Deploying plasma arc reforming to a commercial coal to liquid process: A techno-economic study

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Promoter: Prof. J. I. J. Fick

November 2015

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DECLARATION

I, Liberty Sheunesu Mapamba, hereby declare that the thesis entitled: "**Deploying plasma arc reforming to a commercial coal to liquid process: A techno-economic study**", submitted in fulfilment of the requirements for the degree Doctor of Philosophy in Development and Management Engineering is my own work and has not been submitted to any other tertiary institution in whole or in part. All efforts were made acknowledge other people's work in the text,

Signed at North-West University (Potchefstroom Campus)

Date:

Liberty Sheunesu Mapamba

2016/08/12

ACKNOWLEDGEMENTS

“I write about the power of trying, because I want to be okay with failing. I write about generosity because I battle selfishness. I write about joy because I know sorrow. I write about faith because I almost lost mine, and I know what it is to be broken and in need of redemption. I write about gratitude because I am thankful - for all of it”. - Kristin Armstrong

First, I would like to express my gratitude for the guidance of Prof Johan Fick, to whom I owe a lot of biltong for the patience, invaluable insights and persistent prompts for me to challenge myself and push beyond the average.

Frikkie Conradie, for insightful feedback on some of my articles, I am truly grateful

Tawona, my loving wife, thank you for the encouragement and patience as I put in long hours into the PhD and for being a sounding board for different ideas, I can never repay you

My sincere gratitude is also extended to THRIP, North West University Potchefstroom campus, for financing different activities and providing facilities that enabled me to complete my PhD.

To my friends, colleagues, whose names are too many to include here, and strangers who helped shape the PhD into what it became, I am truly and sincerely grateful.

ABSTRACT

The coal to liquids (CTL) process has played an important role in the supply security of liquid fuels and petrochemicals in South Africa and has the potential of doing the same for coal rich countries globally. Considering the abundance of coal reserves relative to other fossil fuels, coal is probably going to be instrumental as a feedstock for the production of oil for longer than crude oil and gas. However, the CTL process has challenges that include high capital cost, low carbon efficiency and high greenhouse gas emissions. Further, as climate change policies become more widely accepted, the cost implications may threaten the viability and competitiveness of the coal to liquid process. These challenges could be mitigated by the application of cleaner production as a process improvement initiative in commercial coal to liquids. Process redesign to use cleaner and more efficient technology is promising for implementation to coal to liquids.

One re-design option would be to integrate plasma arc reforming (PAR), which converts greenhouse gases in by-product streams to syngas. Redesigning a coal to liquid process to use PAR instead of auto thermal reforming has the potential to improve carbon efficiency, reducing emissions and possibly capital requirements in the process. Though it has such potential, PAR remains at laboratory scale, which brings to question whether it would be feasible and viable to deploy plasma arc reforming to a commercial coal to liquid process. This thesis explores the feasibility and viability of deploying plasma arc reforming to a coal to liquid process. First, a technology assessment was done to evaluate the most suitable configuration for deployment to coal to liquids and evaluating its scalability, commercial development status and efficacy in improving carbon efficiency. After that, the process effects of deploying plasma arc reforming were quantified. Finally, the impact of deploying plasma arc reforming on economic performance of coal to liquids was evaluated.

Technology screening shows that, a plasma reactor using carbon dioxide as a plasma gas has the best balance between performance and compatibility with coal to liquids. The deployment of plasma arc reforming is capable of improving the carbon efficiency of a coal to liquid process by up to 15%. It was also found that it is feasible to scale up plasma reformers to commercial scale using commercially available components. However, complete reformers are not yet ready for commercial applications and require development. Kinetic characterisation is key to the reduction of technology risk.

The improvement in carbon efficiency translates to 15% (by mass) reduction of coal, 32% reduction of oxygen and 20% reduction of steam requirements for process needs. This is accompanied by the reduction of required equipment capacities for gasification, air separation and steam generation equipment. Reduction of required steam generation equipment is accompanied by a substantial reduction in dilute greenhouse gas emissions that would be difficult to manage by sequestration or other means and a reduction of water requirements. However, use of plasma arc reforming requires 49% additional electrical energy and leads to externalised emissions if sourced from fossil powered power plants. Hence, procurement of low carbon electricity would be desirable.

These process changes have an impact on the economic performance of coal to liquids, with impacts on the capital and operating requirements. In the absence of carbon tax, the deployment of plasma arc reforming reduced the break-even price from a baseline cost of $80.95/bbl. to $77.42/bbl. When considering carbon tax equivalent to the proposed regime for South Africa, at an equivalent of $4.80/ton, the PAR modified plant requires an oil price of $81.57/bbl. versus $88.39 required by a conventional plant. For all configurations evaluated, the project net present value was greater than zero and the internal rate of return exceeded the hurdle rate, which was based on the Sasol hurdle rate for a coal to liquid project.

From the findings, it was concluded that it is feasible to deploy plasma arc reforming to a commercial coal to liquid process. The economic measures evaluated in the study support that a plasma arc reforming modified coal to liquids plant would be viable. However, the carbon-pricing regime in act and the cost of low carbon electricity have a significant influence on the crude price that provides sufficient confidence to support investments into such a venture.

KEY WORDS

Carbon efficiency, carbon reclamation, cleaner production, coal to liquid, plasma arc reforming

PREFACE

This thesis was submitted in article format as per the guidelines in Section 3.10 of the North-West University Postgraduate manual.

The work comprises of a collection of three articles that were submitted to the Journal of Cleaner Production (See Appendix A.5 for Author guidelines). All articles were written to be read as standalone articles, however, the connectedness of the three articles means that some information was repeated. The list of articles submitted to the Journal of Cleaner Production, their status and authorship follows below:

Article 1 Title: Technology assessment of plasma arc reforming for greenhouse gas mitigation: A simulation study applied to a CTL process

Status: Published (http://dx.doi.org/10.1016/j.jclepro.2015.07.104)

Authorship: The structure of the article, simulations, analyses and write-up presented in the article were designed and implemented by Liberty S. Mapamba. Frikkie H. Conradie provided expert feedback on the simulation aspects and some editorial input in the initial drafts of the article. Prof J.I.J Fick played an overall advisory role and editorial input into the later drafts. F. Conradie and Prof Fick were acknowledged as second and third authors respectively.

Article 2 Title: The operational implications of using plasma arc reforming as a cleaner production initiative in a coal to liquid process

Status: Under review

Authorship: The structure of the article, simulations, analyses and write-up presented in the article were designed and implemented by Liberty S. Mapamba. Prof J.I.J Fick played an overall advisory role and editorial input into the later drafts Frikkie H. Conradie provided some expert feedback on the simulation aspects and some editorial input in the initial drafts of the article. Prof Fick were acknowledged as second author and F. Conradie was acknowledged for his input.

Article 3 Title: Impact of plasma arc reforming deployment on economic performance of a coal to liquids process

Status: Under review

Authorship: The structure of the article, financial modelling, analyses and write-up presented in the article were designed and implemented by Liberty S. Mapamba. Prof J.I.J Fick played an overall advisory role and editorial input into the later drafts. Prof J Fick was acknowledged as second author to the article.

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1 INTRODUCTION

"Energy security means ensuring that diverse energy resources, in sustainable quantities and at affordable prices, are available to the South African economy in support of economic growth and poverty alleviation, taking into account environmental management requirements and interactions among economic sectors."- Department of Minerals and Energy, South Africa,2011

During the course of this study, the crude oil prices fell from $110/bbl. to $40/bbl. a reduction of almost 65%. The price reduction appears good for oil importers like South Africa as it reduces the expenditure in procurement of oil. However, a strong dependency on imported oil leaves the country vulnerable to supply side disruptions and volatility in the financial markets. To limit the exposure, it is necessary to diversify supply options (Nkomo, 2009). Using local resources such as coal and gas to produce fuels and petrochemical feedstocks is considered as a key strategy for improving energy supply security (DME, 2007).

Historically, South Africa has used Coal to liquids (CTL), through the establishment of Sasol, to make use of cheap coal to provide fuels and petrochemical feedstocks. The use of CTL proved to be helpful when South Africa was placed under sanctions as it offered relief as supply of fuel for the isolated economy dwindled (Murphy, 1979). Gas to liquids (GTL) was introduced into the supply mix more recently through the establishment of a synthetic fuel facility operated by Petro-SA (Knottenbelt, 2002).

Sasol and Petro-SA jointly produce up to 28% of national liquid fuel capacity hence, their contribution to energy security is key (SAPIA, 2014). Sasol has the bigger share of synthetic production capacity contributing 78% to South Africa's synthetic fuel production capacity (SAPIA, 2014). Though the application of synthetic fuels has been viewed in the South African context thus far, the potential applications extend globally as crude oil reserves diminish and coal and gas rich nations seek to boost their oil supply security. The number of synthetic fuel projects has increased significantly in the last decade and this affirms the view that the potential contribution of synthetic fuels is important.

In this thesis, there is a focus on CTL for three reasons. The first is that in the South African context, CTL makes a bigger contribution to synthetic fuel production than GTL. Second, in the global context, coal is expected to outlast oil and gas by up to 70 years (Shafiee & Topal, 2009). Finally, CTL has a greater number of issues that make it unsustainable as an energy supply option. These three reasons suggest that CTL presents a bigger research opportunity in the synthetic fuels production space.

1.1 Rationale

Current syncrude production costs are high compared to conventional crude oil production (Aguilera, 2014) and this may affect the use of CTL as a supply security option. Further, climate change policies are changing the operating landscape in ways that could escalate the production costs of CTL because of its CO_2 emissions. The anticipated high compliance costs have resulted in some CTL projects being shelved. Examples of such projects include Sasol's Mafutha project (Creamer, 2010) and United States Air Force CTL project (Vallentin, 2008). For the CTL to have a chance at continuing to be utilised, it is essential to implement some interventions that will reduce exposure to cost escalating changes. The consequence of failing to be competitive is that CTL will be replaced by cheaper alternatives as was demonstrated when Petro-SA chose Project Mthombo to build a refinery versus a CTL plant (PetroSA, 2015). The choice of cheaper alternatives is consistent with industry practice as can be seen in the oil price- infrastructure deployment trend shown in **Fig. 1-1**.

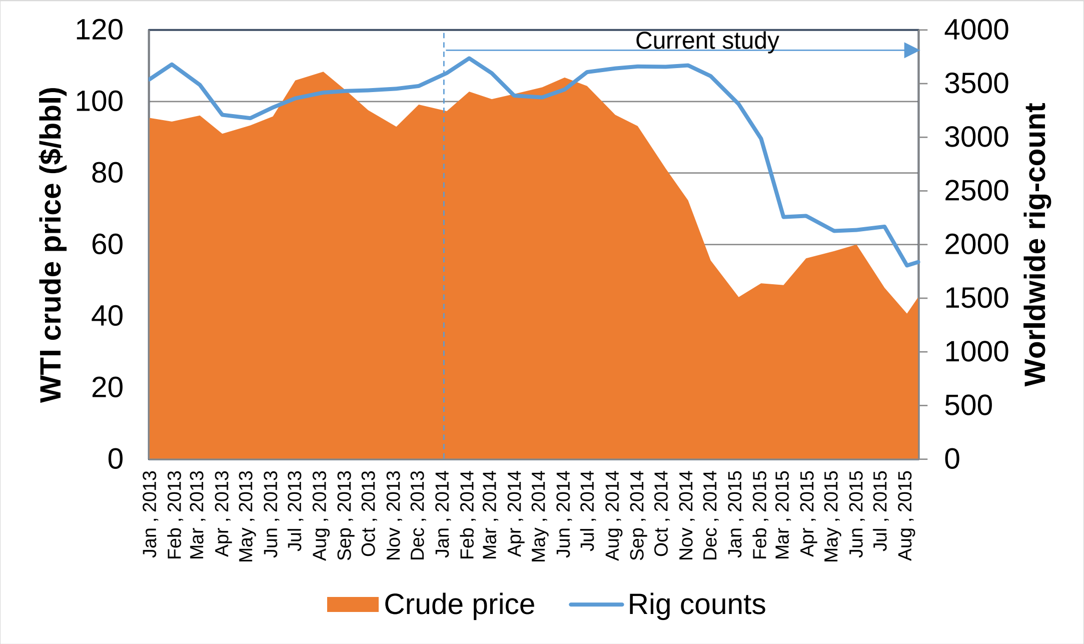

Fig. 1-1: Variation of active rig counts with crude oil price between January 2013 and September 2015 (Source: Baker Hughes)

Fig. 1-1 shows that the deployment of oil production infrastructure as represented by active oilrigs follows the price of crude oil. A more detailed analysis of rig deployment by depth and location also shows that the deep well and offshore rigs, which tend to be expensive, are deactivated first as oil prices go down. The implication is that the cheaper it is to produce oil using specific infrastructure, the better its chances of being utilised for extraction of oil. For CTL to continue to contribute to oil supply security there is a need to mitigate challenges that reduce its cost competitiveness.

There are three main cost drivers in CTL, high capital requirements (De Klerk *et al.*, 2013; Zennaro, 2013), low carbon productivity (Maitlis & de Klerk, 2013) and high greenhouse gas emissions (Miglio *et al.*, 2013). CTL is inherently complex due to the complex composition of coal and that contributes to high capital requirements of CTL (Maitlis & de Klerk, 2013). High greenhouse gas emissions (Miglio *et al.*, 2013) and low carbon efficiency (De Klerk *et al.*, 2013; Mulder, 2009) are often presented as separate issues but they are connected. High greenhouse gas emissions are carbon losses that lower the amount of carbon inputs that are translated into desirable products and the result is a low carbon efficiency. A larger amount of feedstock needs to be processed if the process has low carbon efficiency and that escalates capital and operating costs, which leads to a higher production cost. Overall, the challenges of CTL discussed above fit in the scope of the application of cleaner production.

Cleaner production was developed as an environmental protection initiative that protects the environment by eliminating waste and improving process productivity (Fresner, 1998). Cleaner production tends to have economic benefits for the area of application because of its focus on productivity and elimination of waste. It is likely that if a cleaner production initiative were applied in CTL, the resulting cleaner and more productive process would have better economic performance than the conventional CTL process, if an appropriate strategy were selected. Further, it may be possible to obtain premium prices for cleaner energy in industrialised countries as the position that climate change can be mitigated by decarbonising energy among other initiatives.

