was fed to the gasifier to assist in the conversion of CO_2 produced in the gasifier to CO (Figure 2.8). This resulted in an increase in the CO concentration in the syngas and the H_2/CO ratio was corrected by a supplemental hydrogen stream prior to the F-T reactor. The concept of feeding hydrogen to the gasifier was proposed earlier by Koump (1982) and Katayama (2006).

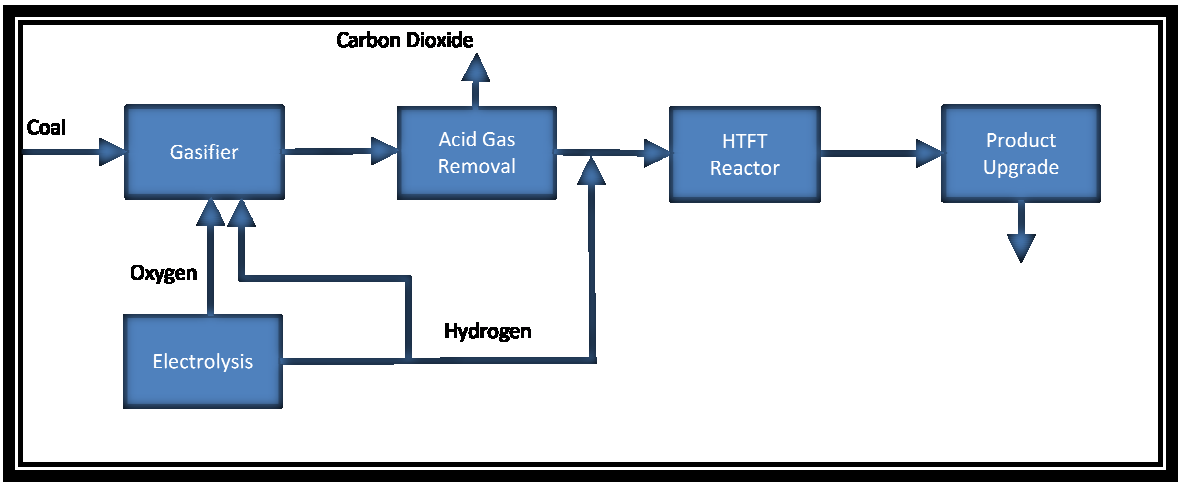


Figure2.8 The utilisation of nuclear hydrogen in CTL 200 (Cherry & Wood, 2008)

A simulated comparison of the three processes CTL 100, CTL 200 and CTL 300 was performed using ASPEN^{TM} and the results are illustrated in the Table 2.5 below.

Table 2.5 A comparison of CTL plant figures-of-merit

	CTL 100	CTL 200	CTL 300
Coal Feed(TPD)	18 800	18 800	18 800
Synfuel Produced(BPD)	26 000	58 200	84 672
Conversion(BPD Fuel/TPD Coal)	1.38	3.09	4.49
Synfuel Yield(% of Carbon Input)	29.5	65.8	95.7

The analysis of Table 2.5 leads to the conclusion that the invention schemes CTL 200 and CTL 300 are possible technological solutions to the sustainability challenges addressed in the current study. However, the recycle of all the carbon-containing gases as proposed in CTL 300 requires a larger than normal gasifier that may not be feasible or economic in the short-term. The recycle of the CO_2 stream is more practical and most likely to have greater performance characteristics than scheme CTL 200.The work presented has been an outright paper study, once again showing simulation effects of various possible schemes without any feasibility or economic studies having been done.

Muradov & Veziroglu (2008) proposed various de-carbonization strategies aimed towards attaining green fuel technology in a possible hydrogen economy. One of the schemes attempted to strip CO_2 from the atmosphere to provide an infinite source of carbon for the production of alternative fuels to be achieved through hydrogenation. The cost of scrubbing atmospheric CO_2 renders the concept technically and economically immature for the short and medium-term although it endeavors to solve the sustainability challenges outlined in the current study. However, the concept can be adopted from the perspective of the CTL plant where there already exits a ready point source of CO_2. It is interesting to note that CO_2 fixation to yield alternative fuels is an extremely attractive idea that has been actively pursued globally by research entities for decades.

Harvego et al (2008) proposed a nuclear-assisted gasification plant and assessed two figures of merit namely production efficiency and carbon utilization. In the proposed scheme, nuclear hydrogen is mixed with the gasifier outlet stream to yield a hydrogen-rich gas mixture. This is a seemingly popular strategy that has been employed by most researchers mentioned earlier in the current study. However, the hydrogen-rich gas is fed to the reverse water gas shift (RWGS) reactor where the CO_2 in the gas mixture is converted to CO as shown in Figure 2.9 below. In their study, a process simulation tool (UniSim^{TM}) was used to

evaluate the performance of the syngas production system proposed. The results of the analysis predicted a syngas feed ratio of 2 and most importantly, a 90.5 % carbon utilization, which is extremely good compared to the 30% carbon utilization that characterizes the conventional CTL plant.

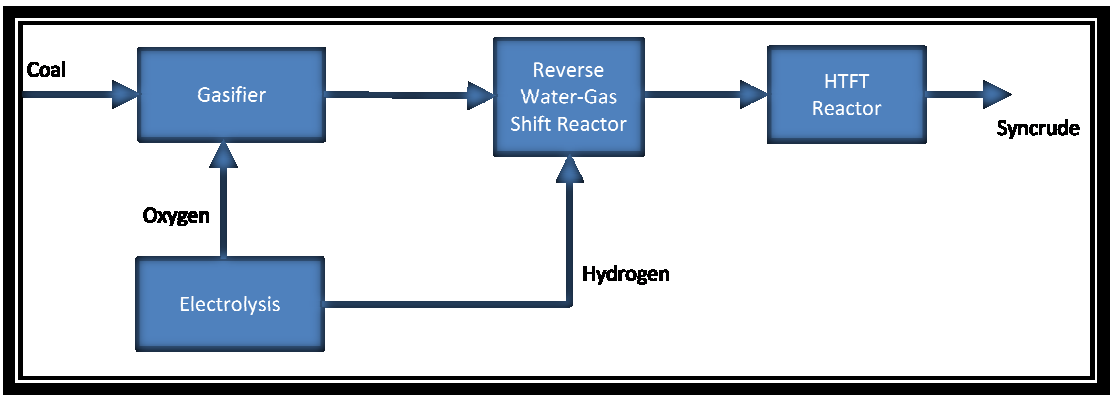


Figure 2.9 Nuclear-assisted syngas production (Harvego E. A., McKellar, Sohal, O'Brien, & Herring, 2008)

It is interesting to note that the carbon utilization achieved by this system is greater than that of the CTL 200 proposed by Cherry & Wood (2008) although the concepts are similar. The difference can be attributed to the huge extent to which the RWGS reactor catalytically converts CO_2 in the Harvego scheme compared to the non-catalytic impulse reaction occurring in the Cherry scheme. The utility-intensive acid gas removal unit has been eliminated as well as the ASU and WGS reactor. These modules are replaced by the RWGS reactor module. However, the RWGS module has a high capital requirement similar to that of the F-T reactor module hence it becomes beneficial to reduce the size of the RWGS reactor. The process in Figure 2.9 requires a large RWGS reactor as a result of the high gas throughput. A retrofit CTL plant would benefit by utilizing the concentrated and relatively small throughput CO_2 stream from acid gas removal unit instead of using the bulky raw gas-hydrogen mixture. The advantage is a much smaller RWGS reactor, a significant result from a process optimization perspective.

The RWGS is an equilibrium reaction whose CO_2 conversion is affected by the initial concentration or partial pressure of CO. Thus, the acid gas removal unit which produces a concentrated CO_2 stream containing a small amount of diluents should not have been eliminated entirely but instead its footprint should have been reduced. The consequential advantage of this incremental development is the possible attainment of greater carbon utilization than the 90.5% achieved in the Harvego scheme due to the higher conversion of the CO_2 to the more useful CO intermediate.

McCormick (2008) reviewed the critical scenario in the US military where the DOD predicted a severe shortage in jet propulsion fuel and started an alternative fuels program. The review proposed the use of an HTR to split water into hydrogen and oxygen whereupon the hydrogen was used in the RWGS reactor with CO_2 to produce CO and H_2O. The CO was mixed with additional hydrogen and fed to an F-T reactor. The coal furnace flue gas and sequestered CO_2 were identified as the possible sources of carbon. This scheme could be useful in the CTL context where the CO_2 emitted directly from the CTL plant is the more concentrated hence cheaper carbon source. The drawback is that the entire process is not commercially available and there is need to determine the feasibility and viability of this scheme.

Schultz et al (2007) captured the possible utilization of coal furnace flue gas and atmospheric CO_2 in synergy with nuclear and renewable technologies to produce synfuels. The study explored the adoptable concepts of using nuclear and renewable energy to solve the simultaneous sustainability challenges mentioned earlier in this thesis. The scheme so proposed is identical to that forwarded by McCormick (2008). The result was an increase in carbon utilization and the economic analysis performed indicated viability. Given that the CO_2 from the conventional CTL plant is approximately eight times more concentrated than that from coal furnace flue gas, it follows that use of CO_2 emissions from CTL plant is predicted to be viable.

Agrawal & Singh (2009) reviewed a biomass-to-liquid (BTL) process where 100% conversion of a lignocellulose material was achieved by recycling all the CO_2 formed to the gasifier. In what may be viewed as a desperate attempt to find a source of CO_2 to suffice requirements, mention of scrubbing of atmospheric CO_2 was made. However, the concentration of CO_2 in air is too low (385ppm) for economic capture. Furthermore, the use of BTL as a technology is limited citing the sustainability of the carbon source.

2.5 Summary and conclusion of literature reviewed

The literature cited outlined, evaluated and analyzed the previous significant studies which represented a true reflection of the worldwide endeavors towards solving the energy and environmental challenges emanating from coal gasification and other processes inherent in synfuels production. It is an important aspect of this study that none of the proposals or schemes provided is commercially available or has been demonstrated at a prototype scale.

Therefore, a need arises to complete process flowsheets and determine feasibility as well as viability of the concepts. An important critique is that most of the concepts proposed centre around the RWGS concept whilst a few are based on supplying the nuclear-process heat directly to the gasifier. This study deviates from the norm and considers a separate process development as well as performs a comparative economic analysis of the conventional and nuclear-assisted CTL plant configurations. Below is a summary of the literature reviewed in this thesis.

Author	Study Design	Main Findings	Comment
Koump(1982)	Achieve clean coal gasification by reducing concentration of polycyclic hydrocarbons	Recycling of syngas to gasifier prevented polymerization of free radicals.	Feasibility of H_2 feed into gasifier
Hishida et al(1997)	Coal reforming to synfuels in methanol production. system	Electrolytic hydrogen mixed with ex-gasifier syngas prior to methanol synthesis reactor	Possible technological solution to CTL environment challenge
Yoshitomo et al (2000)	Method of utilising nuclear heat in gasifier	Effective reduction of CO_2 emissions	Technical challenges in utilising direct heat in the moving-bed gasifier
Katayama et al (2005)	Coal gasification in a methanol production system	A zero CO_2 emission system proposed where solar hydrogen is fed to a methanol synthesis reactor	Capacity factor of solar and nuclear. Use of nuclear would lower significantly the cost of methanol produced
Katayama et al (2006)	Method of gasifying coal. Solar H_2 is split into 2 streams, one for gasifier feed, and the other for feed prior to HTFT.	Very low CO_2 emissions reported	Temp used in test gasifier (>1500) not suitable for moving-bed gasifier operation(Steam /oxygen cut-back above 1200)
Schultz et al (2007) McCormick et al (2008)	Use of coal furnace flue gas and atmospheric CO_2 in synergy with nuclear hydrogen in a RWGS reactor (CO with H_2 fed to HTFT)	Economic analysis reported indicates viability	✓ Process not commercially available ✓ CTL CO_2 8 times more concentrated so should be more viable

Author	Study Design	Main Findings	Comment
Forsberg(2008)	Nuclear process heat application to synfuel production	Efficient reduction of CO_2 emissions	Focus on energy intensive areas of synfuel production e.g. product upgrade
Greyvenstein et al (2008)	Strategies to maximise role of nuclear power in a H_2 economy in SA	Use of nuclear hydrogen results in major capital & operating offsets	Informative study providing terms of reference for future research
Boardman(2008)	Possible integration of nuclear/HyS/CTL technologies. Recycle of CO_2 to gasifier.H_2 fed directly to HTFT.	Increase in carbon utilisation. Hybrid plant uses 70% less coal for the same synfuel output	✓ Result from simulation study. ✓ Gasifier model used is that for entrained bed gasifier
Cherry et al(2008)	Synergistic routes to synfuel production for nuclear and coal	✓ CTL 200:H_2 recycle to gasifier ✓ CTL 300:All C gases recycle ✓ Increase in carbon utilisation(see simulation table next slide)	✓ Simulation effects & concept/s verification required ✓ Recycle of all C-gases could be long term(theoretical) ✓ Recycle of CO_2 only could yield a greater C utilisation than CTL 200(100% in BTL)
Harvego et al(2008)	Proposal scheme of nuclear-assisted gasification plant. Nuclear hydrogen mixed with syngas and fed to RWGS reactor.	✓ 90.5% carbon utilisation better than 30% for conventional CTL ✓ H_2/CO of 2 achieved	✓ Simulation study. Concept feasibility required ✓ RWGS large due to gas throughput. Need for system optimisation.

