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A REVIEW OF THE APPLICABILITY OF INTEGRATED GASIFICATION COMBINED CYCLE IN SOUTH AFRICA

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0202546P

A dissertation submitted to the Faculty of Engineering and Built Environment, University of the Witwatersrand, in fulfilment of the requirements for the degree of Master of Science in Chemical Engineering.

Johannesburg, November 2013

DECLARATION

I declare that this dissertation is my own unaided work. It is being submitted for the degree of Master of Science in Engineering to the University of the Witwatersrand, Johannesburg. It has not been submitted before for any degree or examination to any other University.

……

Fulufhelo Confidence (Nelwamondo) Makananise

…….day of……..year……

day *month* *year*

ABSTRACT

Integrated Gasification Combined Cycle (IGCC) is a technology that combines a number of components with the aim of producing electricity at high cycle efficiencies and near zero emissions. This research focussed on IGCC with coal as a feedstock in an attempt to establish the applicability of this technology in South Africa.

Fluidised bed gasification technology was found to be the fine coal gasification technology in IGCC with greatest potential when considering the qualities of coals currently being used in local power stations. Gasification test work on four selected South African coals was undertaken at the CSIR gasification testing facility, to assess the behaviour and compatibility of these coals with fluidised bed gasification.

A further aspect investigated the likely emissions that would be produced and how these compare to the national limits set by the Department of Environmental Affairs. During the course of the literature survey, it became apparent that the reduction of gaseous emissions from IGCC plant will have a significant impact on the economic and environmental aspects and therefore the attractiveness of the IGCC technology.

For this reason the research direction turned to investigate in greater detail the emissions generated from the combustion of syngas produced from fluidised bed gasification and combusted in a gas turbine. This serves to be an estimation of emissions that may be expected from the syngas combustion turbine in an IGCC technology.

The estimated emissions were used to assess the impact that the selected coals may be expected to have on full scale emissions. It was also established that the agent used in gasifying these coals had an influence on the quality of gas produced. These results are likely to aid in understanding how to control the nature of emissions in future gasification processes with specific application to fluidised bed technology in IGCC processes.

In memory of my father

Zacharia Nelwamondo

ACKNOWLEDGEMENTS

I would like to thank God for giving me the strength to complete this thesis

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- Eskom for allowing me to utilise some of their emission related information
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LIST OF SYMBOLS

kt – kilo tonnes

MMBtu – One million British thermal unit

mt – mega tonnes

MW – Mega Watt

MWe – Mega Watt electrical

MWth – Mega Watt thermal

Nm^3/h – Normal cubic meter per hour

ppmv – Parts per million by volume

NOMENCLATURE

AEO – Annual Energy Outlook

AGR – Acid gas removal

ASU – Air separation unit

BGL – British gas/Lurgi

CCS – Carbon capture and storage/sequestration

CO – Carbon Monoxide

COS – Carbonyl Sulphide

COE – Cost of Electricity

CO_2 – Carbon dioxide

COP – ConocoPhillips

CSIR – Council for Scientific and Industrial Research

CV – Calorific Value

DOE – Department of Energy

EIA – Energy Information Administration

EPRI – Electric Power Research Institute

FBG – Fluidised Bed Gasification

FT – Fischer Tropsch

GE – General Electric

GTI – gas Technology Institute

GHG – Green House Gas

HHV – High Heating Value

HRSG – Heat Recovery Steam Generator

HTW – High Temperature Winkler

IGCC – Integrated gasification combined cycle

IOU – Investor Owned Utilities

ISO – International organisation for standardisation

KBR – Kellogg Brown and Root

KRW – Kellogg-Rust-Westinghouse

LCOE – levelized cost of electricity

MBtu – Million British thermal units

NETL – National Energy Technology Laboratory

NO_X – Nitrogen oxides

O_2 – Oxygen

PC – Pulverised coal

PF – Pulverised fuel

Q – Total quench design

R – Radiant only design

R+C – Radiant plus convective design

R&D – Research and development

RSA – Republic of South Africa

SA – South Africa

SCPC – Supercritical pulverised coal

SNG – Substitute Natural Gas

SNOx – Sulphur oxides and nitrogen oxides

SGC – syngas cooler

SO_X – Sulphur oxides

SO_3 – Sulphur Trioxide

TGA – Thermo Gravimetric Analyser

TGTU – Tail gas treatment unit

TPC – Total Plant Cost.

CHAPTER 1

1. INTRODUCTION

1.1. Introduction

Legislation in South Africa has become stringent with regards to emissions from current pulverised coal based electricity generation. At the same time the electricity demand is increasing sharply year after year requiring more stations to be built. Alternative sources of energy for power generation are being explored; however, coal remains the primary energy source in South Africa due to its abundant coal reserves, and its relatively cheap price. This has therefore led to research on clean coal technologies that can meet the current and projected electricity demand and concurrently complying with the emission standards as required by legislation.

Clean coal technologies are those technologies designed to operate efficiently and to reduce the emission of greenhouse gases and other harmful gases. The clean coal technologies can either be combustion based or gasification based. Gasification based clean coal technologies consist of surface coal gasification and underground coal gasification. Surface coal gasification technologies include technologies such as Fixed bed, Fluidised bed and Entrained flow gasification. Underground coal gasification involves gasifying the coal underground where oxygen or air is injected into the coal seam to react with the coal to produce syngas, which is later used for combustion in a gas turbine for production of electricity.

Coal gasification technologies have been in existence since 1792. The interest in coal gasification was revived by environmental concerns over the burning of coal (Research reports International Inc., 2008). Coal

gasification is considered one of the environmentally friendly coal technologies.

The purpose of this study is therefore to undertake an investigation into a clean coal technology that will be able to operate on South African bituminous coal as a feedstock and offer low emissions per unit power output.

IGCC has been identified as one such technology. It has been in operation in Europe, Japan and the USA and has reported impressive benefits regarding cycle efficiency and emissions. IGCC operation has potential at Eskom with the current underground coal gasification project running next to Majuba power station. It is also of interest to Eskom to explore the combined technology utilising surface coal gasification.

This dissertation is structured as follows:

Chapter 2 provides a comprehensive reference resource for integrated gasification combined cycle technology. This includes assessment of the IGCC technology worldwide, narrowing it down to how it can be applied to the South African power generation industry.

Chapter 3 describes the methodology that was used in the calculation of emissions produced from the combustion of the synthesis gas obtained from the gasification of four selected South African coals at the CSIR fluidised bed gasification testing facility.

Chapter 4 discusses the results obtained from the calculation of the products of combustion of both syngas and pulverised coal. The results obtained are analysed to see the applicability of the technology based on its competitiveness regarding emissions.

Chapter 5 concludes the dissertation based on the findings in the literature review and the emission calculations undertaken.

1.2. Research Questions

- What suitable gasification technologies have been identified for application with SA coal for power generation?
- What are the associated techno-economic implications regarding the implementation of these technologies?
- What time-frames are associated with the introduction of these technologies in South Africa?
- What are the associated risks with these technologies?
- How does the predicted emissions from the IGCC process compare with South African legislated limits?

CHAPTER 2

2. LITERATURE REVIEW

2.1. Introduction

The legislation in South Africa is becoming stringent with regards to emissions from current pulverised coal based electricity generation. At the same time the electricity demand is increasing sharply year after year requiring more stations to be built. The rate of increase of electricity demand globally is three times higher than the rate of total energy produced (Collot, 2002) and therefore there is a need to improve efficiency in the existing electricity generating technologies and, through technology improvement to reduce emissions and to reduce energy consumption as much as possible.

Alternative sources of energy for power generation are being explored however coal remains the primary energy source in South Africa due to its abundant coal reserves, and its relatively cheap price. These have led to research on the clean coal technologies that can meet the current and projected electricity demand and concurrently comply with the emission standards as required by legislation. Clean coal technologies are those technologies designed to operate efficiently and be able to reduce the emission of greenhouse gases and other harmful gases. Gasification technologies, with specific reference to Integrated Gasification Combined Cycle (IGCC), have demonstrated potentiality in terms of improving power generation efficiency and significant reduction in emissions of carbon dioxide (CO_2), sulphur oxides (SO_X), nitrogen oxides (NO_X) and particulate matter. Most of these are removed prior to the combustion process after gasification. The gas produced during gasification is cleaned up before

going into the gas turbine, thereby reducing the volume of gas going into, and the work done by, the emission control technologies after the combustion process.

Attention has already been drawn to the IGCC technology due to its high efficiencies; however interest on this technology will increase with the application of carbon capture and sequestration (CCS) in the future because gasification facilitates easier capture of carbon dioxide, especially in the case of oxygen blown gasification.

IGCC also has the advantage of reduced water consumption and the possibility of cogeneration of electricity with, for example, liquid and gaseous fuels and chemicals.

In general, clean coal technologies can either be combustion based or gasification based. Gasification based clean coal technologies consist of surface coal gasification and underground coal gasification.

Surface coal gasification technologies include technologies such as Fixed bed, Fluidised bed and Entrained flow gasification technologies. The underground coal gasification involves gasifying the coal in situ where oxygen or air is injected into the coal seam to react with the coal to produce syngas, which is later used for combustion in the gas turbine for production of electricity.

This literature review focuses on the coal fired integrated gasification combined cycle (IGCC) technology with surface gasification. This process consists of the gasification technology and the combined cycle technology.

Attention is also drawn to fluidised bed gasification, where some of the coals burnt by Eskom have been tested for suitability in terms of gasification.

2.2. Background on IGCC process

Integrated gasification combined cycle (IGCC) is a technology that combines a number of components employing different kinds of technologies with the aim of producing electricity at high cycle efficiencies. These components include but are not limited to the gasification reactor, cooling systems, cleaning systems, gas turbines, heat recovery systems and steam turbines. This research will focus on IGCC with coal as a feedstock. In this research, the different gasification technologies and cooling systems will be briefly discussed, with more focus on the emissions from the gas turbine.

Coal gasification has progressed from the production of coal gas simply for direct energy generation, to syngas to generate marketable products such as chemicals (45%), Fischer Tropsch (FT) liquids (28%), power (19%) and gaseous fuels (8%) (Research reports International Inc., 2008). IGCC is a proven technology globally which combines gasification technology with both gas and steam turbine technology. The combination of gas and steam turbine is known as combined cycle technology.

In combined cycle technology air is compressed and combusted with fuel to produce gases in a gas turbine; the products of this combustion are then used to drive the gas turbine blades thereby driving the shaft that is connected to the generator to produce electricity. The waste heat is then taken to a heat exchanger where the heat exchange is between the exhaust gases from the gas turbine and water. This heat exchanger is known as a Heat Recovery Steam Generator (HRSG). The steam generated from the HRSG is used in a steam turbine to produce more electricity. It is the integration of these system components that draws attention to this combined cycle technology. (Rajoo, 2003) The exhaust gases are vented into the atmosphere and the steam is condensed. This technology results in high cycle efficiencies. (Ratafia-Brown et al., 2002).

The IGCC technology has proven flexibility regarding the feedstock used. This ranges from a mixture of coal and its blends; coal and petcoke blends; and, coal, coke and biomass blends. (Rousaki & Couch, 2000)

The first coal fired IGCC demonstration plant was in the town of Lunen which operated in 1972 – 1977 in Germany. This was followed by the Cool Water plant from 1984 to 1989 and the Plaquemine plant in 1987 to 1995 both in USA. These demonstration projects were undertaken to provide operational experience and useful information for the improvement of the IGCC technology. This led to a number of large scale demonstration IGCC plants coming into operation from 1995 in Europe and the USA for the purpose of eventually commercialising the IGCC technology. (Rousaki & Couch, 2000)

In a coal fired IGCC plant the coal is subjected to hot steam and oxygen or air in a gasifier under high temperature and pressure to produce syngas. The gasification stage can employ different gasification technologies depending on the feedstock and the products required. The gas produced needs to be cleaned of impurities before going into the gas turbine. The IGCC configuration consists of varying process technologies, which mostly depend on the type of gasification technology used. One type of configuration is illustrated in figure 2.1. Coal is fed into the gasifier together with steam and oxygen (or air). The gas produced is cooled and then cleaned to remove impurities before going into the combustion turbine. The clean gas is combusted in air producing gases that are used to drive the gas turbine to produce electricity. Waste heat is recovered and used to generate steam in a heat recovery steam generator (HRSG); the steam is then used in a steam turbine to further produce electricity. About 60% of electricity is produced in the gas turbine and about 40% in the steam turbine (Henderson, 2008).

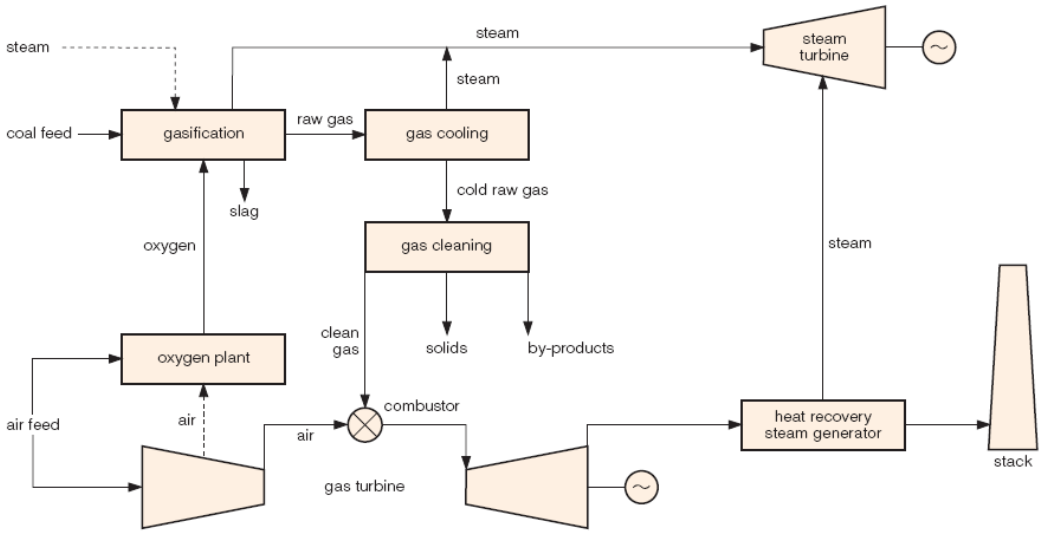


Figure 2.1: Major components of an Integrated Gasification Combined Cycle (**Henderson, 2008**).

Figure 2.2 is an illustration of the energy flow in the IGCC process. This diagram also shows the different energy losses. It can be seen that most of the losses are in the steam/ water cycle. 65% of the chemical energy in the fuel, in this case, coal, goes into producing steam in the heat recovery steam generator. About 70% of this energy goes to losses and only about 30% produces electricity from the steam turbine (Henderson, 2008).

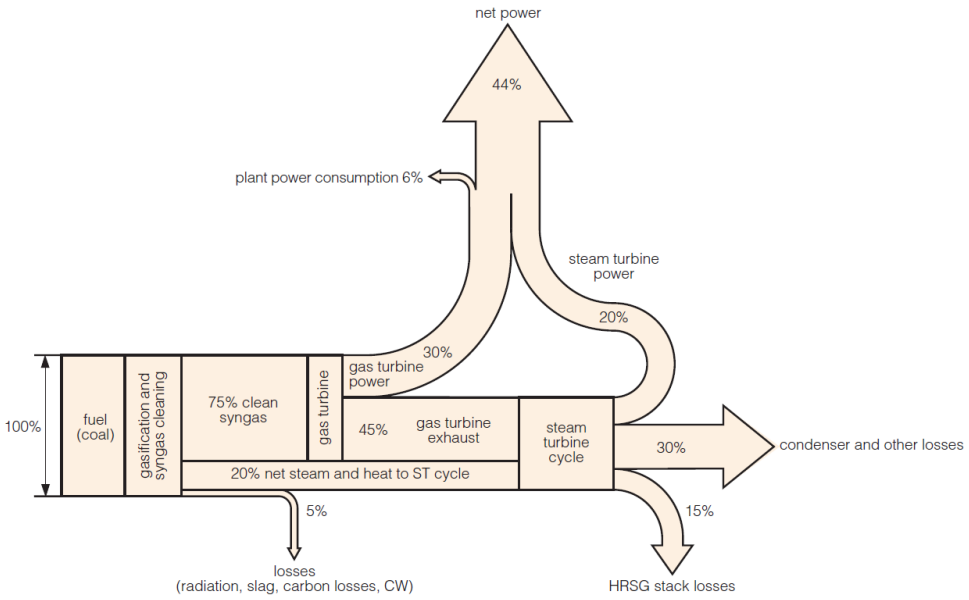


Figure 2.2: Indicative energy flow diagram for IGCC (Henderson, 2008)

The energy/thermal efficiency of the IGCC process can be illustrated further by comparing the conventional cycle and the integrated cycle (*see Figure 2.3*). The conventional cycle uses most of the energy obtained from the coal to convert water into steam, and is able to achieve an overall efficiency of between 33 and 38%; this low efficiency is because most of the energy is lost by evaporation during cooling. Conventional power generation technology uses a considerable amount of water because the whole process is water dependent. The electricity generated from the conventional cycle is produced solely from the steam turbine. The water/steam flow is directly proportional to the amount of electricity generated. The IGCC process on the other hand, can produce up to 55% overall efficiency utilising less water (Engelbrecht et al., 2008).

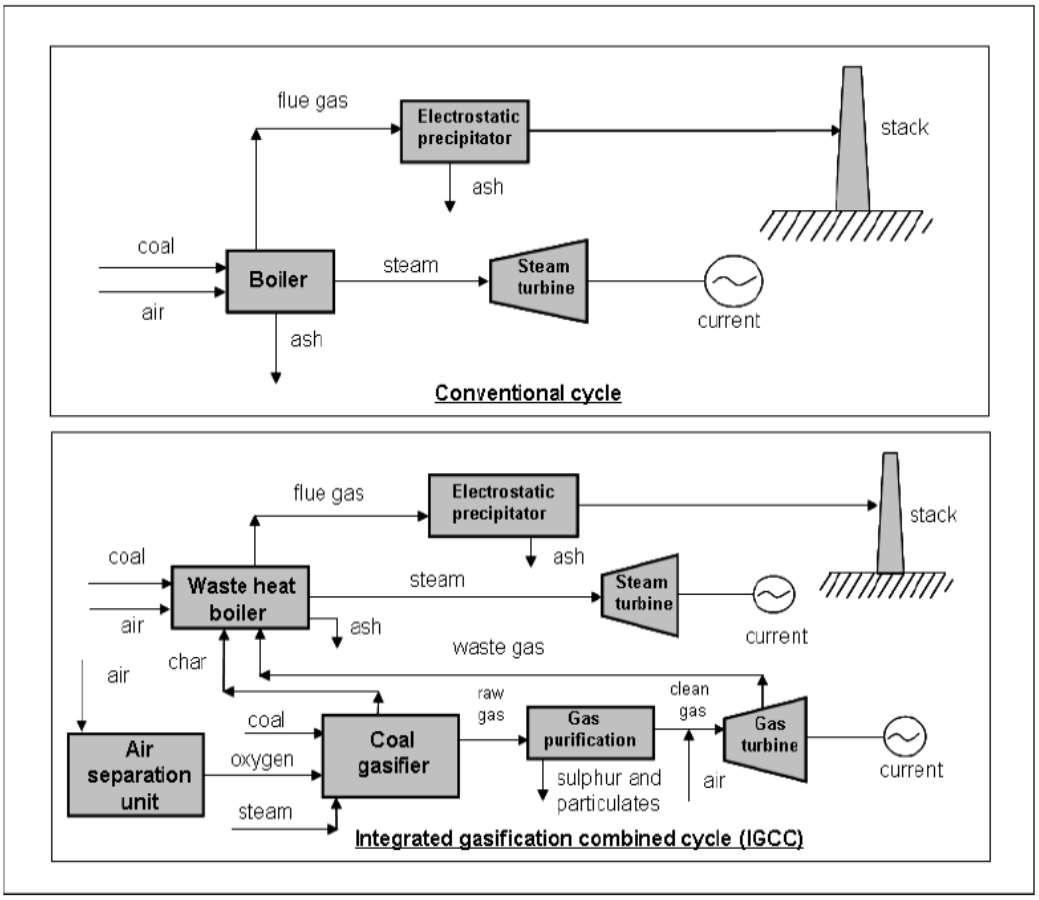


Figure 2.3: Comparison between Conventional cycle and Integrated Gasification Combined (Engelbrecht et al., 2008)

Over and above the IGCC's advantage of good thermal efficiency performance, its emissions are low when compared to the conventional cycle (Engelbrecht et al, 2008); however the IGCC process is accompanied by technical and economic barriers that still need to be overcome. The high capital cost of IGCC technology and the low availability of its operations due to current problems in the plant makes it less competitive compared to other clean coal technologies. The design and manufacturing costs are however expected to reduce as operational experience is gained through more demonstration plants. (Henderson, 2008)

In general, IGCC technology is driven by the following operational drivers,

- High efficiencies
- Low emissions
- Ability to utilize low coal quality
- Utilisation of less water

The economic drivers include emissions control legislation and relatively low operating costs. The newly set standards on the allowable greenhouse gas emissions are putting pressure on the utilities. The penalties enforced in contravening emission limits from utility plants can lead to high costs or even the shutdown of the concerned utility. This therefore encourages the pursuit of thermally efficient operating power generating units. Given that efficiency is inversely proportional to greenhouse gas production, the higher the cycle efficiency, the lower the greenhouse gas emissions are likely to be. For these reasons, it becomes important for utilities to seek alternative technologies that would produce electricity more efficiently thereby resulting in reduced environmental impact.

The applicability of IGCC in South Africa for power generation will depend mostly on the suitability of the feedstock currently available for gasification. This will therefore influence the type of gasification technology to be employed.

2.3. Gasification technologies

2.3.1. Gasification overview

Gasification is a clean energy technology that can utilise low grade fuel and still be able to meet stringent emission standards. It is capable of producing base load electricity, fuels and chemicals. Different feedstock can be used in gasification provided that the gasifier is designed with the

specific feedstock in mind. Gasification utilises a mixture of steam and air or oxygen. The oxygen is usually less than half of that required theoretically for complete combustion (Collot, 2002) and the steam is used for hydrolysis. Gasification converts any feedstock containing carbon into synthesis gas known as syngas, which is a mixture of hydrogen and carbon monoxide. In the case of coal gasification, coal undergoes pyrolysis at temperatures of above 400 ˚C depending on the coal rank, where tars, phenols and hydrocarbon gases are released from the hydrogen-rich volatile matter. Char gasification occurs simultaneously with pyrolysis, where gases, tar vapours and solid residues are released. The gasification of char can be summarised in the following reactions (Collot, 2002):

Combustion with oxygen:

$C + O_2 \leftrightarrow CO_2$ ΔH = -405.9 kJ/mol……2.1

Gasification with oxygen or air (partial combustion):

$2C + O_2 \leftrightarrow 2CO$ ΔH = -123 kJ/mol……..2.2

Gasification with carbon dioxide (Boudouard reaction):

$C + CO_2 \leftrightarrow 2CO$ ΔH = 159.7 kJ/mol……..2.3

Gasification with steam (water gas reaction):

$C + H_2O \leftrightarrow CO + H_2$ ΔH = 118.9 kJ/mol……2.4

Gasification with hydrogen (hydrogasification reaction)

$C + 2H_2 \leftrightarrow CH_4$ ΔH = -87.4 kJ/mol……..2.5

The water gas shift reaction:

$CO + H_2O \leftrightarrow H_2$ ΔH = -40.9kJ/mol……..2.6

The methanation reaction:

$CO + 3H2 \leftrightarrow CH4 + H2O \ \Delta H = -206.3$ kJ/mol……..2.7

Gasification technologies exercise partial oxidation, the amount of air or oxygen used to oxidise the fuel is carefully controlled to ensure that only a relative portion of the fuel burns completely to produce synthesis gas.

The syngas produced can be used for the production of electricity through combustion in the gas turbine and production of fuels or chemicals through further processing.

2.3.2. Underground coal gasification (UCG)

In underground coal gasification, partial oxidation of coal occurs in situ. This reaction is carefully controlled to produce gas that is rich in hydrogen and carbon monoxide. The steam or water used for hydrolysis can be injected into the coal seam.

The UCG process consists of two bore holes on opposite ends of a coal seam. One borehole is used to inject reactants required for the gasification of coal, and the other is used to extract the gases produced during the gasification reaction. The primary products of UCG are H_2, CO, CO_2 and CH_4 (Couch 2009). Figure 2.4 illustrates an overview process of UCG.

Underground coal gasification has the advantage of using unmineable coal deposits, poor grades and deeper seams which would normally be uneconomic to mine or involve high costs if conventionally mined. The second advantage is that this process uses less water for its operation than conventional gasification technologies. However UCG runs the risk of underground water contamination and therefore it is necessary to select sites carefully to avoid contamination of drinking water.

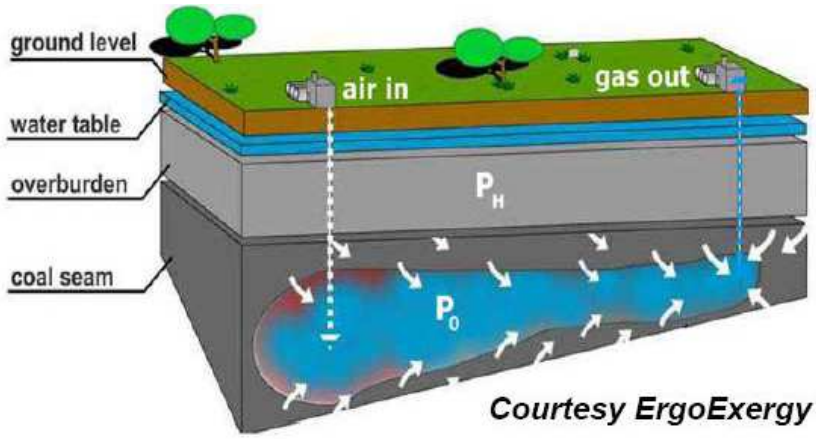


Figure 2.4: Illustration of the UCG process (Bowen, 2008)

The syngas produced from UCG can be used in an IGCC process or it can be co-fired with coal in a conventional boiler for power generation. Eskom is currently operating a pilot UCG plant at Majuba site in Mpumalanga, South Africa. The syngas produced is considered for the demonstration of the applicability of co-firing in the adjacent power station (Gross & Van der Riet, 2011). Exploring IGCC with the use of UCG instead of surface gasification may be a potential option for Eskom.

2.3.3. Surface gasification

2.3.3.1. Entrained flow reactors

Entrained flow gasification technology utilises co-current flow geometry, where the pulverised coal particles and the gas flow at high speed co-currently. The reactants (pulverised fuel, oxidant and steam) are introduced at the top of the reactor. The operating temperatures in this type of reactor are relatively high, usually above 2300˚F (1260˚C) (Rubin et al. 2007). This is above ash slagging conditions enabling high carbon conversion and providing some mechanism of slag removal. The syngas produced from this type of reactor is usually of high quality since it

contains very small amounts of methane and other hydrocarbons. The gases produced consist primarily of H_2, CO and CO2.

The high temperatures in the entrained flow gasification enable use of a wide range of coals since high carbon conversion can be achieved even for less reactive coals. This technology however requires high usage of oxidant. (Rubin et al. 2007).

Examples of currently operating well-known entrained flow gasification technologies are Texaco, Shell, Prenflo, ConocoPhillips and Noell technologies. (Research reports International Inc., 2008).

2.3.3.2. Moving/ fixed bed reactors – counter current design

Moving bed reactors have two types of designs wherein gases flow relatively slowly through the bed of coal feed. In one design, the fuel flow geometry passes co-currently with the oxidant and steam. (Research reports International Inc., 2008). The second design which will be discussed here is the counter current flow. Here the fuel flows counter currently to the oxidant and steam. The fuel enters the reactor at the top while the oxidant together with the steam enters from the bottom. An example of a moving bed gasifier is shown in figure 2.5. The moving bed counter current flow reactor consists of four zones through which the solid fuel particles pass; namely, from top to bottom: first, the drying zone, then the devolatilisation zone, the gasification zone and the combustion zone. The fuel entering the reactor from the top is dried by the heat in the raw syngas leaving the reactor. After the fuel is dried it devolatilises to form tars and oils. During devolatilisation, lighter hydrocarbons are driven off and exit with the syngas. Gasification occurs when the resultant fuel is reacted with the steam and carbon dioxide, thereby forming char and ash, which reacts with oxygen near the bottom of the gasifier, creating

temperatures which lead to the formation of slag. (Research reports International Inc., 2008).

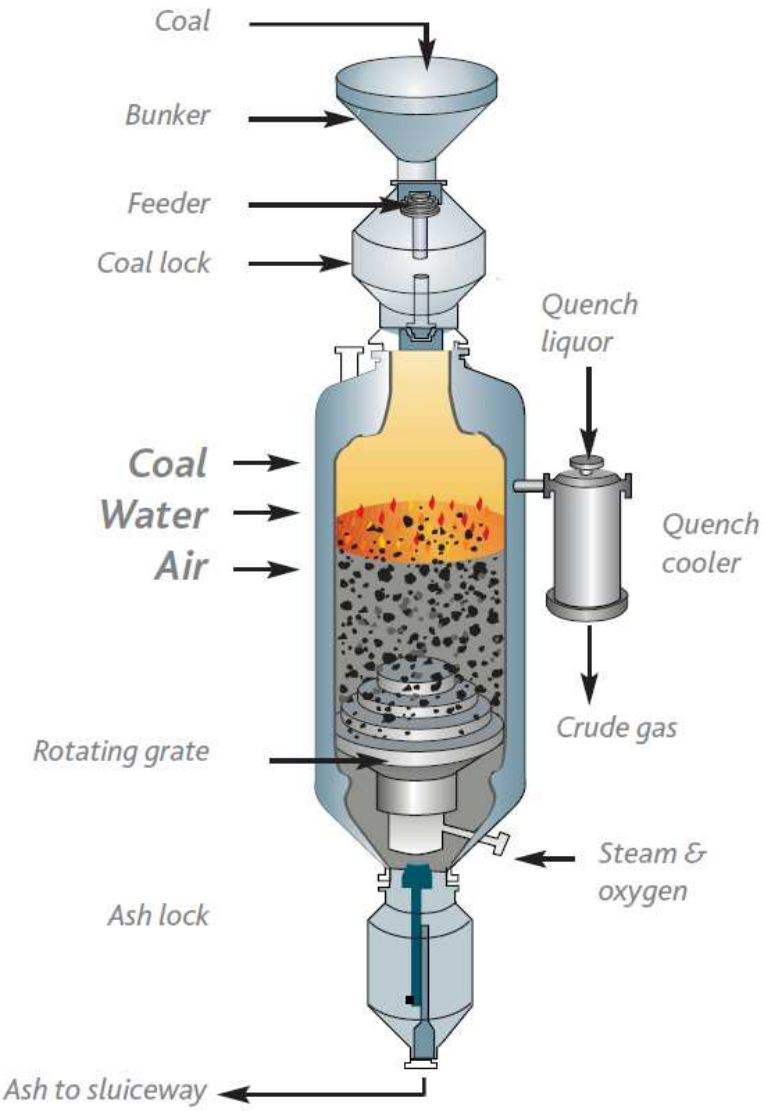


Figure 2.5: The Sasol-Lurgi dry ash gasifier (Collings, 2013)

Examples of currently operating well-known moving/fixed bed gasification technologies are the Lurgi dry ash (Non slagging) technology, which is used by Sasol as shown in figure 2.5. and the British Gas Lurgi (BGL) (slagging) technology (Research reports International Inc., 2008). Sasol

has 97 coal fired gasifiers (in 2008) with about 14 gigawatts thermal of syngas output (Blesl & Bruchof, 2010)

2.3.3.3. Fluidised bed reactors

In fluidised bed gasification, the coal particles are suspended in the gas flow. Turbulence is encouraged to increase contact between the gas and the coal particles. (Collot, 2002). The reactants (pulverised fuel, oxidant and steam) are introduced from the bottom of the reactor with the exception of the transport reactor – which is halfway between a fluidised bed and an entrained flow gasifier (Collot, 2002); these reactants rapidly mix in a fluidised bed. The bed acts like a fluid creating uniform conditions within the reactor. This happens when the minimum air velocity is exceeded creating turbulent conditions within the reactor. The bed is either formed from sand, coke, char sorbent or ash. The temperature in the reactor is uniformly distributed and can range from 900˚C to 1050˚C to avoid ash melting which prevents clinker formation and loss of fluidity of the bed; this concept is shown in figure 2.6. Low temperatures may result in incomplete carbon conversion, which may require recirculation of the residual char (Collot, 2002).