Strategies for implementing cleaner production include product re-design, raw material substitution, waste re-use and process redesign. The most likely strategy for application in CTL is waste reclamation through process redesign. By redesigning CTL to include technology that can convert waste carbon streams into valuable product, the carbon efficiency of the process could be increased. The improvement in carbon efficiency has a chain effect on the other raw materials required by the CTL process that could see the capital and oil requirements being reduced significantly.

Candidate technologies that could be integrated into CTL as part of cleaner production include carbon dioxide co-electrolysis of water (O'Brien *et al.*, 2009), catalysed dry reforming of methane with carbon dioxide (González *et al.*, 2013) and plasma arc reforming of methane with carbon dioxide (Tao *et al.*, 2011). This study focuses on exploring the future application of plasma arc reforming to creating a cleaner and more productive coal to liquids process.

1.2 Problem statement

Plasma arc reforming can be used to convert waste carbon dioxide streams into syngas by reacting it with internally produced methane and that would eliminate some carbon losses. The elimination of carbon losses would result in an improvement in the carbon efficiency of the process and a CTL process with a higher carbon efficiency is likely to have a lower production cost, hence be more competitive. Plasma arc reforming of methane with carbon dioxide remains at laboratory scale despite favourable reviews in literature, which brings to question whether it is feasible and viable to deploy plasma arc reforming to a commercial scale coal to liquid process.

The lack of clarity on the feasibility and viability has probably held back the development of plasma arc reforming to commercial scale. To unlock PAR potential, it is necessary to improve the quality of information available on its feasibility and viability. As a start, a number of questions need to be answered including:

- What is the state of the art in PAR?
- What plasma arc-reforming configuration would be best suited to the deployment in CTL?
- To what degree would deploying PAR improve the carbon efficiency of CTL?
- Can plasma arc reforming be scaled to industrial scale and what are the barriers to the progression?
- What are the operational implications of a coal to liquid process with higher carbon efficiency?
- Could the deployment of plasma arc reforming to a commercial coal to liquids be viable in the future?
- Would the deployment of plasma arc reforming to a commercial coal to liquids make it more competitive than a conventional process?

Answering these questions would shed light on the feasibility of deploying plasma arc reforming to CTL and it would confirm if there are any real benefits to the deployment. The answers create a technical and economic basis upon which it can be decided if it is worthwhile to develop plasma arc reforming for application in industrial scale CTL and defines the boundary conditions under which it makes sense.

1.3 Aims and objectives

The aim for undertaking this research was to evaluate the techno-economic feasibility of deploying plasma arc reforming of methane to a commercial coal to liquids process.

To accomplish this aim, the following objectives were pursued:

- To develop a technical model that allows identification of a plasma arc-reforming configuration most suitable for application in coal to liquids
- To develop a technical framework to assess the scalability and development status of plasma arc reforming technology.
- To develop a technical model to evaluate the impact of deploying plasma arc reforming on the process performance of a commercial coal to liquids process
- To evaluate the impact of the application of plasma arc reforming modification on coal to liquids process economic competitiveness

The alignment of the research questions and objectives are illustrated in **Fig. 1-2**.Since this thesis is presented in article format, as afforded by the academic rules, **Fig. 1-2** also shows how each article addresses specific research objectives in the process of solving the research problem.

1.4 Research design and hypothesis

The research in this thesis was built around testing the hypothesis that it is feasible and viable to deploy plasma arc reforming to a commercial coal to liquid process. The main hypothesis was broken down into two sub-hypotheses to separate the issues that need to be addressed to demonstrate feasibility and viability of deploying plasma arc reforming or the lack thereof. The two sub-hypotheses were:

i. It is technically feasible to deploy plasma arc reforming to a commercial scale coal to liquid process.
ii. Deploying plasma arc reforming in a commercial coal to liquids can be economically viable in the future.

A combination of process simulation, qualitative technical frameworks and literary analysis was used to test the sub-hypotheses. Process simulation was used to screen and evaluate plasma arc reforming options and to quantify the effects of deploying PAR to a CTL process. The process models were developed based on the theory and applications of PAR and CTL processes described in literature. Qualitative technical frameworks and literary analysis were used to assess the technology readiness level (TRL), manufacturability and supportability of PAR technology. **Fig. 1-3** is a graphic summary of the research design.

1.5 Originality claim

The application of the chemistry of dry reforming of methane, which is at the heart of PAR, to a Fischer-Tropsch process, has been proposed by Er-rbib *et al.* (2012). However, their study focused on the application of a catalysed dry reforming system without considering whether it is feasible to implement in a CTL process. Stoker and Conradie (2015) also looked at the application of PAR in CTL with the help of work done by Blom and Basson (2013). They applied a form of PAR to a commercial CTL process as part of improving carbon efficiency using nuclear driven interventions. However, the available information leaves a gap of whether it is really feasible and viable to deploy PAR to commercial CTL process.

While the Stoker and Conradie (2015) study can be said to be the closest evaluation of the application of PAR to a commercial CTL process, PAR is one of many interventions which were part of the study. The study concluded that the combination of initiatives is unlikely to be viable and still leaves the issue of the viability of applying PAR on its own unanswered.

This research challenges what is currently known by changing the perspective and proposing that a CTL process would benefit from the deployment of PAR as a cleaner production initiative, which is not tethered to any other initiatives. In this study, the evaluation of feasibility of in a commercial CTL context was done with a strong focus on how PAR would be deployed as opposed to assuming that it can be deployed. The technical feasibility assessment includes interrogating the compatibility of PAR with CTL, its scalability to commercial scale and its fitness for purpose in CTL. In the re-evaluation, this research contributes a technical model and framework for screening PAR technologies, evaluating scalability and assessing the technology's commercial readiness status.

In addition to change of perspective, there was a focus on deploying only PAR to CTL. Focusing the deployment achieves two things 1) a clearer understanding of the effect of deploying PAR in CTL, 2) making it easier to allocate the financial risks brought about by deploying PAR. If several interventions were to be bundled, the outcome would be a misleading reflection of the value or risk added by the intervention unless the risk of the other interventions is well known. In the current study, the avoidance of blanket risk allocation was achieved by deploying PAR to CTL using low-carbon electricity from a third party who is well positioned to assume the risk of establishing the power plant. This enabled the effect of deploying PAR to CTL at commercial scale to be better evaluated and understood.

Key result contribution to the body of knowledge include:

- Degree of carbon efficiency improvement that is possible when only materials generated within the CTL process are processed with PAR (Article 1: Chapter 3)
- Barriers to deployment of PAR to commercial scale (Article 1: Chapter 3)
- Minimum conversion required for PAR to add benefit to CTL (Article 2: Chapter 4)
- Impact of PAR deployment on the process economics (Article 3: Chapter 5)
- Crude oil price at which a PAR modified CTL will be viable (Article 3: Chapter 5)

A discussion of the implications of the results on the current understanding is presented in Chapter 6.

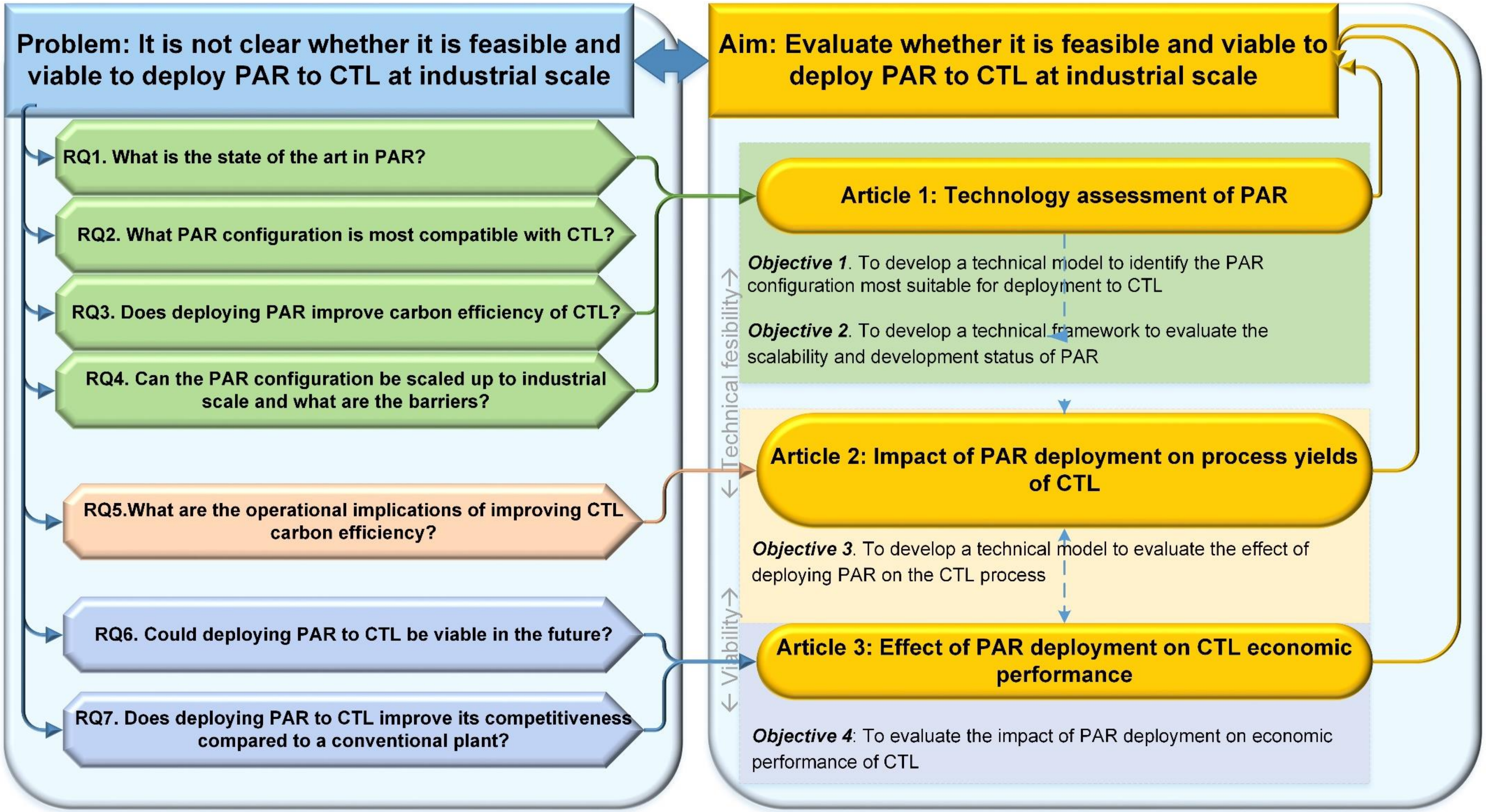

Fig. 1-2: Linkages between problem, research questions, objectives and the article context

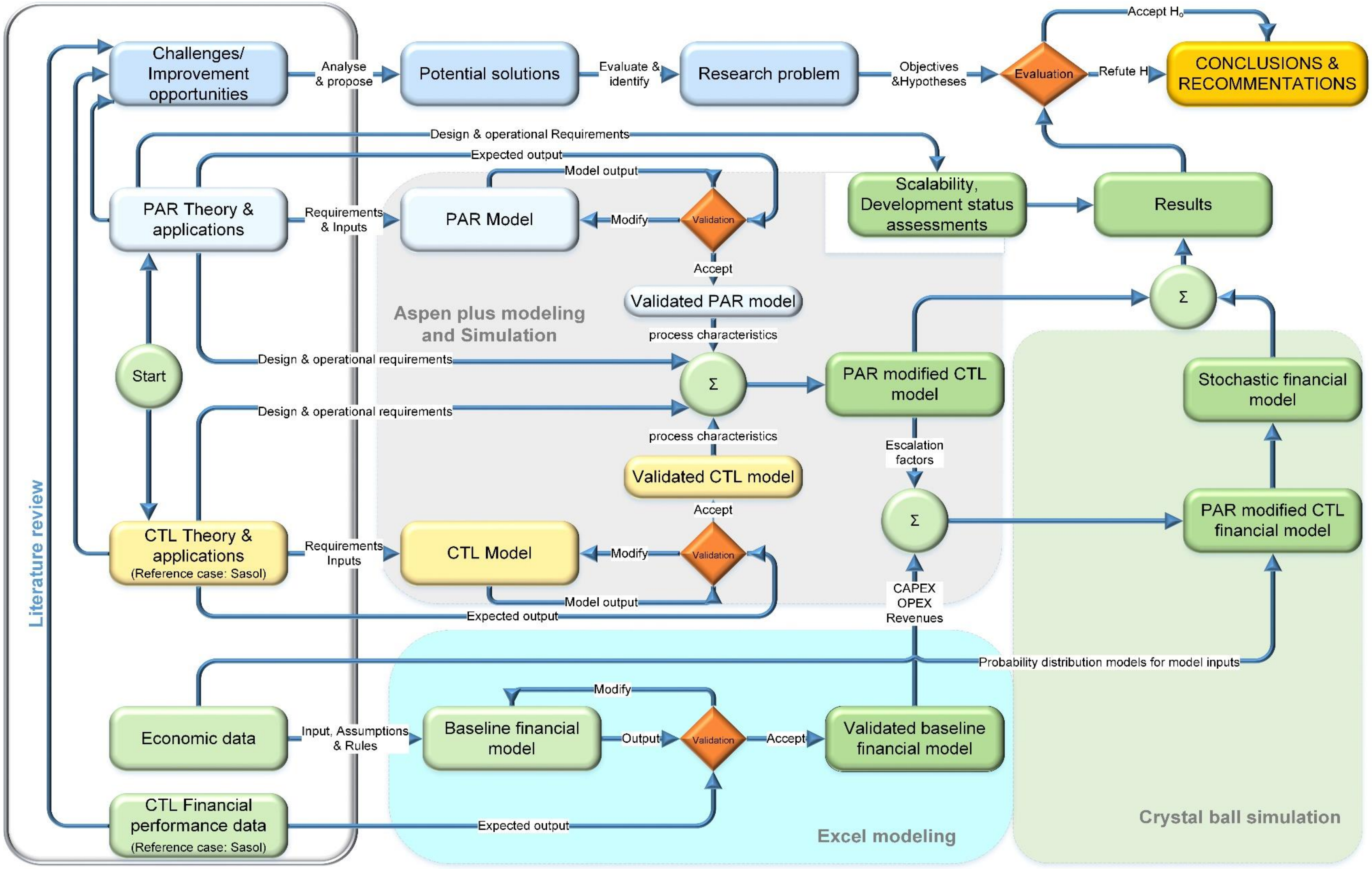

Fig. 1-3: Overall research design

1.6 Thesis outline

This thesis presents the documentation of the feasibility and viability assessment of deploying plasma arc reforming to a commercial coal to liquids processes as a cleaner production initiative. The thesis consists of six chapters, which describe the study from a review of the state of the art of coal to liquids processes to the conclusion of the evaluation of the feasibility of modifying a coal to liquids process with plasma arc reforming. A summary of the remaining chapters is given below:

Chapter 2	In this chapter, a review of the theory and applications of coal to liquid processes and plasma arc reforming is presented. From the review, the opportunities for synergistic application of the two processes are identified and examined.
Chapter 3	A technology assessment of plasma arc reforming is presented in Chapter 3. In the chapter, the technical feasibility of the PAR in CTL is interrogated by examining the state of the art in PAR, the scalability and commercial development status of the plasma arc reforming technologies. The chapter is in the form of an original full-length research article. The article was published in the Journal of Cleaner production.
Chapter 4	Chapter 4 builds on the article in Chapter 3, and examines the implications of improving carbon efficiency of CTL. The impact on raw material requirements, equipment capacities and product throughput of a commercial CTL is analysed and presented as a full-length research article.
Chapter 5	In this chapter, the findings of Chapters 3 and 4 are used to evaluate if the deployment of plasma arc reforming adds economic value to a commercial CTL process and if it plasma arc reforming modified processes could be viable in the future.
Chapter 6	Concluding remarks and recommendations for future work are presented in this chapter. The conclusions and recommendations are based on the initial objectives, experiences met in the course of the study and the eventual findings of the research project.