Chapter 3

Technical analysis of a nuclear-assisted syngas plant

In this section, material balance computations are performed to simulate the production of syngas at a hypothetical CTL facility similar to the Sasol East plant (base case). These are not necessarily fully optimised due to restriction to proprietary information, but are considered realistic enough to provide a fair basis for subsequent computations. On the basis of the base case material analysis, the fundamental aspects to developing a nuclear-assisted syngas plant are established as well as the consequential benefits to be derived investing in the technology.

3.1 Syngas process development

The process description for syngas production has been done in Section 2.2.1 of this study. However, a more detailed process flow diagram is shown in Figure 3.2 below.

3.2 Material balance for a conventional syngas plant

The schematic shown in Figure 3.1 below is a simplified representation of the conventional base case syngas production unit and will be used to perform the mass balance computations.

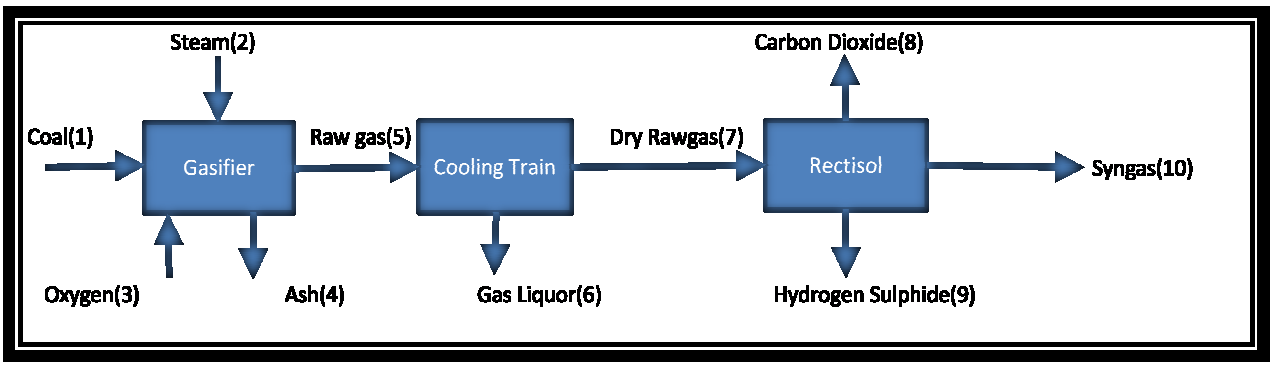


Figure 3.1 Material balance schematic

Table 3.8 outlines the material flows assuming coal feed to a single gasifier. The proximate analysis used in this study is for a coal feed similar to the low rank bituminous coal used at the Sasol CTL plant (Van Dyk, 2006). The Secunda Synfuels factory has a total of 80 gasifiers shared equally between the Sasol East and Sasol West factories. At any one time however, there will be 4 gasifiers on general overhaul. We typically consider an average of 36 gasifiers per factory to give a feed rate of 46 656 tpd (AR) coal feed per factory. Appendix 1 outlines the material balance analysis strategy.

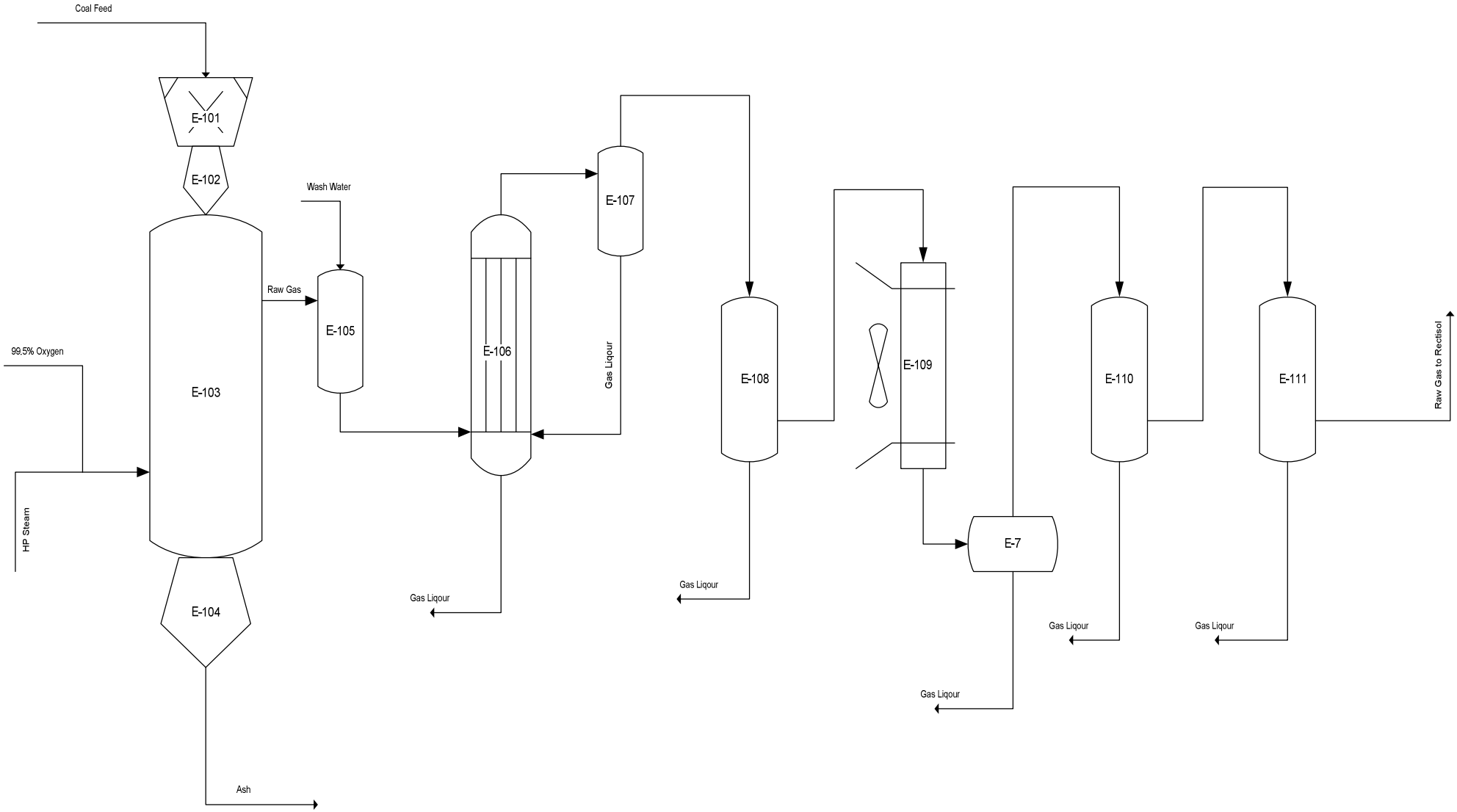


Figure 3.2 Conventional syngas plant process flow scheme

Below is the equipment list for Figure 3.2 above:

Equipment Code	Equipment Name
E-101	Coal Bunker
E-102	Coal Lock
E-103	Gasifier
E-104	Ash Lock
E-105	Wash Cooler
E-106	Waste Heat Boiler
E-107	Knock-out drum
E-108	Pre-cooler
E-109	Air-cooler
E-7	Knock-out drum
E-110	Trim cooler
E-111	Final cooler

The Tables 3.1 to 3.6 below are the basis for the material balance computations performed herein. Volatile matter composition for the low rank bituminous coal considered was determined by a pyrolysis experiment where char and tar were measured and gas captured and analysed (Van Dyk, 2006).

Table3.1 Coal proximate analysis

Component	%wt
Fixed Carbon	46.30
Ash	25.80
Moisture	5.00
Volatiles	22.90

Table 3.2 Volatile matter composition

Component	%wt
H_2O	2.9
N_2	2
H_2	0.14
CH_4	4
CO	0.96
CO_2	7.2
Tars & Oils	5.60

Table 3.3 Raw gas composition (dry basis)

Component	% vol	GHV (BTU/SCF)
CO	21	321.37
H_2	38	325.02
CO_2	30	0
CH_4	9.6	1009
H_2S	0.7	0
C_2H_6	0.7	1 800.00
Steam		0.7 kg/Nm^3 dry raw gas

Table 3.4 Gasifier steady-state operating parameters

Gasifier oxygen consumption	0.243	ton/ton coal
H_2O/O_2	6.50	kg/Nm^3
Raw gas production	1 203.70	Nm^3 dry basis/ton coal
Operating Pressure	2 500.00	kPa
Operating Temperature	1 273.00	K
Residual carbon in Ash	6.00	%wt
Gasifier Nominal Coal Input	54.00	ton/hr
Gasifier Nominal Output	65 000.00	Nm^3/hr(dry basis)

Table 3.5 Estimated miscellaneous parameters

Dry raw gas MW_{avg}	21.82	kg/kmol
Gas constant, R	8.31	kPa m^3/kmol K
Dry raw gas temperature	308.00	K
Raw gas density	0.974	kg/Nm^3 (dry basis)
Syngas density	0.494	kg/Nm^3
Raw gas production	159 648.72	Nm^3/day(dry basis)
Raw gas GHV	300.46	BTU/SCF

Table 3.6 Process basis and specifications

Basis	100.00	TPD (MAF) Coal feed/gasifier
On-stream Factor	0.92	
Availability/year	335.00	Days
Equivalent coal feed	144.51	TPD
On-stream feed-rate	132.63	TPD (AR) Coal feed/gasifier

Table 3.7 Material balance summary at 100 TPD (MAF) gasifier coal feed

Stream No.	1	2	3	4	5	6	7	8	9	10
Stream Name	Coal feed	Steam	Oxygen	Ash	Raw Gas	Gas Liquor	Dry Raw Gas	Carbon Dioxide	Hydrogen Sulphide	Syngas
Component	TPD	TPD	TPD	TPD	TPD	TPD	TPD	TPD	TPD	TPD
C	61.41	0.00	0.00	2.05	0.00	0.00	0.00	0.00	0.00	0.00
Ash	34.22	0.00	0.00	32.17	0.00	0.00	0.00	0.00	0.00	0.00
H_2O	10.48	144.19	0.00	0.00	111.75	111.75	0.00	0.00	0.00	0.00
N_2	2.79	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H_2	0.19	0.00	0.00	0.00	5.41	0.00	5.41	0.00	0.00	5.41
CH_4	5.31	0.00	0.00	0.00	10.94	0.00	10.94	0.00	0.00	10.94
CO	1.27	0.00	0.00	0.00	41.88	0.00	41.88	0.00	0.00	41.88
CO_2	9.55	0.00	0.00	0.00	94.01	0.00	94.01	94.01	0.00	0.00
Tars & Oils	7.43	0.00	0.00	0.00	7.43	7.43	0.00	0.00	0.00	0.00
H_2S	0.00	0.00	0.00	0.00	1.69	0.00	1.69	0.00	1.69	0.00
C_2H_6	0.00	0.00	0.00	0.00	1.50	0.00	1.50	0.00	0.00	1.50
O_2	0.00	0.00	32.23	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	**132.63**	**144.19**	**32.23**	**34.22**	**274.61**	**119.18**	**155.43**	**94.01**	**1.69**	**59.72**

IN

Stream No.	Stream Name	Rate(TPD)
1	Coal	132.63
2	Steam	144.19
3	Oxygen	32.23
		309.05

OUT

Stream No.	Stream Name	Rate(TPD)
4	Ash	34.22
6	Gas Liquor	119.18
8	Carbon Dioxide	94.01
9	Hydrogen Sulphide	1.69
10	Syngas	59.72
		308.83

***** The material balance computations done do not close out perfectly, the small difference being attributed to the exclusion of nitrogen and ammonia in the raw gas composition. In reality, these are present in trace quantities.