The ash is either discharged in agglomerated or dry conditions. The agglomerated ash conditions improve the efficiency of gasifying high rank coal. The dry ash conditions are traditionally used with low rank coals, having the ability to operate at variable loads leading to high turndown flexibility (Collot, 2002).

The raw syngas formed in this process leaves the reactor together with the unconverted char and is transferred to the cyclones where the char is separated from the raw gas.

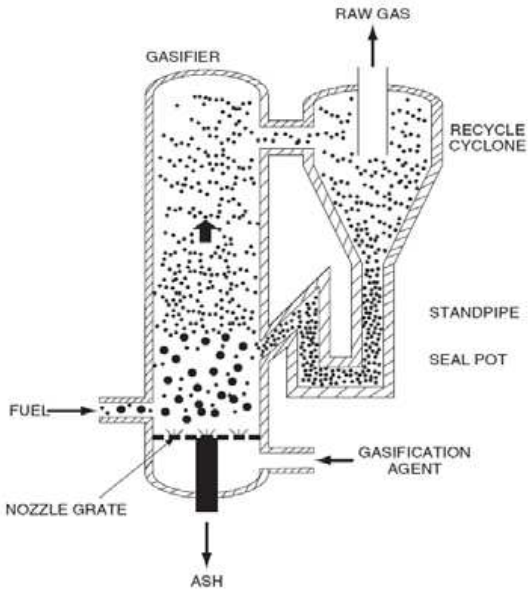


Figure 2.6: The fluidised bed gasification concept (Blesl & Bruchof, 2010)

Examples of currently operating well-known Fluidised bed gasification (FBG) technologies are the High temperature Winkler (HTW) technology, the Kellogg Rust Westinghouse (KRW) technology and the Gas Technology Institute U-gas technology. The HTW will be discussed further in section 2.5.3. (Research reports International Inc., 2008).

2.3.4. Syngas considerations

Gasification technologies have been in use for many years, and are utilised in different industries. Some processes have been in commercial application for more than 50 years in the refining, fertilizers, and chemical industries and more than 35 years in the electric power industry. (Engelbrecht et al., 2008)

Figure 2.7 shows the syngas capacity growth from the year 2000 to present and is projected to 2016. It is estimated that by 2015, the syngas capacity will be just under 125 000 MW_{th}.

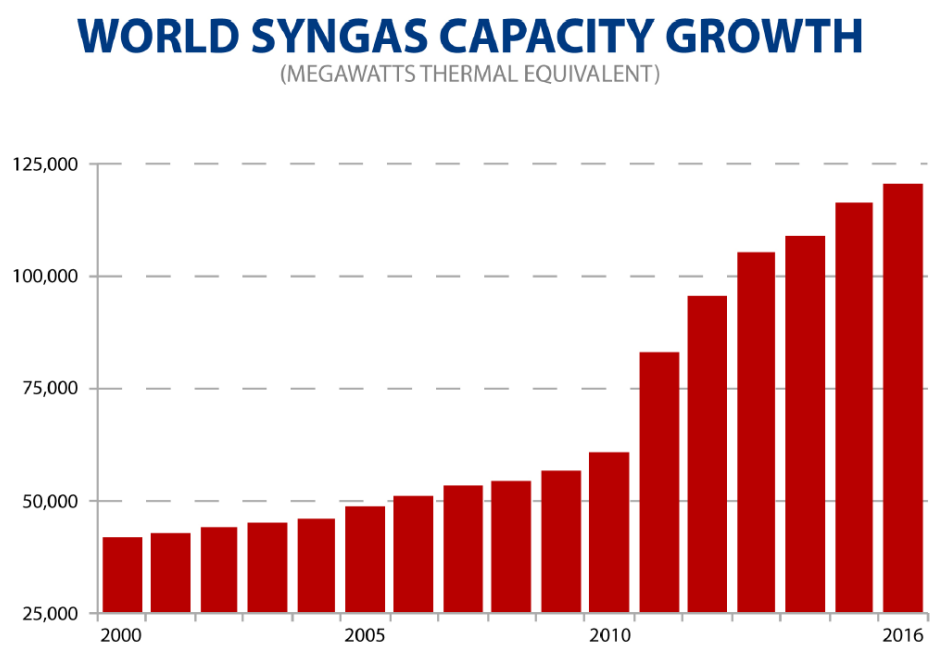


Figure 2.7: World syngas capacity growth

(http://www.gasification.org/what_is_gasification/pop/syngas-capacity-growth.aspx 2013/08/12)

From the graph the rapid increase of syngas production is evident. This data illustrates the increasing levels of confidence in gasification based technologies such as IGCC. The more experience there is in gasification technologies, the more the opportunities to produce better quality syngas.

According to Collot (2002), the chemical composition of the syngas produced and its future use is dependent on the following:

- Coal composition and rank
- Coal preparation (particle size)
- Gasification agents employed (oxygen or air)

- Gasification conditions – temperature, pressure, heating rate and residence time in the gasification reactor.
- Plant configuration which includes,
    - Coal feeding system (fed as either dry powder or slurry with water).
    - Flow geometry – the way by which contact between the fuel and the gasification agents is established.
    - Whether the minerals are removed as dry ash or molten ash
    - The way the heat is produced and transferred
    - The way the syngas is cleaned

2.3.5. Comparison between the different gasification technologies

Entrained flow and fluidised bed gasification technology can use air or oxygen as an oxidant. Examples of air-blown entrained flow designs include Texaco, E-gas, Shell, and Prenflo reactors, whereas the oxygen-blown design includes Mitsubishi reactors. The fluidised bed air and oxygen-blown designs include the HT Winkler and KRW reactors respectively.

Table 2.1 is a comparison of operating conditions between fluidised bed and entrained flow gasifiers. These two types of gasifiers operate on fine coal with a particle size of less than 5mm as illustrated in the table. The fluidised bed gasifier can achieve 75% (Engelbrecht et al., 2008) gasification efficiency operating at less than 1000˚C with longer residence time compared to the entrained flow, while the entrained flow gasifier can achieve 70% (Engelbrecht et al., 2008) gasification efficiency at high temperatures and low residence time.

Examples of moving bed gasifiers include British gas, Lurgi and Lurgi (dry ash) – used by SASOL in South Africa.

Table 2.1: Comparison of operating conditions between fluidised bed and entrained flow gasifiers (Engelbrecht et al., 2008)

	Fluidized bed	Entrained flow
Coal particle size	0.5 mm - 5 mm	< 0.5 mm
Coal moisture	Dry	Dry/slurry
Coal type	Non-caking coals	Low-ash coals
Ash in coal	< 60 %	< 30 %
Gasification agents	Air, oxygen and steam	Oxygen and steam
Temperature	850 °C - 950 °C	1 300 °C - 1 450 °C
Pressure	< 25 bar	< 30 bar
Residence time	0.5 h - 1.5 h	< 10 s
Carbon efficiency	65 % - 85 %	75 % - 90 %
Gasification efficiency	55 % - 75 %	55 % - 70 %
Commercial examples	Winkler	Texaco, Prenflo, Shell and Koppers-Totzek

The quality of coal used for gasification has an impact on the efficiency of the gasifier. (Ramachandran, 2008). Different gasification technologies perform differently with different types of coal. The entrained flow gasifiers perform well with low ash bituminous coals (Ramachandran, 2008). Use of sub bituminous coals and lignites in entrained flow gasifiers is less economic because their oxygen consumption is high and the gasifier cold gas efficiency is low especially for slurry fed gasifiers. Cold gas efficiency is the ratio of the energy in the syngas produced at standard temperature to the energy in the amount of fuel burnt. The cold gas efficiency measures the overall performance of the gasifier. It is not advisable to use high ash coals (ash > 20%) for entrained flow slagging gasifiers. These coals together with the low rank coals are recommended for fluidised bed gasification. (Ramachandran, 2008)

Figure 2.8 shows the installed capacity of the different gasification technologies.

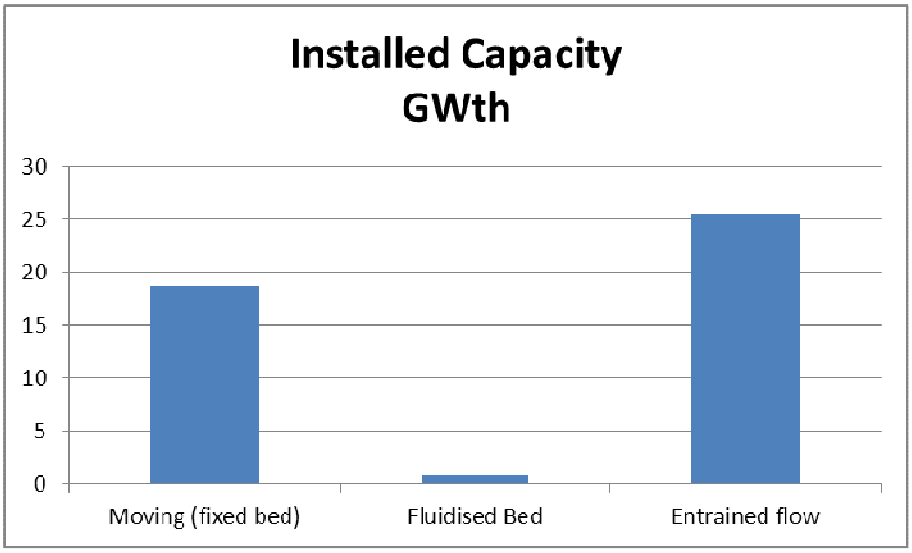


Figure 2.8: Installed gasification capacity

The moving or fixed bed technology was at 42% (18.7 GWth) of the world's total installed gasification capacity before 2011, however it has inherent limitations like relatively high maintenance costs, large capital investment to handle by-products such as tars and ammonia, and these have hindered future installations. (PES, 2013)

The fluidised bed technology although at 2% (0.9 GWth) of the world's total installed gasification capacity - before 2011, may be a feasible alternative especially for low ranked coals. (PES, 2013)

The entrained flow gasification technology is leading the market with 56% (25.4 GWth) of the installed capacity. This technology has dominated the market because of the following (PES, 2013):

- Reliable and proven design (widely used in chemical industry);
- No internal moving parts;
- Compact size compared to other gasifiers;
- Minimal by-products; and
- Ability to supply syngas at higher pressures.

The cost of an IGCC unit is dependent on different factors such as site specific conditions, technology supplier, and coal types. The type and quality of coal influences the design of the gasifiers, the method of storage and the transportation of coal.

Table 2.2 presents a summary on the leading vendors of the three types of gasification technologies. The table suggests that there are more leading vendors providing fluidised bed gasifiers than entrained flow gasifiers and fixed bed gasifiers.

Table 2.2: Technology Summary - Integrated Gasification Combined Cycle (Ramachandran, 2008)

Technologies	Fixed Bed	Fluidized Bed	Entrained Flow	Advanced—Gasification Processes
Leading Vendors	Lurgi	KRW (now KBR), Lurgi, Carbona, Ahlstrom (now Foster Wheeler).	GE Energy, ConocoPhillips, & Shell.	Still in R&D
Major Trends	Pilot plant in Germany in 1936. So. Africa leads after WW II (Sasol). 18 gasifiers by mid-1950s. Late 1970s scaled up over 50%. Sasol produces much of So. Africa motor fuel.	KBR promotes air-blown gasifiers (1) (as opposed to O_2-blown entrained gasifiers).	Standardized designs to reduce cost & construction time. Fuel flexibility.	Higher temperatures in CTs & steam cycle of combined cycle.
Changes to Watch for	There are currently 97 gasifiers at Sasol generating many types of hydrocarbon liquids. British Gas/Lurgi (BGL) is modification/ upgrade to Lurgi. 110 MW BGL IGCC is in Scotland. BGL IGCCs are limited compared to entrained processes.	Carbona & Foster Wheeler sell small Biomass gasifiers. New push associated with small wood mills, farming operations, & other waste Biomass sources for small gasifiers, including small IGCC.	More integration between combustion turbine gas compression & air separation unit (ASU).	Methods to reduce power requirements associated with O_2 production &, if CO_2 emissions become controlled, power for CO_2 removal & compression.
Capital Cost Dec 2007 $/KW 768 (3x256 MW) MW	N/A	N/A	A) 2900 (W/O CO_2 Capture) B) 4000 (W/ CO_2 Capture -2025 time frame).	C) 3250 (W/CO_2 removal and cost and Performance improvements -2025 time frame)
Levelized Cost of Electricity (LCOE, Dec. 2007 Constant $/MWh)	N/A	N/A	A) 70 B) 91 (2025)	C) 77
Other Characteristics	Best suited for coal-to-liquids.	Few commercial installations.	Integration of CT compressor & ASU.	Advanced integration CT, ASU, & emissions controls.
Heat Rate, HHV (Btu/kWh)	N/A	10,500 Btu/kWh (no CO_2 capture).	A) 8980 B) 11000	C) 10,040
Resource Requirements that Impact Technology	Not practical for IGCC.	Increasing price of alloys for pressure parts & vessels. Biomass may become an increasingly more important feedstock.	Increasing price of alloys for pressure parts & vessels. Ability to gasify lower grade coals more cost effectively.	Increasing price of alloys for pressure parts & vessels. Ability to gasify lower grade coals more cost effectively.

2.3.6. Feedstock considerations

Low value feedstock may be an option for gasification due to low prices per ton, and due to the advantageous environmental performance of IGCC technology which has been proven through demonstration projects. When low value coal is used as a feedstock, its impact on the different process units of IGCC need to be assessed as its properties can have adverse impacts on the equipment or the gasification process. For example, coal properties can have an impact on fuel handling, fuel preparation systems, gasifier, gas cooler, gas clean-up, gas turbine, waste heat recovery boiler and the steam turbine (Rousaki & Couch 2000). Most of the current IGCC technologies are designed for high quality coals except for Puertollano in Spain. Coal can be co-fired with biomass to reduce Green House Gas (GHG) emissions; however introduction of biomass is associated with high costs due to biomass preparation and the potential of slagging, fouling and corrosion of downstream components and processes (Klara, 2009).

2.4. IGCC gaseous emissions and CO_2 capture

IGCC allows relatively easier capture of carbon dioxide especially for oxygen-blown gasifiers because the carbon dioxide is concentrated in the flue gas. According to an EPRI report (Ramachandran, 2008), IGCC technology is able to achieve low emissions because of the following:

- The gas clean - up from the gasifier before the combustion turbine allows the removal of emission-forming constituents thereby enabling the technology to meet extremely stringent air emission standards.
- Sulphur removal is greater than 99% using acid gas removal technology with carbonyl sulphide (COS) hydrolysis.
- NO_X emissions were found to be less than 20ppmv at 15% O_2 in the gas turbine exhaust. Combustion modifications in the gas turbine can further reduce these levels.

- CO emissions were found to be 1 – 2ppmv at 15% O_2.
- EPRI also found that CO_2 removal with IGCC is relatively inexpensive, about 15– 20% lower in cost of electricity for IGCC than for PC (pulverised coal) technology.

2.5. IGCC demonstration projects

Coal based IGCC technology for the production of electricity has not been commercially deployed in the past due to unresolved technical issues. In order to advance this technology, three commercial teams were formed in the US to address these issues during the period 2004 – 2005. These teams are:

- GE Energy/Bechtel
- ConocoPhillips/Fluor/Siemens
- Shell/Uhde/Black & Veatch

The teams were expected to develop reference designs that would bring about the application of coal-based IGCC for the commercial generation of electricity and, in so doing, their brief was to provide prices, schedules, performance and emission guarantees. (Holt & Wheeldon, 2007)

Unfortunately all three teams utilised only one type of gasification technology (entrained flow) and gave no reference to fluidised and moving bed technologies.

The teams' first task was to provide an IGCC technology design that would compete with Supercritical Pulverised Coal (SCPC) plant without incorporating carbon dioxide (CO_2) capture. Lately, however, it has become of importance to consider the installation of CO_2 capture to reduce the emissions of CO_2 and therefore a design with CO_2 capture was considered. (Holt & Wheeldon, 2007)

Electric Power Research Institute (EPRI) published a report in 2007 that summarises the IGCC technology presented by the three teams (Holt &

Wheeldon, 2007). The current dissertation will only review two of these entrained flow gasification technologies because the potential candidate technology for IGCC power stations that can utilize high ash South African coals has been identified with fluidised bed gasification (Engelbrecht et al., 2007). The entrained flow gasification technologies selected are reviewed with regards to the following aspects:

- Technical process description
- History – Pilot, demonstration and commercial plants
- Causes of outage at IGCC demonstration plants
- Potential improvements to the technology
- IGCC Reference Plant Design and modifications for CO_2 Capture

Details of IGCC technologies addressed by the three teams can be obtained from an EPRI report titled “Operating experience, risk, and market assessment of clean coal technologies”, report number 1014212. (Holt & Wheeldon, 2007).

It should be noted that IGCC technologies in most cases, differ in gasification technology and cycle configuration. The teams mentioned above, all focus on the entrained flow gasification based IGCC.

2.5.1. Entrained flow gasification based IGCC

2.5.1.1. GE Energy/Bechtel coal gasification technology

2.5.1.1.1. Process description

The GE Energy technology which was formerly known as Texaco gasification technology utilises entrained flow gasification whereby coal is mixed with water fed into a wet grinding mill for pulverisation. The pulverised slurry is then pumped into the entrained flow gasifier. At the same time, 95% pure oxygen from an air separation unit (ASU) is injected into the gasifier. The entrained flow gasifier used is a single stage, down flow and open refractory lined chamber. The syngas produced is mainly hydrogen, carbon monoxide, carbon dioxide

and water. From the gasifier the syngas enters a cooling stage where it is quickly cooled and/or quenched using one of three heat recovery schemes,

- Radiant plus convective design (R+C)
- Radiant only design (R)
- Total quench design (Q)

Figure 2.9 shows a GE Energy gasification process with radiant plus convective heat recovery coolers. The particulate free syngas is fed into a gas turbine for combustion and thereby producing electricity.

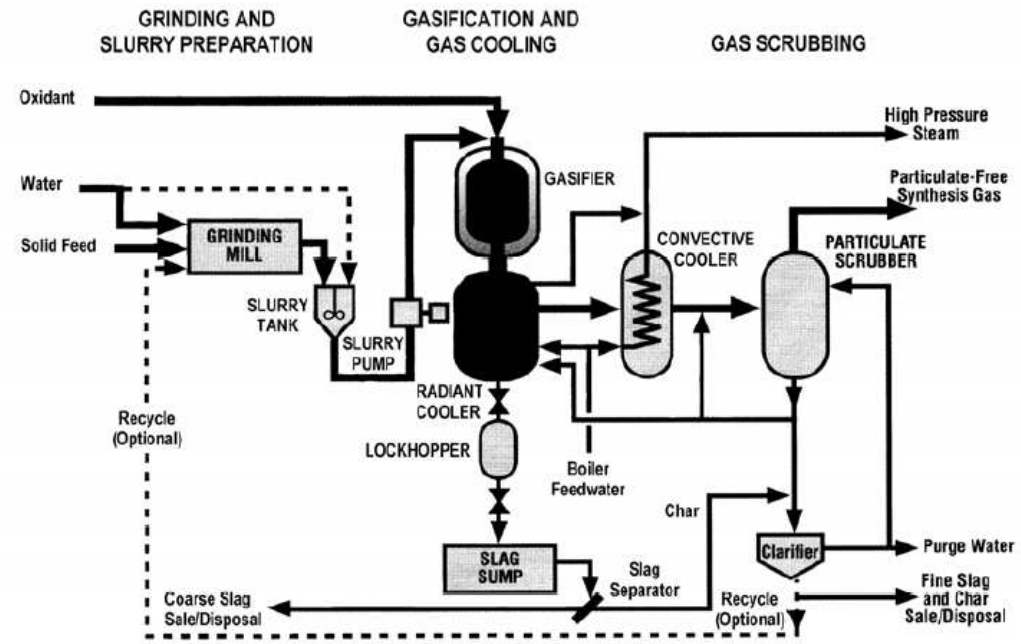


Figure 2.9: Schematic Diagram of the GE (Texaco) Gasification Process – Heat Recovery Mode (with Radiant and Convective Syngas Coolers) (Holt & Wheeldon, 2007)

The radiant plus convective design is configured in such a way that the radiant heat transfer water tube heat exchanger is below the gasification process. This allows for the flue gas from the gasifier to flow down to the radiant syngas cooler (SGC). Heat transfer occurs between the water in the tubes and the gas

passing through. Therefore high pressure steam is produced in the tubes. The slag from the radiant cooler is then collected into a water quench pool before it is removed from the quench vessel via a lock hoppers system for disposal or use afterwards. It is advisable to install a slag crusher before the lock hopper system to avoid blockage caused by large slag pieces (Holt & Wheeldon, 2007).

The radiant only design is configured in the same way as the radiant plus convective design except that both the raw gas and the slag are quenched in water. The slag and any unconverted char is then collected and removed through the lock hopper system. The wet syngas flows to a gas scrubber where particulate matter and chlorides are removed.

In the total quench design, the raw syngas flows straight to a water quench chamber and cooled to the desired temperature depending on the pressure and flow onto the gas scrubbing unit. This reduces the overall height of the structure that is usually brought about by the presence of a radiant syngas cooler. The quench design is illustrated in Figure 2.10 below.

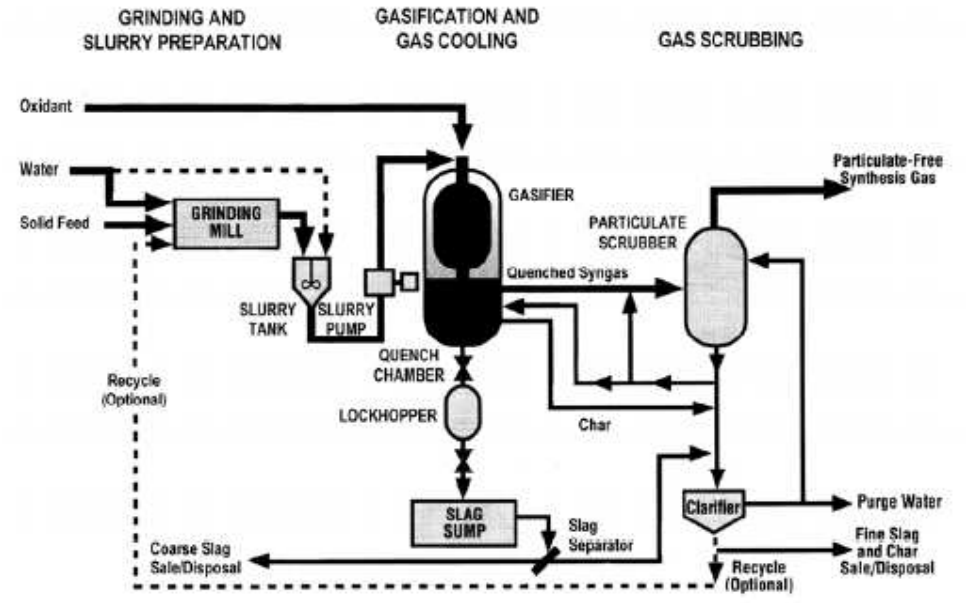


Figure 2.10: Schematic Diagram of the GE (Texaco) Gasification Process – Quench Mode (Holt & Wheeldon, 2007)

The slag sump collects the slag from the lock hoppers. The slag sump then discharges the slag into a separator that separates the coarse and fine slag. The coarse slag contains an insignificant amount of unconverted carbon and it is usually sold to, for example, cement industries. The fine slag contains some unconverted carbon and this is either sold or recycled back to the grinding mill going into the gasifier where the unconverted carbon can be gasified.

The gas is directed to the particulate scrubber where it is washed with water to remove any remaining fine particles of slag and unconverted char. The clean syngas can then be used for combustion in a gas turbine.

2.5.1.1.2. Comparison between the three heat recovery design configurations

Heat recovery configuration has a considerable influence on the overall heat integration or efficiency of the plant. The three heat recovery mechanisms discussed above were compared using same size gasifiers; it was found that the capital cost of the R+C and the R configuration are relatively expensive compared to the Q configuration. The net IGCC efficiency was found to be highest in the R+C design followed by the R design, with the Q design being the least (Holt & Wheeldon, 2007). This usually has an influence on the cost of electricity. The least expensive design usually has the least cost of electricity at the same capacity; in this case the Q design will imply low cost electricity. However, because of the high heat rate of the Q design, it might not be dispatched at the same capacity factor.

2.5.1.1.3. History of GE Energy coal gasification process – pilot, demonstration and commercial plants

In the 1940's, Texaco's first (now GE Energy) reactor was built for the partial oxidation of natural gas to syngas. This reactor was a refractory lined down flow reactor. The syngas was used for production of Fischer – Tropsch liquids. The

same reactor was used for the gasification of heavy oil fractions and for solids such as coal and petroleum coke in the form of slurry in water. Texaco built more than five gasification reactors between 1940 and 1984; however the first IGCC demonstration project was built in 1984, and was operated from 1984 to 1989 producing 100MW net output using a GE 7 E gas turbine with a 1000 ton/day gasifier and a radiant plus convective syngas cooler. This was built at the Southern California Edison Cool Water station near Daggett in California. The next IGCC plant with a Texaco gasifier was the Ube Ammonia for Ammonia production in Ube Japan which was built in 1985; it operated on four 500mt/d of coal/ petroleum coke Quench gasifiers. The Cool Water project was scaled up to a 250MW IGCC plant built for the Department of Energy (DOE) Clean Coal demonstration program for Tampa Electric, making use of a GE 7 FA gas turbine. It has been operating from 1996 to date. In 2007, GE Energy had sold 32 gasification licenses with 21 gasifiers fed on solid feedstock. The first license in China was issued in 1993. (Holt & Wheeldon, 2007).

2.5.1.1.4. Causes of outage at the GE IGCC demonstration plants

Table 2.3 summarises the causes of outages in the 250 MW Tampa IGCC plant. Increased solids in the recycle stream increased the corrosion/ erosion rate which impacted the mills. It was also observed that the use of coal water slurry fed gasifiers tends to decrease the fuel injector tip life, leading to a typical 60 days life which is lower compared to the dry coal fed gasifiers which is normally longer than a year. A hot restart technique was developed in order to recover the plant after minor trips, during which the injector was fully replaced. This has led to a great improvement of reduced forced outages that could have been caused by injector tip failures. This also improved the refractory life from about two years to approximately three years (Holt & Wheeldon, 2007).

Table 2.3: Summary of outage causes in the Tampa 250 MW IGCC plant (Holt & Wheeldon, 2007)

Outage Cause	Notes	Solution/Improvements
Coal Feeding	Minor	Spare pump may be justified
Rod Mills corrosion and rod failures	Problem with increased fines recycle to rod mill	pH control of recycle slurry
Fuel Injector Tip life	Typically 60 days	Hot restart capability has markedly reduced outage hours
Refractory wear	Historical Life ~ 2 years. Now ~3 years in 2006	Improves as plant matures with less temperature cycling. Improved refractories in development
Slag Tap blockage	Yes – often associated with changes in coal blend properties. No recent occurrence	More closely monitor coal slag properties .Install slag crusher below gasifier wet slag outlet
Corrosion/erosion in Circulating Slag water	Yes	Long radius bends. pH control. Minimize chloride content in circulating water
Syngas Cooler fouling and corrosion	Radiant – No Convective – Yes Gas/Gas - Yes	Eliminate gas/gas exchangers. Fouling of Convective firetube cooler has been a significant cause of outage. New GE commercial design is for Radiant only configuration.
Corrosion/Erosion downstream of carbon scrubber	Entrainment of wet particulates	Redesign of top of carbon scrubber and material changes.
AGR Solvent fouling	Initially Yes	Installation of Ion exchange system for removal of heat stable salts (HSS) has largely eliminated the problem
Gas turbine	CT & ST Insulation migration 320/03. Rotor crack 9/2003. CT compressor wreck 1/2005.	All three failures were due to fleet problems with this vintage of 7 FA gas turbines and are not associated with the syngas IGCC application. Ongoing problems require inspection of compressor every 1600 hours.

All possible causes that were identified were addressed and the recommendations were then used for IGCC plants that were in the construction stage and future IGCC plant designs. The issue of erosion/ corrosion alone requires careful consideration and the planning for mitigation techniques, because more than 40% of the outages were connected in one way or another to impacting coal particles (Holt & Wheeldon, 2007).

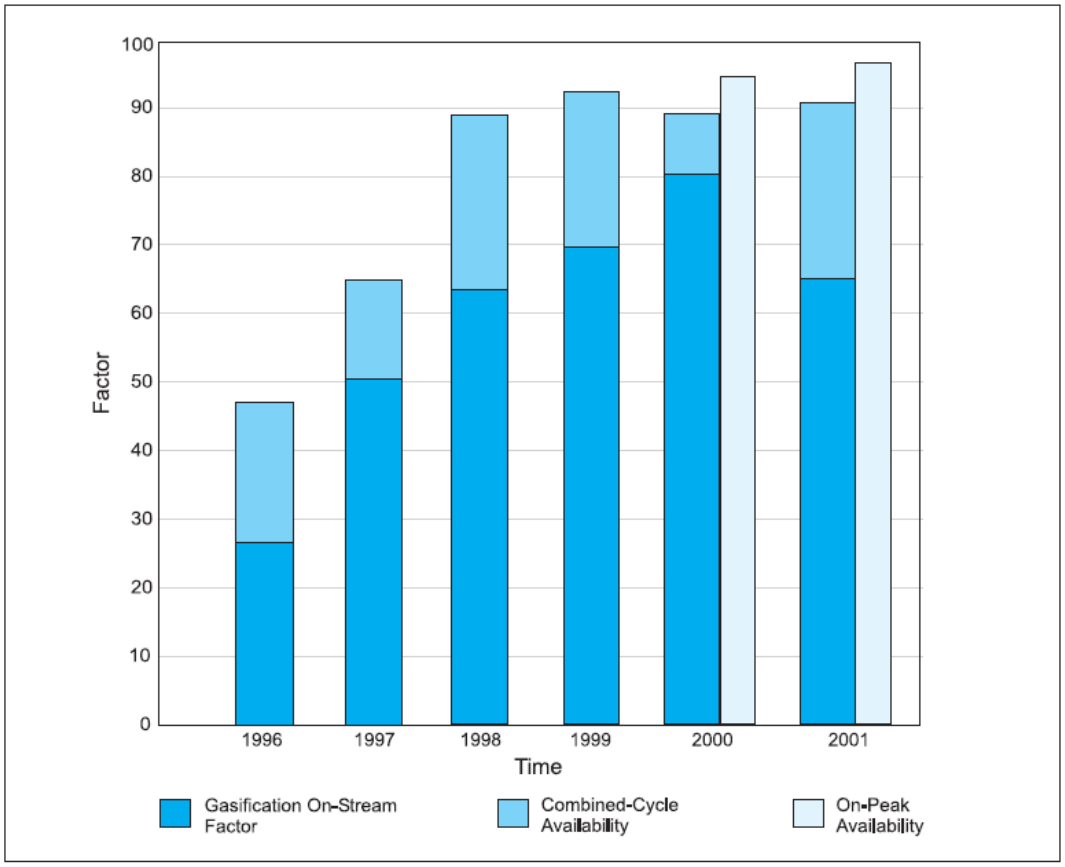


Figure 2.11: Availability of the Tampa IGCC plant (Tampa Electric Company, 2004)

Figure 2.11 shows the availability factor, which is the percentage of time the gasifier and associated systems were available for operation over the total number of hours in the year of operation – 8,760 hours except for leap year (2000) and the partial operating period of 1996. The combined cycle power block was available for about 90% of the time from 1998 to 2001. The on-peak availability during the summer months was over 90% in the year 2000 and 2001 (Tampa Electric Company 2004).