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2 A REVIEW OF COAL TO LIQUIDS AND PLASMA ARC REFORMING PROCESSES

"The notion of the lone genius labouring away in the basement laboratory to invent a future is, by now, one we should all be safely free of. Innovative firms succeed not by breaking free from the constraints of the past but instead by harnessing the past in powerful new ways. The result is an innovation process that thrives by making smaller bets, by building the future from what's already at hand."- Andrew Hargadon

Overview:

Coal to liquids has been contributing significantly to the energy needs of South Africa since 1955, when Sasol opened Sasol 1 (Dry, 2002a). Since then the energy sector has changed as such, the coal to liquids process has had to evolve, through scientific and business innovations, in order to remain viable.

According to Drucker (2002), there are seven things that can create opportunities for the emergence of business innovations, which are: unexpected events, market incongruities, business needs, industry changes, population changes, new knowledge and changes in people's viewpoint. For coal to liquids applications, the incompatibility of the process performance with the market expectations is becoming a major driver for the process to evolve in order to continue meeting the business needs of its operator.

A review of the documented evolution of coal to liquids will probably reveal innovation opportunities that are needed for the coal to liquids process to continue being relevant and viable in a changing economic landscape. This review is an exploration of coal to liquids literature that was done to establish the CTL process state-of-the-art, upon which future CTL processes can be built.

The chapter is structured to examine coal to liquids broadly starting with the communication of some of the process basics and progressing to how the CTL process can be adapted to a future landscape. Sections 2.2 and 2.3 present a big picture view of past and current processes, including a description of the process, drivers, challenges and future prospects. After identifying the issues with the coal to liquids process, Section 2.4 presents a review of possible approaches to some of the significant challenges of coal to liquids. Section 2.5 discusses plasma-reforming basics that create a platform for understanding the opportunity to apply plasma arc reforming to the coal to liquids process. The chapter is summarised in Section 2.6 by mapping out the specific opportunities that will be pursued in the remainder of this thesis.

2.1 Background

In 1923, German scientists, Fischer and Tropsch published their work on a process to produce gasoline from coal and in 1935, the first industrial scale F-T synthesis reactor was built (Schulz, 1999). In the 1940s, Germany and a few other oil-poor countries adopted the use of fuel production technologies from coal. The motivation for most of them was to improve the fuel supply for military transportation. After the World War II, interests in coal to liquid fuels were abandoned after the discovery of cheaper crude oil reserves in the Middle East (Schulz, 1999). However, South Africa was an exception to the trend due to its economic isolation (Dry, 2002a).

Sasol was established in 1955 to provide South Africa, which was an isolated apartheid state, with petroleum products from coal (Olson, 1977). Since then, with the removal of sanctions on South Africa, the application of coal to liquid fuels (CTL) technology ceased to be purely about energy supply security to being also about the economics. High capital requirements and undesirable environmental impact are recurring themes in the evaluation of coal to liquids (De Klerk, 2011; Li & De Klerk, 2013; Vosloo, 2001). A review of the processes is required to understand the capital cost drivers and the sources of negative environmental impact.

The CTL process a number of distinct coal liquefaction processes. On a high level there are two types of CTL processes, direct coal liquefaction (DCL) and indirect coal liquefaction (ICL). Currently, DCL technologies are not being used commercially while ICL, as represented by the Fischer-Tropsch driven process, has become the commercial representative of the CTL process (Liu *et al.*, 2010). DCL and ICL will be explored in more detail in Section 2.2 and Section 2.3 respectively. The discussion of DCL will be presented only for the reader to gain an appreciation. A greater emphasis will be put on reviewing ICL as that currently represents a commercial CTL process. In the rest of the thesis, CTL process is used to represent indirect coal liquefaction. A note to further remove ambiguity on the use of CTL process, most researchers use CTL process to describe processes that produce either of liquid fuels or non-fuel chemicals (De Klerk & Maitlis, 2013; Dry, 2004), but others distinguish processes that produce mostly chemicals by calling them coal to chemicals (CTC) (Li *et al.*, 2012). In this thesis, the distinction is viewed as a minor difference in configuration of the same process.

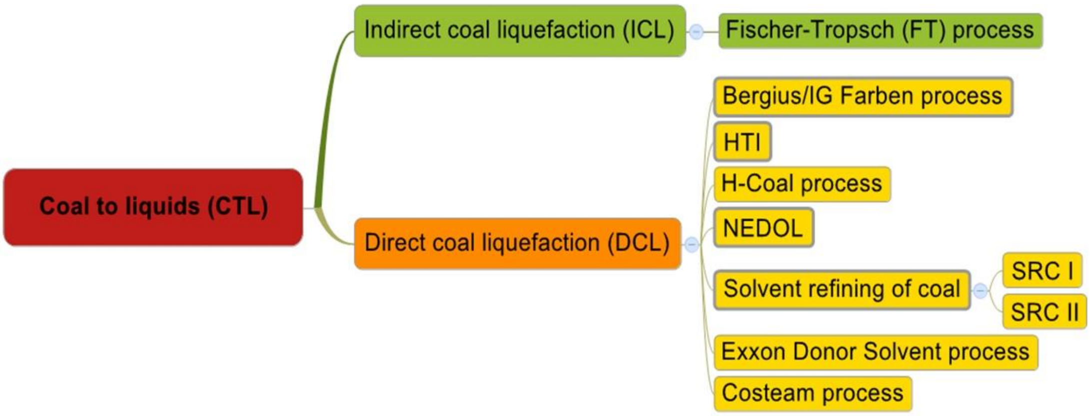

Fig. 2-1: Logic diagram of the different types of coal to liquids processes

Interest in CTL processes has historically been driven by the need for energy security (Nkomo, 2009; Stranges, 1987). This is supported by the fact that research activity on CTL processes has tracked the crude oil cycles, increasing when price is high and waning when prices are low (De Klerk, 2008). DCL has received more attention in China while the rest of the world has pursued Fischer-Tropsch synthesis. Despite notable interest in research circles, the uptake of CTL processes globally has been low. High capital cost (Liu *et al.*, 2010; Olson, 1977) and high emissions of carbon dioxide are the most commonly cited reasons for the low uptake. Other reasons for low uptake are high water resource requirements (De Klerk *et al.*, 2013; Zhou *et al.*, 2011) and long development cycles (Olson, 1977). In some areas such as the USA, competition with simpler, less capital intensive gas to liquids (GTL) technologies has seen GTL being preferred. To address the challenges that influence the prospects of CTL processes such as the Sasol process, a review of the development the CTL process was done to identify persistent challenges.

2.2 Direct Liquefaction

Friedrich Karl Rudolph Bergius submitted several patent applications for his coal liquefaction process in 1914 that would end up being known as the Bergius process (Olson, 1977). The Bergius process faced two challenges; 1) the effect of catalysts on reaction were unknown and 2) having hydrogenation of coal and the subsequent decomposition into petroleum resulted in low process yield and poor quality gasoline. These challenges were solved after Bergius made commercialisation agreement with Baden Aniline and Soda Factory (BASF). BASF and 27 other companies formed the conglomerate IG Farben, which was established to overcome the high capital requirements of commercialising the coal liquefaction process (Stranges, 1984). Under the leadership of Carl Bosch, the catalyst and coal hydrogenation challenges of the Bergius process were overcome. The result was 12 commercial plants being established in Germany by 1944 based on the Bergius/ I.G. Farben technology (Bartis *et al.*, 2008). From 1927 to 1945, Carl Bosch influenced the dominance of the Bergius process over the Fischer-Tropsch process (Stranges, 1984). Despite the liquefied coal being produced at double the cost of imported oil, most of the fuel used in Germany during World War II was supplied by DCL plants in the interest of supply security.

After the war, other direct liquefaction processes were developed in different places also driven by security of fuel supply. Some of the processes include solvent refining of Coal (SRC) (Miller, 2011; Wakeley *et al.*, 1979), NEDOL (Hirano, 2000; Onozaki *et al.*, 2000) H-coal (Miller, 2011), HTI which is also known as H-Coal (Miller, 2011; Schulz, 1999) and Shenhua process (Zhou *et al.*, 2011). Despite being first to market, there are no operational DCL projects at commercial scale. Most of the documented DCL processes are demonstration scale plants in China, Germany, Japan and the United States.

Though DCL is theoretically more efficient than indirect coal liquefaction, it is only true when high quality coal is used (Williams and Larson, 2003; Liu, 2005). The requirement for high quality coal works against DCL. Competing uses for high quality coal raises the cost of feedstock. Since feedstock costs are significant for DCL, a requirement for high quality coal feed reduces the prospects of obtaining favourable process economics. Other challenges include process complexity and lack of clarity in mechanism of reaction, which complicates the reactor design and results in perceived high technology risk (Liu *et al.*, 2010). Given the preference for low risk and cheap energy, the prospects of DCL success at commercial scale appear to be not as good as Fischer-Tropsch based ICL.

2.3 Indirect coal liquefaction

Indirect coal liquefaction is carried out by the Fischer-Tropsch (F-T) process. The F-T process was first reported by Fischer and Tropsch in 1923 (May, 2002). The F-T process is a mature technology with Sasol having operated commercial ICL plants for more than 50years in South Africa. Like DCL, the F-T process is complex (Liu et al., 2010; Zhou et al., 2011; De Klerk, 2012). However, the complexity is better understood unlike DCL complexity. It is known that process complexities lie in oxygen separation, product separations, gasification chemistry, syngas purification and F-T synthesis heat and mass transfer (Mokhatab & Poe, 2012; Onozaki *et al.*, 2000; Schulz, 1999). These process complexities in air separation, syngas purification and gasification chemistry are that contribute to syngas generation requiring the bulk of capital costs in an ICL plant (Liu *et al.*, 2010; Mulder, 2009; Zhou *et al.*, 2011).

Significant progress has been made in leveraging on cost reductions from reactor scale and catalyst performance (Jager, 2003; Leckel, 2010), however, several challenges still exist. A review of the key aspects is presented in Section 2.3.1 to Section 2.3.6 in order to draw attention to some of the remaining challenges.

2.3.1 ICL Feedstock

F-T synthesis decouples syngas generation and hydrocarbon synthesis, which adds flexibility to ICL with respect to the feedstocks that can be used. Currently natural gas and coal are being used at commercial scale (Dry, 2004), but biomass and municipal solid waste (MSW) have been considered as feedstocks. The focus of this thesis is on use of coal as a feedstock but comparisons with gas fed processes will be made occasionally.

Ignoring use of CTL to ensure energy supply security, F-T synthesis has been considered for value adding to remote coal resources where alternative uses are limited by access (Miller, 2011). An example of this is that transportation to industrial customers who are far from source does not make economic sense, as is the case with low-grade coals (Van Dyk *et al.*, 2001). The use of low-grade coals has a number of effects on the performance of F-T plants and the corresponding process economics. The first effect is that low grade coals limit the amount of carbon processed per pass by syngas equipment such as gasifiers. The implication is that larger equipment is required to meet downstream requirements than where higher quality feedstocks are used. This increases capital and operating cost requirements for syngas generation. The second effect is that coal quality influences the performance, stability and lifespan of equipment (Van Dyk *et al.*, 2001), which affects efficiency of gasifiers and results in higher carbon losses. Higher carbon losses also lead to higher capital requirements for syngas generation as more feed needs to be processed to compensate for the losses. Mantripragada and Rubin (2013) corroborate this through their concluding that the performance of an F-T plant using bituminous coals is better than that using lower grade lignite. Hence, prospects of F-T plants using low grade coals getting an investment is less likely unless it achieves higher material and energy utilisation.

Other physical characteristics of coal that can affect the efficiency of syngas generation are the size of coal feed and caking properties (Van Dyk & Waanders, 2007). Use of coals beneath a certain Sauter diameter can cause unstable gasifier performance resulting in loss of carbon conversion efficiency, which influences capital and operational costs (Keyser *et al.*, 2006). Caking coals can influence gasifier performance by affecting pressure drop patterns and causing channel burning (Sha *et al.*, 1990). Pressure drop considerations are used to select the particle size distribution of the feed by methods like the Ergun Sect (Richardson *et al.*, 2002).

When considering competing investments, gasification of coal is less efficient than steam reforming of methane (SMR) due to higher content of hydrogen in methane (Dry, 1996). Processes using coal gasification generate carbon dioxide in generating hydrogen to compensate for the lower hydrogen content of coal-derived syngas (De Klerk, 2011). Generation of large amounts of carbon dioxide means there are high carbon losses in the CTL process (Mulder, 2009), which results in higher feedstock cost when compared to methane reforming. Consequently, larger equipment is required for syngas generation, which implies higher capital cost. This means coal is less desirable as a feedstock for the F-T process than natural gas, which has lower operating costs and capital requirements.

2.3.2 ICL Process description

Six process steps are commonly found in a CTL process: air separation, syngas generation, raw gas cleaning and conditioning, F-T synthesis, and product work-up and utility generation. The relationship between the process steps is illustrated in **Fig. 2-2** and a discussion with more detail follows.