Table 3.8 Material balance summary at nominal gasifier coal feed

Stream No.	1	2	3	4	5	6	7	8	9	10
Stream Name	Coal feed	Steam	Oxygen	Ash	Raw Gas	Gas Liquor	Dry Raw Gas	Carbon Dioxide	Hydrogen Sulphide	Syngas
Component	TPD	TPD	TPD	TPD	TPD	TPD	TPD	TPD	TPD	TPD
C	600.05	0.00	0.00	20.06	0.00	0.00	0.00	0.00	0.00	0.00
Ash	334.37	0.00	0.00	314.31	0.00	0.00	0.00	0.00	0.00	0.00
H_2O	102.38	1 408.94	0.00	0.00	1 092.00	1 092.00	0.00	0.00	0.00	0.00
N_2	27.22	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H_2	1.81	0.00	0.00	0.00	52.89	0.00	52.89	0.00	0.00	52.89
CH_4	51.84	0.00	0.00	0.00	106.89	0.00	106.89	0.00	0.00	106.89
CO	12.44	0.00	0.00	0.00	409.19	0.00	409.19	0.00	0.00	409.19
CO_2	93.31	0.00	0.00	0.00	918.59	0.00	918.59	918.59	0.00	0.00
Tars & Oils	72.58	0.00	0.00	0.00	72.58	72.58	0.00	0.00	0.00	0.00
H_2S	0.00	0.00	0.00	0.00	16.56	0.00	16.56	0.00	16.56	0.00
C_2H_6	0.00	0.00	0.00	0.00	14.61	0.00	14.61	0.00	0.00	14.61
O_2	0.00	0.00	314.93	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	**1 296.00**	**1 408.94**	**314.93**	**334.37**	**2 683.31**	**1 164.58**	**1 518.73**	**918.59**	**16.56**	**583.58**
Temp(K)	**298.00**	**573.00**	**413.00**	**573.00**	**823.00**	**298.00**	**308.00**	**303.00**	**303.00**	**303.00**
Pressure(kPa)	**101.25**	**2 500.00**	**2 500.00**	**101.25**	**2 500.00**	**101.25**	**1 000.00**	**500.00**	**500.00**	**500.00**

IN

Stream No.	Stream Name	Rate(TPD)
1	Coal	1 296.00
2	Steam	1 408.94
3	Oxygen	314.93
		3 019.87

OUT

Stream No.	Stream Name	Rate(TPD)
4	Ash	334.37
6	Gas Liquor	1 164.58
8	Carbon Dioxide	918.59
9	Hydrogen Sulphide	16.56
10	Syngas	583.58
		3 017.68

Table3.9 Syngas plant material balance summary

Stream No.	1	2	3	4	5	6	7	8	9	10
Stream Name	Coal feed	Steam	Oxygen	Ash	Raw Gas	Gas Liquor	Dry Raw Gas	Carbon Dioxide	Hydrogen Sulphide	Syngas
Component	TPD	TPD	TPD	TPD	TPD	TPD	TPD	TPD	TPD	TPD
C	21 601.73	0.00	0.00	722.23	0.00	0.00	0.00	0.00	0.00	0.00
Ash	12 037.25	0.00	0.00	11 315.01	0.00	0.00	0.00	0.00	0.00	0.00
H_2O	3 685.82	50 721.89	0.00	0.00	39 312.00	39 312.00	0.00	0.00	0.00	0.00
N_2	979.78	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H_2	65.32	0.00	0.00	0.00	1 903.98	0.00	1 903.98	0.00	0.00	1 903.98
CH_4	1 866.24	0.00	0.00	0.00	3 848.05	0.00	3 848.05	0.00	0.00	3 848.05
CO	447.90	0.00	0.00	0.00	14 730.82	0.00	14 730.82	0.00	0.00	14 730.82
CO_2	3 359.23	0.00	0.00	0.00	33 069.18	0.00	33 069.18	33 069.18	0.00	0.00
Tars & Oils	2 612.74	0.00	0.00	0.00	2 612.74	2 612.74	0.00	0.00	0.00	0.00
H_2S	0.00	0.00	0.00	0.00	596.25	0.00	596.25	0.00	596.25	0.00
C_2H_6	0.00	0.00	0.00	0.00	526.10	0.00	526.10	0.00	0.00	526.10
O_2	0.00	0.00	11 337.41	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	**46 656.00**	**50 721.89**	**11 337.41**	**12 037.25**	**96 599.11**	**41 924.74**	**54 674.37**	**33 069.18**	**596.25**	**21 008.95**

IN

Stream No.	Stream Name	Rate(TPD)
1	Coal	46 656.00
2	Steam	50 721.89
3	Oxygen	11 337.41
		108 715.30

OUT

Stream No.	Stream Name	Rate(TPD)
4	Ash	12 037.25
6	Gas Liquor	41 924.74
8	Carbon Dioxide	33 069.18
9	Hydrogen Sulphide	596.25
10	Syngas	21 008.95
		108 636.36

3.3 Nuclear-assisted syngas process development

The development of the nuclear-assisted syngas process is based on a first-order mass analysis of the gasification reactions subject to material balance constraints (Table 3.8 & 3.9). In this analysis, the length of the hypothetical moving-bed gasifier hence the residence time is assumed to be sufficient for the raw gas to be in chemical equilibrium (Table 3.10). Van der Burgt & Higmann (2003) specified the difficulty associated with obtaining a gas analysis of the raw gas on leaving the reactor. They proposed a delayed or "post-mortem" strategy whereupon the wet raw gas composition is obtained from the composition of the dry and cool raw gas (Table 3.3). Thus, the analysis is performed for the freeze-in thermodynamic equilibrium of the wet raw gas (Table 3.10) below.

Table 3.10 Wet raw gas composition

Component	Moles (kmol/day)	Mole fraction
H_2O	6 208.33	0.4643
H_2	2 705.00	0.2023
CH_4	683.75	0.0511
CO	1 495.71	0.1119
CO_2	2 136.59	0.1598
Tar Oils	41.74	0.0031
H_2S	49.71	0.0037
C_2H_6	50.00	0.0037

These are the mole fractions as determined from the material balance considerations (Table 3.8).Tar has been defined as $C_{14}H_{10}$, represented in ASPEN Plus™ as phenanthrene (Hamelinck, Faaij, Uil, & Boerrigter, 2004) .The mole fraction of oxygen in the equilibrium mixture is so small to be insignificant and for all practical purposes, no oxygen is present. This is a result of the equilibrium constant being so large of the order 10^{10} hence the combustion reaction is considered irreversible (Smith, Van Ness, & Abbott, 2001). The implication is that all the oxygen fed to the gasifier is consumed by the combustion reaction to yield CO_2. On this basis, we eliminate the combustion reaction from the set of reaction equations and theoretically assume the CO_2 produced by the combustion reaction to be a reactant in the subsequent Boudouard reaction. This amount of CO_2 is evaluated as follows:

The combustion reaction occurring is;

$$C + O_2 \rightarrow CO_2$$

From Table 3.8, mass of O_2 consumed by combustion, $m(O_2)_{consumed}$ = 314.93 TPD

Moles of O_2 consumed, $n(O_2)_{consumed} = \frac{314\,930\,\text{kg}}{32\,\text{kg/kmol}} = 9841.56\,\text{kmol}$

$\therefore n(CO_2)_{produced} = n(O_2)_{consumed} = 9841.56\text{kmol}$

Many reactions occurring inside the gasifier are complex due to the multiple existence of components as both reactants and products in different reactions. This makes it virtually impossible to find the conversions of the individual reactions unless assumptions are specified. Assume devolatilised char for the gasification reactions and also that all oxygen is used up in the combustion process so that no oxygen exists in the gasification zone and that only the following reactions take place;

1. Carbon dioxide gasification (Boudouard): $C+CO_2 \Leftrightarrow 2CO$
2. Steam gasification (water-gas): $C + H_2O \Leftrightarrow CO + H_2$
3. Methanation: $C + 2H_2 \Leftrightarrow CH_4$
4. Water gas shift(WGS): $CO + H_2O \Leftrightarrow CO_2 + H_2$

The combustion of carbon is the fundamental reaction that provides heat for the endothermic gasification reactions. In reality, the reactions do not occur simultaneously, there are some reactions which are consecutive to others (Slaghuis, 1993). The carbon dioxide produced from combustion is utilised in the Boudouard reaction. The WGS reaction corrects the H_2/CO ratio of the syngas by producing hydrogen. In the process, the WGS reaction produces fugitive carbon dioxide emissions. Thus, the WGS reaction is the primary source of carbon dioxide in the moving-bed gasifiers (Van der Burgt & Higmann, 2003; Morgan, 1991).

Let i and j represent the reaction component and reaction number, respectively. Then, the stoichiometric numbers can be arrayed as follows;

i	**CO_2**	**CO**	**H_20**	**H_2**	**CH_4**	
j						**vj**
1	-1	2	0	0	0	**1**
2	0	1	-1	1	0	**1**
3	0	0	0	-2	1	**-1**
4	1	-1	-1	1	0	**0**

For multi-reaction equilibria; $y_i = \frac{n_i}{n} = \frac{n_{io} + \sum_i \sum_j \nu_{i,j} \varepsilon_j}{n_0 + \sum_j \nu_j \varepsilon_j}$

y_i = mol fraction of component i

n_{io} = initial moles of component i

$n_0 = \sum_i n_{i0}$

$\sum_i \nu_{i,j}$ = stoichiometric coefficient of component i in reaction j

ε_j = reaction progress variable

From Table 3.8, $n_{H20,O}$=78 274.44 kmol and $n_{CO2,O}$= 9841.56 kmol

For simplicity of calculations, use $n_{CO2,O}$=1 kmol and $n_{H20,O}$=7.95 kmol

The amount of solid present does not affect the extent of the reaction, hence;

$n_0 = n_{H20,O} + n_{CO2,O} = 8.95\,\text{kmol}$

The composition of the equilibrium mixture is evaluated as follows;

$$y_{CO2} = \frac{1 - \varepsilon_1 + \varepsilon_4}{8.95 + \varepsilon_1 + \varepsilon_2 - \varepsilon_3} \qquad y_{CO} = \frac{2\varepsilon_1 + \varepsilon_2 - \varepsilon_4}{8.95 + \varepsilon_1 + \varepsilon_2 - \varepsilon_3}$$

$$y_{H2O} = \frac{7.95 - \varepsilon_2 - \varepsilon_4}{8.95 + \varepsilon_1 + \varepsilon_2 - \varepsilon_3} \qquad y_{H2} = \frac{\varepsilon_2 - 2\varepsilon_3 + \varepsilon_4}{8.95 + \varepsilon_1 + \varepsilon_2 - \varepsilon_3}$$

$$y_{CH4} = \frac{\varepsilon_3}{8.95 + \varepsilon_1 + \varepsilon_2 - \varepsilon_3}$$

By substituting the equilibrium mole fractions of Table 3.10 into the expressions above, we yield an equation-oriented (EO) model represented by a system of 5 simultaneous equations. These were solved using the SOLVE function of MATLAB™ to yield the following reaction progress variables;

ε_1=0.444 ε_2=1.778 ε_3=0.376 ε_4=1.157

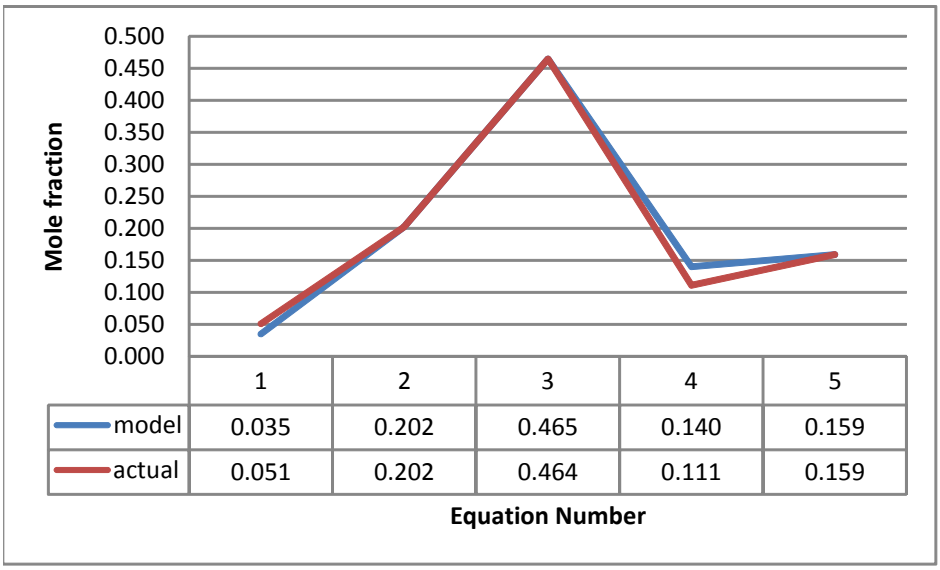


Figure 3.3 Comparison of the actual and EO model mole fractions

The EO model is represented by 5 equations in 4 unknowns. This results in an over-determined system with no unique solution. A best-fit solution is thus sought. For the solution presented, the CH_4 mole fraction equation (equation number 1) is disregarded since it does not include all 4 variables. Fig 3.3 shows a fit of the model mole fractions (derived using the reaction progress variables) and the actual mole fractions given in Table 3.10.The trendlines superimpose for the most part except for the outliers at number 1 and 4 where the model mole fractions deviate slightly from the actual. Other numerical methods such as the Gauss-Seidel iterations could not converge by virtue of the lack of diagonal dominance of the matrix. Thus the values assumed by the reaction progress variables are the best -fit to the theoretical true solution of the simultaneous equations defining the EO model.

$$n_{CO2} = 1 + (-1)(0.444) + (1)(1.157) = 0.556 + 1.157 = 1.713\,\text{kmol}$$

Thus, the EO model predicts the Boudouard reaction contributes 32.4mol % to the CO_2 emissions whilst the WGS reaction contributes 67.6 mol%. These contributions are derived against the 1.713kmol of CO_2 emitted and are the basis for the mass analysis performed.