The GE technology is suited for bituminous coals and petroleum coke and is able to achieve water slurry loading of 60 – 65 weight % dry solids. This is dependent in the moisture and ash content in the coal. If these are high, the oxygen consumption can increase and therefore reduces the gasifier efficiency (Holt & Wheeldon, 2007).

Table 2.4 presents the improvements proposed for the GE technology. The most notable improvements are the use of low cost non fouling convective syngas coolers that will result in reduced capital costs and improve the availability and efficiency of plant. It was also proposed that the replacement of the carbon scrubber with hot gas filter will reduce the operating and maintenance costs and improve availability. The improvement of plant availability and efficiency increases the attractiveness of the technology in the market.

Table 2.4: Suggested improvements to the GE (Holt et al., 2007)

Improvement Description	Impact on Product Cost or COE
New coal feeder with less water injected to gasifier (e.g. Stamet pump for as received coal, flash dryer, Coal in CO_2)	Reduced Oxygen consumption and higher efficiency with PRB and Lignites
Longer injector life. Improved tip cooling.	Reduced outage time
Larger gasifier sizes – particularly for Quench	Match gas turbine fuel needs. Achieve economies of scale in all applications.
Longer life refractory or replace with a cooled membrane wall.	Markedly reduced outage time
Eliminate slag lock hoppers and replace with continuous slag removal system	Reduces height with savings in structural costs. Reduces O&M costs
Improved per pass carbon conversion in the gasifier without increase in operating temperature. Possibly improved injector, multiple injectors and different gasifier dimensions with longer residence time.	Reduced oxygen consumption through reduced fine slag recycle.
Lower cost syngas coolers. More use of platens. Height reduction. Water tube designs are more expensive than fire tube designs.	Reduced capital cost
Non fouling convective syngas coolers.	Improved efficiency and availability
Replace the carbon scrubber with hot gas filter.	Reduce O&M expense. Improve availability.
Warm gas clean-up for sulfur removal	Improved efficiency

2.5.1.1.5. GE Energy/Bechtel IGCC Reference Plant Design for Power Industry

The GE Energy IGCC reference plant is fed on US bituminous coals and uses oxygen as the gasification agent. This plant contains two gas turbines and a steam turbine. The process units in the plant design include the following (Holt & Wheeldon, 2007):

- Slurry preparation (2) and pumping (2)
- Air separation units (2)
- Gasification, radiant cooler (R), water scrubbing, coarse slag handling (2)
- Low temperature gas Cooling (2)
- COS Hydrolysis, Mercury Removal, acid gas removal (AGR) (2)
- Claus plant (2) TGTU(1) or Hydrogenation and Recycle to Selexol (physical solvent)
- Combined Cycle (2 GE 7 FB, 2 HRSG, 1 ST)
- Plot space left for addition of CO_2 capture

The GE reference plant (Illinois basin) performance was estimated at ISO conditions (20˚C and 101.3 kPa) and zero feet elevation at efficiency of 38.5% to 40% to give:

- Coal Feed 4873 megatonne/d (5372 st/d) dry
- Oxygen 4445 megatonne/d (4894 st/d) pure

Plant Power Output MW

- Gas Turbines 464
- Steam Turbine 301
- Total Gross 765
- Aux Power 135
- Net Power 630
- Heat Rate 9250 kJ/kWh (8845 Btu/kWh) HHV

2.5.1.2. Shell/Uhde/Black & Veatch coal gasification technology

2.5.1.2.1. Process description

The Shell technology utilises a dry coal fed oxygen blown entrained flow gasifier, where the raw coal is dried, ground and pressurised in two lock hoppers each being fed into the two horizontally opposite fuel injectors. A high pressure ASU produces 95% pure oxygen which is injected into the gasifier.

The gasification takes place at a temperature of about 1500-1600˚C and a pressure of up to 40 barg. Steam can also be used as a gasification agent replacing a small amount of oxygen depending on the reactivity of oxygen. The gasification temperature is made high enough to melt the coal ashes which are removed as slag at the bottom of the gasifiers, however some of the ash is carried over as fly ash or fly slag.

The gasifier used is a vertical cylindrical pressure vessel that contains tubes with steam providing cooling necessary to prevent overheating of the vessel. The syngas produced is mainly carbon monoxide and hydrogen. The syngas produced is quenched by the recycled syngas to ensure that the fly slag is molten before entering the cooling stage (Holt & Wheeldon, 2007).

The heating value of the cooled syngas is about 80% of the heating value of coal fed. This is generally higher than the syngas heating value from coal/water slurry fed systems. The steam generated is about 16 – 18% of the heating value in the coal fed; this is lower when compared to slurry fed system (Holt & Wheeldon, 2007).

The syngas is cooled further in an economiser to separate the fly slag which is then removed. After the fly slag removal, part of the “solids free” gas is compressed and recycled to the top of the gasifier to quench the raw syngas. The rest is sent to a scrubber to remove halogens and any water soluble components, thereafter sent to the gas cleaning stage. This is illustrated in figure 2.12 below.

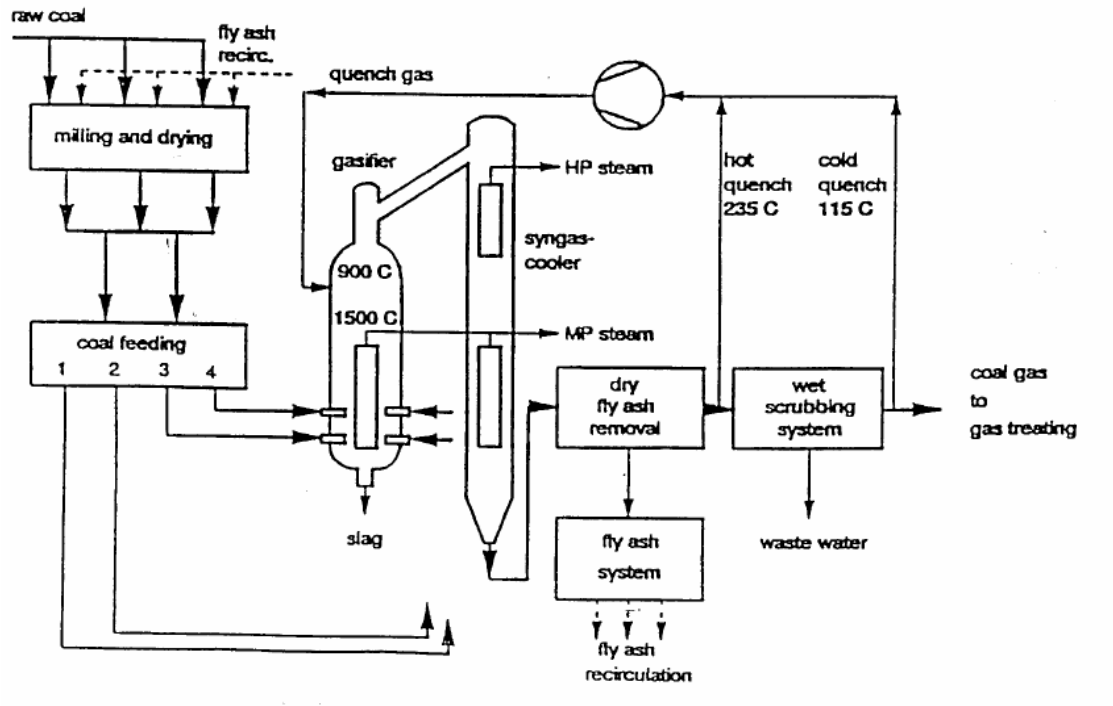


Figure 2.12: Schematic diagram of the Shell gasification process

In September 2007, Shell introduced a partial quench design that eliminates the syngas cooler, this would results in low capital costs for the gasification process unit and allow for carbon capture readiness.

2.5.1.2.2. History of Shell coal gasification process – pilot, demonstration and commercial plants

Shell started as a heavy oil gasification company in the late 1950's to 1960's and licensed many units around the world. The development of a solid fuel gasifier started in the 1970's. It then built a 6 ton/day process development unit in 1976 at the Royal Dutch Shell's Amsterdam laboratories which operated for 20 years. A 150 ton/day unit situated in Deutsche Shell's Harburg refinery followed after agreement for a joint development between Shell and Koppers, this operated for three years from 1979. The partnership ended shortly after the tests were concluded when Krupp took over Koppers. Shell then continued to

build a 250 ton/day advanced coal gasification facility that operated for five years from 1987 on a wide variety of coals in their refinery in Deer park, Texas. Krupp-Koppers also built a 60 ton/day pilot plant which had similar features as the Shell process. This was situated at Furstenhausen in Germany and was called Prenflo technology. It operated for four years from 1988. Both these plants were scaled up to commercial size in the 1990's. Uhde later joined with Krupp to develop and market the Prenflo technology (Holt & Wheeldon, 2007).

The Shell technology was adopted by Nuon's Buggenum 253 MW IGCC plant in the Netherlands. This was originally owned by a consortium of Dutch power companies called Demkolec. The operation started in December 1993 with a variety of international merchant coals and coal blends. Biomass has also been gasified with the coal feed (Holt & Wheeldon, 2007).

The Prenflo technology was adopted by the ELCOGAS European consortium for the 300 MW IGCC plant at Puertollano in Spain. The operation of this plant started in 1998 with Spanish coal and petroleum coke (Holt & Wheeldon, 2007).

The Shell and Prenflo technologies combined in 2002 to be called Shell coal gasification technology. Black & Veatch joined the Shell/Krupp Uhde team for the US market (Holt & Wheeldon, 2007).

2.5.1.2.3. Causes of outage at the Shell IGCC demonstration plants

Table 2.5 summarises the causes of outages in the 250 MW Shell IGCC plant at Buggenum in the Netherlands and the 300 MW plant at Puertollano in Spain. The solutions and improvements to the current problems have also been listed. The two plants experienced problems with slag tap blockage which was mostly associated with coal blends at the Buggenum plant; however this was associated with membrane leaks at the Puertollano plant. The slag tap blockage has nevertheless reduced for the Buggenum plant. At Puertollano,

there are developments to improve the boiler feed water distribution and control of water quality chemistry to mitigate this problem (Holt & Wheeldon, 2007)

Table 2.5: Historical causes of outages in the Buggenum and Puertollano IGCC plants (Holt & Wheeldon, 2007)

Outage Cause	Notes	Solution/Improvements
Coal Feeding	Minor. At Puertollano some mixing and grinding issues with variable feedstocks	Avoid cold temperatures and condensation
Fuel Injector Tip life	>20,000 hours	Life is satisfactory
Leaks in the membrane wall	Minor at Buggenum. BFW distribution and chemistry at Puertollano.	Time to repair minimized. Cool down accomplished quickly in the absence of thick refractory.
Slag fines	Initially higher than design	Added decanter and Vacuum filter to capture fines for recycle. Adjust injectors to produce less bottom slag fines
Slag Tap blockage	Initially at Buggenum– often associated with changes in coal blend properties. Less so more recently. At Puertollano cause was membrane leaks.	More closely monitor coal slag properties. Use of flame monitors. Install slag crusher below gasifier wet slag outlet. At Puertollano better BFW distribution and water quality chemistry control.
Heat skirt failure below slag tap	Problem at Buggenum. No heat skirt at Puertollano	Substitute cooled membrane wall for the refractory lined skirt
Corrosion/erosion in Circulating Slag water	Yes	Long radius bends. pH control. Minimize chloride content in circulating water. Improved materials
Syngas Cooler fouling and corrosion	Minor. Rappers have generally worked well. Increase of fouling with some biomass	Increase rapping frequency. At Puertollano increase gas velocity and improve flow distribution
Corrosion/Erosion of water scrubber and downstream	Entrainment	Monitor pH in Scrubber. Material changes
AGR Solvent fouling	Sulfinol thermal degradation. Initially fouling at Puertollano due to formic and oxalic acid formation in COS hydrolysis	Periodic Vacuum distillation of Sulfinol. Installation of ion exchange on MDEA blowdown.
Gas turbine	Vibration and overheating of burners.	Alternate control system and burner designs at both locations.

There has been minor syngas cooler fouling and corrosion at both plants, this was found to increase with some biomass. The rappers were found to work well in mitigating this problem and therefore the frequency of rapping was increased to mitigate the effects of syngas on the syngas cooler. The pH in the scrubber was monitored and some material changes were made to reduce the corrosion/erosion of water scrubber and downstream components. In 2004 and 2005, fault in the gas turbine main transformer was the main cause of outages (Holt & Wheeldon, 2007).

Table 2.6 shows the potential improvements to the Shell technology. The most notable improvements are the use of lower energy consumption drying technology like RWE MVC (Mechanical Vapour Compression) for high moisture coals which reduces the auxiliary power consumed and thereby leading to better cycle efficiency and low cost of electricity (Holt & Wheeldon, 2007).

Table 2.6: Potential improvements to the Shell gasification technology

Improvement Description	Impact on Product Cost or COE
New coal feeder (e.g. .flash dryer, Coal in CO_2, new as received coal feeder). Enable feed with higher moisture content	Eliminate cost of lock hoppers. Use less conveying gas? Better overall efficiency
Improved lower energy consumption drying technology. E.g. RWE MVC (Mechanical Vapor Compression)	Better efficiency. Lower COE
For synthesis or capture use CO_2 as the feed conveying gas rather than Nitrogen. CO_2 is a reactant whereas Nitrogen is inert	Less inert gas taking up vessel volume in downstream equipment or the synthesis loop. Improved economics.
Higher throughput gasifier. Shell claims a single gasifier could supply two 7 FB gas turbines	Reduced capital cost
Add a second stage to the gasifier.	Reduced oxygen consumption and SGC duty.
Eliminate slag lock hoppers and replace with continuous slag removal system	Reduces height with savings in structural costs. Reduces O&M costs
Lower cost firetube syngas cooler. Water tube designs are more expensive than fire tube designs. Raise 50 bar steam instead of 130 bar.	Reduced capital cost
For hydrogen production or CO_2 capture use partial water quench to 400°C (750°F) and eliminate the recycle gas compressor and the syngas cooler	Marked reduction in capital. Least expensive manner of providing moisture for the shift reaction. Shell now offers partial quench without the syngas cooler but with retention of the syngas recycle for initial gasifier quench
Increase temperature for hot gas filter to 400°C (750°F) for above capture applications	See note above re- CO_2 capture and partial quench design.
Warm gas clean-up for sulfur removal	Improved efficiency

High pressure lock hoppers are costly and become less efficient with increase in pressure since this requires more nitrogen per ton of coal. High pressure feed system is advantageous for CO_2 capturing. In cases where CO_2 is produced as part of the overall process, it can be utilised to convey the gas replacing nitrogen, thereby reducing the volume taken up by the inert gas in downstream equipment.

The syngas cooler and compressor can be eliminated with use of water quench to 400 ˚C and by recycling the syngas. This results in significant cost savings.

Another potential improvement is the use of large gasifiers where one gasifier supplies two 300 MW gas turbines or two gasifiers supply three 300 MW gas turbines which can substantially reduce capital costs (Holt & Wheeldon, 2007).

2.5.1.2.4. Shell IGCC Reference Plant Design for Power Industry

The Shell IGCC reference plant is fed on German lignite and Powder River basin (PRB) coals and uses oxygen as the gasification agent. This plant contains two gas turbines and a steam turbine. The process units in the plant design without carbon capture can be summarised below (Holt & Wheeldon, 2007):

The configuration of the reference Shell IGCC plant for the 60 Hz market without capture can be summarized as:

- Coal Handling (1x100% + 2x 100% conveyors)
- Coal Milling & Drying (3 x 50%)
- Coal Pneumatic Feed Systems (2x 50%)
- Air Separation Units (2x50%) Some Extraction Air from CT Compressor (%?)
- Gasification, Syngas Cooler, Cyclone, Char Filter (2x50%).
- Slag handling (1x100%)
- Low Temperature Gas Cooling (2x 50%)

- COS Hydrolysis, Mercury Removal, Sulfinol M (or other) Acid Gas Removal (2 x 50%)
- Claus Plant (2x66%) Claus Tail Gas Recycle to Sulfinol
- Combined Cycle (2 x STG6-5000F or 2 x GE 7 FB, 2 HRSG, 1 ST (1800 psig/1050F/1050F))
- Net Output ~ 600 MW
- Plot Space left for Addition of CO_2 Capture

The heat rate for the 53% moisture German lignite coal with MVC drying of up to 12% moisture was estimated at 8540 kJ/kWh and that of 30% PRB coal with drying of up to 6% moisture was estimated at 8650 kJ/kWh) on a High Heating Value (HHV) basis.

2.5.2. Fixed/moving bed gasification based IGCC – Vresova

The vresova gasification plant originally produced city gas with an installed capacity of 240,000 m^3 of crude gas from the local brown coal. The production of city gas continued until 1996 after which it was replaced by natural gas from Russia. This gasification plant was then converted to an IGCC plant by installing two 200 MWe gas turbines to two of its units (Mills, 2006).

The gas works of the Vresova IGCC plant in the Czech Republic was originally owned by Sololovska Uhelna (SUAS). This is based on the Lurgi dry ash gasification process, which is a moving bed gasification technology. A mixture of steam and oxygen moves counter current to the flow of coal which descends slowly towards the base of the reactor where ash is discharged. The brown coal is fired into the reactor in particles of 10 – 30mm at a pressure of 2.5 – 2.8 MPa. The syngas exits at a temperature of 200℃ and is then cooled to 30℃. This plant was fed on about 2000t/d of coal and can produce about 4,700,000m^3/day of syngas. The syngas is cleaned and fed into the two units that operate on supercritical steam conditions supplied by Alstom. These two units (1&2) were commissioned in 1995 and 1996 respectively. About 70% of the electricity is produced from a gas turbine and the rest from a steam turbine. The Send out

electricity on each unit is about 185 MWe; the gas turbine produces about 128 MWe and the steam turbine produces about 57 MWe (Mills, 2006).

The gasification reactor is a fixed bed with temperatures highest at the inlet of the gas to the reactor where the ash exits. This is because as the gas moves counter flow through the reactor, the temperature decreases as it comes to contact with the coal flowing downwards. This technology allows for considerable amount of hydrocarbons to be carried out of the reactor with the gas, therefore cleaning is necessary. (Bucko et al., 2000)

This plant consists of 26 fixed bed gasifiers. In addition to the syngas produced, forced by-products were also produced; these are specifically, 90,000 tons of char, 12,000 tons of phenol concentrates, 10,000 tons of ammonia and 8,000 tons of sulphuric acid yearly. (Bucko et al., 2000) and therefore all this requires treatment or cleaning. Hence, this plant is equipped with gas cleaning equipment including rectisol, gas desulphurisation, dephenolation and deammoniation of waste gas works water.

This plant is also coupled with a SNO_X combined control system for the control of nitrogen oxides (NO_X) and sulphur dioxide (SO_2) emissions. The SNO_X principle is based on the SCR followed by the catalytic oxidation of SO_2 to sulphur trioxide (SO_3). This system was provided by Haldor Topsoe A/S in 1993. (Mills, 2006)

The high operating and maintenance costs, low conversion efficiency, lack of fuel flexibility, limited capacity for load regulation and a significant impact on local environment (producing cancerous by-products) of the Vresova plant have opened up opportunities for improvement in economic and environmental performance (Mills, 2006). SUAS and several technology suppliers undertook studies into alternative systems to improve the performance and concluded that the most cost effective option to mitigate these concerns was to replace the existing gasification technology with High Temperature Winkler (HTW) fluidised bed gasification technology. The temperature would increase to up to 1000 ℃ thereby improving the carbon burn out/ conversion to about 93% (Mills, 2006).

The impact of the HTW fluidised bed gasification technology was estimated over a 20 year period and is illustrated in figure 2.13. The emissions of NO_X, SO_2 and particulate matter would be significantly reduced. The SO_2 emissions would be reduced by close to 10,000kt. Natural gas has been used as a secondary fuel to optimise the final power output (Mills, 2006).

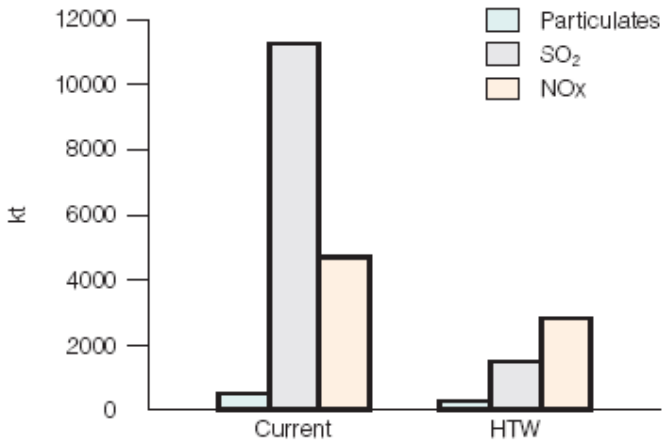


Figure 2.13: Annual emissions for vresova plant (kt) (**Mills, 2006**)

The possibility of co-firing brown coal with 10% biomass was also considered, in order to reduce the emission of CO_2. The impact that raises concerns with use of biomass for combustion/gasification process is the impact on the costs due to biomass preparation and the potential of slagging, fouling and corrosion of downstream components and processes (Klara, 2009).

2.5.3. Fluidised bed gasification based IGCC - High Temperature Winkler (HTW) Vresova IGCC plant, Czech Republic

The HTW Vresova IGCC plant was integrated into the fixed bed Vresova plant discussed in section 2.5.2. This consists of two units as already mentioned each producing close to 200MWe. The syngas is produced from the pressure gas work that was built in 1970 for the Lurgi fixed bed process. The HTW process has a total raw syngas capacity of 2 X 120 000 Nm^3/h. This process avoids the production of by-products compared to the fixed bed technology that produced by-products, so more carbon was converted from to gas.

The HTW was built with the following goals (Bucko et al., 2000):

- To significantly reduce the emissions of CO_2 and other pollutants.
- To improve ecological conditions by reducing the production, storage and distribution of by-products from gasification.
- To improve the economic status of the plant, by improving production, reducing the reproduction of obsolete fixed assets that continuously required repairs and material, and reduction of charges imposed due to impacts on the environment by the plant.
- To remove ineffective technological processes that will not benefit the new fluidised bed gasifiers and optimize the ones that will improve the new process.
- To increase profits from the sales of electricity generated from the low quality coal used in gasification.
- To use the new technology as a demonstration project for possible commercial application in the context of clean coal technologies for power generation utilising low quality coal.

The HTW technology involves feeding pulverised coal into a continuous fluidised bed of particles of ash, semi-coke, and coal. The ash is continuously removed from the bottom of the reactor. This gasification process has the

advantage of being able to utilise different quality coals as well as biomass. The generated gas is low in hydrocarbons such as tar, phenols, and other heavy and substituted aromatics as the outlet temperature is about 900 - 1100˚C. (Bucko et al., 2000). The fluidised bed reactor is characterised by good mixing of coal particles and gasification agents, high reactor temperatures and high conversion of carbon.

2.6. Gas turbine Operation

2.6.1. Gas turbine overview

Gas turbines are internal combustion engines that operate with rotary motion instead of reciprocating motion. Gas turbines consist of three main components, namely the compressor, the combustion chamber and the turbine. The compressor compresses air or oxygen into the combustion chamber, where fuel is also introduced and combustion occurs. The gases produced in the combustion chamber are then transferred to the turbine to drive the turbine blades for power generation. Figure 2.14 shows the main sections of a gas turbine.

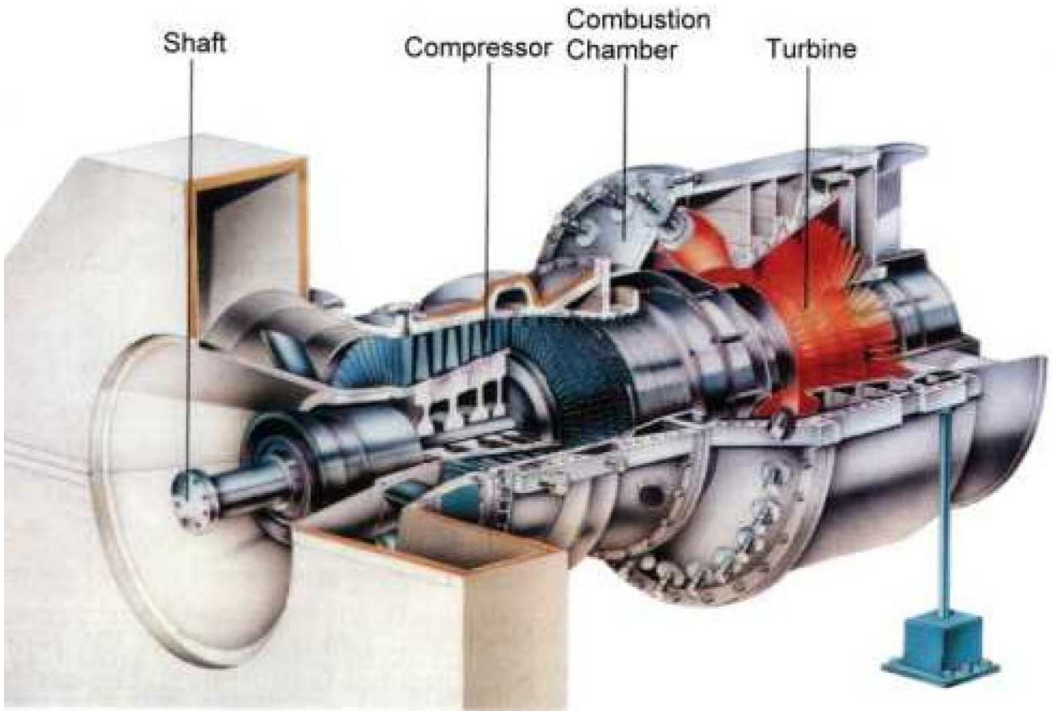


Figure 2.14: Three main sections of a gas turbine (Wartsila.com, 2013)

These sections can be illustrated in a simple cycle shown in figure 2.15; the exhaust gas is then emitted to the atmosphere.

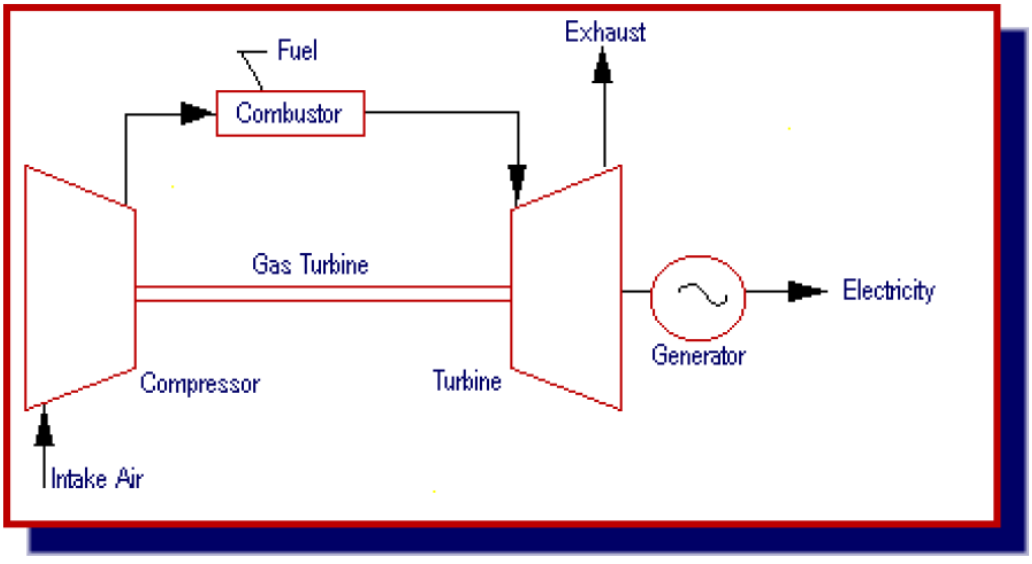


Figure 2.15: Simple cycle gas turbine (cogeneration.net)

The IGCC technology uses a combined cycle technology. For a combined cycle the exhaust gas from the gas turbine is sent to a heat recovery steam generator (HRSG), where steam is generated and sent to a steam turbine to generate more power. Figure 2.16 shows an example of a combined cycle gas turbine. The waste heat boiler shown generates steam by utilising energy from the gas turbine exhaust gas.

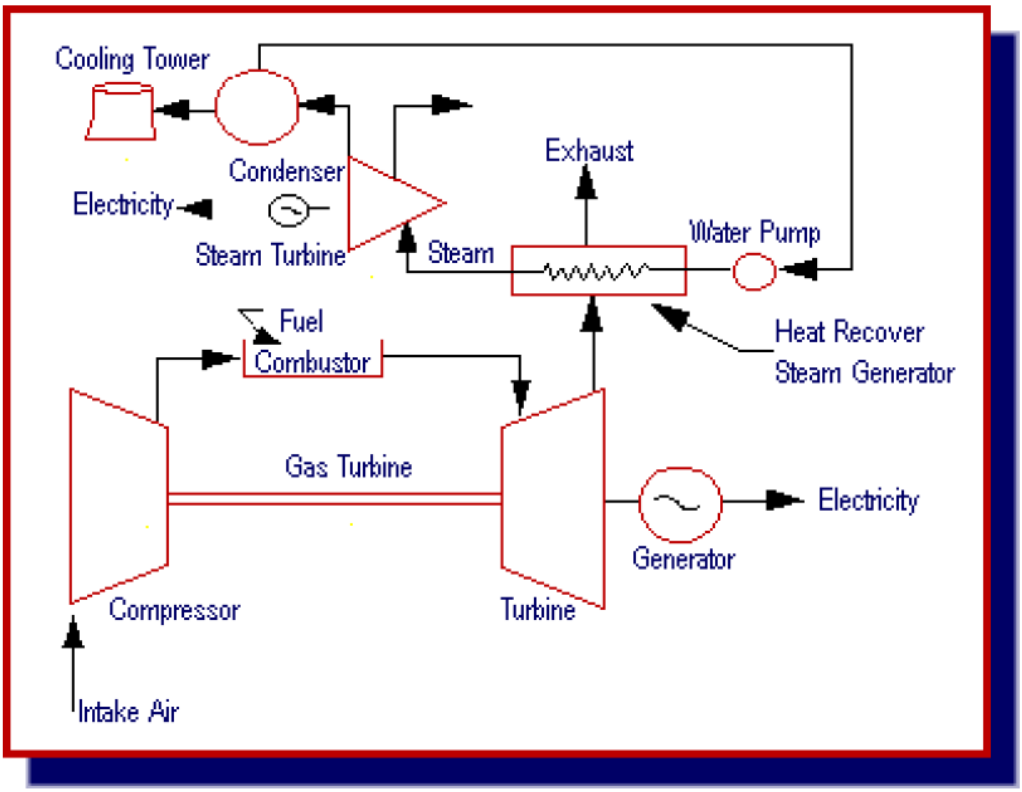


Figure 2.16: Combined cycle gas turbine (cogeneration.net)

The gas turbine offers the following advantages over other combustion engines:

- Low vibration
- High reliability
- No requirement for cooling water
- Suitability for remote operation
- Lower capital costs than reciprocating engines

- Lower capital costs than boiler/ steam turbine based electric power generating plants (US Emission standards division, 1993)

2.6.2. Emissions from gas turbines in an IGCC process

One of the key drivers in the implementation of the IGCC technology is the potential for relatively low emissions. The US environmental protection agency has stipulated the following air pollutants formed from the gasification of coal and other carbonaceous fuels: SO_2, NO_X, Particulates, CO and lead. Lead may be a result of lead containing fuel. These other pollutants are formed when the syngas is combusted in a gas turbine based on the constituents of the syngas and air. (Ratafia-Brown et al., 2002).