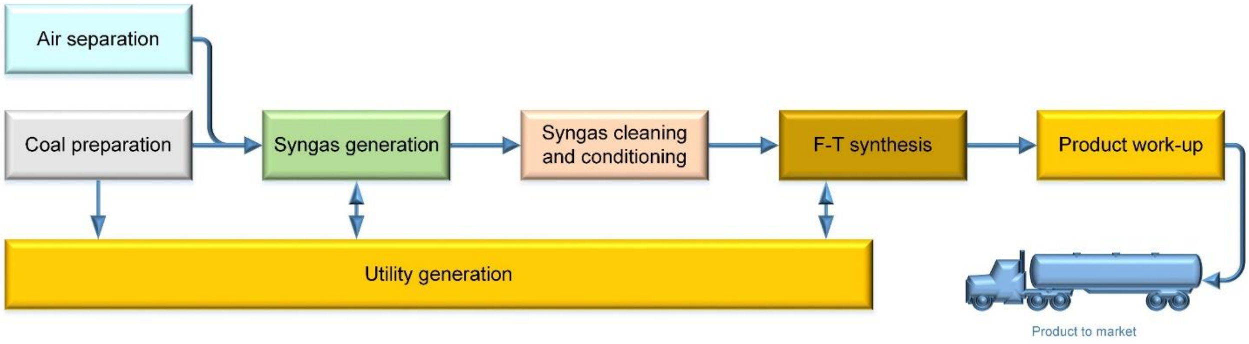

Fig. 2-2: Block flowsheet of an indirect coal to liquids process

2.3.2.1 Air separation

Fischer-Tropsch processes use pure oxygen to avoid the introduction of nitrogen into the process. Nitrogen acts as an inert diluent that affects the efficiency of a CTL process (Li & De Klerk, 2013). Air separation is the process that provides oxygen for gasification and combustion processes within the F-T process and potentially nitrogen for rectisol cooling. Air separation is an important part of the syngas generation section and that is reflected by its contributing 8-10% to total F-T process complex capital requirements (National Petroleum Council, 2007). Cryogenic air separation is the commonly used, as it is the most mature technology but there are alternatives like membrane separation and pressure swing adsorption (Belaissaoui *et al.*, 2014; Zhou *et al.*, 2011). The key steps in the process are air compression, air cleaning, air fractionation (Separates O_2, N_2 and Ar) and produces oxygen of purity ranging from 95%-99.9 % (Yu *et al.*, 2010). Sale of Argon can improve the economics of the process and reuse of N_2 in downstream processes improves the efficiency of the process. Due to the conditions required for cryogenic separation, -192°C (Linde Engineering, 2013) and the compression requirements, cryogenic air separation process requires a lot of energy. This contributes significantly to the electrical consumption of the CTL process and consequently to the operational cost.

2.3.2.2 Syngas generation

Gasification is a key step in the generation of syngas. In the gasification step, coal is fed into one of many gasifier types with a mixture of steam and oxygen, at high temperature and pressure, to produce carbon monoxide and hydrogen. The carbon monoxide and hydrogen are also known as raw gas as it often has impurities such as carbon dioxide, hydrogen sulphide and trace particulates. Sasol the biggest operator of F-T based ICL, uses the Sasol-Lurgi gasifier, which has advantages of high efficiency and feed coal flexibility but consumes a lot of steam and has a high-pressure drop, which can limit throughput (Van Dyk *et al.*, 2001). The temperatures utilised in gasification vary range between 500 and 1500° C. Operating pressures in gasifiers vary between atmospheric pressure and 8 MPa. The operating temperatures dictate whether the ash will be dry or molten (slag) and this has an effect on the thermal efficiency of the gasifier unit. The gasifiers used in the Sasol process are known as dry bottom gasifiers as they operate at temperatures that do not melt the ash (Van Dyk *et al.*, 2001). The use of high temperature and pressure means there are safety concerns and requires additional safety considerations in design. These additional considerations add to the complexity of equipment design.

Gasifier chemistry is complex comprising of several reactions in the gaseous phase and a few solid fluid reactions (Bell *et al.*, 2011a). The quality and size of coal feedstock, the method of solid-fluid contact (counter current or co-current), and the conditions in the reactor influence conversion of reactants, reaction extent, the reaction kinetics and as such the composition of the raw gas (Bell *et al.*, 2011b). Gasification is endothermic and requires some of the feedstock to provide energy for the conversion process through carbon combustion. Combustion results in carbon dioxide being produced instead of the desired carbon monoxide and this represents a carbon loss. Typical carbon efficiency is about 52% because the carbon lost in energy production as carbon dioxide (Dry, 2002b; Mulder, 2009). The implication is that 48% of carbon is consumed in providing energy for the endothermic reactions. Other side products include methane, which is generated by the methanation reaction in gasification, and constitutes 4-10% of the raw gas (Dry, 2002b).

The complexity in gasification chemistry means that the design and operation presents significant technical risk. This is reflected in the high engineering costs in design of gasification plants and the requirements for high contingency costs to buffer against failure to perform at specified levels. Gasification equipment requires 35-37% of total plant investment (Rostrup-Nielsen, 1994). Of the 37%, equipment contribution amounts to 20% and the remainder is the cost of engineering design, procurement and commissioning costs (National Petroleum Council, 2007) which is consistent with the complexity of the gasification chemistry. Based on the large percentage of gasification contribution to capital requirements, reducing the overall capital requirements of the process requires improving the performance of syngas generation and reducing the size of the associated equipment.

Before the raw gas can be used as syngas for synthesis, it has to be conditioned to an appropriate temperature. It is also necessary to remove impurities such as hydrogen sulphide, carbon dioxide, carbonyl sulphide and other trace sulphur compounds capable of poisoning the catalysts.

2.3.2.3 Syngas cleaning and conditioning

When raw gas leaves the gasifier, it is at high temperatures and has impurities such as particulates and acid gases (carbon dioxide, hydrogen sulphide and carbonyl sulphide) which have the potential to poison F-T synthesis catalysts downstream. Raw gas conditioning is the process of recovering excess heat, adjusting H_2: CO ratio and cleaning the gas of impurities. Heat recovery is done using waste heat boilers and gas cleaning is done using a series of stages starting with particulates removal in a cyclone and then acid gas removal. Of the cleaning stages, acid gas removal requires more attention as it contributes significantly to the capital requirements, contributing up to 11% of total investment costs (Kreutz *et al.*, 2008; Zhou *et al.*, 2011). H_2: CO ratio can be adjusted using the water gas shift process, membrane removal of CO or addition of H_2 from a secondary source.

Typical temperatures of raw gas leaving the Sasol-Lurgi gasifier is approximately 500 °C and the gas needs to be cooled to a temperature to 230 °C which corresponds to the temperature required for ratio H_2:CO adjustment (Zennaro *et al.*, 2013). During the cooling process, waste heat recovered in waste heat boiler is used to generate high-pressure steam and this is used in generating electricity, which can be used to offset the electrical demand of the ICL process (De Klerk *et al.*, 2013). After heat recovery, particulates are removed in a cyclone then a portion of the raw gas is passed through a water gas shift reactor (WGS). The WGS converts some carbon monoxide and water into carbon dioxide and hydrogen. The shift reaction adjusts the H_2: CO ratio to a range of 1.79-2.01 (Van Dyk *et al.*, 2001), which is the required ratio for the F-T synthesis reactions. High levels of conversion of the order of 90% are achievable in the shift reactor (Yu *et al.*, 2010). After shift adjustment, the acid gases are removed from the syngas in an acid gas removal process.

Acid gas removal can be achieved by the use of a number of methods but absorption methods are commonly used, particularly selexol (Mohammed *et al.*, 2014) and rectisol (Mohammed *et al.*, 2014). The rectisol process is more effective for removing common components of acid gases to acceptable syngas concentrations (Chen *et al.*, 2013). Rectisol was first applied at Sasol because of its high carbon dioxide absorption capacity and relatively low operating cost (Zhou *et al.*, 2011). The cost advantage of rectisol is debatable. Some researchers have reported that it requires much higher capital than selexol due to higher process complexity (Shu, 2003; Kang, 1999:3-6). The complexity of the rectisol process and its requirements for cryogenic cooling are major sources of criticism for the process. The requirement for cryogenic temperatures raises the capital expenditure and operating cost of the recovery plant (Mokhatab & Poe, 2012). However, when used in plants with cryogenic air plants, rectisol presents opportunities for process integration as by-product nitrogen can be used as a stripping gas (Zhou *et al.*, 2011).

In the Sasol process, sulphur based compounds are recovered in a Claus plant or a modified Stretford plant also known as Sulpholin plant (Collings, 2002). The products of sulphur recovery can be elemental sulphur or sulphuric acid, which can be sold as valuable by-products hence contributing to the plant revenue. Carbon dioxide from rectisol has a purity that makes commercial sense to directly compress to 15 MPa and sent to storage facilities without further processing (Vallentin & Fischedick, 2009). However, currently no CCS plant has been demonstrated at commercial scale and most of the carbon dioxide is emitted to the atmosphere.

2.3.2.4 F-T synthesis

The Fischer Tropsch synthesis step converts carbon monoxide and hydrogen into hydrocarbons on the surface of a catalyst. The conditions in the reactor such as reactant ratios, pressure and temperature influence the composition of the hydrocarbon stream that is produced. The groups of hydrocarbons produced in synthesis are broadly represented by Eq. (2.1) -(2.5) (De Klerk & Furimsky, 2010)

Alkanes: $(2n+1)H_2 + nCO \rightarrow C_nH_{2n+2} + nH_2O$ (2.1)

Alkenes: $2nH_2 + nCO \rightarrow C_nH_{2n} + nH_2O$ (2.2)

Alcohols and Ethers: $2nH_2 + nCO \rightarrow C_nH_{2n+2}O + (n-1)H_2O$ (2.3)

Aldehydes ad Ketones: $(2n-1)H_2 + nCO \rightarrow C_nH_{2n}O + (n-1)H_2O$ (2.4)

Carboxylic acids and Esters: $(2n-2)H_2 + nCO \rightarrow C_nH_{2n}O_2 + (n-2)H_2O$ (2.5)

The synthesis process raises a number of issues, which can affect the efficiency and economics of the ICL. Key issues include reactor choice and configuration, operating conditions catalysts and product distribution and a more detailed discussion of these issues follows.

Reactor choice and configuration

There are two types of reactors that are currently being used in the ICL industry: Multi tubular fixed bed reactors, e.g. Sasol Arge and Shell SMDS, and fluidised bed reactors e.g. Sasol slurry phase reactors) and these are illustrated in **Fig. 2-3**. The fluidised bed reactors can be further classified by phases in contact in the reactor. Circulating Fluidised bed reactors (CFB) and fixed fluidised bed reactors (FFB) are examples of two-phase reactors. Sasol slurry phase reactors facilitate contact of gas-liquid-solid reactions and fit the three-phase reactor class (Dry, 2002a). The FFB are the preferred of the two-phase reactors because of their lower operating costs, construction costs and better volumetric efficiency (Jager, 2003; Steynberg *et al.*, 1999).

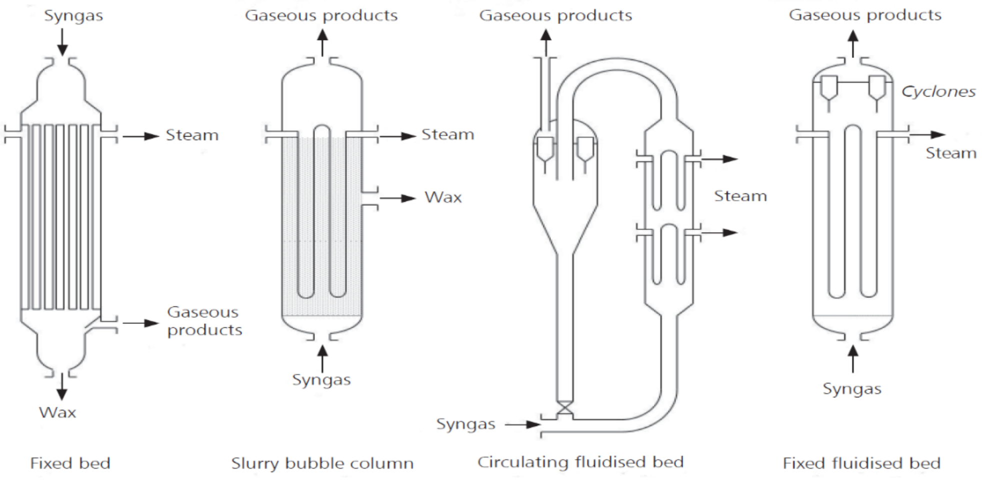

Fig. 2-3: Commonly used F-T synthesis reactors (Jager,2003)

Slurry bed reactors offer improved pressure drop performance and experience less temperature gradients (De Klerk *et al.*, 2013) than CFBs. Ease of replacement of deactivated catalysts lowers the costs associated with catalyst use. The cost reduction is more significant in Cobalt catalysts as they exhibit a lower water inhibition effect (Schulz, 1999). However, slurry reactors have liquid product-catalyst separation challenges because of catalyst fines that are generated by catalyst attrition.

Slurry reactors offer better mass and heat transfer rates than other reactors. Selectivity for longer chain compounds is affected by mass transfer of CO and H_2 in the reactor, higher selectivity has been realised in slurry reactors (Jager, 2003). Removal of heat is key in synthesis reactors hence heat transfer plays a significant role in the selection or design of an F-T synthesis reactor (Dry, 1996). Higher temperatures have a higher selectivity for less valuable low carbon chains (De Klerk *et al.*, 2013). This is supported by product predictions by the Anderson-Schulz-Flory (ASF) distribution model (Masuku *et al.*, 2011). Higher temperatures may also favour the Boudouard reaction, which is responsible for catalyst deactivation via coking and sintering which reduces catalyst life. Short catalyst life increases costs associated with regeneration and replacement of catalysts. Overall, slurry reactors are simpler to design and operate hence they have lower capital requirements (Jager, 2003).

The selection of reactor technology is a delicate balance of economic and operational objectives. Some reactors allow for lower cost operation but perform badly with respect to selectivity of some products. Selection of the wrong reactor technology can have negative effects on the economic and operational performance. Because of the complexity of the selection, reactor selection and design is an obvious source of risk in CTL projects.