$$n_{H2O} = 7.95 + (-1)(1.778) + (-1)(1.157) = 5.015\,\text{kmol}$$

Similarly, the EO model predicts 14.6 mol % of the steam is consumed by the WGS whilst 22.4 mol % is consumed by the steam gasification (water gas) reaction. The excess steam (60mol %) is used to keep the gasifier temperature below the AFT of coal and to cool the ash. The mass analysis computations which follow are based on the EO model results

yielded above and the mass balance constraints as given in Table 3.8. The amount of CO_2 produced by reaction in the gasifier is computed as follows;

$$\mathrm{m}(\mathrm{CO}_2)_{produced} = \mathrm{m}(\mathrm{CO}_2)_{ex-gasifier} - \mathrm{m}(\mathrm{CO}_2)_{coal\ feed} = 918.59 - 93.31 = 825.28\mathrm{TPD}$$

$$\therefore \mathrm{n}(\mathrm{CO}_2)_{produced} = 18756.36\ \mathrm{kmol}$$

Taking note that of the EO model result that 67.6% of the CO_2 produced is generated by the WGS reaction;

$$\mathrm{n}(\mathrm{CO}_2)_{produced\ from\ WGS} = 0.676 \times 18756.36 kmol = 12679.29 kmol$$

From a stoichiometric treatment of the WGS reaction;

$$\therefore \mathrm{n}(\mathrm{CO}_2)_{produced} = \mathrm{n}(\mathrm{H}_2)_{produced} = \mathrm{n}(\mathrm{CO})_{consumed} = \mathrm{n}(\mathrm{H}_2\mathrm{O})_{consumed} = 12679.29\ \mathrm{kmol}$$

$$\therefore \mathrm{m}(\mathrm{H}_2\mathrm{O})_{consumed\ by\ WGS} = 12679.29\ \mathrm{kmol} \times 18\mathrm{kg/kmol} = 228.23\ \mathrm{TPD}$$

$$\therefore \mathrm{m}(\mathrm{CO})_{required\ by\ WGS} = 12679.29\ \mathrm{kmol} \times 28\mathrm{kg/kmol} = 355.02\ \mathrm{TPD}$$

$$\therefore \mathrm{m}(\mathrm{H}_2)_{produced\ by\ WGS} = 12679.29\ \mathrm{kmol} \times 2\mathrm{kg/kmol} = 25.36\ \mathrm{TPD}$$

From Table 3.8, $\mathrm{m}(\mathrm{CH}_4)_{produced\ by\ \mathrm{methanation}} = 106.84 - 51.84 = 55\mathrm{TPD}$

To produce this amount of methane, the following amount of hydrogen was consumed;

$$\mathrm{n}(\mathrm{H2})_{consumed} = 2\mathrm{n}(\mathrm{CH}_4)_{produced} = 2 \times \frac{55000\ \mathrm{kg}}{16\mathrm{kg/kmol}} = 6875\mathrm{kmol}$$

$$\mathrm{m}(\mathrm{H}_2)_{consumed\ by\ \mathrm{methanation}} = 6875\mathrm{kmol} \times 2\ \mathrm{kg/kmol} = 13.75\mathrm{TPD}$$

From Table 3.8, $\mathrm{m}(\mathrm{H}_2)_{producedbyreaction} = 52.89 - 1.81 = 51.08\mathrm{TPD}$

We can therefore quantify the amount of hydrogen produced by the water-gas reaction as;

$$\therefore \mathrm{m}(\mathrm{H}_2)_{producedbysteamgasification} = \mathrm{m}(\mathrm{H}_2)_{producedbyreaction} - \mathrm{m}(\mathrm{H}_2)_{producedbyWGS} + m(H_2)_{consumedbymethanation} = 39.47\mathrm{TPD}$$

$$\mathrm{n}(\mathrm{H}_2)_{produced\ by\ steam\ gasification} = \frac{39472kg}{2kg/kmol} = 19736kmol$$

A stoichiometric treatment of the water-gas reaction demands the following;

$$n(H_2O)_{consumed} = n(CO)_{produced} = n(H_2)_{produced} = 19736\text{kmol}$$

$$\therefore m(CO)_{produced\ by\ steam\ \ gasification} = 19736\text{kmol} \times 28\ \text{kg/kmol} = 552.61\text{TPD}$$

$$\therefore m(H_2O)_{consumed\ by\ steam\ \ gasification} = 19736\text{kmol} \times 18\ \text{kg/kmol} = 355.25\text{TPD}$$

From Table 3.8, $\therefore m(CO)_{produced\ \text{by reaction}} = 409.19 - 12.44 = 396.75\text{TPD}$

Therefore, knowing the total amount of CO produced by all gasification reactions and that produced by the WGS and water-gas reactions respectively, we can compute the amount of CO produced by the Boudouard reaction as;

$$\therefore m(CO)_{bouduard} = m(CO)_{reaction} - m(CO)_{steam\ gasification} + m(CO)_{WGS}$$

$$m(CO)_{bouduard} = 396.75 - 552.61 + 355.02 = 199.16\ \text{TPD}$$

$$n(CO)_{producedbyBouduardreaction} = 199160\text{kmol}/28\text{kg kmol}^{-1} = 7112.928 kmol$$

$$n(CO_2)_{consumedbyBouduardreaction} = 7112.93/2 = 3556.46\text{kmol}$$

As shown in earlier calculations, 9841.56 kmol CO_2 is available initially for the Boudouard reaction. However, 3556.46 kmol CO_2 are used and this implies an excess of 6285.1 kmol CO_2 (276.5 tpd) that manifests as fugitive CO_2 emissions from the gasifier. This is 33.5 mol% of the total gasifier CO_2 emissions which is comparable to the 32.4 mol.% predicted by the EO model. According to material balance (Table 3.8), 419.32 tpd H_2O (30 mol. %) are consumed by this reaction. The EO model gives 583.48 tpd H_2O (41 mol. %) consumption. This inconsistency is attributed to the uncertainties arising from the determination of reaction progress variables as discussed earlier for Figure 3.3.

The availability of nuclear hydrogen to the CTL fraternity presents a unique opportunity to reduce the extent of the WGS reaction and therefore, increase the carbon utilisation of the hypothetical moving-bed gasifier. There arise preliminary indications where advantages are obtained. The direct effects of eliminating the WGS reaction in the gasifier are;

I. The mass analysis above reveals that 355 tpd of CO are required for the WGS reaction. If we were to eliminate the WGS reaction, the 355 tpd of CO would then be available as excess. An increase in carbon utilisation would therefore result and an opportunity exists for increased syngas production on availability of a sufficient external hydrogen source.

$$\mathrm{m(CO)}_{available\ for\ nuclear} = \mathrm{m(CO)}_{base\ case\ ex-gasifier} + \mathrm{m(CO)}_{required\ by\ WGS}$$

$$\mathrm{m(CO)}_{available\ for\ nuclear} = 409.19 + 355.02 = 764.21\,\mathrm{TPD}$$

$$\therefore \mathrm{n(CO)}_{available\ for\ nuclear} = 27293.21\,\mathrm{kmol}$$

The required H_2/CO ratio of syngas remains 1.8 hence the total amount of H_2 required to achieve this F-T feed specification for the nuclear-assisted syngas plant is;

$$\therefore \mathrm{m(H_2)}_{required} = 1.8 \times 27293.21\,\mathrm{kmol} \times 2\mathrm{kg/kmol} = 98.26\mathrm{TPD}$$

The amount of H_2 produced by the gasifier in the nuclear-assisted syngas plant following elimination of the WGS reaction is;

$$\mathrm{m(H_2)}_{produced\ by\ gasifier\ for\ nuclear\ solution} = \mathrm{m(H_2)}_{ex-gasifier\ base\ case} - \mathrm{m(H_2)}_{produced\ by\ WGS}$$

$$\therefore \mathrm{m(H_2)}_{produced\ by\ gasifier\ for\ nuclear\ solution} = 52.89 - 25.36 = 27.53\,\mathrm{TPD}$$

This is the mass of hydrogen that would be present in the raw gas for a gasifier operating in the nuclear-assisted syngas process and the deficit to be supplied externally is;

$$\therefore \mathrm{m(H_2)}_{nuclear\ required} = 98.26 - 27.53 = 70.73\,\mathrm{TPD}$$

This deficit in the hydrogen requirement per gasifier is to be supplied by the HyS process in the turnkey nuclear-assisted syngas process. The total hydrogen requirement for the nuclear-assisted syngas plant consisting of 22 gasifiers is 1556 tpd. A 500MW_{th} reference HTR module produces 170 tpd H_2. Hence, the HyS plant for the nuclear-assisted syngas plant developed herein, requires 9.15 (10) HTR modules for the production of hydrogen.

The HyS process produces oxygen equivalent to eightfold the amount of hydrogen produced (Gorensek & Summers, 2009). For a hydrogen requirement of 1556 tpd, the HyS produces 12 448.48 tpd O_2 .The oxygen requirement per gasifier in the base case is 314.93 tpd hence

for 22 gasifiers, the total oxygen requirement is 6928.46 tpd. Therefore, excess oxygen equivalent to 5520 tpd is produced by the HyS plant. This excess oxygen can be sold to obtain significant by-product credit improving the overall viability of the nuclear-assisted syngas plant. Therefore, the expensive to install and operate ASU becomes obsolete and is eliminated off the process.

The mass of syngas produced by the nuclear-assisted syngas plant is evaluated below.

$$\mathrm{m(syngas\ produced)}_{nuclear} = \mathrm{m(H_2)}_{ex-gasifier\ nuclear} + \mathrm{m(CO)}_{available} + \mathrm{m(CH4)}_{ex-gasifier\ base\ case} + \mathrm{m(C2H6)}_{ex-gasifier\ base\ case}$$

$$\therefore \mathrm{m(syngas\,produced)}_{nuclear} = 98.26 + 764.21 + 106.89 + 14.61 = 983.97\ \mathrm{TPD}$$

Thus, the nuclear-assisted syngas plant produces approximately 1.69 times the syngas produced by the base case (583.58 tpd) per gasifier, from the same coal input. The direct effect is that only 22 gasifiers can be operated for the turnkey nuclear-assisted plant to achieve the same syngas throughput achieved by the 36 gasifiers in the conventional base case syngas plant. This is assuming that each gasifier achieves the nameplate capacity. This translates to approximately 40% reduction in operating costs for a retrofit gasification plant and a reduction of the same magnitude in total installed capital cost for a new-built nuclear-assisted gasification plant.

II. A 40% reduction in coal consumption for the same syngas throughput. Thus, the energy security aspect of this thesis is addressed through preliminary significant savings in the coal resource base proven for the case above.

III. To eliminate the WGS reaction, the steam consumption of the hypothetical gasifier is reduced by 228 tpd. This is the amount of steam required to propagate the WGS in the base case per gasifier. Thus the steam requirement per gasifier in the nuclear-assisted gasification plant is approximately 1180.71 tpd. As mentioned above, the turnkey nuclear-assisted syngas plant will require 22 gasifiers to achieve the same syngas throughput as the base case. This translates to a plant steam requirement of 25 975.62 tpd compared to 50 721.89 tpd for the conventional syngas plant (Table 3.9), a 49% reduction in steam consumption for the same throughput. However, to minimise the WGS reaction by starving the steam may have some serious practical effects in terms of exceeding the coals' AFT. Van Dyk (2006) patented the increase in the AFT of coal by adding mineral species such as kaolinite to the gasifier coal feed. This resulted in the reduction of the steam consumed by the gasifier with a direct effect on the carbon utilisation

(WGS). Van Heerden (2007) revealed that Sasol had endeavoured to develop solutions for reducing the steam consumption of the gasification plant. Thus, nuclear hydrogen brings forth an end-of-pipe solution to reducing the gasification plant steam consumption.

IV. Lower gas liquor production hence reduced gas liquor processing costs as a direct result of a reduction in steam consumption.

V. Reduced load on Rectisol due to reduced CO_2 load. Table 3.11 shows the Rectisol feed ensuing from a single gasifier in the nuclear-assisted and conventional syngas plant. The benefit is a 15% reduction in Rectisol load per gasifier. For the nuclear-assisted syngas plant with 22 gasifiers producing the same syngas throughput as the base case, the rectisol load is 28591.42 tpd. This corresponds to a 48% reduction in Rectisol load when compared to the base case syngas plant in Table 3.9 (54 674.37 tpd). A significant result for the new-built is the 48% reduction in Rectisol plant footprint and capital and operating costs. For the already existing plant, the benefit is a reduced refrigeration duty and methanol requirement.

Table 3.11 Comparison of dry raw gas composition

Component	Nuclear CTL mass-flow(TPD)	Conventional mass-flow (TPD)
CO_2	369.81	918.59
H_2	27.53	52.89
CH_4	106.89	106.89
CO	764.21	409.19
H_2S	16.56	16.56
C_2H_6	14.61	14.62
Total	**1299.61**	**1518.74**

A significant benefit for the nuclear- assisted syngas process is the direct reduction of the atmosphere-bound CO_2 from a daunting 918.59 tpd to 369.81 tpd, a 60% reduction per gasifier. Considering the reduced gasifiers in the nuclear-assisted syngas plant, a total reduction in CO_2 emissions of 75% is achieved. There exists scope for further reduction possibly by reducing the oxygen consumption per gasifier so that the CO_2 contribution by the Boudouard reaction is minimised. This can be the subject of another optimisation study. Thus, the environmental security aspect sought in this study is revealed and addressed.