Table 2.7 gives an overview of the US Commercial IGCC facilities. The IGCC plants presented in this table use oxygen as an oxidant. This has a beneficial impact on the emissions as will be illustrated in the emission calculations.

Table 2.7: Overview of US. Commercial IGCC facilities (Ratafia-Brown et al., 2002).

	Polk Power Station[2]	Wabash River Generating Station[1]	Louisiana Gasification Technology Inc.[3]	Cool Water Gasification Plant[4,5]
Net Power Generation Capacity (MWe)	250	262	160	96
Coal Type	High Sulfur Bituminous	High Sulfur Bituminous	Low Sulfur Subbituminous	Bituminous
Gasification Process Type/Fuel Feed	Texaco Single-Stage Entrained-Bed/ Slurry Fed	E-Gas Two-Stage Entrained-Bed/ Slurry Fed	E-Gas Two-Stage Entrained-Bed/ Slurry Fed	Texaco Single-Stage Entrained-Bed/ Slurry Fed
Oxidant	95% Pure Oxygen	95% Pure Oxygen	95% Pure Oxygen	99.5% Pure Oxygen
Gas Cleanup System Type	Low-Temperature	Low-Temperature	Low-Temperature	Low-Temperature
Particulate Control	Water Scrubber	Metallic Candle Filter System and Water Scrubber	Water Scrubber	Water Scrubber
Acid Gas Cleanup/ Sulfur By-product	Amine Scrubber and H_2SO_4 Plant/Sulfuric Acid	Selectamine™ Scrubber and Claus Plant/ Sulfur	Selectamine™ Scrubber and Selectox™ Plant/ Sulfur	Selexol Absorber
Sulfur Recovery Capability	98% Design	99% Design	85% Design	>97%
NOx Control	Nitrogen and Steam Dilution to Combustion Turbine	Steam Dilution to Combustion Turbine	Steam Dilution to Combustion Turbine	Steam Dilution to Combustion Turbine
Ammonia Control	Water Scrubber	Water Scrubber	Water Scrubber	Water Scrubber
Chloride/ Fluoride Control	Water Scrubber	Water Scrubber	Water Scrubber	Water Scrubber

The sulphur removal capability can go up to 99%. A water scrubber is used for the removal of both ammonia and chlorides/fluorides. Table 2.8 presents the expected emission levels of criteria pollutants (NO_x, SO_x, CO & PM10). The pollutants are below the US Federal New Source Performance Standards (NSPS) for pulverised coal-fired power plants.

Table 2.8: IGCC expected emission levels of criteria pollutants (Ratafia-Brown et al., 2002).

CRITERIA POLLUTANT	EXPECTED IGCC EMISSION LEVELS lb/10^6 Btu (lb/MWh)	NSPS LIMIT lb/10^6 Btu (lb/MWh)
SO_2	< 0.15 (0.5)	1.2 (None)
NOx	< 0.1 (1)	0.15 (1.6)
PM10	< 0.015 (0.14)	0.03 (None)
CO	< 0.033 (0.3)	None (None)

None – these limits were not specified

The South African government under the department of environmental affairs has published the minimum emission standard which stipulates the allowable limits for gaseous emissions and particulate matter. The notice for these limits took effect on the 1st of April 2010. (Government Gazette. Republic of South Africa, 2010). Table 2.9 presents the emission limits from gas combustion installations as stipulated in the South African emission standard at reference conditions of 3% O_2, 273 Kelvin and 101.3 kPa. This apply to gas combustion (including gas turbines burning natural gas) used primarily for steam raising or electricity generation, however, special arrangement for gas turbines reference conditions is stipulated as 15% O_2, 273 Kelvin and 101.3 kPa.

Table 2.9: Minimum emission standards for gas combustion installations (Government Gazette. Republic of South Africa, 2010).

Description:	Gas combustion (including gas turbines burning natural gas) used primarily for steam raising or electricity generation, except reciprocating engines.		
Application:	All installations with design capacity equal to or greater than 50 MW heat input per unit, based on the lower calorific value of the fuel used.		
Substance or mixture of substances		Plant status	mg/Nm^3 under normal conditions of 3% O_2, 273 Kelvin and 101.3 kPa.
Common name	Chemical symbol		
Particulate matter	NA	New	10
		Existing	10
Sulphur dioxide	SO_2	New	400
		Existing	500
Oxides of nitrogen	NO_X expressed as NO_2	New	50
		Existing	300

The following special arrangements shall apply –

i. Reference conditions for gas turbines shall be 15% O_2, 273 Kelvin and 101.3 kPa.

ii. The limit for sulphur dioxide for new installations using low-calorific value gases from coal or refinery waste gasification and coke production shall be 400 mg/Nm^3.

These limits are low when compared to the specified minimum emissions for pulverised coal-fired power plants. See Table 2.10, showing the limits for solid fuel combustion installations.

Table 2.10: Minimum emission standards for solid fuel combustion installations (Government Gazette. Republic of South Africa, 2010)

Description:	Solid fuels (excluding biomass) combustion installations used primarily for steam raising or electricity generation.		
Application:	All installations with design capacity equal to or greater than 50 MW heat input per unit, based on the lower calorific value of the fuel used.		
Substance or mixture of substances		Plant status	mg/Nm^3 under normal conditions of 10% O2, 273 Kelvin and 101.3 kPa.
Common name	Chemical symbol		
Particulate matter	NA	New	50
		Existing	100
Sulphur dioxide	SO_2	New	500
		Existing	3500
Oxides of nitrogen	NO_X expressed as NO_2	New	750
		Existing	1100

The following special arrangement shall apply –

i. Continuous emission monitoring of PM, SO_2 and NO_x is required

Sulphur dioxide emissions produced from gas turbines are usually not a problem because the synthesis gas is cleaned before it can be combusted. However nitrogen oxide emissions are influenced by the operating conditions in the gas turbine. High temperatures encourage formation of thermal NO_x. Gas turbine operations in IGCC technology can go up to 1700˚C (Barnes, 2011).

2.7. IGCC Technology cost summary

2.7.1. Lifecycle costs

There are currently no full commercial operations on coal IGCC plants for power generation globally, therefore most of the costs given are estimates based on the existing demonstration plants. There is more experience in the

entrained flow gasification based technologies than the fluidised bed and fixed bed gasification based IGCC technology. The cost of an IGCC plant differs with process components used. Therefore it is currently difficult to obtain costs that are representative of all coal based IGCC technologies. The limited operating and cost experience of IGCC technology is a barrier to IGCC penetration.

According to an article by the Energy Insider (Energy Insider, July 25 2006) in July 2006, a study was conducted by the state of Wisconsin that showed levelized lifecycle costs without carbon capture. For supercritical pulverised coal units the study showed a cost of 50 – 53 $/MWh and for IGCC units 57 – 60 $/MWh. The inclusion of carbon capture increases the supercritical pulverised coal costs to 82 – 88 $/MWh and those of IGCC to 75 – 78 $/MWh. Therefore IGCC is less expensive than supercritical pulverised coal with carbon capture. It is believed that IGCC has the potential to reduce costs in the long term due to high cycle efficiencies.

2.7.2. Comparison of costs from the EPRI March 2007 and the DOE NETL May 2007 reports (Booras et al., 2008)

The US Department Of Energy (DOE), National Energy Technology Laboratory has three teams working on the project of coal based IGCC. These technologies differ in terms of cycle configuration, process unit technology (e.g. different heat recovery systems) and therefore performance. The results of these technologies are usually reported as an average by the DOE.

The DOE used IGCC capture configurations with syngas coolers for the GE Energy and the ConocoPhillips (CoP) technologies, which is expensive when compared to the direct water quench cooling. The Shell technology used water quench design heat recovery system. The GE system is a high pressure system which gives it an advantage over the other two systems (CoP & Shell). The high pressure reduces the carbon capture and compression costs by use of a physical absorption system (Booras et al, 2008).

The assumptions and economic analysis methodology used differed, however one type of coal was used which is the Illinois #6 coal. Therefore the coal price and the energy input in terms of quality of coal is the same. The differences in the methodology used for economic analysis are as follows (Booras et al., 2008):

- DOE used a 20-year levelized cost of electricity (COE) whereas EPRI used a 30-year levelized COE.
- Delivered Coal Cost - DOE NETL used EIA annual energy outlook (AEO) forecasts of $1.80/MMBtu (2010 cost of coal in 2007 dollars) ($6.14/MWh) and real escalation rate = 0.48%/yr. EPRI assumed a transparent coal cost of $1.50/MMBtu (2006 dollars) ($5.12/MWh) with no real escalation
- CO2 Transportation & Sequestration Cost - DOE NETL varies by case ($3.75 to $4.80/mt CO2). EPRI assumed $10/mt CO2

The key financial assumptions are shown in Table 2.11. This suggests that more interest will be paid for the EPRI technology because the repayment term is longer when compared to the DOE low risk and the DOE high risk technology. The operating and maintenance levelizing factor for the EPRI technology is lower when compared to the DOE low risk and the DOE high risk technology and therefore this will result in lower Levelized Cost of Electricity (LCOE). This can be seen in figure 2.17 and figure 2.18 respectively.

Table 2.11: Key Financial Assumptions DOE NETL and EPRI Studies (*Booras et al., 2008*)

	DOE (Low Risk) PC without CCS	DOE (High Risk) All IGCC and PC with CCS	EPRI (IOU)
Debt % of Total	50	45	55
Cost of Debt, %/yr	9.0	11.0	6.5
Debt term, yrs	15	15	30
Equity % of Total	50	55	45
Return on Equity, %/yr	12	12	11.5
General Inflation Rate %	1.87	1.87	2
Effective Tax Rate %	38	38	39.2
Levelizing period, yrs	20	20	30
Capital Charge Factor	0.164	0.175	0.12 IGCC 0.117 PC
O&M Levelizing Factor	1.1618	1.1568	1.0

A comparison between the EPRI and DOE results is illustrated in figure 2.17 and figure 2.18. The total cost of plant is high for EPRI; however its levelized cost of electricity is low, due to assumptions made. Details of the results can be obtained from the "updated cost and performance estimates for clean coal technologies including CO_2 capture – 2007" (*Booras et al., 2008*).

The cost of plant depends on the different technologies used for the chosen components in the integrated cycle. This also has an effect on the operating costs which eventually determine the cost of electricity.

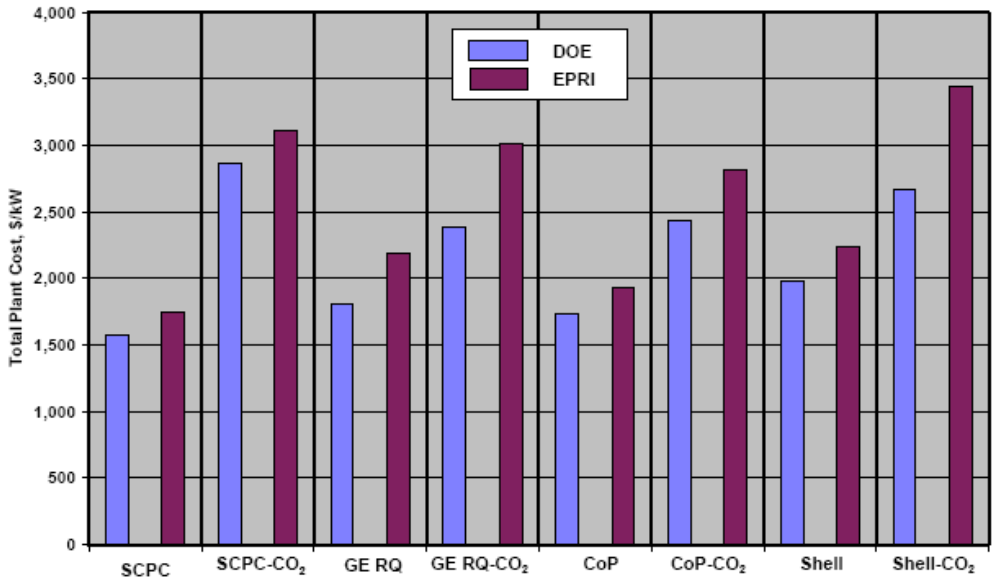


Figure 2.17: Comparison of EPRI and DOE Total Plant Costs TPC (*Booras et al., 2008*)

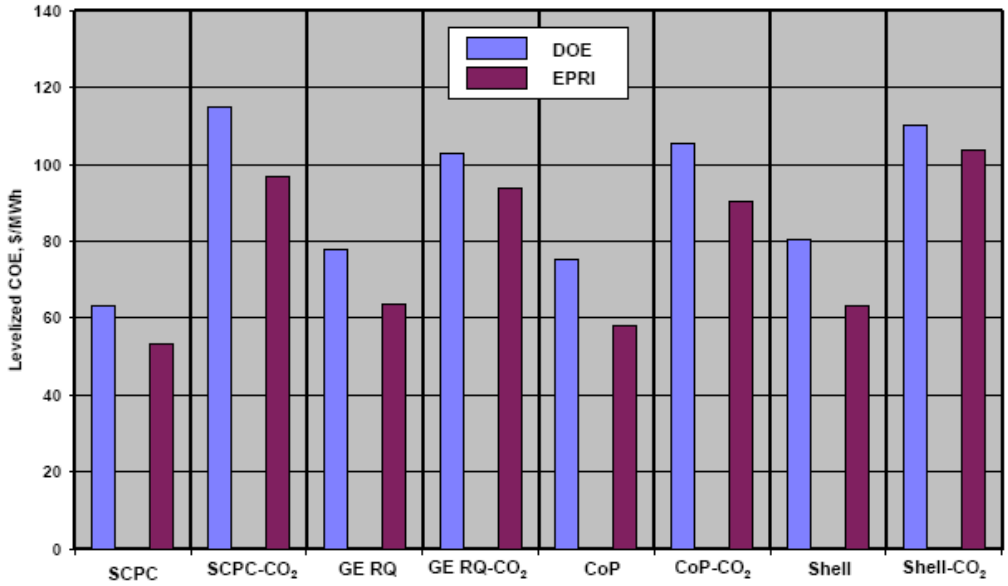


Figure 2.18: Comparison of EPRI and DOE Levelized Cost of Electricity (LCOE) (*Booras et al., 2008*)

2.8. Co-gasification with biomass

Coal can be co-gasified with biomass to reduce the emissions of carbon dioxide (CO_2) since the biomass is considered as almost CO_2 neutral (Henderson, 2008). plants absorb CO_2 from biological materials and it is general view that carbon emitted into the atmosphere from biological materials is carbon neutral. Co-firing with biomass may reduce the combustion or gasification efficiency due to particles with size 1000 µm not being gasified fast enough because of their potentially low reactivity and ending up in wall slag layer (Pruschek, 2000). The calorific value (CV) of biomass is relatively low compared to that of coal therefore more tonnage of the feedstock needs to be fed into the boiler in order to achieve the same electricity output. Commercial trials on co-gasification of coal and biomass have been conducted to determine the performance of biomass at an IGCC plant in Buggenum. It was found that biomass is fairly trouble free at mass percentage of up to 30% in the feed and a net CO_2 reduction of 20% has been realised in these trials. (Henderson, 2008).

An economic review should be conducted on biomass to determine the impact it has on the IGCC process in terms of reducing the electricity generated per ton of feedstock due to its low CV but no such data has been found in literature, this is beyond the scope of this review.

the general view has been that carbon emitted into the atmosphere from biological materials is carbon neutral

2.9. Status of gasification technology in the world

Coal remains the cheapest source of energy in the world. It is therefore not economically viable to forsake coal based power generation technologies. A favourable approach is to investigate clean coal technologies that can reduce the impact coal has on our planet. Interest in coal gasification has been renewed also due to the increasing oil and natural gas prices. As of 2010 the gasification syngas output capacity has grown to 70,817 megawatts thermal

(MW_{th}) at 144 operating plants with 412 gasifiers operating around the world. There are 11 plants with 17 gasifiers under construction, and 37 plants with 76 gasifiers are in the planning stages for operation by 2016. (U.S. DOE, 2010)

Figure 2.19 below illustrates the current status of gasification capacity in the world. Commercial operations are currently in 29 countries falling under the following regions: Africa/Middle east, Asia/Australia, Europe, North America and Central & South America/Caribbean (U.S. DOE, 2010).

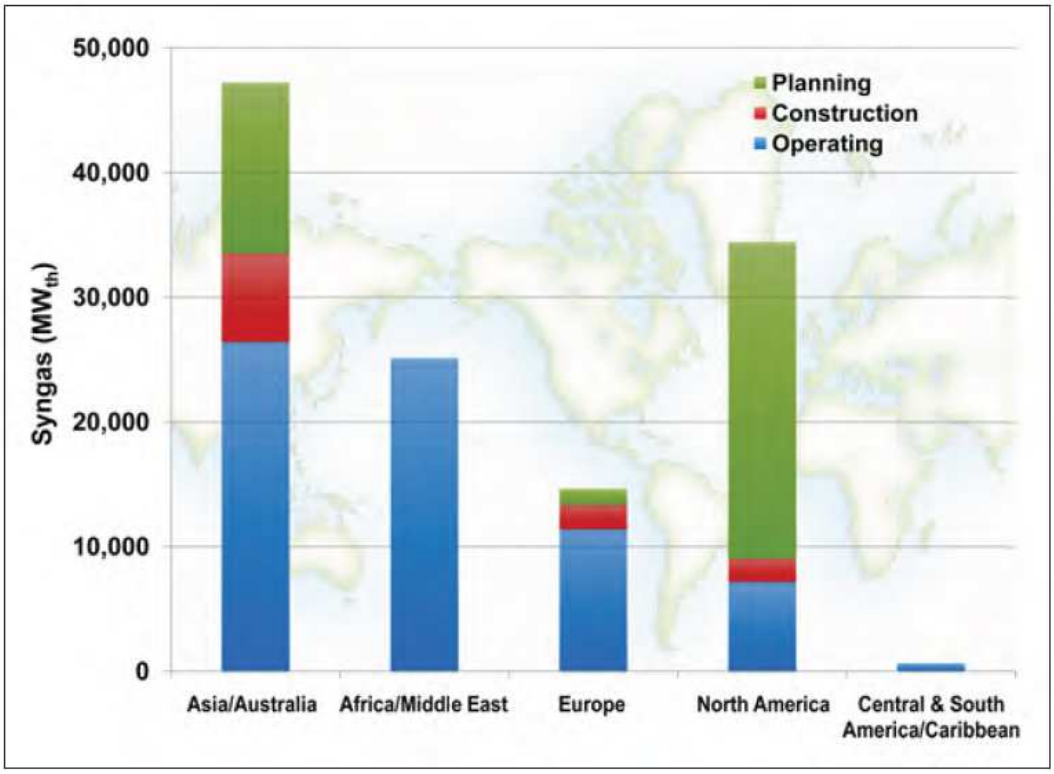


Figure 2.19: World gasification capacity and Planned growth (U.S. DOE, 2010)

Asia/Australia region is currently leading with 37% of the total operating capacity, 65% of the syngas capacity that is currently under construction and 63% of the total planned capacity growth (U.S. DOE, 2010). Africa/Middle East comes in second with the operating syngas capacity. The syngas capacity shown here is generally from all feedstock, and used for different purposes or products.

Figure 2.20 shows the 2010 operating world gasification capacity by feedstock. Coal is the dominating feedstock for gasification contributing 51% of the total syngas capacity on the operating plants and more than 70% on the planned syngas capacity. Petcoke accounts for the remaining planned syngas capacity (U.S. DOE, 2010).

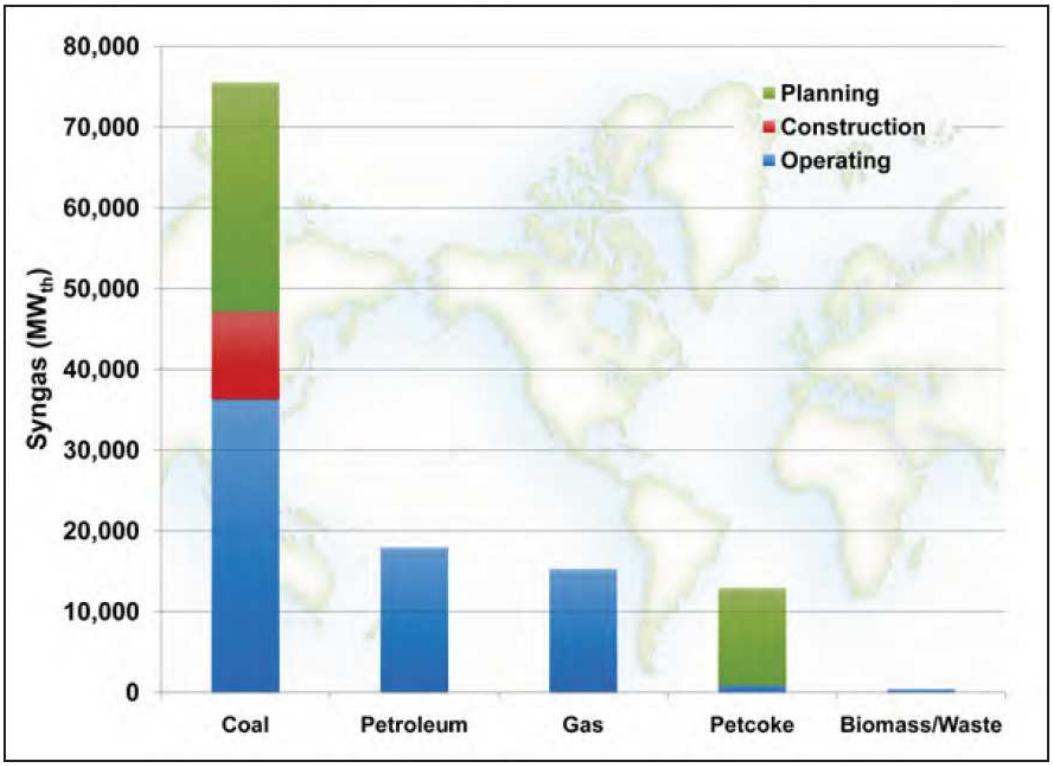


Figure 2.20: 2007 Operating World Gasification Capacities – By Feedstock and Product (U.S. DOE, 2010)

Figure 2.21 illustrates syngas capacity by product. Syngas used for power amounts to 11% of the current operating plants, 36% of the plants under construction and 38% of the planned plants. Gasification for the production of chemicals is currently dominating at 45% of the operating plants, however more plants are planned for syngas to generate power (U.S. DOE, 2010).

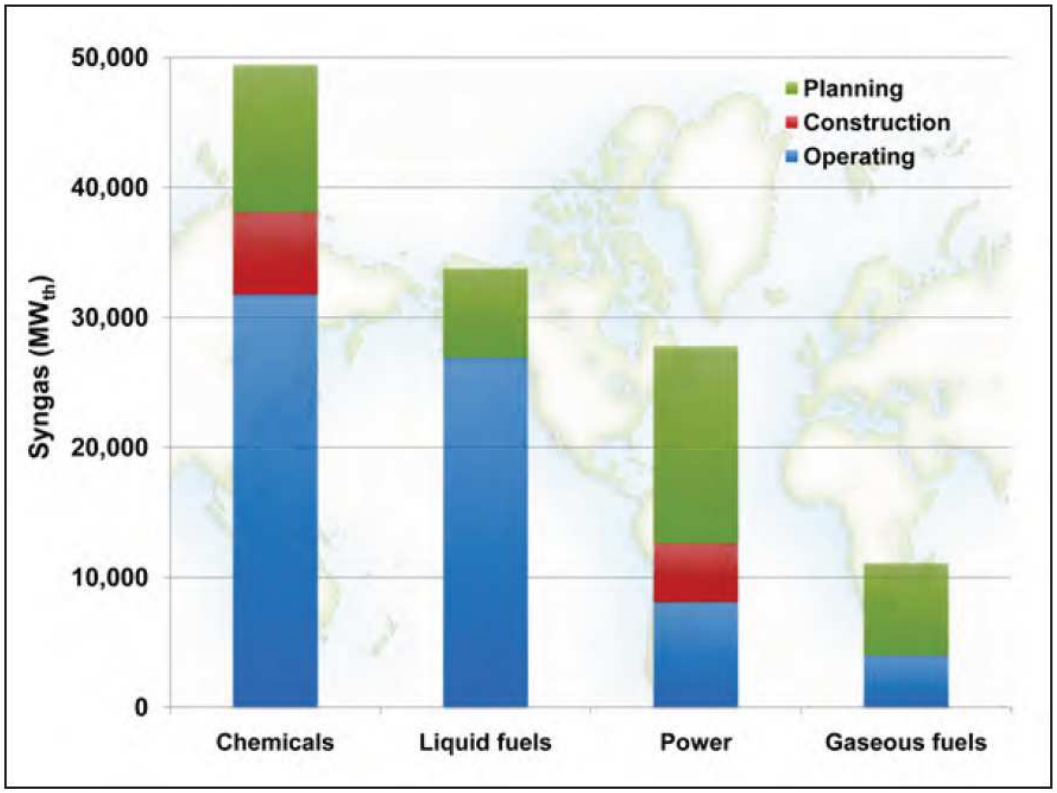


Figure 2.21: World Gasification Capacity and Planned Growth – By Product (U.S. DOE, 2010)

It can be seen from these graphs that the gasification technology is mature; therefore more research and feasibility studies need to be conducted on the other components constituting an IGCC process.

2.10. Gasification experience with South African Coals

IGCC penetration in South Africa (SA) is dependent on the success of gasification of South African low grade coals. South Africa has no experience with gasification of coal for power generation. Most of the coal used for power generation is of low quality and not suitable for use in most of the gasification technologies. There is however potential with fluidised bed gasifiers (Engelbrecht et al., 2008). Research is underway at Eskom's testing facility on fluidised bed combustion with the probability of future fluidised bed gasification tests.

It is necessary for Eskom to test its coals for gasification because there is currently limited experience in South Africa in terms of surface gasification for power generation.

Experiments were conducted by CSIR for gasification reactivity in a thermo gravimetric analyser (TGA) for four South African coals that are currently burnt in some of the Eskom boilers. In the semi- batch TGA experiment, the different coal char samples were weighed before exposing them to specified temperature, pressure and reacting gas. These experiments were conducted at the following conditions: 87.5 kPa, and temperatures of between 875 ˚C and 950 ˚C utilising CO_2 as a reacting gas at 100 vol%. The char from the grootegeluk coal was found to have caking properties which could result in diffusion limitations since the test at 925 ˚C produced the same results as the test at 950 ˚C. The tests on the grootegeluk coal were repeated using prepared char, and did not show caking characteristics. It was found that the reactivity of coal char increases with a decrease in the rank of coal. (Engelbrecht, 2008).

Gasification tests were also conducted on the same coals at the CSIR pilot-scale fluidised bed gasification (FBG) testing facility. These tests were carried out at temperatures of 925 ˚C and 950 ˚C. The factors (oxygen concentration, temperature, particle size and fluidising velocity) that affect diffusion were kept constant for the FBG coal tests. The order of ranking of reactivities was found to correspond with the results of the TGA, however there was less variation in the reactivity index between the four coals in the FBG than that found in the TGA tests. This could be due to the amount of fixed carbon that reacts in the FBG by means of partial combustion which is less sensitive to the reactivity of the char. (Engelbrecht, 2008).

The quality of coal gasified and the gasification conditions in the gasifier have an impact on the quality of syngas produced. The syngas obtained from the gasification of the four South African coals with air and steam was between 2.5 and 3.0 MJ/kg, due to the low volatile matter and the high ash content in the

coals tested. The gasifier had high heat losses and nitrogen dilution which may have also contributed to the quality of the syngas (Engelbrecht, 2008).

The conclusion from these tests was that FBG has potential with high ash South African coals for IGCC technology in power generation despite the coals having relatively low reactivity and low calorific value (Engelbrecht, 2008).

Sasol on the other hand, has considerable gasification experience with South African coals. It contributes largely to the world syngas capacity; in 2008 the estimated syngas capacity was 14GW_{th} from the conversion of 43Mt/y of coal in 97 gasifiers at its plants (Blesl & Bruchof, 2010). Sasol utilises coal as a feedstock to produce syngas for the production of fuels and chemicals from the Sasol-Lurgi fixed bed dry bottom gasification technology. The Sasol-Lurgi fixed bed gasifiers have the ability to handle coal with varying chemical and physical properties however they have limited ability to handle excessive fine coal or coal with high caking propensity (Van Dyk et al., 2001)

Fine coal gasification is the technology of choice for IGCC (Engelbrecht et al., 2008). The limited ability of the Sasol-Lurgi gasifiers to handle excessive fine coal may need to be investigated further to determine the potential for IGCC. The most well-known fine coal gasifiers are the entrained and fluidised bed gasifiers Engelbrecht et al., 2008). However the potential for utilisation of sized coal in gasification may also be considered.

African Explosives and Chemical Industries (AECI) Koppers-Totzek operated their entrained flow gasifiers for over 20 years from 1975 at modderfontein in South Africa. They gasified South African fine coal to produce ammonia. Syngas production was about 100 000 Nm^3/h containing 60% CO. the gasification efficiency was between 60 and 70% (Engelbrecht, 2008). The coal utilised for this process was good quality when compared with coal currently utilised for power generation. More work still needs to be conducted with SA coals on this gasification technology to realise potential for IGCC (Rajoo, 2003).

2.11. Conclusion to literature review

Based upon the literature review conducted the answers to the initial research questions raised are summarised below:

- Fluidised bed gasification has been identified to have potential for application with SA coal for power generation.
- Sasol has considerable gasification experience with South African coals; however their technology is limited when it comes to fine coal gasification. Further studies may need to be conducted to investigate potential for IGCC.
- More work still needs to be conducted on entrained flow gasification utilising the current coal used for power generation in SA.
- There is still some uncertainty regarding the implementation of the IGCC technology because there is no full scale practical experience worldwide. This prevents confidence regarding operation of IGCC technology.
- It is therefore also not possible to estimate risks associated with this process. For the same reason, it is not possible to draw comprehensive reference regarding the techno-economic implications of the IGCC technology.
- In addition, timeframes associated with the introduction of the IGCC technology cannot be estimated with certainty at this stage.