Operating conditions in F-T synthesis reactors

F-T synthesis often happens under high pressure between 2-4 MPa (Steynberg *et al.*, 1999). Pressure affects the productivity synthesis. The temperature used in the synthesis reactor determines whether the process is a low temperature F-T process(LTFT) or high temperature F-T process (HTFT). LTFT plants run synthesis at temperatures between 200 °C and 240 °C, while HTFT is operated at temperatures between 300 °C and 340 °C (Dry, 2002a). The operating temperature influences absorption and desorption onto the catalyst surface which affects the hydrocarbon length of molecules produced (De Klerk *et al.*, 2013). LTFT is used to produce linear long molecules such as waxes, HTFT is used to produce gasoline, and low molecular mass alkenes (Dry, 2002a). All industrial slurry reactors that have been built to date have been used with LTFT processes rather than HTFT (De Klerk *et al.*, 2013). This could be due to the higher selectivity of cobalt catalysts for lighter and less valuable hydrocarbons like methane and ethane.

Because of the ties between influence of conditions, catalyst choice and reactor configuration on product selectivity, the selection of conditions is not a simple matter and has to be done with due consideration of the other connected factors. Since conditions influence the product selectivity, choice of conditions and the control thereof is critical to the successful operation of CTL.

Catalysts for F-T synthesis

F-T synthesis catalysts are subject to three key requirements: activity, selectivity and stability (De Klerk *et al.*, 2013). Research into active, highly selective and long life catalyst is ongoing and catalysis for F-T synthesis is fairly well understood. The selection of catalyst is broadly between iron-based catalysts and cobalt based catalysts and is often influenced by the nature of the desired products.

A guideline on selection of the right catalyst for the process objectives is described in detail by Krishna and Sie (1994). Improved product spectrum would result in fewer separations and as such, a higher efficiency and lower operating costs. Cobalt catalysts have been observed to have a lower selectivity for methane than iron-based catalysts at the same reactor conditions (Leckel, 2010). Of the factors known to affect the selectivity of catalysts, temperature and reactant ratios seem to have the most significant effects whereas pressure has little effect on selectivity for iron-based catalysts but a clear influence on Cobalt catalysts between 0.1- 2 MPa (Dry, 1982). Reactant ratio is often adjusted by the use of a CO_2 recycle to achieve an H_2: CO ratio that is required for a cobalt catalysed F-T synthesis process (Christensen *et al.*, 1998).

Overall, depending on the reactor configuration being used, Cobalt catalysts are preferable where the reactant ratio is between 1.7 and 2.01 whereas iron based catalysts are desirable where higher temperatures are used and water gas shift activity is required. Appropriate selection and management of catalysts is important for the viable operation of CTL.

Models used in predicting F-T synthesis product distribution.

Product distribution models are critical in the techno-economic design and associated evaluation of F-T processes. Estimation of the economic viability is based on these predictions and this influences development of project acceptance criteria. Use of unrealistic predictions could result in escalation of projects that should not be have been considered in the first place, which results in wastage of resources.

In the study of ICL processes, the Anderson Schulz- Flory (ASF) distribution is often used. Researchers have identified deviations of actual product distribution from predictions of the ASF distribution (Madon & Taylor, 1981; Patzlaff *et al.*, 2002). However, liquid phase ASF can adequately predict product composition (Masuku, 2011). Another product distribution model utilizing triple-α model is mentioned by Fox III and Tam (1995) but has not been applied due to complexity and limited adaptability. When using the ASF, there are theoretical limits to the yield of products of a particular chain profile hence the need for upgrading of products (Dry, 1990). Prediction of product distribution in the design of F-T synthesis plants could be another source of technical risk if not done cautiously.

2.3.2.5 Product work-up

Syncrude produced by a Fischer-Tropsch process can be compared to crude oil but is significantly different (De Klerk, 2011). However, much like crude oil, syncrude needs to be processed into a form that the market requires and this is what happens in the product work-up processes. The options include, upgrading, partial refining and full refining depending on the objective. This subject is discussed in more detail by De Klerk (De Klerk, 2012a)

2.3.2.6 Utility generation

Utility generation is a combination of steam generation and electricity generation. F-T synthesis plants can generate power for internal use by use of steam or gas turbines. According to Dry (1999), 33% of an F-T synthesis plant feed coal is used in the steam plant for generation of high-pressure steam (HPS). Additional steam is generated through heat recovery from syngas cooling, water gas shift reactor and cooling of the F-T synthesis reactor, which can be used for electricity generation.

Gas turbines are used for generating electricity using either unconverted syngas or petroleum light gases from the product upgrade section. Use of syngas to generate electricity tends to be economically inefficient as coal can be used directly to generate high-pressure steam, which can generate electricity in cheaper steam turbines (Zennaro, 2013). Theoretically, all F-T plants have the capability of being net exporters of electricity to the grid. However, the highly regulated and localised nature of electricity markets tends to make it unreasonable for capitally intense CTL operations to focus on producing electricity as a primary product.

2.3.3 Efficiency of indirect coal liquefaction

Efficiency in the use of material and energy resources is key to sustainable operation. Carbon efficiency measures how much of carbonaceous feed is converted to desired hydrocarbons. Thermal efficiency measures how well energy is utilised in the conversion of feed to products. There has been a higher focus on thermal efficiencies of F-T processes than with the carbon efficiency (De Klerk, 2011).

According to Rostrup-Nielsen (1994), ICL plants producing only liquid fuels tend to have lower thermal efficiencies than those producing chemicals. The reported averages for gasoline plants is 58% and 63% for diesel producing ICL plants while methanol plants average 72%. This demonstrates that the economic objectives of the CTL plant can influence the efficiencies realised by the process.

The carbon efficiency of CTL plants has not received much attention in literature. In the few instances where carbon efficiency has been reported, the CTL plant carbon efficiency is low ranging between 30% and 52% (De Klerk, 2011; Mulder, 2009). The low efficiencies seem to be connected to greenhouse gas emissions originating from gasification and combustion in the steam plant (De Klerk, 2011). The carbon efficiency necessarily becomes low since the carbon converted to energy is not considered in the product quantities used in the computation of carbon efficiency. Since a lot of literature on the CTL process has been developed as a case for the adoption of CTL, reporting of low carbon efficiency would not work in the favour of the cause. Hence, there appears to be some level of bias in reporting of efficiencies.

Despite the bias in efficiency reporting, both carbon efficiency and thermal efficiency are important parameters when evaluating opportunities for improving CTL processes. Improving the carbon efficiency reduces the process sensitivity to feedstock costs while improving the thermal efficiencies desensitises the process to energy cost shocks (De Klerk *et al.*, 2013). Because of the strong connection between greenhouse gas emissions and carbon efficiency, strategies to improve carbon efficiency have to be centred on minimising carbon losses through emissions.

2.3.4 Process economics of indirect coal liquefaction

Most literature reviewed consists of theoretical studies hence the process economics data supplied is based on projections and not actual costs, which tend to be closely guarded. It is worth mentioning though that there is some general agreement between the plants based data and theoretical projects as to the sections of plant that require the highest capital costs. Syngas generation contributes to 58-70% of the capital investments required for an F-T synthesis based CTL plant (Dry, 2004; Rostrup-Nielsen, 1994; Zhou *et al.*, 2011). There has been very little change to reported capital requirement breakdown over the last two decades. However, some technology developments have been made over this period that should affect the capital requirements distribution. Some of the developments include the use of slurry bed reactors resulting in 40% less capital compared to fixed bed reactors (Jager and Espinoza, 1995) and 70% lower catalyst costs. These changes would imply that the capital cost of syngas generation should be more significant vis-à-vis constituting a bigger percentage of capital breakdown. A possible explanation for this observation is that the capital requirements reported in literature are based on old data, which do not factor in the capital reduction from technological progression.

Since economic analyses presented in literature are theoretical in nature, they tend to have a lot of uncertainty. Operation costs are not usually discussed with the exception of costs of feedstocks. Most other costs tend to be presented as a percentage of the fixed capital cost (Kreutz *et al.*, 2008). This approach has the disadvantage of operating cost projections inheriting the uncertainty in the calculation of capital cost.

Coal consumption is cited as the biggest part of the operating cost in ICL (Zhou *et al.*, 2011). Considering the significant differences in coal costs between China and South Africa, coal cost for the Sasol process is not as significant when compared to China (Sasol limited, 2014). Besides the coal price, electricity price, capacity factor and capital cost have been reported to have a significant impact on the process economics of ICL processes (Zhou *et al.*, 2011). According to Dry (1996), the product mix can make a big difference to the economic viability of F-T synthesis plants, with dedicated liquid fuels plants requiring higher crude oil prices for them to be viable. As an example, the first phase of Sasol's South African ICL operations are said to have survived because of high priced waxes that were being produced alongside the liquid fuels.

As of 2015, prices of crude oil can marginally support the viable operation of a CTL process given Sasol's reported operational costs of $47/bbl. (Sasol limited, 2014). For Sasol, when carbon tax is implemented in 2016, at an effective $10 per CO_2 ton on 40% of emissions, the marginal profits will be eroded. However, there remain some opportunities for improving the economic performance of the process by lowering feed costs and compliance costs related to plant emissions.

2.3.5 Environmental impact of indirect coal liquefaction

Greenhouse gas emissions receive the most attention when discussions of ICL environmental impacts are presented (Bartis *et al.*, 2008; Kreutz *et al.*, 2008; Miglio *et al.*, 2013). Besides greenhouse gas impact, there are other environmental concerns such as the management of solid waste (Furimsky, 1996; Miglio *et al.*, 2013), water and wastewater management and management of toxic air pollutants (Sasol Limited, 2009).

Sasol has been criticised for the release of volatile organic compounds (VOCs) like benzene, carbon monoxide, hydrogen sulphide and sulphur dioxide into the environment. These pollutants have been associated with a rise in respiratory disorders and cancer cases in the surrounding residential areas (Dubey, 2007). The additional cost associated with the environmental impact is often not discussed in literature. As evidenced in Sasol literature (Sasol Limited, 2009), there is a need for ICL operators to invest into the mitigation and that raises the costs of operations.

ICL produces a lot of water from the synthesis reactor (De Klerk, 2011). However, the CTL process is a net consumer of water. Hence, water management is an important concern. Issues that need to be managed include supply security, wastewater quality, specific consumption and cost of water usage (Miglio *et al.*, 2013). Conventionally, CTL plants are located close to source of feedstock but it is clear that a reliable water supply needs to be considered before setting up a plant.

Spent catalysts and ash form the bulk of solid waste that needs to be managed in a CTL plant. Processes have been developed to recover metals from spent catalysts and are often not a real problem in the management of waste (Furimsky, 1996). Course ash has been used as an aggregate in road construction and brick making (Matjie & Van Alphen, 2008).

2.3.6 Future outlook of indirect coal liquefaction

The future prospects of ICL are strongly influenced by the evolution of the factors that enable or challenge the growth of consumption of ICL products and the continued viability of operations. The review of drivers and challenges ICL will face in the future can be grouped into technological, energy resource and policy related influences. The discussion of each of the group of factors is presented in Sections 2.3.6.1 to 2.3.6.3

2.3.6.1 Energy resource related developments

Of the factors that shape the future prospects of coal to liquids technologies, the energy resource dynamics are likely to have the most significant effect on future application of the CTL process. The resource dynamics influence the energy quantities available for supply, the form the energy is available and the cost at which the energy is available to the energy markets.

Resource depletion models by Shafiee and Topal (2010) and Thielemann *et al.* (2007) suggest that oil and gas will be depleted in under three decades while coal reserves will persist for at least a 100 years. A challenge with the depletion models is that they do not account for reserves that will be discovered by improved prospecting technologies or reserves that are currently not considered as viable. In the event that no substantial reserves are discovered, ICL will become more attractive for provision of liquid fuels and chemicals. For the South African case, there are no known viable oil reserves. Gas resources have been found in the Karoo and this may sway investment in synthetic fuels towards the cleaner, cheaper gas to liquids technologies. Given the resource dynamics, prospects of ICL should remain favourable in the long term.

2.3.6.2 Technological developments

The technological factors influencing the applicability of a CTL process in the future are on both the supply side and the demand side.

On the supply side, the drivers are closely connected to some of the CTL process problem areas. As such, advancement of technology that will improve cost competitiveness will be key to the continued application of a CTL process e.g. high performance catalysts, ultra-efficient air separation, zero water-cooling, high efficiency syngas technologies and carbon dioxide reutilisation technologies among others. If capital costs are significantly reduced, operating and clean-up costs of CTL reduced to make it more cost competitive with other alternative processes (Aguilera, 2014), the risks associated with implementing a CTL process will be reduced. Lower operating costs would improve the value created for product market.

The demand side technological factors are most likely going to present hurdles to the application of a CTL process. Some of these technology factors considered include more efficient internal combustion engines, progression of carbon free transportation e.g. electric and hydrogen cars (Kendall, 2015; Lippert, 2015) and preferences for low carbon mass transit systems. Such developments lower demand for synthetic fuels and consequently gives fuel price a higher significance, and more cost competitive sources of energy would then be preferred. Expert opinion in some areas suggests that petroleum driven cars and buses will continue to play a significant role in most cities (Aguiléra & Grébert, 2014). Continued contribution of petroleum driven cars combined with low development rates of alternative fuel infrastructure leaves plenty of room for the application of a CTL process.

2.3.6.3 Policy related developments

A number of policy issues can affect the future prospects of a CTL process, key among them are the general development policy, energy policy and environmental policy, which has received the most attention globally as the decarbonisation agenda gains prominence.

The environmental policy has evolved over the years but maintains a focus on effects of systems on air, land and water quality. In the 1960s and 1970s, ICL was challenged by environmental policies that put pressure on coal mining as the process released particulates, which were perceived to cause climate change and contaminate water supply systems (Olson, 1977:13). In the mid to late 1990s the focus shifted to carbon emissions, which affected the utilisation of coal, including the use of coal based thermal power stations and gasification plants for fuels and chemicals production (Dry, 1999; Schulz, 1999). Currently, there is a shift towards accounting for lifecycle emissions and setting carbon prices. ICL impact on water resources has not been under as much scrutiny as the emissions. However, as pressures on adequacy of freshwater supply grow, the regulation of water impact and cost of cleaning up is bound to affect the viability of ICL in the future.