What remains is to locate the feed point of the nuclear-derived hydrogen. This is to be located after the Rectisol unit at the mixer where the outlet stream of the Rectisol is mixed with the nuclear hydrogen. The sole reason behind this feed-point location is the avoidance of unnecessarily increasing the rectisol load by feeding the hydrogen directly into the Rectisol unit. This is particularly through noting that hydrogen does not contribute in any way to the physical and chemical phenomena occurring in this unit.

Chapter 4

Economic analysis of a nuclear-assisted syngas plant

In this section, a costing model is presented based on the material analyses of the base case and nuclear-assisted syngas plants developed in Chapter 3. The syngas production cost of the 2 plants under consideration are compared with the objective of determining the economic advantage of one plant over the other. Furthermore, an important parameter to be determined is the cost of CO_2 avoided when the nuclear-assisted syngas plant concept is applied.

4.1 Cost analysis methodology

The main objective of the cost analysis performed herein, is to obtain a relative cost comparison of the syngas produced from the 2 processes under investigation rather than to yield accurate estimates. The strategy is to determine the investment and operating costs and then to determine the levelized syngas manufacturing cost over the projected life of the plant. Applying the same cost analysis methodology to the base case and turnkey nuclear-assisted syngas processes leads to an equitable comparison.

Price data on syngas do not exist for the simple reason that syngas is an intermediate product in synfuels production that is not usually marketed. To determine the investment costs, equipment cost data were obtained from previous similar designs (Shaeiwitz, et al., 1999). The costs were assigned to a module (e.g. Rectisol) rather than by evaluating each piece of equipment within the module. To determine the appropriate cost for a module of the desired size, exponential scaling was used. This method of acquiring capital cost data has been used by various authors (Hamelinck & Faaij, 2002; Kreutz, Williams, Consonni, & Chiesa, 2005; Van Vliet, Faaij, & Turkenburg, 2009).

4.2 Economic assumptions

The detailed general specifications and investment parameters for the economic analysis are given in Table 4.1. The prices assumed for the raw materials, products, and by-products are also shown in Table 4.1. It is assumed that all by-products are sold at the indicated price.

4.3 Measures of economic feasibility

The evaluation of overall total investment cost is done on the basis of the cost data as presented in Table 4.2.

Table 4.1 Main investment parameters for costing model

Facility Operating Parameters	
Facility Type	Petrochemical Processing Facility
Operating Mode	Continuous Processing
Load factor	8040 hrs
Plant Lifetime	25 yrs
Tax Rate[a]	28%
Interest/discount rate[b]	15%
Carbon Tax	none
Depreciation Method	Straight line
Cost Data for Feedstock,Products and Utilities(US$/ton)	
Coal[c]	65
Oxygen[d]	26
Steam[e]	16
Hydrogen[f]	3230
Ash[g]	30
Coal tar oils[h]	96
Sulfur[i]	160
Power[j]	$0.08/KWh

[a] Tax rate is based on corporate tax (South Africa) payable on net profit

[b] The interest rate is the weighted average between the prime interest rate of the South African Reserve Bank (11%) and the desired rate of return for shareholders of 20%, based on a debt/equity ratio of 70/30 used by the petrochemical industry.

[c] The average 2009 FOB index price for South Africa thermal coal exports. This is taken as the delivered cost of coal to the conversion plant. Sasol Mining Secunda supplies coal to the Secunda Synfuels. Thus the mining site and conversion plant are at the same location so that the energy and transport costs per ton of coal are insignificant. It is for this difference in supply chain, that the market price of coal is not adopted in this study.

[d] USD_{2010} oxygen credit updated by using CEPCI on USD_{2008} 20/ton assumed by Harvego

[e] USD_{2010} steam price updated by using CEPCI on USD_{2004} 12/ton given by (Sinnott, 2005)

[f] Average cost of hydrogen produced by nuclear HyS process (Elder & Allen, 2009). The HTE process produces hydrogen at a cost of US$3.23/kg (Harvego E. A., McKellar, Sohal, O'Brien, & Herring, 2008). However, a sensitivity analysis is necessary.

[g] FOB price for coal fly ash

[h] FOB price for coal tar oils is USD_{2010} 0.115/litre. The coal condensates have a density of 1.20g/cm^3 at 298K.

[i] USD_{2010} FOB September price. This varies according to market willingness and response to ceiling price.

Table 4.2 Capital cost data for system modules and components

Plant/Module Component	Scaling Unit	Base Capacity	Base Year	Module Cost in Base Year(MM$)	CEPCI in Base Year	Scale factor	Current Capacity	Module Cost in 2010(MM$)	Installation factor	Installed Cost in 2010(MM$)
Coal storage,prep and handling[a]	Raw coal feed, tpd	2367	2002	29.1	395.6	0.67	58 320	368.85	1	368.85
Air Seperation Unit (O_2 at 1.01 bar)[b]	99.5% oxygen,tpd	576	2002	24.552	395.6	0.75	11 337.41	339.80	1.3	441.74
Lurgi Gasification[c]	Coal feed,tpd	17249.4	1992	653.4	359.2	0.65	51 840	2179.19	1	2179.19
Rectisol[c]	Pure CO_2captured,tpd	13 367.48	1992	115.54	359.2	0.65	33 069.18	339.56	1	339.56
Sulfur Recovery(Claus,Beavon)[c]	H_2S input,tpd	374.54	1992	36.1	359.2	0.65	596.25	79.66	1	79.66
Other Compressors[d]	Compression power,MW	97.4	1992	216.6	359.2	0.65	172.67	512.59	1	512.59
Total Estmated Installed Capital Cost										3921.59

[a] Module base cost given by (Kreutz, Williams, Consonni, & Chiesa, 2005). It is assumed that 25% of the gasifier coal feed is rejected as fines in the coal preparation module. Thus the raw coal feed to this module is 1.25 times that of the gasifier coal feed.

[b] Hamelinck et al (2004) state that the costs quoted in literature range significantly. Their study is based on costs given by Tijmensen et al (2002) since it was closely related to the real cost price of oxygen. The cryogenic oxygen plant module does not include the inlet air or outlet oxygen compressors.

[c] Costs for the Lurgi gasification plant module is inclusive of the syngas cooling train (Shaeiwitz, et al., 1999). The installed cost in 2010 for the gasifiers includes the standby 4 gasifiers which were assumed to be on general overhaul. The cost data for the Rectisol module and sulphur recovery module are given by (Shaeiwitz, et al., 1999). The sulphur recovery module is composed of the Claus and Beavon units, whilst the COS hydrolysis unit has been assumed to have an insignificant cost.

[d] Air compressor is a single stage with a pressure ratio of 5 and consuming 81.4MW (Shaeiwitz, et al., 1999). This is the same compressor, usually of the Brown-Boveri type by ABB as in most cryogenic oxygen plants. The outlet oxygen compressor used is a multi-stage compressor with interstage cooling and consuming 16MW for an outlet pressure of 28bar. Both the power consumptions for the base ASU plant are adjusted according to a direct proportionality between power, flowrate, and pressure ratios.

* The unit investments depend on the size of the components (which follow from the technical analysis of chapter 3), by scaling from known scales in literature (see Table4.2), using the equation below:

$Cost_{2010} = Cost_{base\ year}(Size_{2010}/Size_{base\ year})^{R}\ (CEPCI_{2010}/CEPCI_{base\ year})$; R= scale factor

In evaluating the cost of synfuels, Tillman (1987) highlighted the importance of understanding the cost structure of products in addition to the final costs associated with the produced commodities. In particular, the cost of acquiring capital was also a cost component of the total annualised cost used in determining the annual production cost. This methodology has been used by various authors. Hamelinck & Faiij (2002) evaluated the methanol and hydrogen production costs by dividing the total annual costs of a system by the produced amount of fuel. Van Vliet et al (2009) evaluated the cost of fuel by dividing the total annual costs by the synfuels production. In both cases, the total annual cost consists of annualised investment, operating and maintenance, raw material and by-product credit.

Similarly, this study defines the manufacturing cost as the sum of the raw materials and operating costs plus a capital recovery annuity, minus by-product credits. This model simply amortizes the installed capital investment over the anticipated life of the plant at the given interest rate. Besides utilities, the operating costs also include maintenance, insurance, plant overhead, and sustaining capital charges. These latter costs are estimated to be equivalent to 18% of the total installed capital (Peters & Timmerhaus, 1991).

Table 4.3 Annual manufacturing cost for conventional syngas plant

Total Estimated Installed Capital Cost(MM$)	3 921.59	
Annuity factor for amortization	6.464	
Capital Recovery Factor	0.155	
Capital Recovery Annuity(MM$/yr)		**606.67**
Total Estimated Operating Cost(MM$/yr)		1 975.80
Coal	1 269.92	
Steam[a]	271.87	
Other Expenses	434.02	
Total Estimated Credits (MM$/yr)[b]		235.08
Ash	120.97	
Coal Tar Oils	84.03	
Sulfur	30.08	
Net Operating Cost (MM$/yr)		**1 740.73**
Total Annualised Costs(MM$/yr)		**2 347.39**
Synthesis gas production(Nm^3/yr)		14 227 490 822.28
Total Annual Production Cost($/$Nm^3$)		**0.165**

[a] Steam is assumed to be a utility as well as a raw material. The oxygen cost is inherent in the ASU and associated compression installed costs.

[b] The total estimated credit is not corrected for the CO_2 emissions trading scheme. At the EU allocated credit of US$$_{2008}$35/ton CO_2, the total carbon penalty is MM$387.73/yr. The total estimated credit decreases to MM$-152.66/yr and the total annual production cost for syngas increases to US$0.192/$Nm^3$ syngas.

Table 4.4 Nuclear-assisted syngas capital cost data

Plant/Module Component	Scaling Unit	Base Capacity	Base Year	Module Cost in Base Year(MM$)	CEPCI in Base Year	Scale factor	Current Capacity	Module Cost in 2010(MM$)	Installation factor	Installed Cost in 2010(MM$)
Coal storage,prep and handling	Raw coal feed, tpd	2367	2002	29.1	395.6	0.67	35 640	265.18	1	265.18
Air Seperation Unit (O_2 at 1.01 bar)	99.5% oxygen,tpd	576	2002	24.552	395.6	0.75	0.00	0.00	1.3	0.00
Lurgi Gasification	Coal feed,tpd	17249.4	1992	653.4	359.2	0.65	31 104	1563.49	1	1563.49
Rectisol	Pure CO_2captured,tpd	13 367.48	1992	115.54	359.2	0.65	8 135.82	136.47	1	136.47
Sulfur Recovery(Claus,Beavon)	H_2S input,tpd	374.54	1992	36.1	359.2	0.65	364.32	57.83	1	57.83
Other Compressors[a]	Compression power,MW	16	1992	15	359.2	0.65	16.1	24.57	1	24.57
Total Estmated Installed Capital Cost[b]										2047.54

[a] Compressor duty is only for the HyS oxygen compression to S-L FBDB™ gasifier operating pressure. No air is to be compressed at any stage.

[b] The total installed capital cost estimated is a pseudo-cost that does not include the installed capital cost of the nuclear- HyS plant. This latter cost is inherent in the hydrogen cost as is given in the Harvego analysis (Harvego E. A., McKellar, Sohal, O'Brien, & Herring, 2008). The hydrogen production cost assumed, takes into account capital and operating costs as well as maintenance costs inherent in the HTR-HyS plant.

Table 4.5 Annual manufacturing cost for nuclear-assisted syngas plant

Total Estimated Installed Capital Cost(MM$)	2 047.54	
Annuity factor for amortization	6.464	
Capital Recovery Factor	0.155	
Capital Recovery Annuity(MM$/yr)		**316.75**
Total Estimated Operating Cost(MM$/yr)		2 708.46
Coal	776.06	
Hydrogen	1 563.84	
Steam	139.23	
Other Expenses	229.33	
Total Estimated Credits (MM$/yr)[a]		191.74
Ash	73.93	
Coal Tar Oils	51.35	
Oxygen	48.08	
Sulfur	18.38	
Net Operating Cost (MM$/yr)		**2 516.72**
Total Annualised Costs(MM$/yr)		**2 833.47**
Synthesis gas production(Nm^3/yr)		14 227 490 822.28
Total Annual Production Cost($/$Nm^3$)		**0.199**

[a] The total estimated credit is not inclusive of CO_2 credit from the emissions trading scheme. At a carbon credit of US$35/ton$CO_2$, the total carbon penalty is MM$95.39/yr. Total estimated credit becomes MM$96.35/yr and the total annual production cost for syngas increases to US$0.206/$Nm^3$ syngas.