During the course of the literature survey, a far more relevant aspect became apparent which could affect the introduction of IGCC more rapidly in future, namely, it became apparent that the reduction of gaseous emissions from IGCC plant will have a significant impact on the economic and environmental aspect and therefore the attractiveness of the IGCC technology.

For this reason the research direction turned to investigate in greater detail the emissions generated from the combustion of synthesis gas produced from fluidised bed gasification and combusted in a gas turbine. This serves to be an

estimation of emissions that may be expected from the syngas combustion turbine in an IGCC technology.

CHAPTER 3

3. METHODOLOGY

3.1. Introduction

Gaseous emissions were calculated from the combustion of synthesis gas produced from the fluidised bed gasification of four low grade coals that are currently being fed into the Eskom power stations. A methodology developed by John Keir at Eskom to calculate gaseous emissions from the combustion of pulverised coal was manipulated in order to estimate gaseous emissions from the combustion of syngas in a gas turbine. The gasification test work was undertaken at the Council for Scientific and Industrial Research (CSIR) as part of a previous Masters project (Engelbrecht, 2008). The results from that work form the basis of the current study.

3.2. Sample selection

Four coals were selected from four different coalfields in three different provinces in South Africa. These coals include the New Vaal coal from the Free State province, Matla and Duvha coals from Mpumalanga and Grootegeluk coal from Limpopo. Table 3.1 presents the location of the selected coals and the estimated life of the respective mines.

The gaseous emissions to be calculated from the combustion of synthesis gas produced from the gasification were CO_2, SO_2 and NO_x as NO_2. These were calculated with the aim of comparing them to emissions from the combustion of conventional pulverised coal and to the South African emissions standards published by the Department Of Environmental Affairs.

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Table 3.1: Background information on four South African coals (Engelbrecht, 2008)

Colliery	New Vaal	Matla	Grootegeluk	Duvha
Location of mine	Free State	Mpumalanga	Limpopo	Mpumalanga
Coal field	Sasolburg	Highveld	Waterberg	Witbank
Production rate (Mt/a)[1]	15.2	14.0	15.0	16.0
Started production	1985	1979	1985	1979
Expected lifetime (years)[1]	30 - 40	40 - 50	40 - 50	30 - 40
Coal preparation	Washed	Raw coal	Washed	Raw coal
Receiving power station	Lethabo	Matla	Matimba	Duvha
Power station rating (GWe)	3.6	3.6	3.6	3.5

A proximate, an ultimate and a calorific value (CV) analysis were undertaken on the selected coals and the results are shown in Table 3.2 below. Of specific note is the fact that all four coals are high in ash and variable in CV.

The synthesis gases produced from the four coals under investigation were produced in a bubbling fluidised bed pilot scale gasifier under the following conditions: 90 kPa absolute pressure, bed temperature from 921˚C and bed pressure from 2115 Pa.

Table 3.2: Composite sample results (Engelbrecht, 2008)

		New Vaal	Matla	Grootegeluk	Duvha
Proximate analysis	Standard				
Ash content (%)	ISO 1171	40.40	33.40	34.90	32.50
Inherent moisture (%)	SABS 925	5.80	3.50	1.60	1.80
Volatile matter (%)	ISO 562	19.20	21.00	24.90	19.90
Fixed carbon (%)	By diff.	34.60	42.10	38.60	45.80
Ultimate analysis					
Carbon (%)	ISO 12902	42.58	50.66	51.96	58.70
Hydrogen (%)	ISO 12902	2.19	2.65	3.15	3.33
Nitrogen (%)	ISO 12902	0.89	1.07	0.99	1.27
Sulphur (%)	ISO 19759	0.69	0.74	1.58	1.10
Oxygen (%)	By diff.	7.54	7.97	5.85	3.14
Calorific value					
Calorific value (MJ/kg)	ISO 1928	15.07	18.60	19.80	21.10

On the assumption that these synthesis gases were then fed into a combustion/ gas turbine, emissions were calculated from the combustion process in the gas turbine. The emissions calculation will consider the quality of coal fed into the IGCC process and the resulting emissions from the gas turbine.

3.3. Emissions calculation from gas turbines

In order to calculate the gaseous emissions in mg/Nm^3, the products of combustion per kg of fuel combusted need to be calculated. The following is required in order to calculate the products of combustion:

- An ultimate analysis of the fuel. This is generated from the fuel volume composition.
- Theoretical air. This is the amount of air theoretically required to fully combust the fuel.
- Excess air. Excess air is required to increase the combustion efficiency and reduce the formation of carbon monoxide. In practice more than the

theoretical amount of air is required to obtain complete combustion (Perry et.al, 1997).

3.3.1. Determination of ultimate synthesis gas analysis

Table 3.3 presents the composition of the synthesis gas obtained from gasifying the selected coals in a bubbling fluidised bed gasifier using air and steam. (Engelbrecht, 2008).

Table 3.3: Summary of fluidised bed gasification tests results with air and steam (Engelbrecht, 2008).

	New Vaal		Matla		Grootegeluk		Duvha	
Test number	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
Dry gas composition								
CO (%)	NR[1]	11.1	10.8	11.6	8.7	10.2	8.8	9.9
H_2 (%)	NR	8.6	10.0	9.6	9.4	9.5	8.5	9.3
CH_4 (%)	NR	0.7	0.8	0.7	1.1	1.1	0.8	0.7
CO_2 (%)	NR	15.8	14.8	14.6	15.0	14.9	15.3	15.0
N2 + others[2] (%)[3]	NR	63.7	63.5	63.4	65.7	64.2	66.5	65.0
O_2 (%)	NR	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Gas calorific value[4] (MJ/Nm[3])	-	2.8	3.0	3.0	2.7	2.9	2.5	2.7

1 NR - no reading

2 Others are < 0.4 % and include H2S, NH3, HCN and $C2^+$

3 (N2 + others) by difference

4 The estimated error in the calculated gas calorific value is given in Appendix B.6.2 of Engelbrecht's thesis

Table 3.4 shows the composition of gas obtained from gasifying the Matla and Duvha coal in a fluidised bed gasifier using oxygen and steam.

Table 3.4: Summary of fluidised bed gasification tests results with oxygen and steam (Engelbrecht et.al, 2008)

Coal tested	Matla	Duvha
Dry gas composition		
CO (%)	19.0	22.1
H_2 (%)	27.6	28.4
CH_4 (%)	2.0	2.2
CO_2 (%)	46.1	36.6
N2 + others[1] (%)[2]	5.2	10.6
O_2 (%)	0.1	0.1
Gas calorific value[4] (MJ/Nm^3)	6.9	7.4

1 Others are < 0.8 % and include H2S, NH3, HCN and $C2^+$

2 (N2 + others) by difference

The dry flue gas compositions in table 3.3 and table 3.4 are presented in volume percentage. These were converted to a mass percentage by first multiplying the given volume percentage by the molecular weight of the respective compound and then summing up the products of the respective compounds. Thereafter a percentage of each product was obtained from the sum of all the products. This was taken as the mass percentage. The molecular weight fraction of each element in the respective compound was multiplied by the mass percentage obtained for the respective compound to achieve the ultimate analysis by mass.

3.3.2. Determination of theoretical air and excess air

3.3.2.1. Theoretical air calculation

Theoretical air was calculated based on the oxygen required to react with the individual elements. The individual elements involved are Carbon (C) which reacts to form carbon dioxide, Hydrogen (H) which reacts to form moisture, Sulphur (S) which reacts to form Sulphur dioxide and Nitrogen (N) which reacts to form Nitric oxide. The Nitric oxide is quickly converted to nitrogen dioxide

(NO_2) when emitted to the atmosphere and therefore NO_x is reported as Nitrogen dioxide.

The following assumptions were made to enable calculation of the theoretical air required and the products of combustion from combustion in a gas turbine:

- All the carbon in the fuel gas is converted to carbon dioxide in a fuel lean mixture.
- According to the General Electric's experience with the gas turbine, all sulphur in the fuel gas is converted to sulphur oxides in the form of Sulphur dioxide (SO_2) and Sulphur trioxide (SO_3), however Sulphur trioxide exists in very small amounts (Pavri & Moore, 2012). It is therefore assumed that the concentration of SO_3 in the flue gas is negligible and all the sulphur in the fuel gas converts to sulphur dioxide. Therefore the theoretical air required must be able to combust all the sulphur in the fuel to sulphur dioxide.
- The determination of the amount of NO_x formed in the flue gas is complicated due to the fact that NO_x is formed from two sources of nitrogen, i.e. The fuel and the combustion air. In order to simplify the calculation of NO_x, only the NO_x formed from the nitrogen in the fuel was considered. This is because the combustion temperatures in the gas turbine are below 1700K and as a rule of thumb, at temperatures below 1700K, the residence time is not long enough to enable formation of significant thermal NO_x in combustion turbine (Richards et.al, 2012).
- It is further assumed that the fuel NO_x emissions are due to the nitrogen that is chemically bound in the fuel and the conversion percentage is 100% at low fuel bound nitrogen contents (Pavri et.al, 2012).
- Emissions from gas turbines are reported under normal conditions of 15% O_2, 273K and 101.3 kPa (Government Gazette RSA, 2010).

The following reactions are used in the combustion process to determine the amount of oxygen required. The molecular weights used are shown in table 3.5.

Table 3.5: Molecular weights used in the products of combustion calculation (Perry et.al, 1997)

Molecular weights (kg/kmol)	
Carbon (C)	12
Oxygen (O_2)	32
Hydrogen (H_2)	2
Sulphur (S)	32
Nitrogen (N_2)	28
Methane (CH_4)	16
Carbon monoxide (CO)	28
Carbon dioxide (CO_2)	44
Moisture (H_2O)	18
Sulphur dioxide (SO_2)	64
Nitric oxide (NO)	30
Nitrogen dioxide (NO_2)	46
Hydrogen Sulphide (H_2S)	34
Ammonia (NH_3)	17

Carbon combustion:

$$C + O_2 \rightarrow CO_2$$

12 kg of Carbon reacts with 32kg of Oxygen to form 44kg of Carbon dioxide

$$12C + 32O \rightarrow 44CO_2$$

Therefore, 1 kg of Carbon reacts with 2.67 kg Oxygen to form 3.67 kg of Carbon dioxide

$$1C + \frac{32}{12}O \rightarrow \frac{44}{12}CO_2$$

$$1C + 2.67O \rightarrow 3.67CO_2$$

Hence Oxygen required to combust Carbon is expressed as follows:

$$O_C = 2.67C$$ ..... (*3.1*)

Hydrogen combustion:

$$2H_2 + O \rightarrow 2H_2O$$

4 kg of Hydrogen reacts with 32kg of Oxygen to form 36kg of Moisture

$$4C + 32O \rightarrow 36H_2O$$

Therefore, 1 kg of Hydrogen reacts with 8 kg of Oxygen to form 9 kg of Moisture

$$1H + \frac{32}{4}O \rightarrow \frac{36}{4}H_2O$$

$$1H + 8O \rightarrow 9H_2O$$

Hence Oxygen required to combust Hydrogen is expressed as follows:

$$O_H = 8H$$ ..... (*3.2*)

Sulphur combustion:

$$S + O_2 \rightarrow SO_2$$

32kg of Sulphur reacts with 32kg of Oxygen to form 64kg of Sulphur dioxide

$$32S + 32O \rightarrow 64SO_2$$

Therefore, 1 kg of Sulphur reacts with 1 kg of Oxygen to form 2 kg of Sulphur dioxide

$$1S + \frac{32}{32}O \rightarrow \frac{64}{32}SO_2$$

$$1S + 1O \rightarrow 2SO_2$$

Hence Oxygen required to combust Sulphur is expressed as follows:

$$O_S = 1S \quad \text{..... (3.3)}$$

Nitrogen combustion:

$$N_2 + O_2 \rightarrow 2NO$$

28kg of Nitrogen reacts with 32kg of Oxygen to form 60kg of Nitrous oxide

$$28N + 32O \rightarrow 60NO$$

Therefore, 1 kg of Nitrogen reacts with 1.14 kg of Oxygen to form 2.14 kg of Nitric oxide

$$1N + \frac{32}{28}O \rightarrow \frac{60}{28}NO$$

$$1N + 1.14O \rightarrow 2.14NO$$

Hence Oxygen required to combust Nitrogen is expressed as follows:

$$O_N = 1.14N \quad \text{..... (3.4)}$$

Therefore the total theoretical mass of oxygen required is obtained by adding equations *3.1* to *3.4*:

$$O_{theoretical} = 2.67C + 8H + S + 1.14N \quad \text{..... (3.5)}$$

Where C,H,S and N are expressed in percentage in 1 kg of fuel.

However, in a case where the fuel used contains oxygen, the total oxygen required is expressed by equation *3.6*.

$$O_{theoretical} = 2.67C + 8H + S + 1.14N - O_{fuel} \quad \text{..... (3.6)}$$

Where O_{fuel} is the percentage of oxygen in the fuel.

Air contains 20.9% (Gagnon, 1993) of oxygen and 79.1% of Nitrogen by volume, then mass percentage of oxygen in air can be calculated as follows,

$$m_{O2} = 20.9kmol \times 32\frac{kg}{kmol} = 668.8kg$$

$$m_{N2} = 79.1kmol \times 28\frac{kg}{kmol} = 2214.8kg$$

$$m_{air} = m_{O2} + m_{N2} = 2883.6kg$$

$$\%O_2 = \frac{668.8kg}{2883.6kg} \times 100 = 23.2\%$$

Therefore air contains *23.*2% of oxygen by mass, so, oxygen in air is:

$$O_{air} = \frac{23.2}{100} air$$

Hence, theoretical oxygen is:

$$O_{theoretical} = \frac{23.2}{100} air_{theoretical} \quad \ldots\ldots\ldots\

Taking into account the conversion percentages, equation 3.9 can be expressed as,

$$air_{theoretical} = \frac{100}{23.2}\left[2.67C + 8H + 1S \times SC + 1.14N \times NC - O_{fuel}\right] \quad \text{…….. (3.10)}$$

Where SC and NC is the sulphur and nitrogen conversion respectively.

3.3.2.2. Excess air calculation

Excess air is calculated from the required excess O_2 percentage at the stack exit. Formula 3.11 obtained from the Babcock & Wilcox notebook (Babcox & Wilcox, 1986) was used to calculate excess air:

$$air_{excess}\,\% = \frac{100}{f}\left[\frac{O_2}{20.9 - O_2}\right] \quad \text{…….. (3.11)}$$

And,

$$f = \frac{1 + 3K}{1 + 2.37K + 0.09n}$$

Where,

$$K = \frac{H - \frac{O}{8}}{C + \frac{3}{8}S}$$

and,

$$n = \frac{N}{C + \frac{3}{8}S}$$

C, H, O, N & S is carbon, hydrogen, oxygen and sulphur percentages in the fuel.

3.3.3. Products of combustion from syngas combustion

The products of combustion are calculated per kg of fuel combusted. The main focus in this investigation will be on three products, namely, CO_2, SO_2 and NO_x. NO_x is calculated in the form of NO and later converted to NO_2. This is because all NO_x originates as NO and this further reacts in the atmosphere with oxygen to form the stable NO_x in the form of NO_2 (US emissions standards division, 1993).

As stated in section 3.3.2.1, for the purpose of the calculation, complete combustion is assumed for carbon and sulphur in the fuel gas. For nitrogen, only the organically bound nitrogen in the fuel is assumed to react. The percentage conversion of nitrogen will then depend on the amount of nitrogen chemically bound in the fuel. This is obtained by determining the percentage of nitrogen chemically bound to hydrogen (NH_3).

The following steps were followed in calculating the products of combustion:

- The fuel dry gas composition was converted to an ultimate fuel gas analysis.
- The combustion products formed were determined from the ultimate analysis and the combustion reactions were derived from section 3.3.2.1.
    - 1 kg of carbon reacts to form 3.67 kg of CO_2.
    - 1 kg of sulphur reacts to form 2 kg of SO_2.
    - 1 kg of nitrogen reacts to form 2.14 kg of NO.
- The mass percentage for each of these products in the flue gas is calculated from the sum of all products formed.
- The mass percentages were then converted to volume percentage using molecular weights of each product. This was then converted to ppm.
- The densities of these products were calculated at standard temperature and pressure, where the molar volume is 22.4 m^3/mol
- The product of the density and the volume in ppm calculated then gives emissions in mg/Nm^3.

3.3.4. Products of combustion from pulverised coal combustion

Emissions from combustion of the four coals were calculated. A procedure similar to that of gas turbine emissions calculations was used however the following was considered:

- The coal composition given in table 3.2 is on an air dried basis, and therefore these results require conversion to as-received basis because the coal is fired as it is in pulverised fuel boilers. The conversion to as-received basis was calculated based on the British standard for analysis and testing of coal and coke (Part 16 method for reporting results, 1981). Average total moisture in the coal for the four Eskom stations in 2007 was used (Eskom Holdings SOC, 2007).
- The carbon conversion in this case is not 100% since there is usually unburnt carbon in the ash produced from the pulverised fuel boilers. The unburnt carbon used in the calculations is the average unburnt carbon from the four Eskom power stations burning the chosen coals. (Eskom Holdings SOC, 2007).
- The sulphur in the fuel is not completely oxidised, the percentage conversion will depend on the type of mills used. Coal fired from vertical spindle mills is believed to have a relatively low conversion of sulphur since some sulphur can be found in mill rejects. However sulphur conversion for tube mills is slightly high because there are no mill rejects and therefore no residual sulphur. A 90% sulphur conversion was used in the calculation as stated in combustion engineering handbook (Singer, 1981).
- As already stated, calculation of NOx is complicated due to the different sources of NOx in the combustion process. In this case, only fuel NOx was calculated. Fuel NOX amounts to 70 - 80% of the total NO_X emissions in pulverised fuel combustion power generation (Wu, 2002). Approximately 80% of NOx formed is due to about 20% (Innovative combustion, 2011) of nitrogen in the fuel that converted.

- Emissions from pulverised fuel combustion are reported under normal operating conditions of 273 K and 101.3 kPa at 10% O_2 (Government Gazette RSA, 2010).

3.3.5. Hydrogen Sulphide and ammonia composition in the syngas

According to Engelbrecht from CSIR, the "others" in the syngas produced consist of H_2S, NH_3, HCN and C2+ and these are ± 0.4 vol % for air-blown gasification, where H_2S was assumed to be about 0.3% and therefore NH_3 was assumed to be 0.1% (1000 ppm). Some SO_x and COS were found to be present in the syngas but at much lower concentrations. The NH_3 and HCN amounts were not measured, however it was noted that the HCN amount is a lot lower that the NH3 amount (Engelbrecht, 2008).

For oxygen blown gasification the gas flow is lower (± 50% lower) and the CV higher due to the absence of N_2 in the gas. The H_2S will therefore be ± 0.6 % and the NH_3 0.2 % (2000 ppm) (Engelbrecht, 2008).

This is in accordance with the typical gasifier gas composition given by Ke Liu et.al. The H_2S typical volume percentage was given as ranging from 0.2 – 1 vol % and that of NH_3 (including HCN) was given as ranging from 0 – 0.3 vol % (Liu et.al, 2010).

Stiegel et.al (2012), gives the typical volume percentages for H_2S ranging from 0.02 – 0.5% and for NH_3 ranging from 0.9 – 1.3%. These however are specified for entrained and moving bed gasifiers with Illinois no.5 & 6 coals.

CHAPTER 4

4. RESULTS & DISCUSSIONS

The results obtained from emissions calculations undertaken will be presented below, followed by a discussion on overall observations and results. The emissions calculations were calculated for an IGCC operation and for the conventional coal fired combustion operation and then compared.

4.1. Results

4.1.1. Emissions from the combustion of syngas from gasification with air and steam

Emissions from IGCC were estimated and compared to the requirements of the South African emissions standard. The emissions were calculated for an IGCC system with and without an H_2S and NH_3 removal system. It is however assumed that all particulates have been removed both systems. IGCC plants as already discussed in the literature review involve removal of sulphur and particulates before the synthesis gas can be combusted in a gas turbine. Two gasification tests were conducted by Engelbrecht (Engelbrecht, 2008) per type of coal and the emissions from these are shown in table 4.1. Only one test for the New Vaal coal was undertaken because the gas analysers were not yet installed at the time the first test was done.

Table 4.1: Emissions obtained from an IGCC operation without pre-cleaning the fuel gas

IGCC	mg/Nm3 @ 15% O2, 273K, 101.3kPa												
	Standard		New Vaal		Matla			Grootegeluk			Duvha		
	New	existing	1	2	3	4	Average	5	6	Average	7	8	Average
CO2			NR	112,131	121,873	123,739	122,806	117,261	120,457	118,859	120,898	121,596	121,247
SO2	400	500	NR	1,773	2,015	2,008	2,011	2,064	2,006	2,035	2,119	2,073	2,096
NO			NR	276	314	313	313	321	313	317	330	323	326
NO2	50	300	NR	424	481	479	480	493	479	486	506	495	501

1 NR – no reading

Table 4.1 compares SO_2 and NO_2 emissions obtained from synthesis gas combustion with the limits from the South African government emissions standard. The emissions calculated are higher than what has been set as a standard for both new and existing operations. This is because no emission control was considered in calculating these emissions, these calculations were conducted to illustrate the advantage of pre-cleaning the synthesis gas before combustion and further illustrate the amount of SO_2 and NO_2 that may need to be removed compared to the conventional coal fired operations without emission control technologies. The emissions reduction amount required has an influence on the size of the emissions control plant and hence the cost of that plant. The detailed results for the un-cleaned syngas combustion can be seen in appendices A.1, B.1, C.1 and D.1 for the New Vaal, Matla, Grootegeluk and Duvha coals respectively.

The emission limits given in table 4.1 are for gas turbine operations because the emissions are calculated from synthesis gas combustion in a gas turbine assuming that the heat recovery steam generator (HRSG) is not supplemented by combustion of coal.

Table 4.1 suggest the need for control technologies. The incorporation of control technologies however has a negative impact on the overall process of producing electricity. The inclusion of a Flue Gas Desulphurisation (FGD) plant and a NOx control plant increases the auxiliary power consumed by the unit, thereby decreasing the overall efficiency of the unit. This relationship is illustrated by formula 4.1 below. The inclusion of emission control technologies also negatively impacts the cost of electricity as it increases both the capital and the operational cost of the plant.

$$eff = \frac{Power_{gen} - Power_{aux}}{Coal \times CV} \quad \text{..... (4.1)}$$

Where *eff*, is the overall thermal efficiency of the plant in %,
$Power_{gen}$, is the total generated power in MW,
$Power_{aux}$, is the auxiliary power consumed by the unit in MW,
Coal, is the coal flow in kg/s, and
CV, is the caloric value of the coal in MJ/kg

In general an IGCC plant would have gas pre-cleaning technologies installed and this would have the advantage of cleaning the gas before combustion in a gas turbine which reduces the costs associated with installing post combustion emission control technologies. It is the pre-cleaning that gives it an environmental performance advantage over other clean coal technologies.

Table 4.2 illustrates the effect of pre-cleaning fuel gas on emissions. It was assumed that 95% (Ratafia-Brown et al., 2002) of the hydrogen sulphide (H_2S) and 88% (Henderson, 2008) of ammonia removal was achieved before entering the gas turbine. The detailed results can be seen on appendices A.2, B.2, C.2 and D.2 for the New Vaal, Matla, Grootegeluk and Duvha coals respectively.

Table 4.2: Emissions obtained from an IGCC operation with combustion of pre-cleaned fuel gas

IGCC pre-cleaned fuel gas, mg/Nm3 @ 15% O2, 273K, 101.3kPa										
	Standard		New Vaal		Matla		Grootegeluk		Duvha	
	New	existing	1	2	3	4	5	6	7	8
CO2			NR	114,320	124,579	126,478	119,945	123,121	123,768	124,397
SO2	400	500	NR	90	103	103	106	103	108	106
NO			NR	34	39	38	39	38	41	40
NO2	50	300	NR	52	59	59	61	59	62	61

Sulphur dioxide emissions were reduced well below the required new limit. However, nitrogen dioxide emissions were slightly above the required new limit. This therefore requires additional NO_x control in the form of either primary or secondary NO_x control technologies. Primary control technologies affect the combustion process and secondary control technologies control emissions post combustion. With primary controls, the fuel gas can either be humidified or the turbine inlet temperatures can be increased. These however have the disadvantage of increasing the moisture levels in the flue gas and encouraging the formation of thermal NO_x respectively. Another primary alternative method which controls both thermal and fuel NO_x is the dry low NO_x combustion design which utilises a rich/quench/lean staged combustion process. This method uses three stages of combustion, which are, fuel-rich primary stage, quenching stage and fuel-lean secondary stage. The primary stage is oxygen-lean which inhibits NO_x formation and the quenching stage reduces the temperature and increases oxygen levels. The temperature in the secondary stage is therefore well below the NO_x formation temperature and the combustion environment is fuel-lean due to excess oxygen. This technology however is still under development (US Emission standards division, 1993). Secondary controls like the Selective Catalytic Reduction (SCR) and Selective Non-Catalytic Reduction (SNCR) are well established and can become an alternative.

4.1.2. Emissions from the combustion of pulverised fuel in existing boilers

In this section, emissions from coal fired combustion were estimated and compared to the requirements of the South African emissions standard. Table 4.3 shows a summary of emissions calculated to be generated from the combustion of the four selected South African coals in a PF boiler. Refer to appendices A.3, B.3, C.3 and D.3 for detailed results on emission calculations from pulverised coal combustion.

Table 4.3: Emissions obtained from a PF fired operation without emissions control technologies

PF	mg/Nm3 @ 10% O2, 273 K, 101.3 kPa					
	Standard		New Vaal	Matla	Grootegelul	Duvha
	New	Existing				
CO2			194,986	194,749	187,888	188,639
SO2	500	3500	1,561	1,402	2,816	1,092
NO			479	482	420	478
NO2	750	1100	734	739	643	733

The emissions obtained are well within the limits for existing operations. The SO_2 emissions from the Grootegeluk coal were found to be high when compared to emissions from the other coals as illustrated in figure 4.1. The higher sulphur dioxide is due to the high sulphur in the coal.

Figure 4.2 shows that the NO_2 emissions obtained from the combustion of the selected coals results in emissions that are within the limits specified by the South African government for existing plant.

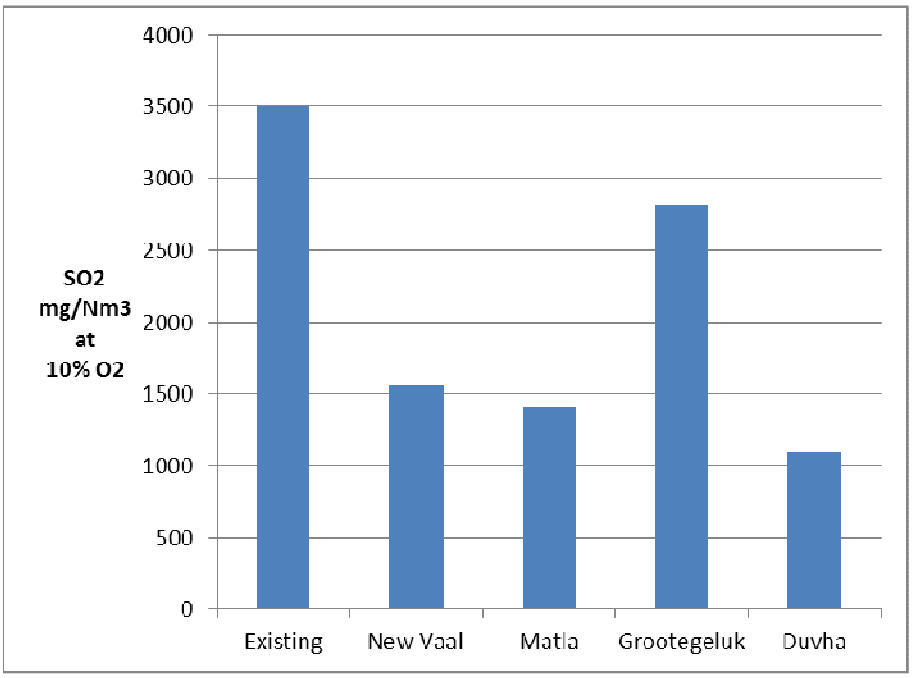


Figure 4.1: Comparison between SO_2 emissions obtained from existing plant and the limits set for existing plant by the RSA government

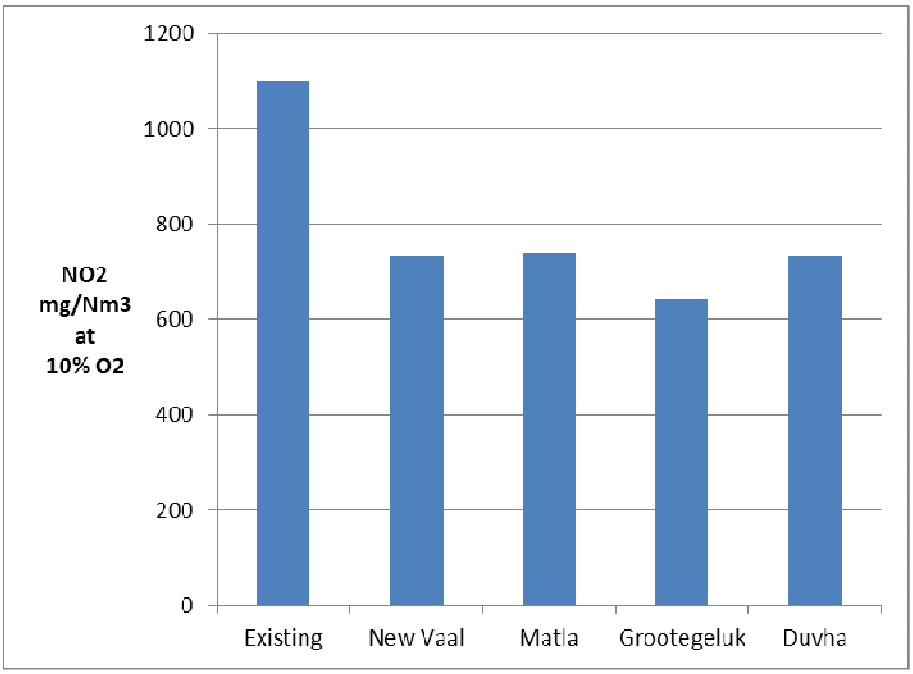


Figure 4.2: Comparison between NO_2 emissions obtained from existing plant and the limits set for existing by the RSA government

The fact that existing plant operations meet the government emission standards poses a challenge to new technologies, because they remain cheaper and yet are able to meet the emission requirements without the need to retrofit emission control technologies. However the South African government stipulates in the emission standard (Government Gazette. Republic of South Africa, 2010) that the existing plant should comply with the minimum emission limits for new plant ten years after the publication of the standard, this would be in 2020. The RSA emission limits set for new plant are significantly low when compared to the existing plant limits. The existing PF plant would require emissions control technologies to meet the new plant limits for SO_2, as seen on figure 4.3. IGCC then becomes advantageous as it not only meet the SO_2 emissions but also reports high cycle efficiencies (Engelbrecht et al., 2008). The cycle efficiency of up to 38% on the conventional cycle is already low when compared to about 47% cycle efficiency on the IGCC plant and introducing emissions control technologies on the conventional cycle may further decrease the cycle efficiency. On the other hand the increase in electricity demand (Collot, 2002) would require more power plants to be built and these plants would need to adhere to even more stringent emission limits and yet be able to obtain high efficiencies.