Most environmental policy directives tend to come with capital and operating cost requirements for businesses. With current policy, carbon-pricing policies affect the economics of the process. Mitigation of emissions has extra equipment needs to minimise emissions and to reduce land and water contamination. Such additional costs in ICL processes include carbon capture and sequestration (CCS) equipment. According to Yoshino *et al.* (2012), equipment costs for mitigating carbon dioxide could add as much as 10% to product cost. In practice the added cost will probably be higher. However, not investing in mitigation solutions can be associated with operating costs in the form of carbon taxes. As of 2015, South Africa has a carbon policy that is still under review. Knoope *et al.* (2013) suggests that the cost of CO_2 avoidance is of the order $15-20 which may have no advantage over paying the carbon tax in its current design of $4-10/ t CO_2 (South Africa National Treasury, 2013). However, payment of this carbon tax adds $3.7/bbl.- $9.1/ bbl. to the operating costs based on the current tax regime design.

Not all policy issues affect the prospects of ICL negatively as the energy policy and resource development policies will likely be enablers and drivers of ICL implementation. Historically, ICL development in South Africa, Germany, Japan and China was driven by the need for fuel supply security (Zhou *et al.*, 2011). The pursuit of energy security can, as in the case of Germany (Stranges, 1984) and South Africa during isolation phases, supersede the economic performance criteria. As crude oil and natural gas diminish, the need for supply security may enhance the prospects of ICL processes (Rong & Victor, 2011).

ICL is one of the few ways of adding value to coal (Bell *et al.*, 2011c). Hence, the adoption of pro- resource development policies would improve the future prospects of ICL but that would be dependent on competitive economic performance of ICL processes. A holistic analysis of the economic benefit, such as was carried out by Qi *et al.* (2012), of ICL plants could help boost the future ICL prospects. According to Rong and Victor (2011), conventional economic analysis fails to capture the full benefits of ICL plants and this was corroborated by Qi *et al.* (2012). An ICL techno-economic analysis of a Chinese plant implies investment returns of 500 jobs/$ million invested as well as economic stimulation of the order of $3.50/ $1 invested (Qi *et al.*, 2012) and these are not usually captured in conventional economic analyses. Further, benefits like improving energy security are difficult to quantify. If the economic value added of ICL improves with the lowering of the environmental footprint then, the future prospects are bound to improve.

2.3.7 Research and development opportunities

After reviewing developments of F-T synthesis in the last three decades, a number of research and development opportunities emerge.

- Reducing the overall capital cost of ICL with major opportunities in syngas generation
- Improving the carbon efficiency of indirect coal liquefaction
- Reducing greenhouse gas emissions, which can also be viewed as minimising process carbon losses.
- Development of cheaper CO_2 compliance cost avoidance solutions, from the $15- $85/ ton CO_2 range (Chiesa & Lozza, 1999)
- Development of high activity catalysts with low selectivity for CH_4, high selectivity for middle distillates and high coking temperatures
- Improving mass transfer rates for reactants and improving heat transfer rate in the removal of Fischer Tropsch reaction heat.
- Low cost gas separations for H_2, O_2 and CO_2
- Integration of internal processes to improve utilisation of energy from exothermic reactions and cold utilities from cryogenic air separation

The risks of implementing ICL are increased by the number of processing steps in the liquefaction process. If the complexity is accepted as an inherent part of using ICL, then the biggest opportunity to improve ICL lies in improving the carbon efficiency.

Improving the carbon efficiency will probably improve the economic performance of indirect coal liquefaction (De Klerk *et al.*, 2013). To improve carbon efficiency, it is necessary to reduce carbon losses from the process. The biggest carbon loss in ICL is in the form of greenhouse gas emissions. Recovery and re-utilisation of carbon from greenhouse gases will result in smaller syngas equipment requirements. Smaller syngas generation equipment means the capital requirements of the most capital intense section of ICL will be reduced. However, the capital savings would be a trade off with the cost of recycling CO_2.

Reduction of emissions by redesigning the process coincides with the cleaner production philosophy (Ashford, 1994; Fresner, 1998; Kjaerheim, 2005). Hence, ICL would benefit from the application of cleaner production principles. Details of cleaner production principles are discussed by Fresner (1998).

2.4 Improving carbon efficiency of indirect coal liquefaction

Since most of the carbon loss in ICL is in the form of greenhouse gases, recycling carbon dioxide and redirecting it to product formation will improve carbon efficiency. This study focuses on methods of recycling greenhouse gases as a way of improving carbon efficiency of ICL.

In principle, many methods can be used to convert carbon dioxide to desired products. Examples include carbon dioxide thermolysis (Lyman & Jensen, 2001), photo electrolysis (Lee *et al.*, 2014), low and high temperature co-electrolysis of carbon dioxide (Graves *et al.*, 2011; Stoots *et al.*, 2010) and dry reforming of methane with carbon dioxide (Lavoie, 2014; Swapnesh *et al.*, 2014). Of the listed conversion processes, only dry reforming converts the two most significant greenhouse gases from ICL, hence dry reforming is the focus of this thesis.

Dry reforming is similar to conventional steam reforming with the exception that steam is substituted with carbon dioxide as the oxidant. One of the most common challenges inherent in the dry reforming process is endothermic nature of the reaction (Tao *et al.*, 2011). Use of methane combustion to provide energy for dry reforming had been previously proposed by Treacy and Ross (2004) in a thermodynamic study but the net greenhouse gas consumption was marginal. When Sudiro and Bertucco (2009) proposed use of dry reforming in ICL, they proposed the use of unconverted syngas, in F-T synthesis tail gas, combustion as a source of heat for the reaction. However, syngas combustion generates more carbon dioxide that limits the potential to improve carbon efficiency. In addition to the endothermic challenge, unfavourable thermodynamics of the reaction (Oyama *et al.*, 2012) and catalyst coking (Aziznia *et al.*, 2012) have been cited as potential challenges. The coking has been reported to be avoidable under certain conditions. Tao *et al.* (2011) reported that it is possible to have high conversions of both carbon dioxide and methane in their review of laboratory scale plasma assisted dry reforming.

Plasma reformers have a challenge of high electricity consumption but Xu *et al.* (2013) have demonstrated that the plasma synergistic effect can reduce the specific energy consumption if the reactor is correctly configured. The high electrical consumption will contribute to a higher operating cost for plasma reactors but the benefit may be greater than the cost. If the electrical energy is supplied from a fossil fuelled source, use of plasma reforming would result in externalisation of carbon dioxide emissions.

Section 2.5 presents some basic concepts of plasma and plasma-assisted chemistry to give the reader some background and appreciation of some of the challenges of applying plasma arc reforming.

2.5 Introduction to plasma technology

2.5.1 The basics of plasma technology

The term plasma was first used in physics to describe gases in a state beyond its critical conditions by Irving Langmuir in 1928 (Fridman, 2008). Plasma is considered by some as the fourth state of matter (Fauchais & Rakowitz, 1979). The composition of a plasma varies depending on the degree of ionisation of the plasma and the method used in the creation of the plasma.

Plasma can be formed by heating a gas to a very high temperature or exposing the gas to a strong electromagnetic field or both. This causes electrons to be dislodged out of their normal molecular orbits and the gas ionises to form a mixture of electrons, ions and neutral molecules. The electrons are sometimes called light particles while the ions and neutral molecules are called heavy particles. The degree of approach to thermodynamic equilibrium of light and heavy particles can be used as the basis of classification. The differences in the approach to equilibrium can explained by the mechanism of plasma formation and the relative proportion of the different particle classes.

Plasmas are generally separated into two types that are differentiated by the extent of thermal equilibrium between heavy particles and light particles. If a plasma establishes equilibrium at a point where the temperature of electrons is very different from the heavy particles, then the plasma is classified as a non-equilibrium or cold plasma (Venkatramani, 2002). If the electrons and heavy particles achieve thermal equilibrium, the plasma is then classified as a thermal plasma (Fridman, 2008). A more detailed description of the two plasma classes is presented in Section 2.5.1.1 and 2.5.1.2.

2.5.1.1 Cold plasma:

Cold plasmas are also known as non-equilibrium plasmas and are characterised by the existence of a large temperature gradient between heavy particles and light particles. The electron temperature can be of the order of 10000 K whereas the heavy particle temperature is at room temperature. This normally occurs because the electrons receive energy from the electrical field first due to their low mass. The dislodged electrons subsequently dislodge other electrons in a chained process known as the electron avalanche effect, which was first proposed by John Sealy Townsend in 1897 (Roth, 1995). Because the avalanche effect is significant for cold plasmas the most important mechanism of ionisation is direct ionisation by electron impact (Fridman, 2008).

The collision and interaction between particles in plasma has two effects. The first is that the collisions between electrons cause Joule heating, which results in the temperature of electrons rising rapidly to very high values. The second is that collisions between electrons and the heavy particles result in energy being transferred from electrons to ions and neutral particles, which results in the overall plasma temperature rising.

Cold plasmas are normally generated at low pressures and low power of pulsed discharge systems hence the overall rise in temperature due to light and heavy particle interaction is limited. Due to the overall low temperature of cold plasmas, they tend to be applied where there is a requirement for ion selectivity but no energy intensity. These applications include areas where the glow discharge from ionisation is significant such as in neon lights or visual plasma devices. Other examples of cold plasmas include some medical plasmas, plasmas in neon lights, in plasma screens etc.

2.5.1.2 Hot plasma /equilibrium plasma

Hot plasmas are also known as equilibrium plasmas, as the temperature of the electron cloud and the bulk gas temperature are in thermal equilibrium. The methods and conditions used in the production of hot plasmas are usually high temperature and pressure and that influences the overall temperatures of both the light and heavy particles in the plasma. Examples of such methods include use of electric arc discharges where a gas is passed through a high voltage arc to ionise the gas.

Hot plasmas are very powerful and can generally be applied in situations that require high power intensity (Roth, 1995). Examples of hot plasmas are the plasma arcs used in metallurgy for smelting, plasma arcs in cutting torches, destruction of hazardous wastes among others.

2.5.2 Components of plasma and their influence on applications of plasmas

Research into applications of plasma started in the late 18th century (Fauchais & Rakowitz, 1979). However, a lack of understanding of plasma characteristics made it difficult to correlate the observed results to the type of plasma discharge applied. The implication of this was that it was not possible to specify the plasmas that could be used for a particular application as it was difficult to reproduce the plasma discharges. In the context of chemical processing, it meant that conditions in plasma reactors could not be reproduced at different scales and this limited the areas of industrial application (Fauchais & Vardelle, 1997). However, as the understanding of plasma composition and characteristics has grown, it has become possible to specify and reproduce plasmas for different applications.

The composition of a plasma depends on the degree of ionisation of the gases used in its formation. Most plasma discharges are mixtures of electrons, ions and neutral particles. In the formation phase, there is production of ultraviolet radiation that can influence reactive processes or cause some gases to glow such as in neon lights (Fridman, 2008). Since the composition of a plasma influences the application, it is necessary to briefly discuss the role of different components in determining plasma characteristics prior to a discussion of some of the applications.

Electrons are usually the first components to receive energy from electric fields that are used in the ionisation of gases to plasma. These electrons subsequently play the role of redistributing the energy to the heavier components like ions and the remaining neutral particles. Redistribution may take the form of vibrational excitation of atoms and molecules, which could lead to formation of free radicals. Influencing the density, temperature or energy distribution functions of the plasma’s electron cloud gives users finer control on the effectiveness of a plasma on the effectiveness of a plasma in a specific application.

Ions contribute to applications in two ways. 1) Due to their relatively heavier mass, they carry and transmit their sensible energy, which can provide a heating effect if they are high energy ions. 2) Ions are capable of suppressing activation barriers of chemical reactions as their charged nature influences the behaviours of reagents by interacting with electrons of neutral particles (Fridman, 2008). These effects result in plasmas having a catalytic effect in chemical processing applications such as flame stabilisation, destruction of hazardous chemicals and treatment of living tissue as in plasma skin therapy (Roth, 1995).

Besides the effect of electrons and ions, photons and transient particles can influence the properties of a plasma, which in turn affects the applications of the plasma. Photons tend to be important in plasmas applied in visual applications such as glow discharges used in neon lights and plasma televisions. Transients include particulate transients such as free radicals and transient energy states that have a potential to participate in plasma chemistry. Transient energy states include translation of electron kinetic energy into vibrational energy. This vibrational energy has the potential of contributing to the formation of free radicals and other metastable particles that have reactive properties such as has been observed in plasma stimulation of carbon dioxide (Fridman, 2008). Vibrational stimulation presents the highest opportunity for energy efficiency in complex molecules in cold plasma processes (Gallagher Jr & Fridman, 2011). Carbon dioxide transfers most of the energy from electrons to vibrational energy, if the vibrational energy is used to stimulate the reaction, then the process is more efficient.

As mentioned before, though there are two basic types of plasma, there are many different plasma discharges that have different properties. The differences in properties presents the opportunity for many applications. Examples of plasma uses include thermal decomposition of coatings, flame stabilisation, water sterilisation, destruction of hazardous chemicals, microelectronics processing, plasma etching and wound treatment among many other applications. Plasma gasification of waste presents the best design lessons for ICL applications hence, lessons from plasma gasification will be applied in the development of plasma reforming for application to ICL. Because the application of plasmas in ICL falls under chemical processing, the remainder of the plasma application focuses on plasma applications in chemical processing.

In chemical processing applications, plasma was conventionally considered to be attractive for high temperatures and high energy densities of the components and by implication only hot plasmas were considered applicable. As the understanding of plasma has expanded, it has been realised that plasmas can influence chemical reactions in more ways than providing high temperature and as a result, both hot and cold plasmas are now considered important for chemical processing. In cold plasmas the chemical process could be enhanced by atoms that have been excited by electrons. The electron excitation of atoms and molecules becomes significant in chemical applications if the lifetime of excited particles is long. An example of this is the case of metastable oxygen encountered in oxidative plasma discharges.

The rationale, design considerations, historical application, application performance evaluation, challenges and opportunities of plasma application in chemical processing as represented by ICL are discussed in Sections 2.5.3 to 2.5.8

2.5.3 Rationale of plasma reforming application in ICL

The attractiveness of applying plasma reforming in ICL can be demonstrated by comparing the overall chemical reactions for dry reforming of methane with carbon dioxide and steam methane reforming (SMR).