The syngas production in Tables 4.3 and 4.5 has been evaluated as follows;

$$\text{Syngas production} = \frac{\text{syngas mass} \times \text{plant load factor}}{\text{syngas density}} = \frac{2100895\,TPD \times 1000\,kg/ton \times 335\,days}{0.4946\,kg/Nm^3}$$

The installed capital cost of the nuclear-assisted syngas plant excluding the nuclear hydrogen production island is shown in Table 4.4 above. The economic analyses performed indicate the use of nuclear hydrogen in syngas production as a practical and environmentally conscious solution to the immensely huge CTL footprint. In addition, it allows syngas to be produced with a 21% cost increase over coal-based synfuel production. The extra cost to be incurred by investing into the nuclear-assisted syngas plant is evaluated as the cost of CO_2 avoided;

$$\text{Cost of } CO_2 \text{ avoided} = \frac{\text{Cost}_{\text{nuclear}} - \text{Cost}_{\text{base case}}}{\text{Emissions}_{\text{base case}} - \text{Emissions}_{\text{nuclear}}}$$

But from the economic analyses above;

$$\text{Cost}_{\text{nuclear}} - \text{Cost}_{\text{base case}} = 0.199 - 0.165 = US\$0.034/Nm^3$$

And from the material analyses of both plants;

$$\text{Emissions}_{\text{base case}} - \text{Emissions}_{\text{nuclear}} = \frac{(11\,078\,175.30 - 2\,725\,499.70)\,\text{tpy}}{14\,227\,490\,822.28\,\text{Nm}^3/yr} = 0.000587\,\text{ton CO}_2/\text{Nm}^3$$

At the initial assumed parameters to the costing model (Table 4.1), the cost of avoided CO_2 is therefore US$58.2. However, sensitivity analyses are required to ascertain the extent of economic feasibility under various critical assumptions.

4.4 Sensitivity analyses

The economic analyses performed were based on a set of common cost assumptions given in Table 4.1 above. The hydrogen production cost assumed was the average price of hydrogen produced by a nuclear integrated HyS plant. This does not imply the cost of producing hydrogen with HyS technology is fixed but instead can decrease depending on technology development and maturation. Against this background, there arises need to vary the assumptions to test the sensitivity of costs to the most critical assumptions. In this study, the critical assumptions were taken to be the hydrogen cost, delivered coal cost and the interest rate (capital charge). Hydrogen cost was considered to vary from $1.5/kg to $4/kg

meanwhile the coal prices have a history of volatility hence a broader cost range was considered ($50/ton -$160/ton). Capital charge varied from 10% to 20%, a common range in the global financial market.

4.4.1 Cost sensitivity to hydrogen production cost

Figures 4.1 and 4.2 below illustrate the sensitivity of the cost of syngas and cost of avoided CO_2 to the variation in the production cost of hydrogen.

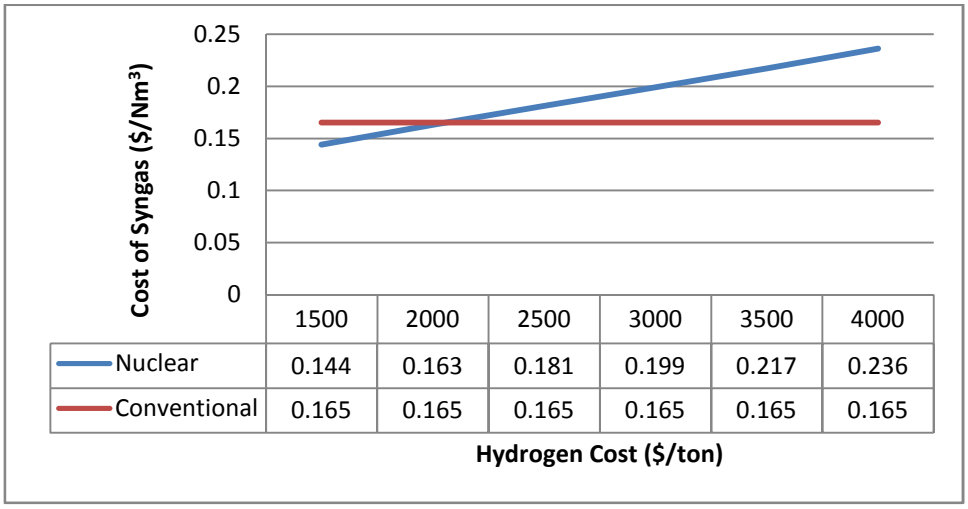


Figure 4.10 Syngas cost sensitivity to hydrogen cost

The cost of syngas from the conventional plant is understandably insensitive to the hydrogen production cost since hydrogen is not a raw material for the plant. However, the cost of syngas from the nuclear-assisted syngas plant varies linearly the hydrogen cost. There is a hydrogen cost at which the cost of syngas from the nuclear-assisted syngas plant equals that from the conventional syngas plant. At this critical hydrogen cost, the cost of avoided CO_2 is zero. Figure 4.2 below shows this cost at US$2.07/kg H_2.

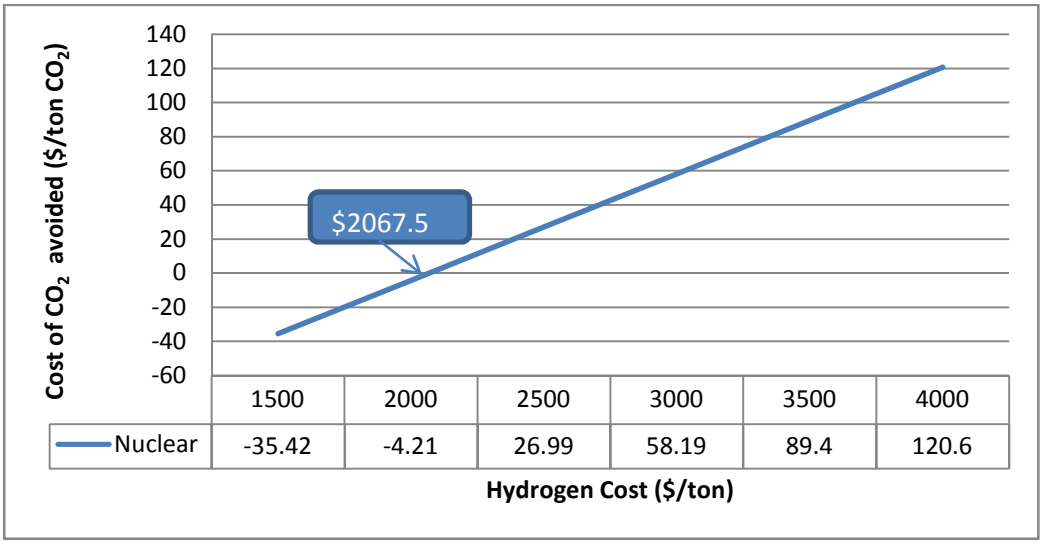


Figure 4.2 Sensitivity of the cost of CO_2 avoided to hydrogen cost

Below the hydrogen production cost of \$2.07/kg H_2, a credit becomes intrinsic in the nuclear-assisted syngas plant and a return is imminent for the investment. Thus, the turnkey nuclear-assisted syngas process becomes the technology of choice for the CTL plant.

4.4.2 Cost sensitivity to coal cost

Figures 4.3 and 4.4 below illustrate the sensitivity of the cost of syngas and cost of avoided CO_2 to the delivered cost of coal.

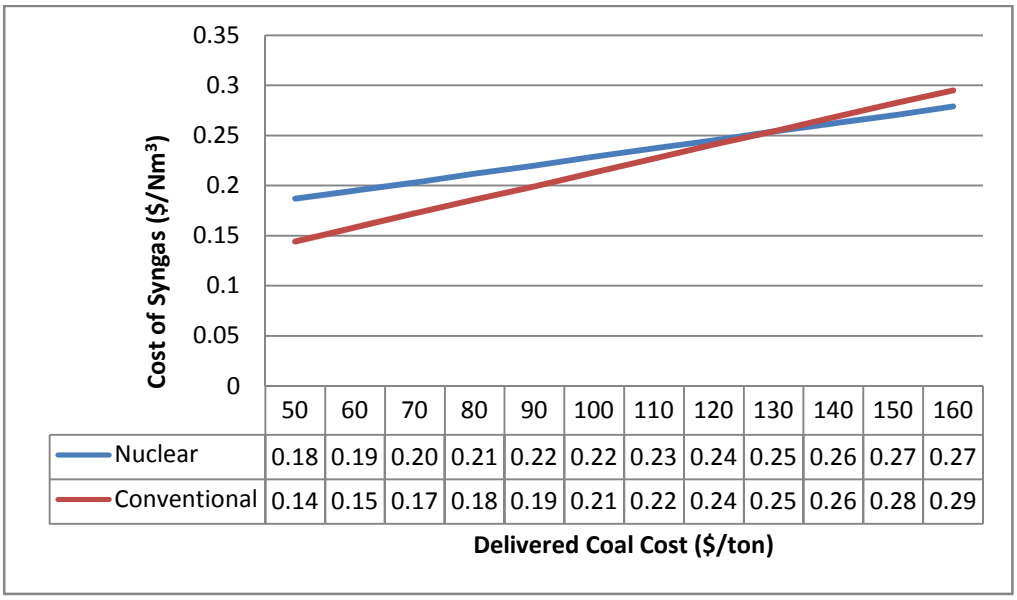


Figure 4.3 Syngas cost sensitivity to delivered coal cost

In contrast to the case with hydrogen production cost, the cost of syngas from both plants is sensitive to the delivered cost of coal since coal is feedstock to both plants. The trend is for the cost of syngas from the conventional plant to be more sensitive to the delivered coal cost

in comparison with the nuclear-assisted plant. At some instant, the costs of producing syngas from both the plants become equal. At this delivered coal cost, the cost of avoided CO_2 is zero. Figure 4.4 shows this cost at US$128.97/ton.

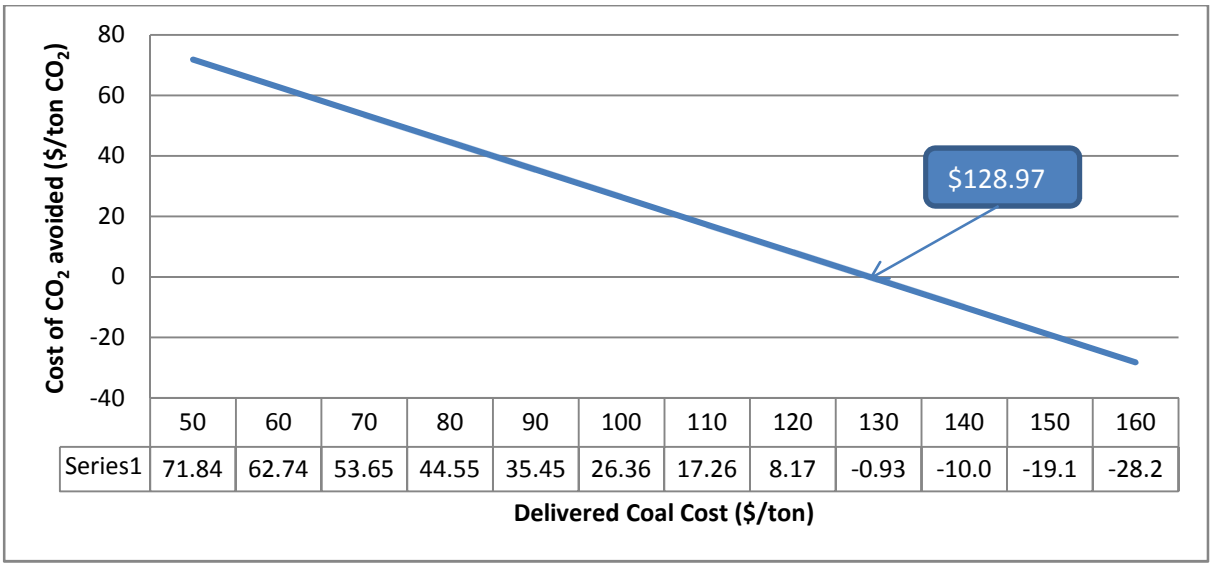


Figure 4.4 Sensitivity of the cost of CO2 avoided to delivered coal cost

Above this threshold delivered coal cost, it becomes expensive to manufacture syngas using the conventional base case plant.

4.4.3 Cost sensitivity to interest rate

Figure 4.5 below shows that both plants are sensitive to the interest rate but the trends are inconclusive with respect to the relative cost of syngas for all practical purposes. Therefore, the significance of the interest rate as a critical assumption ceases so that there exists only two assumptions worth considering in the sensitivity analyses namely, the hydrogen cost and delivered coal cost.