Figure 4.4 shows that the NO_2 emissions calculated to be generated from the existing PF plant would still be within the limits for new plant when implemented in 2020.

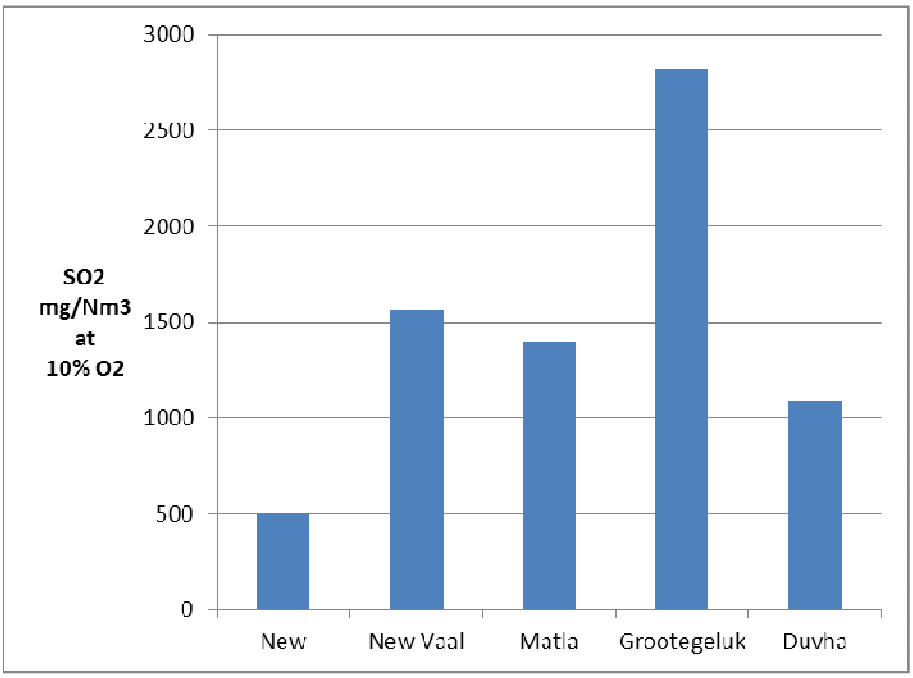


Figure 4.3: Comparison between SO2 emissions obtained from existing plant and the limits set for new plant by the RSA government

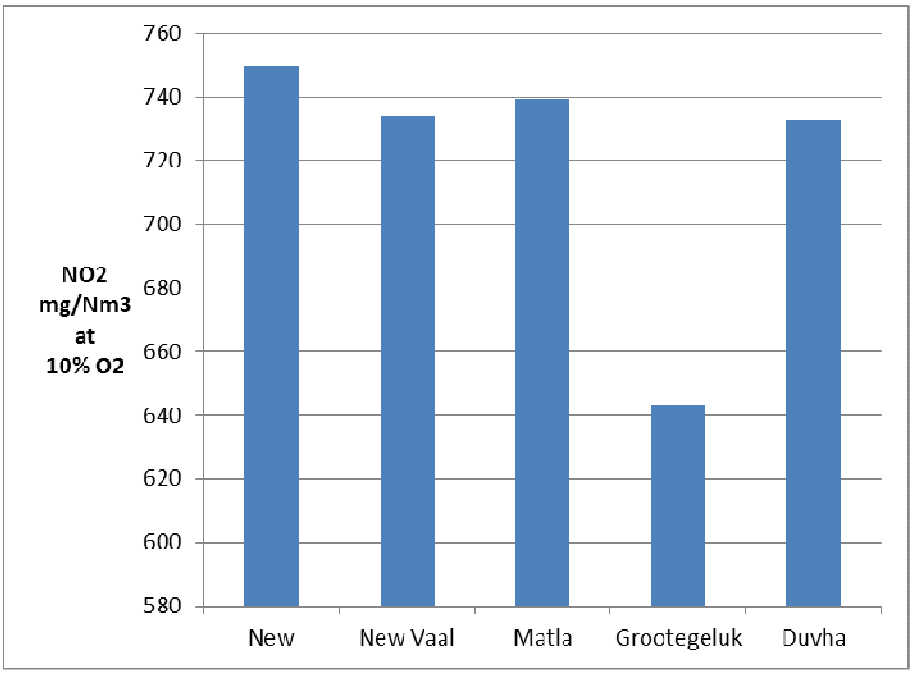


Figure 4.4: Comparison between NO2 emissions obtained from existing plant and the limits set for new plant by the RSA government

NO_2 from the combustion of grootegeluk coal was found to be significantly low when compared with the NO_2 from the combustion of the other coals; this is because the increase in SO_2 concentration decreases the concentration of other constituents in the flue gas, and therefore the NO concentration decreases.

Table 4.4: Flue gas volume % on a dry basis

PF	Vol% dry @ 10% O2, 273 K, 101.3 kPa			
	New Vaal	Matla	Grootegelul	Duvha
CO2	9.9243	9.9122	9.5630	9.6013
SO2	0.0546	0.0490	0.0985	0.0382
NO	0.0357	0.0360	0.0313	0.0357

This is seen in table 4.4, where the concentration of CO_2 and NO decrease because of an increase in SO_2 concentration.

4.1.3. Synthesis gas from gasification with oxygen and steam

The gasification of Matla and Duvha coals was conducted by CSIR (Engelbrecht et.al, 2008), this time with oxygen and steam instead of with air and steam. From table 3.4 in chapter 3 it can be seen that utilising oxygen instead of air has a positive impact on the quality of gas produced. The calorific value (CV) of syngas obtained shows a significant improvement. Gasification with air gave synthesis gas with a CV of 3 MJ/Nm3 for Matla coal and an average of 2.6 MJ/Nm3 for Duvha coal which is relatively low when comparing it with a CV of 6.86 MJ/Nm3 and 7.4 MJ/Nm3 for Matla and Duvha coal respectively gasified with oxygen. This is said to be due to the absence of Nitrogen and the increased rate of steam – char gasification reaction (Engelbrecht et.al, 2008). The CV for synthesis gas obtained from using air as a gasification agent, is even lower than the CV of 4.2 MJ/Nm3 (Gross & Van der Riet, 2011) obtained from utilising air on underground coal gasification (UCG).

The higher the calorific value of the syngas the more power will be generated at constant thermal efficiency.

The syngas obtained from gasification of coal with oxygen was also subjected to the same conditions in the gas turbine for the purpose of calculating emissions.

Table 4.5 shows the emissions obtained from combustion of this syngas. See appendices B.4 and D.4 for detailed calculations. Carbon dioxide emissions were found to significantly increase, as illustrated in figure 4.5. This is influenced by the increased concentration of CO_2 that went into the combustion chamber with the fuel gas as was shown previously in table 3.3 and table 3.4. The CO_2 % for Matla coal was an average of 14.7% from an air blown gasifier and 46.1% from an oxygen blown gasifier. The CO_2 from oxygen blown gasifier is more than double the CO_2 from air blown gasifier. This is due to absence of the dilution effect of nitrogen in the air.

Table 4.5: Emissions obtained from combustion of syngas fired from oxygen

IGCC oxygen fired gasification, mg/Nm3 @ 15% O2, 273K, 101.3kPa						
	Standard		Matla		Duvha	
	New	existing	without pre-cleaning	with pre-cleaning	without pre-cleaning	with pre-cleaning
CO2			207,361	213,225	181,657	186,582
SO2	400	500	2,697	139	2,604	134
NO			420	52	406	50
NO2	50	300	644	80	622	77

It can also be noted that CO_2 concentration increases with implementation of gas clean-up. This is because the removal of the SO_2 and NO_x forming constituents increases the concentration of carbon in the syngas.

Figure 4.5 compares the CO_2 emissions obtained from the combustion of syngas that was acquired from gasification with air and with oxygen.

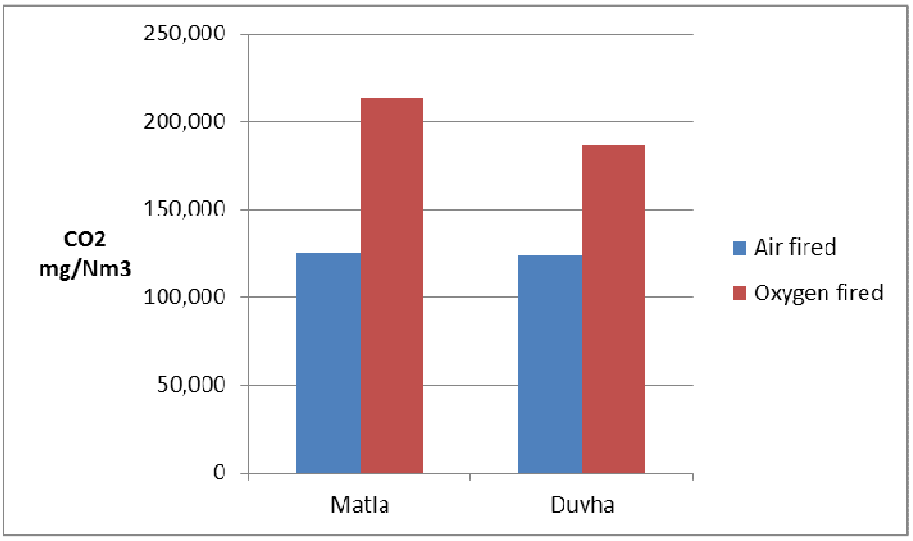


Figure 4.5: CO2 emissions obtained from the combustion of syngas with both air and oxygen blown gasifiers

Figure 4.5 confirms the findings in literature (Breault, 2010), that the CO_2 from IGCC with oxygen blown gasifiers is high in concentration with typical CO_2 syngas composition from a sub bituminous coal fed dry bottom moving bed of 30.4% for oxygen blown and 14.8% for air blown. This allows for easier capture for sequestration in the carbon capture and storage process.

It was also found that gasifying with oxygen instead of air increases SO_2 and NO_2 emissions. Figure 4.6 and Figure 4.7 illustrates the difference between emissions obtained from an IGCC operation with air and with oxygen blown gasifiers. A 35% and 25% increase in SO_2 emissions was obtained from combustion of syngas from Matla and Duvha coal gasification respectively.

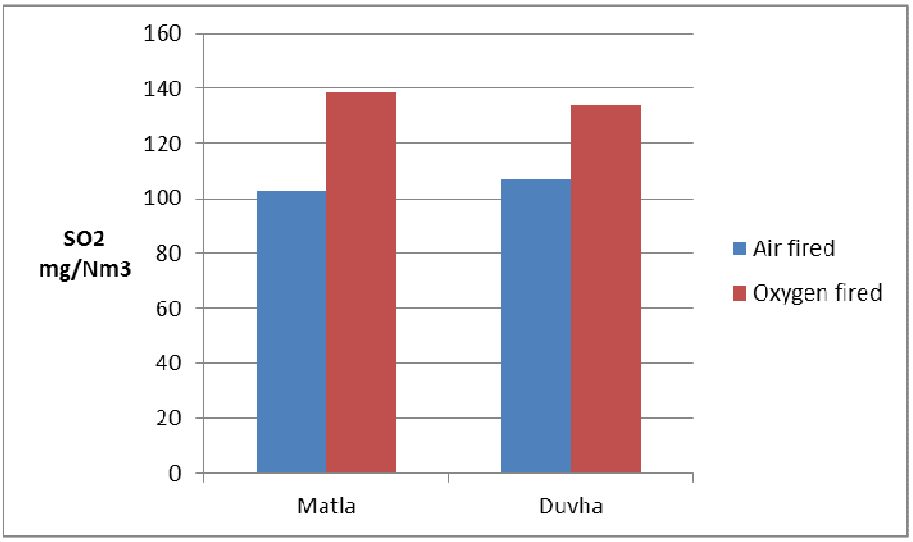


Figure 4.6: : SO2 emissions obtained from the combustion of syngas with both air and oxygen blown gasifiers

The concentration of H_2S and NH_3 in the fuel gas increased, due to the absence of N_2 from air in the gas. The same H_2S and NH_3 removal efficiencies used for syngas from air-blown gasification were used in this case. For NO_2, an increase of 36% and 24% was obtained from combustion of syngas from Matla and Duvha coal gasification respectively.

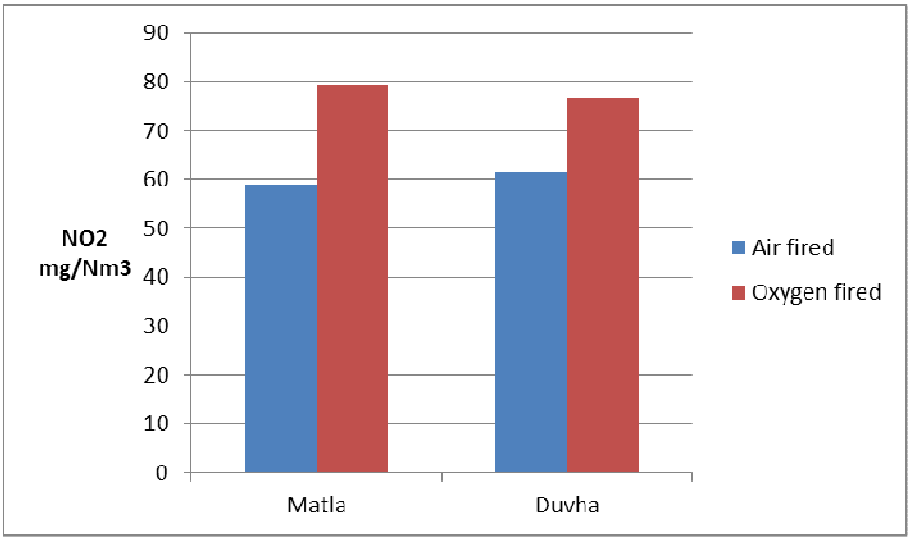


Figure 4.7: NO2 emissions obtained from the combustion of syngas with both air and oxygen blown gasifiers

The NO_2 emissions are even higher than what has been put as the limits by the South African Government with oxygen used as a gasification agent. See figure 4.8. It is therefore necessary to include combustion based NO_x control for the IGCC gas turbine in order to meet the NO_x emission limits. This will nevertheless depend on the amount of NH_3 in the fuel gas and the percentage removal achieved.

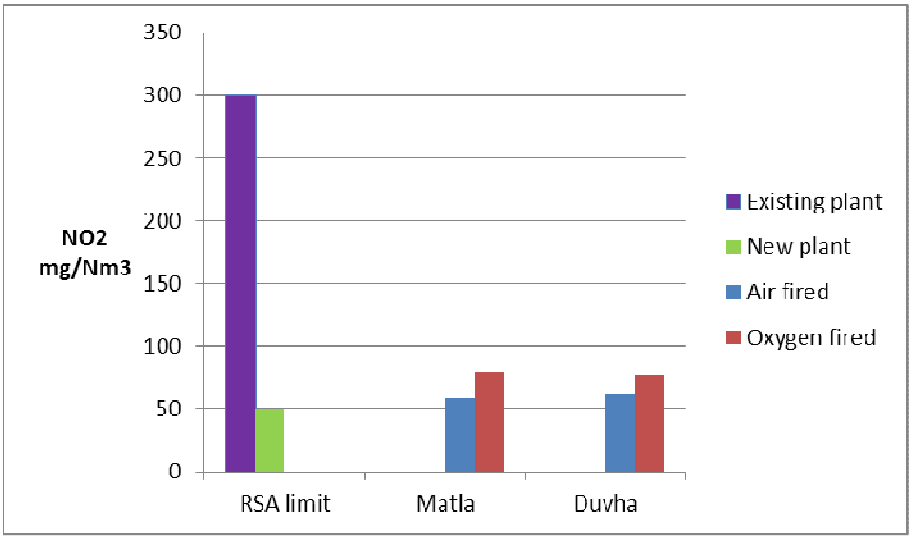


Figure 4.8: Comparison of NO2 emissions between the RSA limits and the emissions obtained from combustion of syngas with both air and oxygen blown gasifiers

Figure 4.9 shows the comparison between the SO_2 emission limits and what was obtained from the combustion calculations conducted.

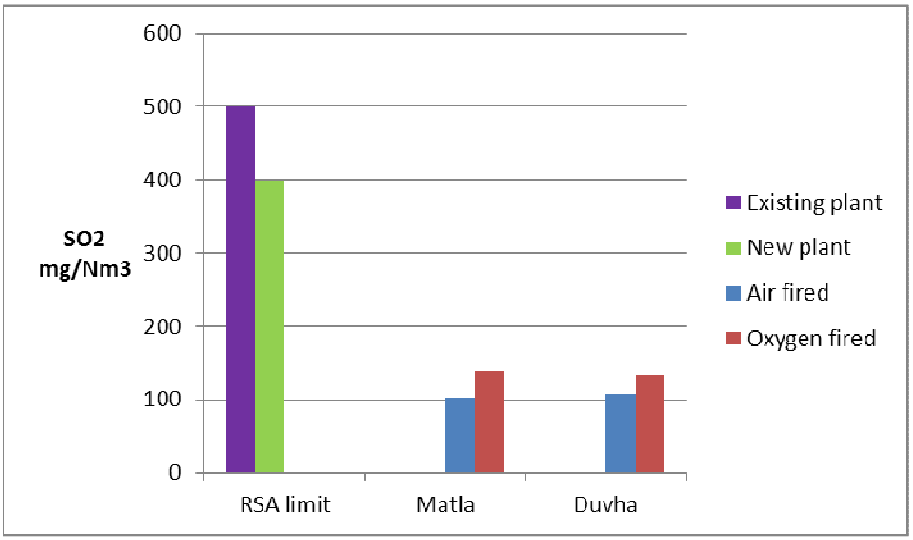


Figure 4.9: Comparison of SO2 emissions between the RSA limits and the emissions obtained from combustion of syngas with both air and oxygen blown gasifiers

The SO_2 emissions calculated for both air- and oxygen-blown gasification are well within the limits set by the South African government.

4.2. Discussions

The initial intention of this research was to undertake the techno economic review of IGCC, however during the process of research it became obvious that the most important aspect which would lead eventually into the economic features was the environmental impact of the emissions arising from the IGCC process. This is more important considering the penalties on exceeded limits in emissions that could soon be implemented.

The emphasis of this research has therefore become environmentally focussed which would hopefully lead to an economic study on a PHD level.

Coal fired IGCC technology for power generation has not been fully established commercially, and therefore there is not enough operating history to refer back to. Power plant owners and financiers require assurance that operational

problems will be limited based on proven operational experience. Very few IGCC technologies are close to full commercial stage; however they still need to overcome technical problems associated with the integration of the different systems of an IGCC plant which generally lead to plant availability problems.

IGCC has potential in the future when carbon capture is implemented because according to a study conducted by the state of Wisconsin, the inclusion of carbon capture increases the levelized lifecycle costs, however, these are relatively cheaper for IGCC at 75 – 78 $/MWh when compared to the supercritical pulverised coal units at 82 – 88 $/MWh (Energy Insider, July 25 2006). IGCC has drawn attention due to its proven ability to attain high cycle efficiencies and a significant reduction in emissions.

The results obtained in this study suggest that IGCC can lead to significant success in the reduction of emissions through combusting pre-cleaned synthesis gas. Nevertheless more effort needs to be put in meeting the emissions standards and keeping the high efficiencies because the more process units are included in the production process the less efficient the overall process becomes.

It was found that the gasification agent used has an effect on the reduction of emissions. The emissions were found to be better when utilising air as a gasification agent than when utilising oxygen as a gasification agent. This is because the concentration of the gas species in the flue gas increases in the absence of N_2 from air. The absence of N_2 from air results in better quality of syngas when compared to the syngas obtained from an air blown gasifier. The CO_2 from an oxygen-blown gasifier is more concentrated and therefore the CO_2 recovered is higher; higher concentrations of CO_2 are good for carbon capture and storage. Using oxygen blown gasifiers would require inclusion of an air separation unit (ASU) which is expensive and may affect the overall efficiency of the unit.

UCG gas for combustion in a gas turbine may also be explored where emissions and costs can be compared with surface gasification technologies.

Unfortunately emissions from combustion of the gas produced from the Eskom UCG project could not be calculated due to unavailability of gas composition/specification data.

It was also found that, based on the calculations undertaken; IGCC technology would require either improvement in ammonia removal efficiency or the inclusion of primary measures to control NO_x emissions in order to meet the South African Government emission standards for NO_x.

Coal gasification technologies are well established and the technology manufacturers are already marketing these technologies. But there is still some uncertainty about pursuing IGCC technology for power generation. Most companies are waiting for someone to initiate a full scale plant and then others will follow. This is understandable because it comes with reduced risk of loss in case it is not productive; however someone needs to take the first step.

CHAPTER 5

5. CONCLUSIONS & RECOMMENDATIONS

5.1. Conclusions

Based upon the results of the review and research undertaken in this project, the following conclusions may be drawn:

- The success of IGCC in South Africa depends largely on the success of gasifying the low grade South African coals.
- Coal gasification technologies are well established worldwide, however they still need to be explored for power generation utilising high ash South African coals.
- Sasol has extensive gasification experience with South African coals; however their gasifiers have limited ability to gasify excessive fine coal – fine coal gasification has been identified as the technology of choice for power generation.
- More work still need to be conducted for entrained flow gasification utilising the current coal used for power generation in SA in order to realise potential with IGCC.
- Fluidised bed gasification has been identified to have potential for application with SA coal for power generation.
- The gasification agent has an impact on the quality of gas produced and therefore the emissions produced.
- Coal fired IGCC technology for power generation has not been fully established commercially, and therefore there is not enough operating history to provide confidence in the process and timeframe, and for risk and reference purposes.

- The complexity in the integration of the IGCC systems result in technical issues that reduce plant availability, and therefore this largely affects the success of this technology.
- IGCC has considerable techno-economic potential in the future when carbon capture is implemented because IGCC allows for easier capture of CO_2.
- More specifically, IGCC technology has the potential to meet emission limits set by the South African government.
- The limited operating and cost experience of IGCC technology is a barrier to IGCC penetration

5.2. Recommendations

It is recommended that a similar type of study be done in five to ten years' time to assess the progress of coal fired IGCC for power generation before any major decision to implement this process in South Africa is taken. In the meantime, gasification experiments/test work can help in identifying a suitable surface gasification technology for South African coals.

Sasol has considerable gasification experience with South African coals in the chemical and refining industry, however this is not enough for application in power generation. This experience can nevertheless be utilised to investigate further the limitation of utilising fine coal for the Sasol-Lurgi gasification technology and identify a way around it.

Biomass gasification could also be explored, to determine the impact this would have on the IGCC process both economically and technically. An economic review would assist in terms of the impact biomass would have on the cost of electricity based on the preparation required before gasification and the low energy content. A technical review would assist in terms of the impact it would have on the downstream components of the IGCC process. Its availability should be considered before any decision about pursuing it is taken.

The integration of the IGCC systems and the impact of syngas from SA coals on the downstream process units should be closely investigated, because this seems likely to be where most technical problems lie in the IGCC process. This could start with underground coal gasification (UCG) at the Majuba site as gasification is already established at that location and the constituents of the syngas produced are known. This would assist in selecting the appropriate gas cleaning technology.

The high efficiency of the IGCC technology should be investigated for plant specific conditions in South Africa. This will be affected by the number of process units required which is plant specific. Supplementary firing for the HRSG should be investigated regarding steam raising for steam turbine. The inclusion of supplementary firing in an HRSG may result in increased energy input into the system versus the send out power.

The IGCC technology has a lot of uncertainties and therefore its potential currently cannot be confirmed for application in South Africa. Its penetration in South Africa will largely depend on the identification of a suitable coal gasification technology for South African coals and its performance in terms of meeting stringent SA emission limits when compared to current PC technology. The high costs for the IGCC technology creates a barrier for financiers considering the limited experience in the technology and they may require increased guarantees. A pre-feasibility study would need to be conducted before sufficient confidences could be gained to implement this technology.

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APPENDICES

Appendices A through to D show the calculations of emissions from the combustion of both un-cleaned and pre-cleaned syngas in a gas turbine and the combustion of coal in a PF boiler. The syngas combusted for all four coals was obtained from the gasification of coal utilising air as a gasification agent. The syngas used in appendices B4 and D4 was obtained from the gasification of matla and Duvha coals utilising oxygen as a gasification agent.

The H_2S and NH_3 compositions were assumed to be 0.3 and 0.1 vol% respectively for gasification with air and 0.6 and 0.2 vol% for gasification with oxygen. These typical values were obtained from CSIR.

APPENDIX A: NEW VAAL COAL RESULTS

Appendix A.1: Combustion of un-cleaned syngas

Species	Molar Mass (kg/kmol)	Volume Fraction (%)	mass (kg)	mass%
Carbon monoxide (CO)	28.01	11.10	310.91	11.01
Hydrogen (H2)	2.02	8.60	17.34	0.61
Methane (CH4)	16.04	0.70	11.23	0.40
Carbon dioxide (CO2)	44.01	15.80	695.36	24.63
Nitrogen (N2) & others	28.02	63.30	1773.67	62.82
Hydrogen Sulphide (H2S)	34.08	0.30	10.22	0.36
Ammonia (NH3)	17.03	0.10	1.70	0.06
Oxygen (O2)	32.00	0.10	3.20	0.11
Total		100.00	2823.63	100.00

	Molar mass (kg/kmol)	Ultimate analysis by mass (%)
Total Moistu	18.02	0
Ash	-	0
Carbon	12.01	11.74
Hydrogen	1.01	0.75
Nitrogen	14.01	62.86
Sulphur	32.06	0.34
Oxygen	16.00	24.31
Total		100.00
N from NH3		0.05
N from N2		62.77
Fuel N conversion		0.08

Assumptions

For N_2, the others are mostly H_2S and NH_3 which amount to 0.4%. It is further assumed that the H2S is 0.3% and NH3 is 0.1%

Equations used

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

NEW VAAL

ULTIMATE COAL ANALYSIS

	Dry gas composition	
Total moisture:	0.00	
Ash	0.00	
Carbon	11.74	
Hydrogen	0.75	
Nitrogen	62.86	
Sulphur	0.34	
Oxygen	24.31	
	100.00	
Carbon conversion	100	%
Fuel Nitrogen conversion (NC)	0.08	%
Sulphur conversion	100	%

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

	100/23.2	(2.67C	+8H	+1S	+1.14N*NC	-O fuel)
	4.3103	0.3134	0.0597	0.0034	0.0006	0.2431

0.58 kg/kg fuel

EXCESS AIR

K = -0.1932
n = 5.2974
f = 0.4126

Exhaust g 15.00 %

100/f (O2/(20.9-02)
242.34 2.54
616.12 %

3.56 kg/kg fuel

TOTAL AIR 4.14 kg/kg fuel

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION			PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
$C+2.67O_2$	3.67CO2	0.117	3.670	0.431	8.388	44.01	0.191	5.586	5.71	57072	1.96	112130.55	CO2
$H+8O_2$	9H2O	0.007	9.000	0.067	1.307	18.02	0.073	2.127					
$S+O_2$	2SO2	0.003	2.000	0.007	0.133	64.06	0.002	0.061	0.06	620	2.86	1773.05	SO2
$N+1.14O_2$	2.14NO	0.629	2.140	0.001	0.021	30.01	0.001	0.020	0.02	206	1.34	276.35	NO
N_2	N2	0.629	0.999	0.628	12.229	28.02	0.436	12.792	13.07				N2
Excess O_2	EXCESS O2	3.559	0.232	0.826	16.074	32.00	0.502	14.722	15.04				O2
N_2 AIR	N2 AIR	4.137	0.768	3.177	61.848	28.02	2.207	64.693	66.10				
H_2O	H2O	0.000	1.000	0.000	0.000	18.02	0.000	0.000	0.00				
TOTAL				5.137	100.00		3.41	100.00	100.00				

Appendix A.2: Combustion of pre-cleaned syngas

Species	Molar Mass (kg/kmol)	Volume Fraction (%)	mass (kg)	mass%	pre-cleaned gas mass - 95% H2S & 88% NH3 removed	pre-cleaned gas mass %
Carbon monoxide (CO)	28.01	11.10	310.91	11.01	310.91	11.05
Hydrogen (H2)	2.02	8.60	17.34	0.61	17.34	0.62
Methane (CH4)	16.04	0.70	11.23	0.40	11.23	0.40
Carbon dioxide (CO2)	44.01	15.80	695.36	24.63	695.36	24.72
Nitrogen (N2) & others	28.02	63.30	1773.67	62.82	1773.67	63.07
Hydrogen Sulphide (H2S)	34.08	0.30	10.22	0.36	0.51	0.02
Ammonia (NH3)	17.03	0.10	1.70	0.06	0.20	0.01
Oxygen (O2)	32.00	0.10	3.20	0.11	3.20	0.11
Total		100.00	2823.63	100.00	2812.42	100.00

	Molar mass (kg/kmol)	Ultimate analysis by mass (%)
Total Moisture	18.02	0
Ash	-	0
Carbon	12.01	11.79
Hydrogen	1.01	0.72
Nitrogen	14.01	63.07
Sulphur	32.06	0.02
Oxygen	16.00	24.41
Total		100.00

N from NH3		0.01
N from N2		63.02
Fuel N conversion		0.01

Assumptions

For N_2, the others are mostly H_2S and NH_3 which amount to 0.4%. It is further assumed that the H2S is 0.3% and NH3 is 0.1%

95% of H2S and 88% of NH3 is removed during gas cleaning

Equations used

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

NEW VAAL

ULTIMATE COAL ANALYSIS

	Dry gas composition
Total moisture:	0.00
Ash	0.00
Carbon	11.79
Hydrogen	0.72
Nitrogen	63.07
Sulphur	0.02
Oxygen	24.41
	100.00

Carbon conversion	100 %
Fuel Nitrogen conversion (NC)	0.01 %
Sulphur conversion	100 %

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

100/23.2	(2.67C	+8H	+1S	+1.14N*NC	-O fuel)
4.3103	0.3147	0.0575	0.0002	0.0001	0.2441

0.55 kg/kg fuel

EXCESS AIR

K =	-0.1977	
n =	5.3484	
f =	0.4017	
Exhaust gas O2 dry	15.00	%
100/f	(O2/(20.9-02)	
248.93	2.54	
632.87	%	
3.50	kg/kg fuel	

TOTAL AIR 4.06 kg/kg fuel

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIOMETRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
$C+2.67O_2$	3.67CO2	0.118	3.670	0.433	8.555	44.01	0.194	5.697	5.82	58186	1.96	114319.82	CO2
$H+8O_2$	9H2O	0.007	9.000	0.065	1.280	18.02	0.071	2.083					
$S+O_2$	2SO2	0.000	2.000	0.000	0.007	64.06	0.000	0.003	0.00	32	2.86	90.38	SO2
$N+1.14O_2$	2.14NO	0.631	2.140	0.000	0.003	30.01	0.000	0.002	0.00	25	1.34	33.81	NO
N_2	N2	0.631	1.000	0.631	12.473	28.02	0.445	13.047	13.32				N2
Excess O_2	EXCESS O2	3.503	0.232	0.813	16.072	32.00	0.502	14.721	15.03				O2
N_2 AIR	N2 AIR	4.056	0.768	3.115	61.611	28.02	2.199	64.446	65.82				
H_2O	H2O	0.000	1.000	0.000	0.000	18.02	0.000	0.000	0.00				
TOTAL				5.056	100.00		3.41	100.00	100.00				

Appendix A.3: Combustion of pulverised coal

	Molar mass (kg/kmol)	Ultimate analysis by mass AD (%)	Ultimate analysis by mass AF (%)
Total Moisture	18.02	5.91	10.83
Ash	-	40.2	38.10
Carbon	12.01	42.58	40.35
Hydrogen	1.01	2.19	2.08
Nitrogen	14.01	0.89	0.84
Sulphur	32.06	0.69	0.65
Oxygen	16.00	7.54	7.15
Total		100.00	100.00

Assumptions

Sulphur conversion depends on the type of mills used, for tube mills the sulphur converted will be more compared to the sulphur converted in vertical spindle mills. This is due to the fact that vertical spindle mills have rejects and some of the sulphur will be in the rejects. EPRI gives a sulphur conversion of 94% while the combustion engineering's handbook gives a conversion of 90%. in this case a worse case scenario of 94% will be used

It is assumed that the nitrogen in the fuel converting is 20% (innovative combustion technologies inc., 2011). It should be noted however that the fuel nitrogen conversion will be influenced by the type of burner orientation. Tangentially fired boilers produce less NOx compared to wall fired.