Steam reforming: $CH_4 + nH_2O \rightarrow CO + 3H_2$ ΔH = 206 kJ/mol. (2.6)

Dry reforming: $CH_4 + CO_2 \rightarrow 2CO + 2H_2$ ΔH = 247kJ/mol. (2.7)

Both steam reforming and dry reforming are endothermic reactions, hence, dry reforming has a disadvantage with respect to energy requirements. However, when comparing the raw material requirements, dry reforming requires 75% of the methane required by steam reforming to produce 1 mole of carbon monoxide (Tao *et al.*, 2011). Another advantage is that dry reforming in a plasma reformer recycles a waste carbon dioxide stream and internally generated methane to improve yield of syngas. Further, if a renewable or low carbon power source is used in plasma reforming, dry reforming produces no greenhouse gases as opposed to SMR that converts a third of the methane to carbon dioxide.

Because dry reforming is energy intensive, efficiency of energy use is more critical in plasma reforming applications. PAR would be more energetically effective if the active species generated in the plasma are capable in participating in chemical reaction (Benilov & Naidis, 2006). It therefore follows that for dry reforming, the process will probably be more efficient if either carbon dioxide or methane is used as the plasma gas as opposed to using air or an inert gas as the plasma gas. It can be argued by some that complex molecules cannot be used as plasma gases, however if the trade-offs are considered, neither atomic nor complex gases have a distinct advantage in their use as a plasma gas. Theoretically, the arc losses are the same for atomic and complex molecules (Roth, 1995). On the other hand, complex molecules have higher heat capacities, which gives them an advantage in chemical reaction applications that requires high enthalpy transfers (Venkatramani, 2002). Hence, it should be advantageous to use a plasma reformer with a complex molecule like carbon dioxide as the plasma gas.

There is no record of plasma arc reforming application in the coal to liquid space with the exception of a study by Stoker and Conradie (2015), which was done in the context of creating a nuclear assisted coal to liquid process. In their study they concluded that the combined use of nuclear heat and nuclear hydrogen in a commercial process would not likely be viable. Two drawbacks to their study are 1) it assumes it is feasible to apply PAR at commercial scale even though it is unproven in the CTL process context and 2) the lumping of several initiatives in the analysis makes it difficult to attribute observed effects to a particular initiative. As a result, the issue of feasibility and viability of applying PAR to a CTL process remains unclear.

2.5.4 Useful measures in evaluating performance of plasma applications

A few parameters are key to the evaluation and application of plasma in chemical processing. These parameters form the fundamental criteria by which the effectiveness of a plasma reactor configuration can be measured on a macro scale and these are the electron density, plasma temperature, specific energy input and energy conversion efficiency.

i) *Electron density*:

The electron density is a measure of the number of electrons per unit volume occupied by plasma.

ii) *Plasma temperature:*

Plasma temperature refers to either the temperature of the electron cloud in a plasma or the temperature of the heavy particles (ions, excited atoms or molecules) in a plasma. For thermal plasma, there is no need to provide reference of temperature as temperature is the same for all species.

iii) *Specific energy input:*

Specific energy input (SEI) is the energy required to produce one mole of product. SEI has potential to show the impact of synergistic effect on the energy requirements of a chemical conversion process.

iv) *Energy conversion efficiency:*

Energy conversion efficiency (ECE) is the ratio of energy contained by products to the energy contained by inputs to the reactor. ECE considers all forms of energy changes in determining the efficiency of conversion.

2.5.5 Performance of existing experimental reactors in chemical applications

Several plasma reactors that have the potential of being made plasma reformers have been reported in literature (Fauchais & Rakowitz, 1979), however their performance differs with application. Some of the plasma reactors with the highest potential for application to plasma assisted dry reforming are shown in **Table 2-1**.

Table 2-1: Performance of some experimental plasma reactors

Reactor type	Conversion (%)	Selectivity (%)	ECE (%)	Source
Cold plasma jet + Ni/Al_2O_3 catalyst	CH_4:**60**;CO_2:**40**	CO:**97**;H_2:**97**	80	(Long *et al.*, 2008)

Cold plasma jet	CH_4:**46**;CO_2:**34**	CO:**85**;H_2:**78**	63	(Long *et al.*, 2008)
Binode thermal plasma	CH_4:**79**;CO_2:**65**	CO:**97**;H_2:**83**	57	(Xu *et al.*, 2013)
Single anode thermal plasma+ Ni/Al_2O3 catalyst	CH_4:**92**;CO_2:**82**	CO:**90**;H_2:**82**	54	(Tao *et al.*, 2008)
Single anode thermal plasma (H_2 plasma gas)	CH_4:**87**;CO_2:**84**	CO:**75**;H_2:-	36	(Zhang *et al.*, 2002)
Single Anode thermal plasma (N_2 plasma gas)	CH_4:**89**;CO_2:**80**	CO:**88**;H_2:**68**	48	(Tao *et al.*, 2008)

From **Table 2-1**, it is evident that both cold and thermal plasmas have the potential to achieve high selectivity for syngas. However, the conversion for the cold plasma reactors is much lower than that of thermal plasmas. High conversion combined with high selectivity results in thermal plasmas achieving better syngas yields and that confirms claims, by Xu et al (2013), that thermal plasmas have better results for chemical processing. The performance in terms of energy efficiency is more difficult to compare because of differences in design of lab reactors and differences in calculation methods. Because of better yield, thermal plasma was applied in this thesis.

2.5.6 Industrial scale plasma reformer design considerations

If lessons from experimental plasma reactors are considered in industrial scale reactor design, a number of considerations are apparent. The three most important considerations are;

- Mixing of reactants and plasma, which can be a special challenge since the residence times tend to be small (Fauchais & Vardelle, 1997)
- Achieving the desired product distribution can be complicated and kinetic parameters of plasma reactions are not readily available and are complex to determine (Fauchais *et al.*, 1997)
- Quenching is sometimes necessary to remove excess energy of newly formed species (Fauchais & Rakowitz, 1979). This is achievable by a number of means including cold gas injection, cold wall quenching, fluidized bed, and adiabatic expansion and impinging into a liquid spray/bath (Sundstrom & DeMichiell, 1971)

2.5.7 Historical application of plasma reformers at Commercial scale

The Union Steel Corporation of South Africa (USCO) is reported to have operated plasma arc heated methane reformer at industrial scale in 1985 (Jones et al., 1993). Their plasma arc reformer had a plasma heater, developed by Hüls, heating carbon dioxide, which was being used as an oxidant in the reformer. High temperature carbon dioxide, preheated by the plasma heater, was then introduced into the reactor vessel where it reacted with a mixture of methane and steam to produce syngas for iron reduction (Jones et al., 1993). During the two years of operation, the USCO reformer (Jones et al., 1993) represented one of the first successful industrial implementation cases of a gas phase plasma reformer. However, the plasma reactor had to be stopped due to upstream equipment challenges.

At present, there are no commercial plasma reformers due to challenges in scaling up (Xu et al., 2013). Hence, scaling up of plasma arc reformers is an important area of study if plasma arc reforming is to be applied at industrial scale.

2.5.8 Challenges and opportunities of industrial plasma application

The application of plasma has a number of grey areas that challenge the application to dry reforming from being a precise science. Significant among the grey areas is the lack of established scaling up procedures for plasma equipment especially in chemical applications (Fridman, 2008; Roth, 1995). This is symptomatic of the lack of full characterisation of plasma assisted chemistry mechanisms. One important drawback resulting from the incomplete characterisation is that it is difficult to predict accurately the product composition of a plasma driven chemical process. As a result, optimisation of process cost and power consumption of plasma driven process is difficult (Nozaki & Okazaki, 2013).

2.6 Summary

A review of literature on Fischer-Tropsch ICL processes from the last three decades shows that the capital requirements for the implementation of the CTL process has been a significant hurdle due to the current availability of cheaper oil and gas resources. Additionally, emissions of greenhouse gases have also been deemed unacceptably high. The capital requirements and emissions of greenhouse gases are connected and are in essence different sides of the same problem. The greenhouse gas emissions are raw material losses that result in the larger process equipment being required to deliver the required throughput of required products, which results in higher capital requirements.

The use of dry reforming in a plasma reformer has the potential to abate the capital requirements, through reducing the material loss problem. However, the dry reforming reaction is a highly endothermic reaction which requires external energy. Use of fossil energy to energise the dry reforming reaction is counter-productive because it reduces the effectiveness of the process by producing greenhouse gases.

Application of plasma reforming opens the door to the application of clean and renewable energy in producing transportation fuels and petrochemical feedstocks. This presents an opportunity for the creation of ICL processes with a lower environmental footprint and better economic performance. These improvements can be achieved by targeting to improve the process carbon efficiency.

The design and scale-up of plasma reactors still presents some significant technical risk to CTL process operators. Hence, there has been an aversion to scaling them up to industrial scale. Because of this challenge, there is little information on the economic performance of plasma reformers for application in coal to liquids. This presents an opportunity to close the existing knowledge gap in the design and scale-up of plasma reformers and the techno-economic performance of the application of such plasma reformers to ICL processes.

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3 TECHNOLOGY ASSESSMENT OF PLASMA ARC REFORMING FOR GREENHOUSE GAS MITIGATION: A SIMULATION STUDY APPLIED TO A COAL TO LIQUIDS PROCESS.

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Abstract

Coal to liquids processes contribute significantly to coal rich countries like South Africa. However, their sustainability is affected by high greenhouse gas emissions and low carbon productivity. This paper explores the future possibility of applying plasma arc reforming to turn waste carbon dioxide into a useful chemical feedstock. This was achieved through a technology assessment that was performed by applying existing modelling techniques to an existing industrial liquid fuel from coal process. The approach was: 1) the selection of an appropriate plasma reforming technology, 2) evaluation of the potential impact on an industrial coal to liquids process and 3) assessment of commercial status of the chosen technology. Simulation results showed that carbon dioxide based plasma arc reformers are most compatible with coal to liquids processes. Plasma arc reforming of methane is capable of improving carbon efficiency of the coal to liquids process by up to 14% by carbon recovery from carbon dioxide. However, non-catalytic reforming of methane is not yet ready for commercial implementation, with a technology readiness level of 4. High electrical energy consumption and high technical risk in scale-up were identified as key barriers to technology commercialisation. The potential for success of plasma arc reformers would be enhanced by availability of low carbon electricity and characterisation of plasma reforming kinetics to minimise technical risk. This paper highlights the opportunity to derive value from intense, high purity waste carbon dioxide streams by the application of plasma arc reforming. It also identifies the areas technology developers should focus on to bring the technology to commercially readiness.

Keywords

Technology assessment, Plasma arc reforming, coal to liquids, greenhouse gas mitigation

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Highlights

- Plasma arc reforming technology selection for coal to liquids was done.
- An assessment of technology status of plasma arc reforming technology was done.
- Application of PAR improves carbon efficiency and footprint of coal to liquids.

Abbreviations

ATR	Auto Thermal Reforming
CE	Carbon Efficiency
CTL	Coal to Liquids
DMR	Dry Methane Reforming
ECE	Energy Conversion Efficiency
GTL	Gas To Liquids
IRL	Integration Readiness Levels
NASA	National Aeronautics and Space Administration
$R\&D^3$	Research and Development Degree of Difficulty
SEI	Specific Energy Input
SRL	System readiness level
TRL	Technology Readiness Level
TRRA	Technology Readiness and Risk Assessment
US DoD	United States Department of Defence
US DoE	United States Department of Energy
WGS	Water Gas Shift

3.1 Introduction

The sustainability of coal to liquid fuel production is affected by challenges such as high capital requirements and high emissions (Rong and Victor, 2011; Zhou et al., 2011) when compared with conventional crude refining. The biggest capital cost in a conventional coal to liquids (CTL) production plants is the synthesis gas generation section, which accounts for approximately 60% of plant costs (Dry, 2002; Williams and Larson, 2003). Synthesis gas, also called syngas, is a mixture of hydrogen and carbon monoxide that is used to produce hydrocarbons in the Fischer-Tropsch process. In a typical CTL process, only 52% of available carbon in the syngas section ends up in desirable product streams and the rest is lost as carbon dioxide emissions (Mulder, 2009). Recovering carbon from the carbon dioxide downstream will reduce the size of the process equipment, which corresponds to reduction of capital expenditure.

Processes that have been identified to have potential to use carbon dioxide as a feedstock in the production of syngas include dry methane reforming (DMR)(Yang and Wang, 2014) and high temperature co - electrolysis of water with carbon dioxide (O'Brien et al., 2010). DMR was chosen as the focus of this paper as it mitigates both carbon dioxide and methane, the primary CTL greenhouse gas emissions, at the same time. DMR makes use of an endothermic reaction between methane and carbon dioxide to produce syngas. The potential of catalysed DMR has been assessed by several researchers including Er-rbib et al. (2012) and Gangadharan et al. (2012) who studied the process with the use of Nickel based catalysts. The use of catalysts presents key challenges and still needs significant development to achieve commercially acceptable performance (González et al., 2013; Oyama et al., 2012) . Several researchers have described the use of plasma reactors to study plasma enhancement of DMR (Aziznia et al., 2012; Tao et al., 2011). These reports show that several configurations of plasma enhanced DMR are possible. The simplest case for plasma assisted reforming is when a thermal plasma source is coupled with DMR to form a plasma arc reformer (PAR).

This article is a primer to the future possibility of turning waste carbon dioxide back into a useful chemical feedstock, with the attendant reduction of carbon dioxide released directly to the atmosphere. The authors chose to illustrate the possibility by applying the theoretical concept via a simulation model to an existing and relevant industrial process. The choice of demonstration process fell on the Fisher Tropsch process employed by Sasol at the Secunda coal to liquid (CTL) fuel plant in South Africa. The plant produces 160 kbpd of synthetic fuel with a concomitant release of 70 million tons of carbon dioxide per annum, making this plant one of the largest point source of CO_2 on the planet (Mulder, 2009). This requirement was balanced with a need to provide convincing evidence that the possible application of plasma arc reforming of methane with carbon dioxide did fall within the bounds of thermodynamic and practical feasibility.

Sasol and PetroSA jointly produce up to 40% of national liquid fuel demand from coal and natural gas (Greyvenstein et al., 2008). Contribution of liquid fuels from coal is more than 60% of synthetic fuel production in South Africa, which makes CTL significant to the South African economy. As a result, ensuring the sustainability of CTL is a strategic issue for South Africa. The importance of sustainable CTL production extends beyond South Africa as global coal reserves are forecast to outlast both natural gas and crude oil (Shafiee and Topal, 2009; Thielemann et al., 2007) as a potential future liquid fuel feedstock.

The technology assessment reported in this study creates a technological case for the industrial application of plasma arc reforming of methane in CTL processes. The aim of the study was to identify the interventions required to set plasma arc reforming on its development path from being a theoretical solution at lab scale to an industrially ready solution. The paper has been structured to introduce CTL, plasma arc reforming in Sections 3.2 and 3.3, a presentation of the approach to the assessment follows in Section 3.4 and the results, discussion, and conclusions are presented in Sections 3.5 and 3.6.