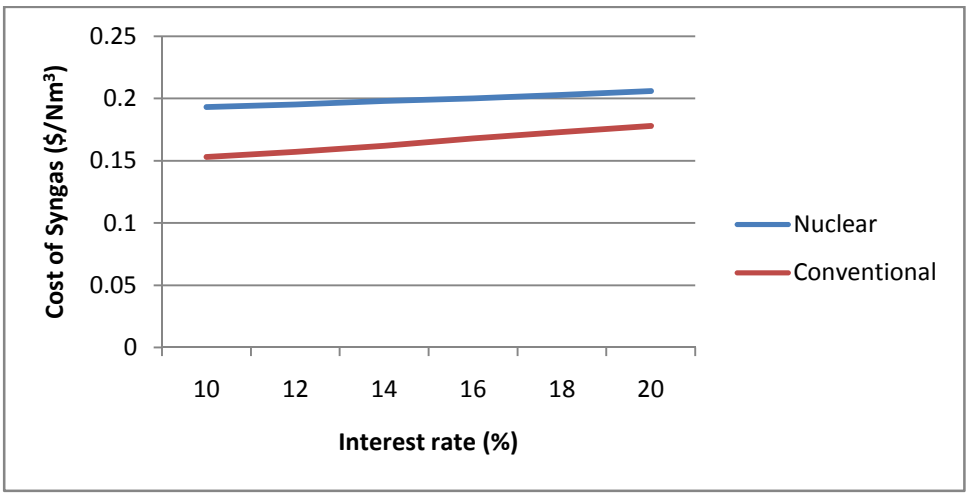


Figure 4.5 Syngas cost sensitivity to capital charge rate

Chapter 5

Conclusions and Recommendations

5.1 Conclusions

The production of coal-based synfuels was found to have contributed immensely to the global warming phenomenon resulting from the huge CO_2 footprint inherent in CTL facilities. The large CO_2 footprint revealed the energy inefficiency, vis'-a-vis', the low carbon utilisation exhibited by the CTL facilities. The CTL predicament was further exacerbated by the limited lifespan of coal reserves. Thus two (2) simultaneous problems of environmental and energy security giving rise to an untenable scenario were defined in this study. The primary objective of this study was to investigate the consequential benefits arising from using nuclear-derived hydrogen in CTL facilities.

Meanwhile existing past studies used the reaction between supplemental hydrogen and CO_2 to reduce or eliminate the CTL carbon footprint, this study proposed a unique strategy that significant reduced additional plant equipment. In comparison to past studies, this study performed detailed feasibility aspects and proceeded to evaluate the economics of the proposed concept. In this study, a reference CTL facility similar to the Sasol East plant was taken as the base-case CTL facility and the moving-bed gasifier was identified as the fundamental CO_2 emission point-source. Thus, the study focused on the syngas production plant of the CTL facility.

The study investigated the techno-economic aspects of the proposed nuclear-assisted syngas production plant of a CTL facility. The proposed system used supplemental nuclear hydrogen and oxygen derived from a HyS plant powered by ten (10) units of the HTGR such as the South African PBMR. In the analysis, a simple stoichiometric treatment of the gasification reactions was considered and the WGS reaction emerged as the primary contributor to the CO_2 generation. The elimination of the WGS reaction from the set of gasification reactions was crucial in reducing the CO_2-generating capacity of the gasifier and the study predicted the reduction in the steam to starve and eliminate the WGS reaction. The result was a hydrogen-poor raw gas exiting the gasifier at a very low H_2/CO ratio of 0.5 which would have been unsuitable for subsequent F-T conversion to syncrude were it not for the external hydrogen source. In addition, the hydrogen-poor raw gas so produced is similar

to that produced by entrained bed gasifiers such as the Shell gasifier. In this aspect, it becomes paramount for the new-built nuclear-assisted CTL plants to base their gasification module on entrained-bed gasifier technology. Meanwhile from a cost perspective, retrofit nuclear-assisted CTL plants will remain with moving-bed gasifiers as the technology of choice.

However, the elimination of the WGS reaction significantly reduced the quantity of CO_2 in the gasifier raw gas by 549 tpd per gasifier. It is important to note there would not have been any value-addition were it not for the alternative hydrogen source. The nuclear hydrogen was introduced at the additional mixer after the Rectisol unit to tailor the previously hydrogen-deficient syngas to the required ratio of 1.8. The following benefits accruing from implementing the nuclear-assisted syngas plant concept were noted;

I. A total reduction in CO_2 emissions of 75% was achieved mainly due to the nuclear-assisted plant having 14 less gasifiers. The existing CTL facilities have struggled to curb the emissions despite a number of efforts. The nuclear-assisted CTL signifies and presents a realistic implementation opportunity to reduce the CO_2 footprint of CTL facilities. Based on this significant result, CTL technology could go a long way in the sustainable alleviation of the current global energy and environmental crisis as most nations are predicted to invest in it. On this basis, CTL players such as Sasol could begin to market their novel technologies to populous nations like China without any form of environmentalist hindrance.
II. High capital offsets were also realised. The nuclear-assisted syngas plant proposed eliminated the ASU due to the capability of the HyS process to produce more than sufficient oxygen as a by-product. In addition, the nuclear-assisted plant required 14 less gasifiers to achieve the same syngas output as the conventional syngas plant. Furthermore, the reduced CO_2 load implied a reduction in the Rectisol plant footprint. The study predicted a 50% reduction in installed capital investment for the nuclear-assisted syngas plant excluding the nuclear island consisting of the integrated HTR and HyS plants.
III. An increase in carbon utilisation resulting in a 69% increase in syngas output for the same coal input as the conventional CTL plant.
IV. The extension of the coal reserve lifespan resulting from a 40% reduction in coal usage for the same syngas output.
V. A 49% reduction in steam consumption for the same syngas output. Sasol are still involved in research to reduce the water consumption of the gasification plant. Thus,

the nuclear-assisted CTL plant brings forth an end-of-pipe solution to address this problem.

An important aspect of the study was to demonstrate the reduction of CO_2 emissions from the CTL facilities could be economically supported with HTR technology integration. Thus, an economic analysis was performed to obtain the relative cost comparison of the syngas produced by the 2 processes under investigation. The manufacturing cost of the coal-based (conventional) syngas was US\$0.165/Nm^3 compared to US\$0.199/Nm^3 for the nuclear-assisted syngas, when the average nuclear hydrogen cost of US\$3/kg. Thus, a 21% cost increase existed for the nuclear-assisted syngas plant.

The cost of CO_2 avoided was the most important economic parameter evaluated to obtain the extra cost that would be incurred by the investor in reducing the CO_2 emissions using the turnkey nuclear-assisted syngas plant. The hydrogen cost was defined as the most critical assumption and a sensitivity analysis performed on this basis. The cost of CO_2 avoided of US\$100/ton CO_2 was taken as the economic threshold forming the basis of a strategic decision analysis (SDA) tool. According to the SDA, a decision to invest into the nuclear-assisted syngas plant presented negative economics above this threshold cost. The cost of CO_2 avoided was US\$58/ton $CO_2$for the assumed hydrogen cost of US\$3/kg. For the most part of the assumed hydrogen cost, the cost of CO_2 avoided was well below the threshold cost implying economic feasibility of the nuclear-assisted syngas plant. A significant bonus was that the cost of CO_2 avoided assumed the value of zero when the hydrogen cost was US\$2.07/kg. Economic studies have indicated the hydrogen cost from a HyS plant to be between US\$3-5/kg H_2.The hydrogen cost is expected to be lower as a result of the hydrogen production system optimisation currently being done at different institutes around the world.

To conclude, the study shows that nuclear-assisted synfuels production has attractive economics and has realistic implementation opportunities that would induce governments and private industry alike, to support various HTR technology development programs. In the South African context, this study provides the opportunity for the resuscitation of the PBMR program whose closure was based primarily on the unavailability of an anchor customer for the technology. As both an energy player and planner, the South African government would

be interested in PBMR redeployment in order to meet global emissions targets as well as to avert the global energy crisis, as has been epitomised in the study. Meanwhile, Sasol and other CTL players worldwide are sole beneficiaries of the nuclear-assisted CTL technology in that the turnkey technology provides a gateway to implement investment plans that were otherwise halted on the basis of failure to adhere to environmental obligations.

5.2 Recommendations

The study performed herein is a preliminary techno-economic assessment contributing further knowledge to the field. Theoretically, the nuclear-assisted syngas plant concept is stimulating and if successful could have momentous impact on the energy sector. Thus, there exists scope for scale-up of the study to experimental phase in order to progress the theoretical concept predicted. The recommended experimental set-up uses a bed of coal particles packed in either a thermo-gravimetric analyser (TGA) or a pipe reactor .The coal bed is heated to a temperature of 1000^{o}C to simulate the temperature distribution in the moving-bed gasifiers and the blast introduced. This completes the control experiment simulating a hypothetical gasification process. The gas analysis may be measured by chromatography. In this analysis, we measure the H_2/CO ratio as well as the CO_2 concentration of the off-gas. The second experiment involves variation of the blast flows into the TGA by reducing H_2O/O_2 ratio and the H_2/CO ratios and CO_2 concentrations compared with those obtained in the control experiment. Once the predictions of the study are proved, experimental studies on the test gasifier are recommended. If these tests are successful, the study would have proved, beyond doubt, the technical feasibility of the nuclear-assisted CTL facility and indeed, reinforce the establishment of a significant niche' market for the hydrogen economy.

In addition, the gasification reactions considered in developing the nuclear-assisted syngas plant (Chapter 3) were assumed to take place in a certain order which might not correspond to reality. Furthermore, gasification is an extremely complex phenomenon and the analysis done, herein, simplifies the chemical reactions. This is not to say the analysis done cannot be relied upon but refining of the computations using thermodynamic modelling software like Chemical Equilibrium with Applications (CEA) and FactSage is also recommended, perhaps before the progression of the concept to experimentation phase.

Bibliography

Agrawal, R., & Singh, N. R. (2009). Synergistic Routes to Liquid Fuel for a Petroleum-Deprived Future. *A.I.ChE , 55* (7), 1898-1905.

Anderson, R. (1952). Fischer-Tropsch Synthesis. *Industrial and Engineering Chemistry , 44* (2).

Anderson, R. (1956). Kinetics and Reaction Mechanism for the Fischer-Tropsch Synthesis. *Catalysis , 4*, 350.

Boardman, R. (2008). Nuclear Hybrid Energy Systems. *4th International Topical Meeting on High Temperature Reactor Technology.* Washington D.C: American Society of Mechanical Engineers.

Cherry, R. S., & Wood, R. A. (2008). *Patent No. US20080103220A1 .* USA.

Cover, A., Schreiner, W., & Skarpedas, G. (1973). Coal Gasification Process. *Chemical Engineering Progress , 69* (3), 32-36.

Detman, R. (1977, March). Economics of Six Coal-to-SNG Processes. *Hydrocarbon Processing* , 115-118.

Earthlife. (2009, September 7). *NGO Pulse.* Retrieved January 8, 2010, from www.earthlife.org.za: http://www.sangopulse.net

EIA. (2006). Retrieved October 10, 2009, from http://www.eia.doe.gov

Elder, R., & Allen, R. (2009). Nuclear heat for hydrogen production: Coupling a very high/high temperature reactor to a hydrogen production plant. *Progress in Nuclear Energy , 51*, 500-525.

Engelbrecht, A., Golding, A., Hietkamp, S., & Scholes, B. (2004). *The Potential for Sequestration of Carbon Dioxide in South Africa.* Council for Scientific and Industrial Research.

Forsberg, C. (2005). Futures for Hydrogen Produced using Nuclear Energy. *Progress in Nuclear Energy , 47* (1-4), 484-495.

Forsberg, C. (2008). High Temperature Reactors for Liquid Fuels Production. *4th International Topical Meeting on High Temperature Reactor Technology.* Washington D.C: American Society of Mechanical Engineers.

Gibson, P. (2007). Coal to Liquids at SASOL. *Kentuck Energy Security Summit CAER's 30th Anniversary* (pp. 1-3). Kentucky,USA: SASOL Technology R & D.

Gorensek, M. B., & Summers, W. A. (2009). Hybrid Sulfur Fowsheets using PEM Electrolysis and a Bayonet Decomposition Reactor. *International Journal of Hydrogen Energy , 34*, 4097-4114.

Greyvenstein, R., Correia, M., & Kriel, W. (2008). South Africa's Opportunity to Maximise the Role of Nuclear Power in a Global Hydrogen Economy. *Nuclear Engineering and Design , 238*, 3031-3040.

Hamelinck, C. N., & Faaij, A. P. (2002). Future Prospects for Production of Methanol and Hydrogen from Biomass. *Journal of Power Sources , 111*, 1-22.

Hamelinck, C. N., Faaij, A. P., den Uil, H., & Boerrigter, H. (2004). Production of FT transportation fuels from biomass;technical options,process analysis and optimisation, and development potential. *Energy , 29*, 1743-1771.

Hamelinck, C. N., Faaij, A. P., Uil, H. d., & Boerrigter, H. (2004). Production of FT transportation fuels from biomass;technical options,process analysis and optimisation, and development potential. *Energy , 29*, 1743-1771.

Harvego, E. A., McKellar, M. G., Sohal, M. S., O'Brien, J. E., & Herring, J. S. (2008). Economic Analysis of a Nuclear-Powered High Temperature Electrolysis Hydrogen Production Plant. *2nd International Conference on Energy Sustainability* (pp. 1-11). Jacksonville,Florida: Idaho National Laboratory.

Harvego, E., McKellar, M., & O'Brien, J. (2008). System Analysis of Nuclear-Assisted Syngas Production from Coal. *Proceedings of the 4th International Topical Meeting on High Temperature Reactor Technology. 2.* Washington DC: American Society of Mechanical Engineers.