The total moisture used is the average from Eskom for 2007

Equations used

Unburnt carbon = (Carbon in ash%/100)*(Ash%/(100-carbon in ash))

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

NEW VAAL COAL

ULTIMATE COAL ANALYSIS

	Coal composition	
Total moisture:	10.83	
Ash	38.10	
Carbon	40.35	
Hydrogen	2.08	
Nitrogen	0.84	
Sulphur	0.65	
Oxygen	7.15	
	100.00	
Carbon conversion	100	%
Fuel Nitrogen conversion (NC)	20.00	%
Sulphur conversion	90	%
Carbon in ash	0.73	%
Unburnt carbon (UC)	0.0028	kg/kg fuel

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

	100/23.2	(2.67(C-UC)	+8H	+1S*SC	+1.14N*NC	-O fuel)
	4.3103	1.0700	0.1660	0.0059	0.0019	0.0715
	5.05	kg/kg fuel				

EXCESS AIR

K =	0.0291	
n =	0.0208	
f =	1.0154	
Exhaust gas	10.00	%
100/f	(O2/(20.9-02)	
98.48	0.92	
90.35	%	
4.57	kg/kg fuel	
TOTAL AIR	9.62	kg/kg fuel

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION			PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
$C+2.67O_2$	3.67CO2	0.401	3.670	1.4707	14.370	44.01	0.327	9.628	9.92	99243	1.96	194985.93	CO2
$H+8O_2$	9H2O	0.021	9.000	0.1868	1.825	18.02	0.101	2.987					
$S+O_2$	2SO2	0.006	2.000	0.0118	0.115	64.06	0.002	0.053	0.05	546	2.86	1560.55	SO2
$N+1.14O_2$	2.14NO	0.008	2.140	0.0036	0.035	30.01	0.001	0.035	0.04	357	1.34	478.62	NO
N_2	N2	0.008	0.800	0.0067	0.066	28.02	0.002	0.069	0.07				N2
Excess O_2	EXCESS O2	4.566	0.232	1.0593	10.350	32.00	0.323	9.537	9.83				O2
N_2 AIR	N2 AIR	9.619	0.768	7.3874	72.181	28.02	2.576	75.959	78.30				
H_2O	H2O	0.108	1.000	0.1083	1.058	18.02	0.059	1.732	1.79				
Unburnt sulphur	S2	0.0065392	0.1	0.0007									
Ash			0.381	0.3810									
Unburnt carbon			0.003	0.0028									
TOTAL				10.619	100.00		3.39	100.00	100.00				

APPENDIX B: MATLA COAL RESULTS

Appendix B.1: Combustion of un-cleaned syngas

Species	Molar Mass (kg/kmol)	Volume Fraction (%)	mass (kg)	mass%
Carbon monoxide (CO)	28.01	10.80	302.51	10.92
Hydrogen (H2)	2.02	10.00	20.16	0.73
Methane (CH4)	16.04	0.80	12.83	0.46
Carbon dioxide (CO2)	44.01	14.80	651.35	23.51
Nitrogen (N2) & others	28.02	63.10	1768.06	63.83
Hydrogen Sulphide (H2S)	34.08	0.30	10.22	0.37
Ammonia (NH3)	17.03	0.10	1.70	0.06
Oxygen (O2)	32.00	0.10	3.20	0.12
Total		100.00	2770.04	100.00

	Molar mass (kg/kmol)	Ultimate analysis by mass (%)
Total Moistur	18.02	0
Ash	-	0
Carbon	12.01	11.45
Hydrogen	1.01	0.88
Nitrogen	14.01	63.88
Sulphur	32.06	0.35
Oxygen	16.00	23.45
Total		100.00
N from NH3		0.05
N from N2		63.83
Fuel N conversion		0.08

Assumptions

For N2, the others are mostly H2S and NH3 which amount to 0.4%. It is further assumed that the H2S is 0.3% and NH3 is 0.1%

Equations used

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

MATLA 1

ULTIMATE COAL ANALYSIS

	Dry gas composition	
Total moisture:	0.00	
Ash	0.00	
Carbon	11.45	
Hydrogen	0.88	
Nitrogen	63.88	
Sulphur	0.35	
Oxygen	23.45	
	100.00	
Carbon conversion	100	%
Fuel Nitrogen conversion (NC)	0.08	%
Sulphur conversion	100	%

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

	100/23.2	(2.67C	+8H	+1S	+1.14N*N	-O fuel)
	4.3103	0.3056	0.0702	0.0035	0.0006	0.2345
	0.63	kg/kg fuel				

EXCESS AIR

K =	-0.1775	
n =	5.5180	
f =	0.4346	
Exhaust gas	15.00	%
100/f	(O2/(20.9-02)	
230.11	2.54	
585.03	%	
3.66	kg/kg fuel	
TOTAL AIR	4.29	kg/kg fuel

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIOMETRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
$C+2.67O_2$	3.67CO2	0.11	3.67	0.42	9.03	44.01	0.21	6.03	6.20	62031	1.96	121873.39	CO2
$H+8O_2$	9H2O	0.01	9.00	0.08	1.70	18.02	0.09	2.77					
$S+O_2$	2SO2	0.00	2.00	0.01	0.15	64.06	0.00	0.07	0.07	704	2.86	2014.70	SO2
$N+1.14O_2$	2.14NO	0.64	2.14	0.00	0.02	30.01	0.00	0.02	0.02	234	1.34	313.79	NO
N_2	N2	0.64	0.001	0.00	0.01	28.02	0.00	0.01	0.01				
Excess O_2	EXCESS O2	3.66	0.23	0.85	18.27	32.00	0.57	16.79	17.26				
N_2 AIR	N2 AIR	4.29	0.77	3.30	70.82	28.02	2.53	74.31	76.43				
H_2O	H2O	0.00	1.00	0.00	0.00	18.02	0.00	0.00	0.00				
TOTAL				4.653	100.00		3.40	100.00	100.00				

Species	Molar Mass (kg/kmol)	Volume Fraction (%)	mass (kg)	mass%
Carbon monoxide (CO)	28.01	11.60	324.92	11.69
Hydrogen (H2)	2.02	9.60	19.35	0.70
Methane (CH4)	16.04	0.70	11.23	0.40
Carbon dioxide (CO2)	44.01	14.60	642.55	23.13
Nitrogen (N2) & others	28.02	63.00	1765.26	63.53
Hydrogen Sulphide (H2S)	34.08	0.30	10.22	0.37
Ammonia (NH3)	17.03	0.10	1.70	0.06
Oxygen (O2)	32.00	0.10	3.20	0.12
Total		100.00	2778.43	100.00

	Molar mass (kg/kmol)	Ultimate analysis by mass (%)
Total Moisture	18.02	0
Ash	-	0
Carbon	12.01	11.63
Hydrogen	1.01	0.83
Nitrogen	14.01	63.58
Sulphur	32.06	0.35
Oxygen	16.00	23.61
Total		100.00
N from NH3		0.05
N from N2		63.53
Fuel N conversion		0.08

Assumptions

For N_2, the others are mostly H_2S and NH_3 which amount to 0.4%. It is further assumed that they are each 0.2%

Equations used

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

MATLA 2

ULTIMATE COAL ANALYSIS

	Dry gas composition
Total moisture:	0.00
Ash	0.00
Carbon	11.63
Hydrogen	0.83
Nitrogen	63.58
Sulphur	0.35
Oxygen	23.61
	100.00
Carbon conversion	100 %
Fuel Nitrogen conversion (NC)	0.08
Sulphur conversion	100 %

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

100/23.2	(2.67C	+8H	+1S	+1.14N*NC	-O fuel)
4.3103	0.3105	0.0665	0.0035	0.0006	0.2361

0.62 kg/kg fuel

EXCESS AIR

K = -0.1804

n = 5.4080

f = 0.4333

Exhaust gas O2 15.00 %

100/f (O2/(20.9-02)

230.81 2.54

586.80 %

3.66 kg/kg fuel

TOTAL AI 4.29 kg/kg fuel

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIOMETRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
C+2.67O_2	3.67CO2	0.12	3.67	0.43	9.17	44.01	0.21	6.13	6.30	62980	1.96	123739.48	CO2
H+8O_2	9H2O	0.01	9.00	0.07	1.61	18.02	0.09	2.62					
S+O_2	2SO2	0.00	2.00	0.01	0.15	64.06	0.00	0.07	0.07	702	2.86	2007.53	SO2
N+1.14O_2	2.14NO	0.64	2.14	0.00	0.02	30.01	0.00	0.02	0.02	233	1.34	312.67	NO
N_2	N2	0.64	0.001	0.00	0.01	28.02	0.00	0.01	0.01				
Excess O_2	EXCESS O2	3.66	0.23	0.85	18.27	32.00	0.57	16.80	17.25				
N_2 AIR	N2 AIR	4.29	0.77	3.29	70.77	28.02	2.53	74.34	76.34				
H_2O	H2O	0.00	1.00	0.00	0.00	18.02	0.00	0.00	0.00				
TOTAL				4.653	100.00		3.40	100.00	100.00				

Appendix B.2: Combustion of pre-cleaned syngas

Species	Molar Mass (kg/kmol)	Volume Fraction (%)	mass (kg)	mass%	pre-cleaned gas mass - 95% H2S & 88% NH3 removed	pre-cleaned gas mass %
Carbon monoxide (CO)	28.01	10.80	302.51	10.92	302.51	10.97
Hydrogen (H2)	2.02	10.00	20.16	0.73	20.16	0.73
Methane (CH4)	16.04	0.80	12.83	0.46	12.83	0.47
Carbon dioxide (CO2)	44.01	14.80	651.35	23.51	651.35	23.61
Nitrogen (N2) & others	28.02	63.10	1768.06	63.83	1768.06	64.09
Hydrogen Sulphide (H2S)	34.08	0.30	10.22	0.37	0.51	0.02
Ammonia (NH3)	17.03	0.10	1.70	0.06	0.20	0.01
Oxygen (O2)	32.00	0.10	3.20	0.12	3.20	0.12
Total		100.00	2770.04	100.00	2758.83	100.00

	Molar mass (kg/kmol)	Ultimate analysis by mass (%)
Total Moi	18.02	0
Ash	-	0
Carbon	12.01	11.49
Hydroge	1.01	0.85
Nitroge	14.01	64.09
Sulphur	32.06	0.02
Oxygen	16.00	23.55
Total		100.00
N from NH3		0.01
N from N2		64.04
Fuel N conversion		0.01

Assumptions

For N_2, the others are mostly H_2S and NH_3 which amount to 0.4%. It is further assumed that the H2S is 0.3% and NH3 is 0.1%

95% of H2S and 88% of NH3 is removed during gas cleaning

Equations used

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

MATLA 1

ULTIMATE COAL ANALYSIS

	Dry gas composition
Total moisture:	0.00
Ash	0.00
Carbon	11.49
Hydrogen	0.85
Nitrogen	64.09
Sulphur	0.02
Oxygen	23.55
	100.00
Carbon conversion	100 %
Fuel Nitrogen conversion (NC)	0.01 %
Sulphur conversion	100 %

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

100/23.2	(2.67C	+8H	+1S	+1.14N*NC	-O fuel)
4.3103	0.3069	0.0680	0.0002	0.0001	0.2355

0.60 kg/kg fuel

EXCESS AIR

K =	-0.1820
n =	5.5737
f =	0.4241

Exhaust g 15.00 %

100/f	(O2/(20.9-02)
235.78	2.54

599.44 %

3.61 kg/kg fuel

TOTAL AIR 4.21 kg/kg fuel

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIOMETRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
$C+2.67O_2$	3.67CO2	0.11	3.67	0.42	9.23	44.01	0.21	6.17	6.34	63408	1.96	124579.33	CO2
$H+8O_2$	9H2O	0.01	9.00	0.08	1.67	18.02	0.09	2.73					
$S+O_2$	2SO2	0.00	2.00	0.00	0.01	64.06	0.00	0.00	0.00	36	2.86	102.97	SO2
$N+1.14O_2$	2.14NO	0.64	2.14	0.00	0.00	30.01	0.00	0.00	0.00	29	1.34	38.52	NO
N_2	N2	0.64	0.0001	0.00	0.00	28.02	0.00	0.00	0.00				
Excess O_2	EXCESS O2	3.61	0.23	0.84	18.32	32.00	0.57	16.83	17.31				
N_2 AIR	N2 AIR	4.21	0.77	3.23	70.76	28.02	2.53	74.26	76.34				
H_2O	H2O	0.00	1.00	0.00	0.00	18.02	0.00	0.00	0.00				
TOTAL				4.569	100.00		3.40	#######	100.00				

Species	Molar Mass (kg/kmol)	Volume Fraction (%)	mass (kg)	mass%	pre-cleaned gas mass - 95% H2S & 88% NH3 removed	pre-cleaned gas mass %
Carbon monoxide (CO)	28.01	11.60	324.92	11.69	324.92	11.74
Hydrogen (H2)	2.02	9.60	19.35	0.70	19.35	0.70
Methane (CH4)	16.04	0.70	11.23	0.40	11.23	0.41
Carbon dioxide (CO2)	44.01	14.60	642.55	23.13	642.55	23.22
Nitrogen (N2) & others	28.02	63.00	1765.26	63.53	1765.26	63.79
Hydrogen Sulphide (H2S)	34.08	0.30	10.22	0.37	0.51	0.02
Ammonia (NH3)	17.03	0.10	1.70	0.06	0.20	0.01
Oxygen (O2)	32.00	0.10	3.20	0.12	3.20	0.12
Total		100.00	2778.43	100.00	2767.22	100.00

	Molar mass (kg/kmol)	Ultimate analysis by mass (%)
Total Moisture	18.02	0
Ash	-	0
Carbon	12.01	11.67
Hydrogen	1.01	0.80
Nitrogen	14.01	63.80
Sulphur	32.06	0.02
Oxygen	16.00	23.71
Total		100.00
N from NH3		0.01
N from N2		63.75
Fuel N conversion		0.01

Assumptions

For N_2, the others are mostly H_2S and NH_3 which amount to 0.4%. It is further assumed that the H2S is 0.3% and NH3 is 0.1%

95% of H2S and 88% of NH3 is removed during gas cleaning

Equations used

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

MATLA 2

ULTIMATE COAL ANALYSIS

	Dry gas composition
Total moisture:	0.00
Ash	0.00
Carbon	11.67
Hydrogen	0.80
Nitrogen	63.80
Sulphur	0.02
Oxygen	23.71
	100.00
Carbon conversion	100 %
Fuel Nitrogen conversion (NC)	0.01
Sulphur conversion	100 %

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

	100/23.2	(2.67C	+8H	+1S	+1.14N*NC	-O fuel)
	4.3103	0.3117	0.0643	0.0002	0.0001	0.2371

0.60 kg/kg fuel

EXCESS AIR

K =		-0.1849
n =		5.4615
f =		0.4228
Exhaust gas O2 d		15.00 %
100/f		(O2/(20.9-02)
	236.51	2.54
	601.28 %	
	3.61	kg/kg fuel
TOTAL AIR	4.21	kg/kg fuel

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIOMETRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
C+2.67O_2	3.67CO2	0.12	3.67	0.43	9.38	44.01	0.21	6.27	6.44	64374	1.96	126477.80	CO2
H+8O_2	9H2O	0.01	9.00	0.07	1.58	18.02	0.09	2.59					
S+O_2	2SO2	0.00	2.00	0.00	0.01	64.06	0.00	0.00	0.00	36	2.86	102.60	SO2
N+1.14O_2	2.14NO	0.64	2.14	0.00	0.00	30.01	0.00	0.00	0.00	29	1.34	38.38	NO
N_2	N2	0.64	0.0001	0.00	0.00	28.02	0.00	0.00	0.00				
Excess O_2	EXCESS O2	3.61	0.23	0.84	18.32	32.00	0.57	16.85	17.30				
N_2 AIR	N2 AIR	4.21	0.77	3.23	70.71	28.02	2.52	74.29	76.26				
H_2O	H2O	0.00	1.00	0.00	0.00	18.02	0.00	0.00	0.00				
TOTAL				4.570	100.00		3.40	100.00	100.00				

Appendix B.3: Combustion of pulverised coal

	Molar mass (kg/kmol)	Ultimate analysis by mass AD(%)	Ultimate analysis by mass AF (%)
Total Moisture	18.02	3.51	8.96
Ash	-	33.4	31.51
Carbon	12.01	50.66	47.80
Hydrogen	1.01	2.65	2.50
Nitrogen	14.01	1.07	1.01
Sulphur	32.06	0.74	0.70
Oxygen	16.00	7.97	7.52
Total		100.00	100.00

Assumptions

Sulphur conversion depends on the type of mills used, for tube mills the sulphur converted will be more compared to the sulphur converted in vertical spindle mills. This is due to the fact that vertical spindle mills have rejects and some of the sulphur will be in the rejects. EPRI gives a sulphur conversion of 94% while the combustion engineering's handbook gives a conversion of 90%. in this case a worse case scenario of 94% will be used

It is assumed that the nitrogen in the fuel converting is 20% based on ref(innovative combustion technologies). It should be noted however that the fuel nitrogen conversion will be influenced by the type of burner orientation. Tangentially fired boilers produce less NOx compared to wall fired.

The total moisture used is the average from Eskom for 2007

Equations used

Unburnt carbon = (Carbon in ash%/100)*(Ash%/(100-carbon in ash))

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

MATLA COAL

ULTIMATE COAL ANALYSIS

	Coal composition	
Total moisture:	8.96	
Ash	31.51	
Carbon	47.80	
Hydrogen	2.50	
Nitrogen	1.01	
Sulphur	0.70	
Oxygen	7.52	
	100.00	
Carbon conversion	100	%
Fuel Nitrogen conversion (NC)	20.00	%
Sulphur conversion	90	%
Carbon in ash	0.73	%
Unburnt carbon (UC)	0.0023	kg/kg fuel

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

	100/23.2	(2.67(C-UC)	+8H	+1S*SC	+1.14N*NC	-O fuel)
	4.3103	1.2700	0.2000	0.0063	0.0023	0.0752
	6.05	kg/kg fuel				

EXCESS AIR

K =	0.0325	
n =	0.0210	
f =	1.0172	
Exhaust gas	10.00	%
100/f	(O2/(20.9-02)	
98.31	0.92	
90.19	%	
5.46	kg/kg fuel	
TOTAL AIR	11.51	kg/kg fuel

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIOMETRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
$C+2.67O_2$	3.67CO2	0.476	3.670	1.7457	14.324	44.01	0.325	9.612	9.91	99122	1.96	194748.76	CO2
$H+8O_2$	9H2O	0.025	9.000	0.2250	1.846	18.02	0.102	3.027					
$S+O_2$	2SO2	0.006	2.000	0.0126	0.103	64.06	0.002	0.048	0.05	490	2.86	1402.03	SO2
$N+1.14O_2$	2.14NO	0.010	2.140	0.0043	0.035	30.01	0.001	0.035	0.04	360	1.34	482.04	NO
N_2	N2	0.010	0.800	0.0081	0.066	28.02	0.002	0.070	0.07				N2
Excess O_2	EXCESS O2	5.456	0.232	1.2658	10.386	32.00	0.325	9.585	9.88				O2
N_2 AIR	N2 AIR	11.505	0.768	8.8361	72.503	28.02	2.588	76.418	78.80				
H_2O	H2O	0.090	1.000	0.0896	0.735	18.02	0.041	1.205	1.24				
Unburnt sulphur	S2	0.00698203	0.1	0.0007									
Ash			0.315	0.3151									
Unburnt carbon			0.002	0.0023									
TOTAL				12.505	100.00		3.39	100.00	100.00				

Appendix B.4: Combustion of pre-cleaned oxygen fired syngas

Species	Molar Mass (kg/kmol)	Volume Fraction (%)	mass (kg)	mass%	pre-cleaned gas mass - 95% H2S & 88% NH3 removed	pre-cleaned gas mass %
Carbon monoxide (CO)	28.01	19.00	532.19	19.01	532.19	19.17
Hydrogen (H2)	2.02	27.60	55.64	1.99	55.64	2.00
Methane (CH4)	16.04	2.00	32.08	1.15	32.08	1.16
Carbon dioxide (CO2)	44.01	46.10	2028.86	72.48	2028.86	73.07
Nitrogen (N2) & others	28.02	4.40	123.29	4.40	123.29	4.44
Hydrogen Sulphide (H2S)	34.08	0.60	20.45	0.73	1.02	0.04
Ammonia (NH3)	17.03	0.20	3.41	0.12	0.41	0.01
Oxygen (O2)	32.00	0.10	3.20	0.11	3.20	0.12
Total		100.00	2799.12	100.00	2776.70	100.00

	Molar mass (kg/kmol)	Ultimate analysis by mass (%)
Total Moistur	18.02	0
Ash	-	0
Carbon	12.01	29.02
Hydrogen	1.01	2.30
Nitrogen	14.01	4.45
Sulphur	32.06	0.03
Oxygen	16.00	64.19
Total		100.00

N from NH3		0.01
N from N2		4.44
Fuel N conversio		0.27

Assumptions

For N_2, the others are mostly H_2S and NH_3 which amount to 0.8%. It is further assumed that the H2S is 0.6% and NH3 is 0.2%

95% of H2S and 88% of NH3 is removed during gas cleaning

Equations used

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

MATLA 2

ULTIMATE COAL ANALYSIS

	Dry gas composition
Total moisture:	0.00
Ash	0.00
Carbon	29.02
Hydrogen	2.30
Nitrogen	4.45
Sulphur	0.03
Oxygen	64.19
	100.00

Carbon conversion 100 %

Fuel Nitrogen conversion (NC) 0.27

Sulphur conversion 100 %

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

	100/23.2	(2.67C	+8H	+1S	+1.14N*NC	-O fuel)
	4.3103	0.7749	0.1839	0.0003	0.0001	0.6419

1.37 kg/kg fuel

EXCESS AIR

K = -0.1972

n = 0.1533

f = 0.7475

Exhaust gas O2 dry 15.00 %

100/f (O2/(20.9-02)

133.79 2.54

340.13 %

4.65 kg/kg fuel

TOTAL AIR 6.02 kg/kg fuel

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIOMETRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
C+2.67O_2	3.67CO2	0.29	3.67	1.07	15.27	44.01	0.35	10.32	10.85	108526	1.96	########	CO2
H+8O_2	9H2O	0.02	9.00	0.21	2.97	18.02	0.16	4.90					
S+O_2	2SO2	0.00	2.00	0.00	0.01	64.06	0.00	0.00	0.00	48	2.86	138.68	SO2
N+1.14O_2	2.14NO	0.04	2.14	0.00	0.00	30.01	0.00	0.00	0.00	39	1.34	51.88	NO
N_2	N2	0.04	0.00	0.00	0.00	28.02	0.00	0.00	0.00				
Excess O_2	EXCESS O2	4.65	0.23	1.08	15.47	32.00	0.48	14.39	15.13				
N_2 AIR	N2 AIR	6.02	0.77	4.62	66.28	28.02	2.37	70.38	74.01				
H_2O	H2O	0.00	1.00	0.00	0.00	18.02	0.00	0.00	0.00				
TOTAL				6.977	100.00		3.36	100.00	######				

APPENDIX C: GROOTEGELUK COAL RESULTS

Appendix C.1: Combustion of un-cleaned syngas

Species	Molar Mass (kg/kmol)	Volume Fraction (%)	mass (kg)	mass%
Carbon monoxide (CO)	28.01	8.70	243.69	8.75
Hydrogen (H2)	2.02	9.40	18.95	0.68
Methane (CH4)	16.04	1.10	17.65	0.63
Carbon dioxide (CO2)	44.01	15.00	660.15	23.70
Nitrogen (N2) & others	28.02	65.30	1829.71	65.69
Hydrogen Sulphide (H2S)	34.08	0.30	10.22	0.37
Ammonia (NH3)	17.03	0.10	1.70	0.06
Oxygen (O2)	32.00	0.10	3.20	0.11
Total		100.00	2785.27	100.00

	Molar mass (kg/kmol)	Ultimate analysis by mass (%)
Total Moisture	18.02	0
Ash	-	0
Carbon	12.01	10.69
Hydrogen	1.01	0.87
Nitrogen	14.01	65.74
Sulphur	32.06	0.35
Oxygen	16.00	22.35
Total		100.00
N from NH3		0.05
N from N2		65.69
Fuel N conversion		0.08

Assumptions

For N2, the others are mostly H2S and NH3 which amount to 0.4%. It is further assumed that the H2S is 0.3% and NH3 is 0.1%

Equations used

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

GROOTEGELUK 1

ULTIMATE COAL ANALYSIS

	Dry gas composition
Total moisture:	0.00
Ash	0.00
Carbon	10.69
Hydrogen	0.87
Nitrogen	65.74
Sulphur	0.35
Oxygen	22.35
	100.00
Carbon conversion	100 %
Fuel Nitrogen conversion (NC)	0.08 %
Sulphur conversion	100 %

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

	100/23.2	(2.67C	+8H	+1S	+1.14N*N-O fuel)	
	4.3103	0.2855	0.0698	0.0035	0.0006	0.2235
	0.59	kg/kg fuel				

EXCESS AIR

K =	-0.1775	
n =	6.0742	
f =	0.4152	
Exhaust gas O2	15.00	%
100/f	(O2/(20.9-O2)	
240.85	2.54	
612.34	%	
3.59	kg/kg fuel	
TOTAL AIR 4.17	kg/kg fuel	

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIOMETRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
$C+2.67O_2$	3.67CO2	0.11	3.67	0.39	8.69	44.01	0.20	5.80	5.97	59683	1.96	117260.95	CO2
$H+8O_2$	9H2O	0.01	9.00	0.08	1.74	18.02	0.10	2.83					
$S+O_2$	2SO2	0.00	2.00	0.01	0.15	64.06	0.00	0.07	0.07	722	2.86	2063.51	SO2
$N+1.14O_2$	2.14NO	0.66	2.14	0.00	0.02	30.01	0.00	0.02	0.02	240	1.34	321.39	NO
N_2	N2	0.66	0.001	0.00	0.01	28.02	0.00	0.01	0.01				
Excess O_2	EXCESS O2	3.59	0.23	0.83	18.43	32.00	0.58	16.91	17.40				
N_2 AIR	N2 AIR	4.17	0.77	3.20	70.96	28.02	2.53	74.36	76.52				
H_2O	H2O	0.00	1.00	0.00	0.00	18.02	0.00	0.00	0.00				
TOTAL				4.515	100.00		3.41	100.00	#######				

Species	Molar Mass (kg/kmol)	Volume Fraction (%)	mass (kg)	mass%
Carbon monoxide (CO)	28.01	10.20	285.70	10.27
Hydrogen (H2)	2.02	9.50	19.15	0.69
Methane (CH4)	16.04	1.10	17.65	0.63
Carbon dioxide (CO2)	44.01	14.90	655.75	23.58
Nitrogen (N2) & others	28.02	63.80	1787.68	64.28
Hydrogen Sulphide (H2S)	34.08	0.30	10.22	0.37
Ammonia (NH3)	17.03	0.10	1.70	0.06
Oxygen (O2)	32.00	0.10	3.20	0.12
Total		100.00	2781.05	100.00

	Molar mass (kg/kmol)	Ultimate analysis by mass (%)
Total Moisture	18.02	0
Ash	-	0
Carbon	12.01	11.31
Hydrogen	1.01	0.88
Nitrogen	14.01	64.33
Sulphur	32.06	0.35
Oxygen	16.00	23.13
Total		100.00
N from NH3		0.05
N from N2		64.28
Fuel N conversion		0.08

Assumptions

For N2, the others are mostly H2S and NH3 which amount to 0.4%. It is further assumed that the H2S is 0.3% and NH3 is 0.1%

Equations used

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

GROOTEGELUK 2

ULTIMATE COAL ANALYSIS

	Dry gas composition
Total moisture:	0.00
Ash	0.00
Carbon	11.31
Hydrogen	0.88
Nitrogen	64.33
Sulphur	0.35
Oxygen	23.13
	100.00

Carbon conversion	100	%
Fuel Nitrogen conversion (NC)	0.08	
Sulphur conversion	100	%

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

	100/23.2	(2.67C	+8H	+1S	+1.14N*f	-O fuel)
	4.3103	0.3021	0.0705	0.0035	0.0006	0.2313
	0.63	kg/kg fuel				

EXCESS AIR

K =	-0.1757	
n =	5.6213	
f =	0.4341	
Exhaust gas O2	15.00	%
100/f	(O2/(20.9-O2)	
230.35	2.54	
585.62	%	
3.67	kg/kg fuel	
TOTAL AI 4.29	kg/kg fuel	

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIOMETRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
$C+2.67O_2$	3.67CO2	0.11	3.67	0.42	8.93	44.01	0.20	5.96	6.13	61310	1.96	120457.43	CO2
$H+8O_2$	9H2O	0.01	9.00	0.08	1.70	18.02	0.09	2.78					
$S+O_2$	2SO2	0.00	2.00	0.01	0.15	64.06	0.00	0.07	0.07	702	2.86	2006.49	SO2
$N+1.14O_2$	2.14NO	0.64	2.14	0.00	0.02	30.01	0.00	0.02	0.02	233	1.34	312.51	NO
N_2	N2	0.64	0.001	0.00	0.01	28.02	0.00	0.01	0.01				
Excess O_2	EXCESS O2	3.67	0.23	0.85	18.29	32.00	0.57	16.80	17.28				
N_2 AIR	N2 AIR	4.29	0.77	3.30	70.89	28.02	2.53	74.36	76.48				
H_2O	H2O	0.00	1.00	0.00	0.00	18.02	0.00	0.00	0.00				
TOTAL				4.652	100.00		3.40	100.00	100.00				

Appendix C.2: Combustion of pre-cleaned syngas

Species	Molar Mass (kg/kmol)	Volume Fraction (%)	mass (kg)	mass%	pre-cleaned gas mass - 95% H2S & 88% NH3 removed	pre-cleaned gas mass %
Carbon monoxide (CO)	28.01	8.70	243.69	8.75	243.69	8.78
Hydrogen (H2)	2.02	9.40	18.95	0.68	18.95	0.68
Methane (CH4)	16.04	1.10	17.65	0.63	17.65	0.64
Carbon dioxide (CO2)	44.01	15.00	660.15	23.70	660.15	23.80
Nitrogen (N2) & others	28.02	65.30	1829.71	65.69	1829.71	65.96
Hydrogen Sulphide (H2S)	34.08	0.30	10.22	0.37	0.51	0.02
Ammonia (NH3)	17.03	0.10	1.70	0.06	0.20	0.01
Oxygen (O2)	32.00	0.10	3.20	0.11	3.20	0.12
Total		100.00	2785.27	100.00	2774.06	100.00