Hatch, L. F., & Matar, S. (2000). *Chemistry of Petrochemical Processes.* Houston,Texas: Gulf Publishing Company.

Hebden, D., & Stroud, H. (1981). *Chemistry of Coal Utilisation* (Vol. Second Supplementary Volume). New York: John Wiley and Sons.

Hersh, D., & Abrardo, J. (1977). Air Seperation Plant Design. *Cryogenics , 17* (7), 383-390.

Hishida, M., Fumizawa, M., Inaba, Y., Aritomi, M., Nomura, S., Kosaka, S., et al. (1997). Nuclear Energy Conversion Systems for Arresting Global Warming. *Energy Conversion Management , 38* (10-13).

Hobbs, L., Radulovic, T., & Smoot, D. (1992). Modelling Fixed-Bed Coal Gasifiers. *AIChE , 38* (5), 681-702.

Johnson, P., & Conger, W. (1981). Availability Analysis of Coal Gasification Processes. *Fuel Process Technology* (5), 1140-1156.

Katayama, Y. (2006). *Patent No. US 6 997 965 B2.* Japan.

Katayama, Y., & Tamaura, Y. (2005). Development of New Green-Fuel Production Technology by Combination of Fossil Fuel and Renewable Energy. *Energy , 30*, 2179-2185.

Kosky, P. (1981). Nuclear Process Heat Application to Coal Gasification. *Nuclear Engineering and Design , 66* (3), 331-342.

Kotanigawa, T., Chakrabartty, S., & Berkowitz, N. (1981). Behaviour of Iron Catalysts in Hydrocarbon Synthesis from Carbon Monoxide and Steam. *Fuel Processing Technology* , 79-90.

Koump, V. V. (1982). *Patent No. 4 312 638.* USA.

Kreutz, T., Williams, R., Consonni, S., & Chiesa, P. (2005). Co-production of hydrogen,electricity and carbon dioxide from coal with commercially ready technology.Part B:Economic Analysis. *International Journal of Hydrogen Energy , 30*, 769-784.

Kuhr, R. (2008). HTR's Role in Process Heat Applications. *Nuclear Engineering and Design , 238*, 3013-3017.

Lahoda, E., McLaughlin, D., Mulik, R., Kriel, W., Kuhr, R., Bolthrunis, C., et al. (2006). Estimated Costs for the Improved HyS Flowsheet. *Proceedings of the Third International Topical Meeting on High Temperature Reactor Technology*, (p. Paper C00000068).

Lee, B. (1982). Synfuels from Coal. *AIChE , 78*, 14.

Mahalingham, R. (1985). *Studies in Tar Formation and Seperation in Coal Gasification Systems.* Washington State University, Chemical Engineering. Washington D.C: U.S Department of Energy.

McCormick, J. L. (2008). High Temperature Reactor:Driving Force to Convert Carbon Dioxide to Fuel. *Proceedings of the 4th International Conference on High Temperature Reactor Technology. 2.* Washington DC: American Society of Chemical Engineers.

Meyers, R. (1981). *Coal Handbook.* New York: Dekker.

Morgan, P. (1991). *An Experimental and Modelling Study of Coal Pyrolysis in a Lurgi Gasifier.* Johannesburg: University of the Witswatersrand.

Muradov, N. Z., & Veziroglu, N. T. (2008). Green Path from Fossil-based to Hydrogen Economy:An Overview of Carbon-neutral Technologies. *International Journal of Hydrogen Energy , 33*, 6804-6839.

Mwakasonda, S., & Winkler, H. (2005). Carbon Capture and Storage in South Africa. *Growing in the Greenhouse:Protecting the Climate by Putting Development First* , pp. 95-109.

Peters, M. S., & Timmerhaus, K. D. (1991). *Plant Design and Economics for Chemical Engineers* (4th ed.). New York: McGraw-Hill.

Pollaert, T. (1979). Coal Gasification-Commercial Production of Synfuels Today. *Coal Technology* , 27-49.

Ranwell, P. (1997). *A Numerical Model of the Moving Bed Gasifier.* Potchefstroom University for CHE, Mechanical Engineering. Potchefstroom: Potchefstroom University for CHE.

Rao, V., Stiegel, G., Cinquegrane, G., & Srivastava, R. (1992). Iron-based Catalysts for Slurry-phase Fischer-Tropsch Process. *Fuel Processing Technology , 30*.

Ricketts, T. (1963, October). The Operation of the Westfield Lurgi Plant. *Institute of Gas Engineering Journal* , 563-588.

Schilling, H., Bonn, B., & Krauss, U. (1981). *Coal gasification-existing processes and new developments.* London: Graham & Trotman.

Schultz, K. R., Bogart, L. S., & Noceti, R. P. (2007). *Synthesis of Hydrocarbon Fuels using Renewable and Nuclear Energy.* San Diego: General Atomics.

Shaeiwitz, J., Turton, R., Torries, T., Gautam, M., Bata, R., Whiting, W., et al. (1999). *The Economical Production of Alcohol Fuels from Coal-Derived Synthesis Gas.* U.S Dept. of Energy Report no. DE-AC22-91PC91034--25, Union Carbide Technical Center, West Virginia.

Sinnott, R. K. (2005). *Chemical Engineering Design* (Vol. 6). (4th, Ed.) Elsevier.

Slaghuis, J. H. (1993). *Coal Gasification.* Sasol Synfuels Secunda: SASTECH R&D Division.

Smith, J. M., Van Ness, H. C., & Abbott, M. M. (2001). *Introduction to Chemical Engineering Thermodynamics* (6th ed.). New York: McGraw-Hill.

Smoot, L., & Smith, P. (1985). *Coal Combustion and Gasification.* New York: Plenum Press.

Song, X., & Guo, Z. (2007). Production of Syngas by Co-gasifying Coke and Natural Gas in a Fixed-Bed Reactor. *Energy , 32*, 1972-1978.

Steynberg, A., & Nel, H. (2004). Clean Coal Conversion Options Using Fischer-Tropsch Technology. *Fuel , 83*, 765-770.

Steynberg, A., Espinoza, R., Jager, B., & Vosloo, A. (1999). High Temperature Fischer-Tropsch Synthesis in Commercial Practice. *Appl Catal A , 186*, 41-54.

Tijmensen, M. J., Faaij, A. P., van Hardeveld, M. R., & Hamelinck, C. N. (2002). Exploration of the possibilities for production of Fischer-Tropsch liquids via biomass gasification. *Biomass and Bioenergy , 23*, 129-152.

Tillman, D. A. (1987). The Costs of Coal Liquefaction:Influences of Technical/Economic Risk. *Fuel Processing Technology , 16*, 19-33.

Van der Burgt, M., & Higmann, C. (2003). *Gasification* (4th Edition ed.). New York: Elsevier.

Van Dyk, J. C. (2006). *Manipulation of gasification coal feed in order to increase the ash fusion temperature of the coal to operate the gasifiers at higher temperatures.* Nort-West University, Chemical Engineering. Potchefstroom: North-West University.

Van Heerden, J. (2005). *Aspects of the Clean Coal Technology Research and Development Program in SASOL.* Sasolburg: SASOL Technology Pvt Ltd.

Van Heerden, J. (2007). *Aspects of the Clean Coal Technology Research and Development Program in SASOL.* Sasolburg: SASOL Technology Pvt Ltd.

Van Nierop, P., Erasmus, H., & Van Zyl, J. (2000). SASOL'S achievements in the 20th century as a building block for the 21st. *Gasification Technologies Council* (pp. 4-7). San Francisco,California: Sasol Technology.

Van Vliet, O. P., Faaij, A. P., & Turkenburg, W. C. (2009). Fischer-Tropsch diesel production in a well-to-wheel perspective:A carbon,energy flow and cost analysis. *Energy Conversion and Management , 50*, 855-876.

Vogt, E., & Van der Burgt, M. (1980). Status of the Shell-Koppers process. *Chemical Engineering Progress , 76* (3), 65-72.

Winkler, H. (2007, March). Energy Policies for Sustainable Development in South Africa. *Energy for Sustainable Development , XI* (1).

Wolff, F., Eyre, D., & Grenier, M. (1979). Oxygen Plants:10 years of Development and Operation. *Chemical Engineering Progress , 75* (7), 83-87.

Yoshitomo, I., Motoo, F., Makoto, T., & Yutaka, T. (2000). Coal Gasification System using Nuclear Heat for Ammonia Production. *Applied Energy , 67*, 395-406.

Appendix 1

In the material balance scheme (Table 3.6), the gasifier has a nominal input of 100 tons per stream day of MAF coal. This is adjusted to establish the on-stream or as-received (AR) coal feed.

Assume the total period of anticipated maintenance and unscheduled interruptions at 30 days so that the gasifier achieves a 92% on-stream operation;

Equivalent coal feed (assuming 100% on-stream factor) =

$$\frac{100TPD}{100-(25.8+5.0)}\times 100 = 144.51TPD$$

Therefore, actual coal feed/gasifier$=144.51\times 0.92 = 132.63$tons per calendar day

These are the results shown in Table 3.6

The mass flow of coal as determined from the proximate analysis (Table 3.1) and volatile matter composition (Table 3.2) can be normalised to a required mass flow, 132.63 tpd in this case.

The gasifier operates at an oxygen consumption of approximately 0.243 ton/ton of coal (Van Dyk, 2006).This is within the range of the oxygen to coal ratio given for fixed bed gasifiers (Hobbs, Radulovic, & Smoot, 1992).

Amount of oxygen required = $0.243\times 132.63 = 32.23\,\mathrm{TPD}$

The gasifier operates at a steam/oxygen ratio of between 5.5 and 6.5 kg/Nm^3 (Ranwell, 1997).The density of oxygen at room temperature and pressure (rtp) is 1.331 kg/m^3. A normal cubic meter is defined at atmospheric pressure and 273K temperature. Therefore, the temperature corrected density of oxygen is 1.452kg/Nm^3.

Volumetric oxygen flow required= 32230/1.453 =22 183.426 Nm^3/day

Amount of steam required = $6.5\times 22183.426 = 144.19\mathrm{TPD}$

The gasifier nominal coal input of 54 tons/hr has a nominal gas output of 65000Nm^3/hr dry raw gas (Van Nierop, Erasmus, & Van Zyl, 2000). This corresponds to a raw gas production of 1203.7Nm^3/ton coal. Therefore, a coal feed of 132.63 tpd produces 159 648.72 Nm^3/day dry raw gas.

Density of dry raw gas = $\frac{\mathrm{MW}_{\mathrm{avg}}P}{RT}$

Average Molecular Weight of dry raw gas, $\mathrm{MW}_{\mathrm{avg}} = \sum_{i=1} y_i MW_i = 21.82\mathrm{kg/kmol}$

y_i = mole fraction of component i in gas mixture (given in Table 3.3)

MW_i = molecular weight of component i

$$\rho_{\text{dry raw gas}} = \frac{\mathrm{MW}_{\mathrm{avg}} P}{RT} = \frac{21.82 \times 101.25}{8.314 \times 273} = 0.974\mathrm{kg/Nm}^3$$

Dry raw gas mass flow = $0.974\ \mathrm{kg/m}^3 \times 159648.72 Nm^3/day$ =155.43TPD

Total moles of dry raw gas produced, n = 155 430(kg/day)/21.82kg/kmol =7121.77 kmol/day

Component mass flow, $m_i = \sum_{i=1} y_i n(MW_i)$

The mass flows of components in the dry raw gas stream are the same as the raw gas with exception of the water component. Ranwell (1997) specifies the composition of water in the raw gas as 0.7kg/Nm^3 raw gas.

Therefore, amount of water in ex-gasifier raw gas = 0.7 *159 648.72 = 111.75TPD.

Amount of tar and oils in raw gas = 7.43TPD

Thus, the amount of raw gas = 111.75 + 7.43 + 155.43 = 274.61 TPD

The raw gas leaving the gasifier is quenched with water to solidify entrained ash that would otherwise agglomerate on the WHB(Waste Heat Boiler).In the process, the raw gas is steam saturated (spray cooling)and condensation occurs to yield a crude condensate called gas liquor. Thus the quench water is used effectively for spray cooling the gas and ash cooling.

Spray cooling and ash cooling water requirements are specified as 8.4L/GJ and 71.7L/GJ, respectively (Vogt & Van der Burgt, 1980; Schilling, Bonn, & Krauss, 1981). The raw gas obtained herein, is estimated to have a gross heating value (GHV) of 300.46BTU/SCF (0.011GJ/m^3).The GHV are extracted from (Hatch & Matar, 2000).

Wash water requirement = $0.011\mathrm{GJ/m}^3 \times 159648.72\mathrm{Nm}^3/\mathrm{day} \times (8.4 + 71.7)\mathrm{L/GJ} = 143.18\mathrm{TPD}$

Gas liquor produced is the amount of water and black products (tar and oils) in the raw gas. Ammonia is also dissolved, and in reality is a component of gas liquor. This goes directly to the phenolsolvan and tar recovery plants.

Tables 3.8 and 3.9 are scale-up computations of Table 3.7

The Rectisol plant is assumed to achieve 100% separation although in reality the separation efficiency is in the range >99%.