	Molar mass (kg/kmol)	Ultimate analysis by mass (%)
Total Mol	18.02	0
Ash	-	0
Carbon	12.01	10.74
Hydroge	1.01	0.85
Nitroge	14.01	65.96
Sulphur	32.06	0.02
Oxygen	16.00	22.44
Total		100.00
N from NH3		0.01
N from N2		65.91
Fuel N conversio		0.01

Assumptions

For N_2, the others are mostly H_2S and NH_3 which amount to 0.4%. It is further assumed that the H2S is 0.3% and NH3 is 0.1%

95% of H2S and 88% of NH3 is removed during gas cleaning

Equations used

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

GROOTEGELUK 1

ULTIMATE COAL ANALYSIS

	Dry gas composition	
Total moisture:	0.00	
Ash	0.00	
Carbon	10.74	
Hydrogen	0.85	
Nitrogen	65.96	
Sulphur	0.02	
Oxygen	22.44	
	100.00	
Carbon conversion	100	%
Fuel Nitrogen conversion (NC)	0.01	%
Sulphur conversion	100	%

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

	100/23.2	(2.67C	+8H	+1S	+1.14N*NC	-O fuel)
	4.3103	0.2867	0.0676	0.0002	0.0001	0.2244
	0.56	kg/kg fuel				

EXCESS AIR

K =	-0.1824	
n =	6.1399	
f =	0.4043	
Exhaust gas O2 (	15.00	%
100/f	(O2/(20.9-02)	
247.37	2.54	
628.91	%	
3.53	kg/kg fuel	
TOTAL AIR 4.09	kg/kg fuel	

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIOMETRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
$C+2.67O_2$	3.67CO2	0.11	3.67	0.39	8.89	44.01	0.20	5.93	6.10	61049	1.96	119945.16	CO2
$H+8O_2$	9H2O	0.01	9.00	0.08	1.72	18.02	0.10	2.80					
$S+O_2$	2SO2	0.00	2.00	0.00	0.01	64.06	0.00	0.00	0.00	37	2.86	105.54	SO2
$N+1.14O_2$	2.14NO	0.66	2.14	0.00	0.00	30.01	0.00	0.00	0.00	29	1.34	39.48	NO
N_2	N2	0.66	0.0001	0.00	0.00	28.02	0.00	0.00	0.00				
Excess O_2	EXCESS O2	3.53	0.23	0.82	18.48	32.00	0.58	16.96	17.45				
N_2 AIR	N2 AIR	4.09	0.77	3.14	70.90	28.02	2.53	74.30	76.44				
H_2O	H2O	0.00	1.00	0.00	0.00	18.02	0.00	0.00	0.00				
TOTAL				4.431	100.00		3.41	#######	100.00				

Species	Molar Mass (kg/kmol)	Volume Fraction (%)	mass (kg)	mass%	pre-cleaned gas mass - 95% H2S & 88% NH3 removed	pre-cleaned gas mass %
Carbon monoxide (CO)	28.01	10.20	285.70	10.27	285.70	10.31
Hydrogen (H2)	2.02	9.50	19.15	0.69	19.15	0.69
Methane (CH4)	16.04	1.10	17.65	0.63	17.65	0.64
Carbon dioxide (CO2)	44.01	14.90	655.75	23.58	655.75	23.67
Nitrogen (N2) & others	28.02	63.80	1787.68	64.28	1787.68	64.54
Hydrogen Sulphide (H2S)	34.08	0.30	10.22	0.37	0.51	0.02
Ammonia (NH3)	17.03	0.10	1.70	0.06	0.20	0.01
Oxygen (O2)	32.00	0.10	3.20	0.12	3.20	0.12
Total		100.00	2781.05	100.00	2769.84	100.00

	Molar mass (kg/kmol)	Ultimate analysis by mass (%)
Total Moisture	18.02	0
Ash	-	0
Carbon	12.01	11.36
Hydrogen	1.01	0.85
Nitrogen	14.01	64.55
Sulphur	32.06	0.02
Oxygen	16.00	23.22
Total		100.00

N from NH3	0.01
N from N2	64.49
Fuel N conversion	0.01

Assumptions

For N_2, the others are mostly H_2S and NH_3 which amount to 0.4%. It is further assumed that the H2S is 0.3% and NH3 is 0.1%

95% of H2S and 88% of NH3 is removed during gas cleaning

Equations used

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

GROOTEGELUK 2

ULTIMATE COAL ANALYSIS

	Dry gas composition	
Total moisture:	0.00	
Ash	0.00	
Carbon	11.36	
Hydrogen	0.85	
Nitrogen	64.55	
Sulphur	0.02	
Oxygen	23.22	
	100.00	
Carbon conversion	100	%
Fuel Nitrogen conversion (NC	0.01	
Sulphur conversion	100	%

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

	100/23.2	(2.67C	+8H	+1S	+1.14N*NC	-O fuel)
	4.3103	0.3033	0.0683	0.0002	0.0001	0.2322
	0.60	kg/kg fuel				

EXCESS AIR

K	=	-0.1802
n	=	5.6785
f	=	0.4237

Exhaust gas O2	15.00	%
100/f	(O2/(20.9-02)	
236.00	2.54	
599.99	%	
3.61	kg/kg fuel	
TOTAL AIR 4.21	kg/kg fuel	

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIOMETRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
$C+2.67O_2$	3.67CO2	0.11	3.67	0.42	9.13	44.01	0.21	6.09	6.27	62666	1.96	123121.24	CO2
$H+8O_2$	9H2O	0.01	9.00	0.08	1.68	18.02	0.09	2.74					
$S+O_2$	2SO2	0.00	2.00	0.00	0.01	64.06	0.00	0.00	0.00	36	2.86	102.54	SO2
$N+1.14O_2$	2.14NO	0.65	2.14	0.00	0.00	30.01	0.00	0.00	0.00	29	1.34	38.36	NO
N_2	N2	0.65	0.0001	0.00	0.00	28.02	0.00	0.00	0.00				
Excess O_2	EXCESS O2	3.61	0.23	0.84	18.34	32.00	0.57	16.85	17.32				
N_2 AIR	N2 AIR	4.21	0.77	3.24	70.84	28.02	2.53	74.31	76.40				
H_2O	H2O	0.00	1.00	0.00	0.00	18.02	0.00	0.00	0.00				
TOTAL				4.569	100.00		3.40	100.00	100.00				

Appendix C.3: Combustion of pulverised coal

	Molar mass (kg/kmol)	Ultimate analysis by mass AD(%)	Ultimate analysis by mass AF (%)
Total Moisture	18.02	1.57	10.22
Ash	-	34.9	31.83
Carbon	12.01	51.96	47.39
Hydrogen	1.01	3.15	2.87
Nitrogen	14.01	0.99	0.90
Sulphur	32.06	1.58	1.44
Oxygen	16.00	5.85	5.34
Total		100.00	100.00

Assumptions

Sulphur conversion depends on the type of mills used, for tube mills the sulphur converted will be more compared to the sulphur converted in vertical spindle mills. This is due to the fact that vertical spindle mills have rejects and some of the sulphur will be in the rejects. EPRI gives a sulphur conversion of 94% while the combustion engineering's handbook gives a conversion of 90%. in this case a worse case scenario of 94% will be used
It is assumed that the nitrogen in the fuel converting is 20% (innovative combustion technologies inc., 2011). It should be noted however that the fuel nitrogen conversion will be influenced by the type of burner orientation. Tangentially fired boilers produce less NOx compared to wall fired.
The total moisture used is the average from Eskom for 2007

Equations used

Unburnt carbon = (Carbon in ash%/100)*(Ash%/(100-carbon in ash))

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

GROOTEGULUK COAL

ULTIMATE COAL ANALYSIS

	Coal composition	
Total moisture:	10.22	
Ash	31.83	
Carbon	47.39	
Hydrogen	2.87	
Nitrogen	0.90	
Sulphur	1.44	
Oxygen	5.34	
	100.00	
Carbon conversion	100	%
Fuel Nitrogen conversion (NC)	20.00	%
Sulphur conversion	90	%
Carbon in ash	0.73	%
Unburnt carbon (UC)	0.0023	kg/kg fuel

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

	100/23.2	(2.67(C-UC)	+8H	+1S*SC	+1.14N*NC	-O fuel)
	4.3103	1.2592	0.2299	0.0130	0.0021	0.0534

6.25 kg/kg fuel

EXCESS AIR

K =	0.0460
n =	0.0188
f =	1.0246

Exhaust gas 10.00 %

100/f (O2/(20.9-02)

97.60 0.92

89.54 %

5.60 kg/kg fuel

TOTAL AIR 11.85 kg/kg fuel

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIOMETRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
$C+2.67O_2$	3.67CO2	0.472	3.670	1.7308	13.813	44.01	0.314	9.240	9.56	95630	1.96	187887.54	CO2
$H+8O_2$	9H2O	0.029	9.000	0.2586	2.064	18.02	0.115	3.373					
$S+O_2$	2SO2	0.013	2.000	0.0259	0.207	64.06	0.003	0.095	0.10	985	2.86	2816.07	SO2
$N+1.14O_2$	2.14NO	0.009	2.140	0.0039	0.031	30.01	0.001	0.030	0.03	313	1.34	419.56	NO
N_2	N2	0.009	0.800	0.0072	0.058	28.02	0.002	0.061	0.06				N2
Excess O_2	EXCESS O2	5.599	0.232	1.2990	10.367	32.00	0.324	9.538	9.87				O2
N_2 AIR	N2 AIR	11.852	0.768	9.1023	72.645	28.02	2.593	76.330	78.99				
H_2O	H2O	0.102	1.000	0.1022	0.816	18.02	0.045	1.333	1.38				
Unburnt sulphur	S2	0.0144115	0.1	0.0014									
Ash			0.318	0.3183									
Unburnt carbon			0.002	0.0023									
TOTAL				12.852	100.00		3.40	100.00	100.00				

APPENDIX D: DUVHA COAL RESULTS

Appendix D.1: Combustion of un-cleaned syngas

Species	Molar Mass (kg/kmol)	Volume Fraction (%)	mass (kg)	mass%
Carbon monoxide (CO)	28.01	8.80	246.49	8.75
Hydrogen (H2)	2.02	8.50	17.14	0.61
Methane (CH4)	16.04	0.80	12.83	0.46
Carbon dioxide (CO2)	44.01	15.30	673.35	23.90
Nitrogen (N2) & others	28.02	66.10	1852.12	65.75
Hydrogen Sulphide (H2S)	34.08	0.30	10.22	0.36
Ammonia (NH3)	17.03	0.10	1.70	0.06
Oxygen (O2)	32.00	0.10	3.20	0.11
Total		100.00	2817.06	100.00

	Molar mass (kg/kmol)	Ultimate analysis by mass (%)
Total Moisture	18.02	0
Ash	-	0
Carbon	12.01	10.62
Hydrogen	1.01	0.76
Nitrogen	14.01	65.80
Sulphur	32.06	0.34
Oxygen	16.00	22.49
Total		100.00
N from NH3		0.05
N from N2		65.75
Fuel N conversion		0.08

Assumptions

For N2, the others are mostly H2S and NH3 which amount to 0.4%. It is further assumed that the H2S is 0.3% and NH3 is 0.1%

Equations used

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

DUVHA 1

ULTIMATE COAL ANALYSIS

	Dry gas composition
Total moisture:	0.00
Ash	0.00
Carbon	10.62
Hydrogen	0.76
Nitrogen	65.80
Sulphur	0.34
Oxygen	22.49
	100.00
Carbon conversion	100 %
Fuel Nitrogen conversion (N	0.08 %
Sulphur conversion	100 %

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

	100/23.2	(2.67C	+8H	+1S	+1.14N*	(-O fuel)	
	4.3103	0.2834	0.0604	0.0034	0.0006	0.2249	
	0.53	kg/kg fuel					

EXCESS AIR

K =	-0.1914	
n =	6.1242	
f =	0.3879	
Exhaust gas O2 d	15.00	%
100/f	(O2/(20.9-02)	
257.78	2.54	
655.36	%	
3.47	kg/kg fuel	
TOTAL AIR 4.00	kg/kg fuel	

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIOMETRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
$C+2.67O_2$	3.67CO2	0.11	3.67	0.39	8.97	44.01	0.20	6.00	6.15	61534	1.96	120897.90	CO2
$H+8O_2$	9H2O	0.01	9.00	0.07	1.56	18.02	0.09	2.55					
$S+O_2$	2SO2	0.00	2.00	0.01	0.16	64.06	0.00	0.07	0.07	741	2.86	2118.97	SO2
$N+1.14O_2$	2.14NO	0.66	2.14	0.00	0.02	30.01	0.00	0.02	0.02	246	1.34	330.03	NO
N_2	N2	0.66	0.001	0.00	0.01	28.02	0.00	0.01	0.01				
Excess O_2	EXCESS O2	3.47	0.23	0.81	18.54	32.00	0.58	17.05	17.50				
N_2 AIR	N2 AIR	4.00	0.77	3.07	70.74	28.02	2.52	74.29	76.24				
H_2O	H2O	0.00	1.00	0.00	0.00	18.02	0.00	0.00	0.00				
TOTAL				4.345	100.00		3.40	100.00	100.00				

Species	Molar Mass (kg/kmol)	Volume Fraction (%)	mass (kg)	mass%
Carbon monoxide (CO)	28.01	9.90	277.30	9.93
Hydrogen (H2)	2.02	9.30	18.75	0.67
Methane (CH4)	16.04	0.70	11.23	0.40
Carbon dioxide (CO2)	44.01	15.00	660.15	23.64
Nitrogen (N2) & others	28.02	64.60	1810.09	64.82
Hydrogen Sulphide (H2S)	34.08	0.30	10.22	0.37
Ammonia (NH3)	17.03	0.10	1.70	0.06
Oxygen (O2)	32.00	0.10	3.20	0.11
Total		100.00	2792.65	100.00

	Molar mass (kg/kmol)	Ultimate analysis by mass (%)
Total Moisture	18.02	0
Ash	-	0
Carbon	12.01	11.01
Hydrogen	1.01	0.80
Nitrogen	14.01	64.87
Sulphur	32.06	0.34
Oxygen	16.00	22.97
Total		100.00

N from NH3		0.05
N from N2		64.82
Fuel N conversion		0.08

Assumptions

For N2, the others are mostly H2S and NH3 which amount to 0.4%. It is further assumed that the H2S is 0.3% and NH3 is 0.1%

Equations used

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

DUVHA 2

ULTIMATE COAL ANALYSIS

	Dry gas composition	
Total moisture:	0.00	
Ash	0.00	
Carbon	11.01	
Hydrogen	0.80	
Nitrogen	64.87	
Sulphur	0.34	
Oxygen	22.97	
	100.00	
Carbon conversion	100	%
Fuel Nitrogen conversion (	0.08	
Sulphur conversion	100	%

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

100/23.2	(2.67C	+8H	+1S	+1.14N*NC	-O fuel)
4.3103	0.2940	0.0644	######	0.0006	0.2297
0.57	kg/kg fuel				

EXCESS AIR

K =	-0.1856	
n =	5.8236	
f =	0.4088	
Exhaust gas O2	15.00	%
100/f	(O2/(20.9-02)	
244.60	2.54	
621.86	%	
3.55	kg/kg fuel	
TOTAL AI 4.13	kg/kg fuel	

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIOMETRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
$C+2.67O_2$	3.67CO2	0.11	3.67	0.40	9.02	44.01	0.20	6.03	6.19	61889	1.96	121595.59	CO2
$H+8O_2$	9H2O	0.01	9.00	0.07	1.62	18.02	0.09	2.64					
$S+O_2$	2SO2	0.00	2.00	0.01	0.15	64.06	0.00	0.07	0.07	725	2.86	2072.92	SO2
$N+1.14O_2$	2.14NO	0.65	2.14	0.00	0.02	30.01	0.00	0.02	0.02	241	1.34	322.86	NO
N_2	N2	0.65	0.001	0.00	0.01	28.02	0.00	0.01	0.01				
Excess O_2	EXCESS O2	3.55	0.23	0.82	18.41	32.00	0.58	16.93	17.37				
N_2 AIR	N2 AIR	4.13	0.77	3.17	70.76	28.02	2.53	74.29	76.24				
H_2O	H2O	0.00	1.00	0.00	0.00	18.02	0.00	0.00	0.00				
TOTAL				4.479	########		3.40	100.00	######				

Appendix D.2: Combustion of pre-cleaned syngas

Species	Molar Mass (kg/kmol)	Volume Fraction (%)	mass (kg)	mass%	pre-cleaned gas mass - 95% H2S & 88% NH3 removed	pre-cleaned gas mass %
Carbon monoxide (CO)	28.01	8.80	246.49	8.75	246.49	8.78
Hydrogen (H2)	2.02	8.50	17.14	0.61	17.14	0.61
Methane (CH4)	16.04	0.80	12.83	0.46	12.83	0.46
Carbon dioxide (CO2)	44.01	15.30	673.35	23.90	673.35	24.00
Nitrogen (N2) & others	28.02	66.10	1852.12	65.75	1852.12	66.01
Hydrogen Sulphide (H2S)	34.08	0.30	10.22	0.36	0.51	0.02
Ammonia (NH3)	17.03	0.10	1.70	0.06	0.20	0.01
Oxygen (O2)	32.00	0.10	3.20	0.11	3.20	0.11
Total		100.00	2817.06	100.00	2805.85	100.00

	Molar mass (kg/kmol)	Ultimate analysis by mass (%)
Total Moi	18.02	0
Ash	-	0
Carbon	12.01	10.66
Hydroge	1.01	0.73
Nitroge	14.01	66.02
Sulphur	32.06	0.02
Oxygen	16.00	22.58
Total		100.00

N from NH3	0.01
N from N2	65.96
Fuel N conversion	0.01

Assumptions

For N_2, the others are mostly H_2S and NH_3 which amount to 0.4%. It is further assumed that the H2S is 0.3% and NH3 is 0.1%

95% of H2S and 88% of NH3 is removed during gas cleaning

Equations used

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

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ULTIMATE COAL ANALYSIS

	Dry gas composition	
Total moisture:	0.00	
Ash	0.00	
Carbon	10.66	
Hydrogen	0.73	
Nitrogen	66.02	
Sulphur	0.02	
Oxygen	22.58	
	100.00	
Carbon conversion	100	%
Fuel Nitrogen conversion (NC)	0.01	%
Sulphur conversion	100	%

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

	100/23.2	(2.67C	+8H	+1S	+1.14N*NC	-O fuel)
	4.3103	0.2846	0.0582	0.0002	0.0001	0.2258
	0.51	kg/kg fuel				

EXCESS AIR

K =	-0.1964	
n =	6.1902	
f =	0.3763	
Exhaust gas O2 d	15.00	%
100/f	(O2/(20.9-02)	
265.75	2.54	
675.64	%	
3.41	kg/kg fuel	

TOTAL AIR 3.92 kg/kg fuel

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIO METRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
C+2.67O_2	3.67CO2	0.11	3.67	0.39	9.18	44.01	0.21	6.14	6.30	62995	1.96	123767.61	CO2
H+8O_2	9H2O	0.01	9.00	0.07	1.54	18.02	0.09	2.51					
S+O_2	2SO2	0.00	2.00	0.00	0.01	64.06	0.00	0.00	0.00	38	2.86	108.46	SO2
N+1.14O_2	2.14NO	0.66	2.14	0.00	0.00	30.01	0.00	0.00	0.00	30	1.34	40.57	NO
N_2	N2	0.66	0.0001	0.00	0.00	28.02	0.00	0.00	0.00				
Excess O_2	EXCESS O2	3.41	0.23	0.79	18.60	32.00	0.58	17.10	17.55				
N_2 AIR	N2 AIR	3.92	0.77	3.01	70.67	28.02	2.52	74.23	76.15				
H_2O	H2O	0.00	1.00	0.00	0.00	18.02	0.00	0.00	0.00				
TOTAL				4.260	100.00		3.40	#######	100.00				

Species	Molar Mass (kg/kmol)	Volume Fraction (%)	mass (kg)	mass%	pre-cleaned gas mass - 95% H2S & 88% NH3 removed	pre-cleaned gas mass %
Carbon monoxide (CO)	28.01	9.90	277.30	9.93	277.30	9.97
Hydrogen (H2)	2.02	9.30	18.75	0.67	18.75	0.67
Methane (CH4)	16.04	0.70	11.23	0.40	11.23	0.40
Carbon dioxide (CO2)	44.01	15.00	660.15	23.64	660.15	23.73
Nitrogen (N2) & others	28.02	64.60	1810.09	64.82	1810.09	65.08
Hydrogen Sulphide (H2S)	34.08	0.30	10.22	0.37	0.51	0.02
Ammonia (NH3)	17.03	0.10	1.70	0.06	0.20	0.01
Oxygen (O2)	32.00	0.10	3.20	0.11	3.20	0.12
Total		100.00	2792.65	100.00	2781.43	100.00

	Molar mass (kg/kmol)	Ultimate analysis by mass (%)
Total Mois	18.02	0
Ash	-	0
Carbon	12.01	11.05
Hydroge	1.01	0.78
Nitroge	14.01	65.08
Sulphur	32.06	0.02
Oxygen	16.00	23.07
Total		100.00

N from NH3	0.01
N from N2	65.03
Fuel N conversior	0.01

Assumptions

For N_2, the others are mostly H_2S and NH_3 which amount to 0.4%. It is further assumed that the H2S is 0.3% and NH3 is 0.1%

95% of H2S and 88% of NH3 is removed during gas cleaning

Equations used

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

DUVHA 2

ULTIMATE COAL ANALYSIS

Dry gas composition

Total mo	0.00
Ash	0.00
Carbon	11.05
Hydrogen	0.78
Nitrogen	65.08
Sulphur	0.02
Oxygen	23.07
	100.00
Carbon convers	100 %
Fuel Nitrogen c	0.01
Sulphur convers	100 %

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

	100/23.2	(2.67C	+8H	+1S	+1.14N*NC	-O fuel)
	4.3103	0.2951	0.0622	0.0002	0.0001	0.2307
	0.55	kg/kg fuel				

EXCESS AIR

K =		########
n =		5.8844
f =		0.3977
Exhaust gas O2	15.00	%
100/f		(O2/(20.9-02)
	251.43	2.54
	639.24	%
	3.50	kg/kg fuel
TOTAL AIR	4.04	kg/kg fuel

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIOMETRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
$C+2.67O_2$	3.67CO2	0.11	3.67	0.41	9.23	44.01	0.21	6.17	6.33	63315	1.96	124396.78	CO2
$H+8O_2$	9H2O	0.01	9.00	0.07	1.59	18.02	0.09	2.60					
$S+O_2$	2SO2	0.00	2.00	0.00	0.01	64.06	0.00	0.00	0.00	37	2.86	106.03	SO2
$N+1.14O_2$	2.14NO	0.65	2.14	0.00	0.00	30.01	0.00	0.00	0.00	30	1.34	39.66	NO
N_2	N2	0.65	0.0001	0.00	0.00	28.02	0.00	0.00	0.00				
Excess O_2	EXCESS O2	3.50	0.23	0.81	18.47	32.00	0.58	16.98	17.42				
N_2 AIR	N2 AIR	4.04	0.77	3.11	70.70	28.02	2.52	74.24	76.15				
H_2O	H2O	0.00	1.00	0.00	0.00	18.02	0.00	0.00	0.00				
TOTAL				4.394	100.00		3.40	100.00	99.91				

Appendix D.3: Combustion of pulverised coal

	Molar mass (kg/kmol)	Ultimate analysis by mass AD (%)	Ultimate analysis by mass AF (%)
Total Moisture	18.02	0.37	6.69
Ash	-	32.5	30.44
Carbon	12.01	58.70	54.98
Hydrogen	1.01	3.33	3.12
Nitrogen	14.01	1.27	1.19
Sulphur	32.06	0.69	0.65
Oxygen	16.00	3.14	2.94
Total		100.00	100.00

Assumptions

Sulphur conversion depends on the type of mills used, for tube mills the sulphur converted will be more compared to the sulphur converted in vertical spindle mills. This is due to the fact that vertical spindle mills have rejects and some of the sulphur will be in the rejects. EPRI gives a sulphur conversion of 94% while the combustion engineering's handbook gives a conversion of 90%. in this case a worse case scenario of 94% will be used

It is assumed that the nitrogen in the fuel converting is 20% based on ref(innovative combustion technologies). It should be noted however that the fuel nitrogen conversion will be influenced by the type of burner orientation. Tangentially fired boilers produce less NOx compared to wall fired.

The total moisture used is the average from Eskom for 2007

Equations used

Unburnt carbon = (Carbon in ash%/100)*(Ash%/(100-carbon in ash))

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

DUVHA COAL

ULTIMATE COAL ANALYSIS

	Coal composition	
Total moisture:	6.69	
Ash	30.44	
Carbon	54.98	
Hydrogen	3.12	
Nitrogen	1.19	
Sulphur	0.65	
Oxygen	2.94	
	100.00	
Carbon conversion	100	%
Fuel Nitrogen conversion (NC)	20.00	%
Sulphur conversion	90	%
Carbon in ash	0.73	%
Unburnt carbon (UC)	0.0022	kg/kg fuel

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

100/23.2	(2.67(C-UC)	+8H	+1S*SC	+1.14N*NC	-O fuel)	
4.3103	1.4619	0.2495	0.0058	0.0027	0.0294	
	7.29	kg/kg fuel				

EXCESS AIR

K =	0.0498	
n =	0.0215	
f =	1.0263	
Exhaust gas O2 dry	10.00	%
100/f	(O2/(20.9-02)	
97.44	0.92	
89.39	%	
6.51	kg/kg fuel	
TOTAL AIR	13.80	kg/kg fuel

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION	ULTIMATE COAL ANALYSIS	STOICHIOMETRY	PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
$C+2.67O_2$	3.67CO2	0.548	3.670	2.0094	13.865	44.01	0.315	9.297	9.60	96013	1.96	188639.01	CO2
$H+8O_2$	9H2O	0.031	9.000	0.2807	1.937	18.02	0.107	3.172					
$S+O_2$	2SO2	0.006	2.000	0.0116	0.080	64.06	0.001	0.037	0.04	382	2.86	1092.00	SO2
$N+1.14O_2$	2.14NO	0.012	2.140	0.0051	0.035	30.01	0.001	0.035	0.04	357	1.34	477.91	NO
N_2	N2	0.012	0.800	0.0095	0.066	28.02	0.002	0.069	0.07				N2
Excess O_2	EXCESS O2	6.514	0.232	1.5112	10.427	32.00	0.326	9.616	9.93				O2
N_2 AIR	N2 AIR	13.800	0.768	10.5988	73.129	28.02	2.610	77.019	79.54				
H_2O	H2O	0.067	1.000	0.0669	0.462	18.02	0.026	0.756	0.78				
Unburnt sulphur	S2	0.0064623	0.1	0.0006									
Ash			0.304	0.3044									
Unburnt carbon			0.002	0.0022									
TOTAL				14.800	100.00		3.39	100.00	100.00				

Appendix D.4: Combustion of pre-cleaned oxygen fired syngas

Species	Molar Mass (kg/kmol)	Volume Fraction (%)	mass (kg)	mass%	pre-cleaned gas mass - 95% H2S & 88%	pre-cleaned gas mass %
Carbon monoxide (CO)	28.01	22.10	619.02	23.59	619.02	23.79
Hydrogen (H2)	2.02	28.40	57.25	2.18	57.25	2.20
Methane (CH4)	16.04	2.20	35.29	1.34	35.29	1.36
Carbon dioxide (CO2)	44.01	36.60	1610.77	61.39	1610.77	61.92
Nitrogen (N2) & others	28.02	9.80	274.60	10.46	274.60	10.56
Hydrogen Sulphide (H2S)	34.08	0.60	20.45	0.78	1.02	0.04
Ammonia (NH3)	17.03	0.20	3.41	0.13	0.41	0.02
Oxygen (O2)	32.00	0.10	3.20	0.12	3.20	0.12
Total		100.00	2623.98	100.00	2601.56	100.00

	Molar mass (kg/kmol)	Ultimate analysis by mass (%)
Total Mc	18.02	0
Ash	-	0
Carbon	12.01	28.11
Hydroge	1.01	2.55
Nitroge	14.01	10.57
Sulphu	32.06	0.04
Oxygen	16.00	58.73
Total		100.00

N from NH3	0.01
N from N2	10.55
Fuel N conver	0.12

Assumptions

For N_2, the others are mostly H_2S and NH_3 which amount to 0.8%. It is further assumed that the H2S is 0.6% and NH3 is 0.2%

95% of H2S and 88% of NH3 is removed during gas cleaning

Equations used

Theoretical air = 100/23.2*(2.67C+8H+1S+1.14N-O fuel)

Excess air = $100/f*(O_2/20.9-O_2)$

f = (1+3K)/(1+2.37K+0.09n)

K = (H-O/8)/(C+(3/8)*S)

n = N/(C+(3/8)*S)

DUVHA

ΓIMATE COAL ANALYS

	Dry gas composition
Total m	0.00
Ash	0.00
Carbon	28.11
Hydrogen	2.55
Nitrogen	10.57
Sulphur	0.04
Oxygen	58.73
	######

Carbon conve 100 %

Fuel Nitrogen 0.12

Sulphur conve 100 %

TOTAL AIR REQUIREMENT PER ULTIMATE ANALYSIS

THEORETICAL AIR REQUIRED PER KG OF FUEL

100/23 (2.67C +8H +1S +1.14N*I -O fuel)

4.3103 0.7507 0.2037 0.0004 0.0001 0.5873

1.58 kg/kg fuel

EXCESS AIR

K : ######

n : 0.3757

f : 0.7758

Exhaus 15.00 %

100/f (O2/(20.9-02)

128.90 2.54

327.71 %

5.19 kg/kg fuel

TOTAL A 6.78 kg/kg fuel

PRODUCTS OF COMBUSTION PER KG OF FUEL COMBUSTED

	PRODUCT OF COMBUSTION			PRODUCT FORMED (kg)	% BY MASS	MOL WEIGHT OF PRODUCT	KMOL	Vol % WET	VOL % DRY	PPM	DENSITY OF GAS AT STP	mg/Nm3 @ 15% O2	
$C+2.67O_2$	3.67CO2	0.28	3.67	1.03	13.45	44.01	0.31	9.03	9.50	94965	1.96	186581.52	CO2
$H+8O_2$	9H2O	0.03	9.00	0.23	2.99	18.02	0.17	4.90					
$S+O_2$	2SO2	0.00	2.00	0.00	0.01	64.06	0.00	0.00	0.00	47	2.86	133.71	SO2
$N+1.14O_2$	2.14NO	0.11	2.14	0.00	0.00	30.01	0.00	0.00	0.00	37	1.34	50.02	NO
N_2	N2	0.11	0.00	0.00	0.00	28.02	0.00	0.00	0.00				
Excess O_2	XCESS O	5.19	0.23	1.20	15.70	32.00	0.49	14.50	15.25				
N_2 AIR	N2 AIR	6.78	0.77	5.20	67.84	28.02	2.42	71.55	75.24				
H_2O	H2O	0.00	1.00	0.00	0.00	18.02	0.00	0.00	0.00				
TOTAL				7.671	######		3.38	######	99.99				