3.2 Coal to liquids overview

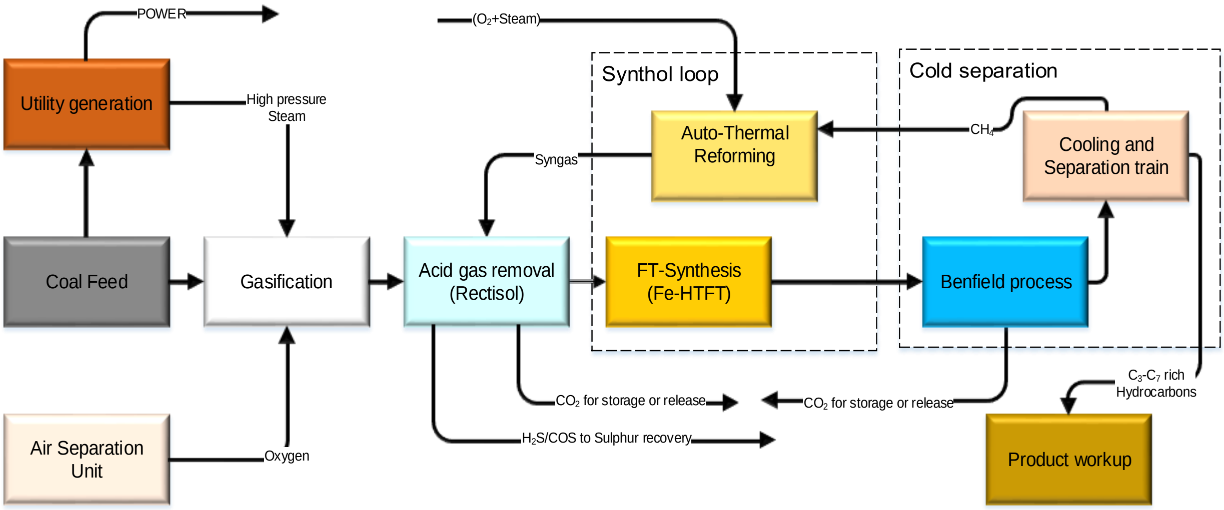
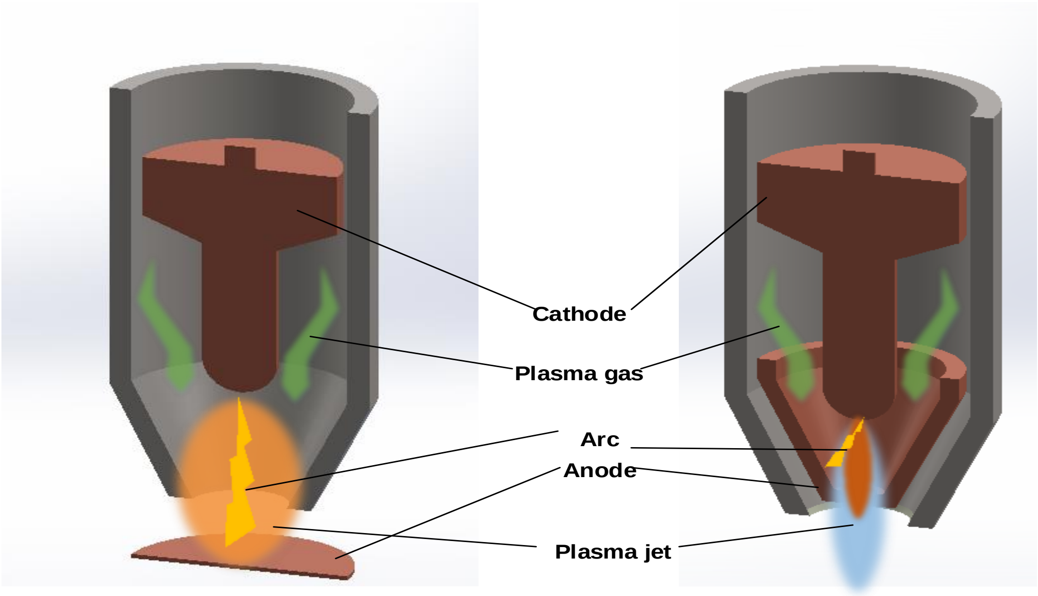


Fig. 3-1: Block flow diagram of a conventional CTL process.

Fig. 3-1 is an illustration of a simplified block flow diagram of a typical CTL. Coal is prepared to a size range that is suitable for gasification. The gasifier converts coal to synthesis gas (Zennaro et al., 2013) with the use of oxygen and steam under high temperature and pressure. Conditions in the gasifier influence the amount of greenhouse gases present in the raw syngas stream (Bell et al., 2011). After gasification, syngas, sulphur based compounds and carbon dioxide are removed by rectisol (Sun and Smith, 2013) or selexol (Mohammed et al., 2014). If necessary, the ratio of hydrogen to carbon monoxide in the syngas is adjusted through the water gas shift (WGS) (Zennaro et al., 2013). Purified syngas is then used to produce synthetic hydrocarbons, which are also known as syncrude, under high pressure with the help of a cobalt or iron catalyst (De Klerk, 2011). The syncrude is processed in the product work-up section in preparation for refining, upgrading or shipping to different product markets (De Klerk, 2011).

3.3 Plasma arc reforming basic concepts

Plasma is a state of matter that is similar to a gas but is highly ionised and is sometimes called the fourth state of matter (Bosmans et al., 2013). Plasma is created in arc reactors by passing a gas through an electric arc between two electrodes (Huang and Tang, 2007). Arc reactors can be classified into transferred arc reactors and non-transferred arc reactors (Roth, 1995).



(a) Transferred arc **(b) Non-transferred arc**

Fig. 3-2: Illustration of the two types of plasma arc torches

As shown in the simplified torch illustrations in **Fig. 3-2**, the main difference between transferred arc and non-transferred arc torches is in the anode (Barcza, 1986). Transferred arc torches have one internal electrode and use the material to be processed as the anode whereas non-transferred arc torches have both electrodes in the torch body. Vessels using non-transferred arc technology are commonly used in waste processing (Roth, 1995) and have been applied for gas heating in steel production (Jones et al., 1993). The remainder of this paper refers to non-transferred arc reactors when it discusses plasma arc reformers, as transferred arc reactors are not well suited to gas processing applications.

Since plasma gasifiers also utilise non-transferred arc technology and are technically reformers, it is necessary to exclude them from this paper by focusing on only gas phase reformers. Though similar in principle, gasifiers and gas phase reformers have different design issues, where plasma gasifiers are now a commercially proven technology (Solena Group, 2002) gas phase reformers are not as established at industrial scale.

Sections 3.3.1 to 3.3.3 give a high-level description of the plasma arc reformers that are being proposed for use as methane reformers in coal to liquids plants.

3.3.1 Chemistry

Plasma arc reforming of methane creates an important mechanism for generating valuable syngas from waste carbon dioxide through the endothermic reaction in Eq.(3.1)

$$CH_{4(g)} + CO_{2(g)} \rightarrow 2CO_{(g)} + 2H_{2(g)} \qquad \Delta\mathrm{H} = 247\ \mathrm{kJ/mol} \tag{3.1}$$

Eq. (2.1) is also known as dry reforming of methane. Heat needs to be supplied since the reaction is endothermic.

3.3.2 The basic elements of a plasma arc reactor

In principle, a plasma arc reactor consists of 1) a plasma source, 2) reaction volume and 3) a heat recovery unit. Treating the three components as separate elements that interact makes it simpler to model plasma arc reactors. The process flow relationship of the reactor elements is illustrated in **Fig. 3-3**. The key inputs and outputs of each stage are shown.

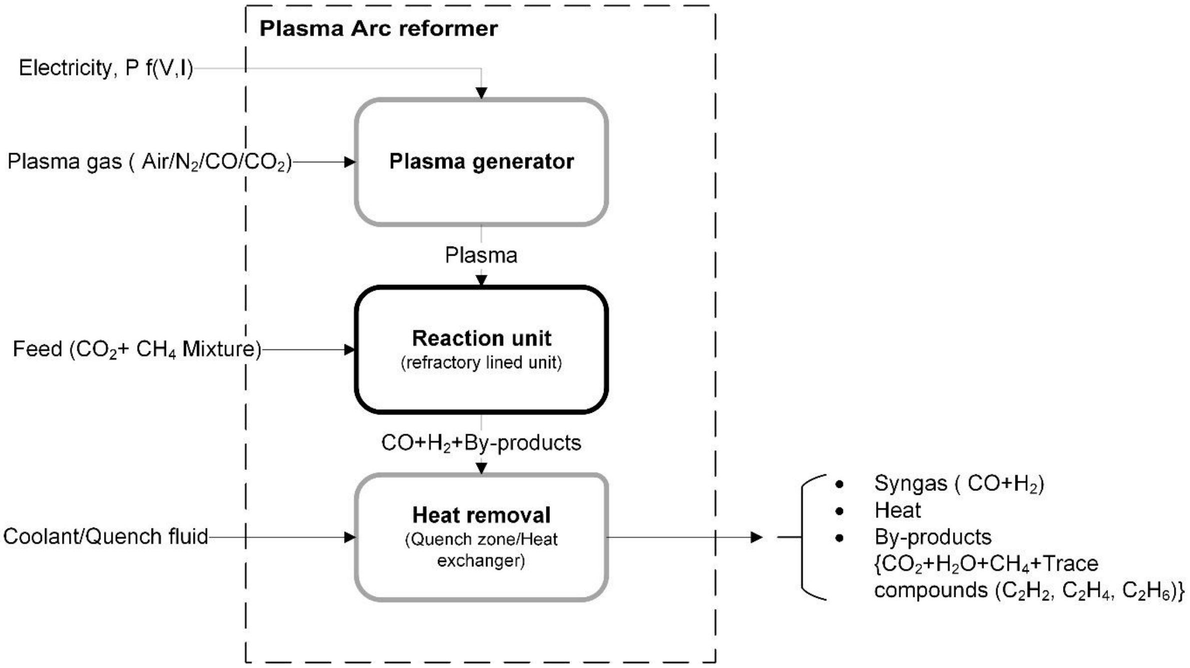


Fig. 3-3: Process flow relationship of the components of the proposed plasma arc reformer

The plasma source used in the reactor could be either a non-equilibrium plasma (Aziznia et al., 2012; Long et al., 2008) or an equilibrium plasma also known as a thermal plasma (Tao et al., 2011). Cold plasmas are generally reported to have more reactive species (Fridman, 2008) but thermal plasmas are more effective for chemical processing (Tao et al., 2011). Therefore, the more effective thermal plasma source was chosen for this study.

The reaction unit is essentially a containment space that ensures that all reactants have sufficient contact time under the required conditions. Sizing of the reaction unit is critical as it is essential for the complete conversion of reactants (Peacock and Richardson, 2012).

Plasma arc reactors create very high temperature conditions for dry reforming to occur. Since dry reforming is an endothermic reaction, high temperatures favour the formation of syngas. Lowering temperatures would favour the reverse reaction hence, an effective heat removal method ensures that the selectivity of the reactor is not reduced by the reverse reaction (Sundstrom and DeMichiell, 1971).

3.3.3 Industrial implementation of plasma arc reforming

The Union Steel Corporation of South Africa (USCO) is reported to have operated plasma arc heated methane reformer at industrial scale in 1985 (Jones et al., 1993). Their plasma arc reformer had a plasma heater, developed by Hüls, heating carbon dioxide, which was being used as an oxidant in the reformer. High temperature carbon dioxide, preheated by the plasma heater, was then introduced into the reactor vessel where it reacted with a mixture of methane and steam to produce syngas for iron reduction (Jones et al., 1993). During the two years of operation, the USCO reformer (Jones et al., 1993) represented one of the first successful industrial implementation cases of a gas phase plasma reformer.

The plasma arc reformer proposed in this paper differs from the USCO reformer in two ways. Whereas the USCO process used steam and carbon dioxide as reforming oxidants, the current proposition uses carbon dioxide as the only oxidant. The second difference is that, the plasma arc reformer proposed in this paper allows direct interface of the plasma jet with the reagents in the reformer.

The plasma arc reformer envisioned in this paper will be implemented at industrial scale by use of a refractory lined vessel with a number of thermal plasma torches mounted to it. The quenching zone or heat recovery section can be integrated into the main vessel as internal coiling or by installation of liquid spray nozzles or externally as a waste heat boiler.

3.4 Approach

It has been established that plasma arc reformers are not being applied at industrial scale, especially so in the CTL context. In order for the PAR to be applied successfully in CTL, it is essential to identify the appropriate plasma system for CTL, quantify the impact of the application and determine the commercial status of the technology. The methods used to carry out those functions in this paper are described in Sections 3.4.1 to 3.4.3.

3.4.1 Selection of plasma arc reforming technology

The selection of an appropriate plasma technology was done by assessing the performance of different systems through simulation studies. This section describes the modelling philosophy, the process modelling, thermodynamic package used and the performance criteria used to select the appropriate plasma arc reforming system for application to CTL.

3.4.1.1 Modelling philosophy

Gibbs free energy minimisation (Demidov et al., 2011; Janajreh et al., 2013) was used in this study to determine the equilibrium conversions and subsequently the equilibrium compositions from the plasma arc reformer. It was then assumed that it is possible for the plasma arc-reforming reactor to achieve and maintain a uniform temperature to allow equilibrium to be achieved.

3.4.1.2 Thermodynamic property package

The thermodynamic property package of a simulator contains properties and rules for computing chemical interactions of materials in a reactive process. The Carlson algorithm (Carlson, 1996) for property selection was used to ensure the selection of an appropriate property model. Using the algorithm, the recommended property method for dry reforming is the Peng Robinson method (Peng and Robinson, 1976). Use of the Peng-Robinson method, or derivatives of it, for modelling dry reforming of methane was corroborated by other researchers such as Øi (2007) and Özkara-Aydınoğlu (2010). Er-rbib et al. (2012) used the Peng Robinson with the Boston Mathias mixing rules and obtained equally satisfactory thermodynamic property predictions.

3.4.1.3 Aspen plus process flow sheet description.

The process model used to model the reactor system in this study was developed in Aspen Plus v 7.2. **Fig. 3-4** is an illustration of the flow sheet placed alongside the reactor concept.

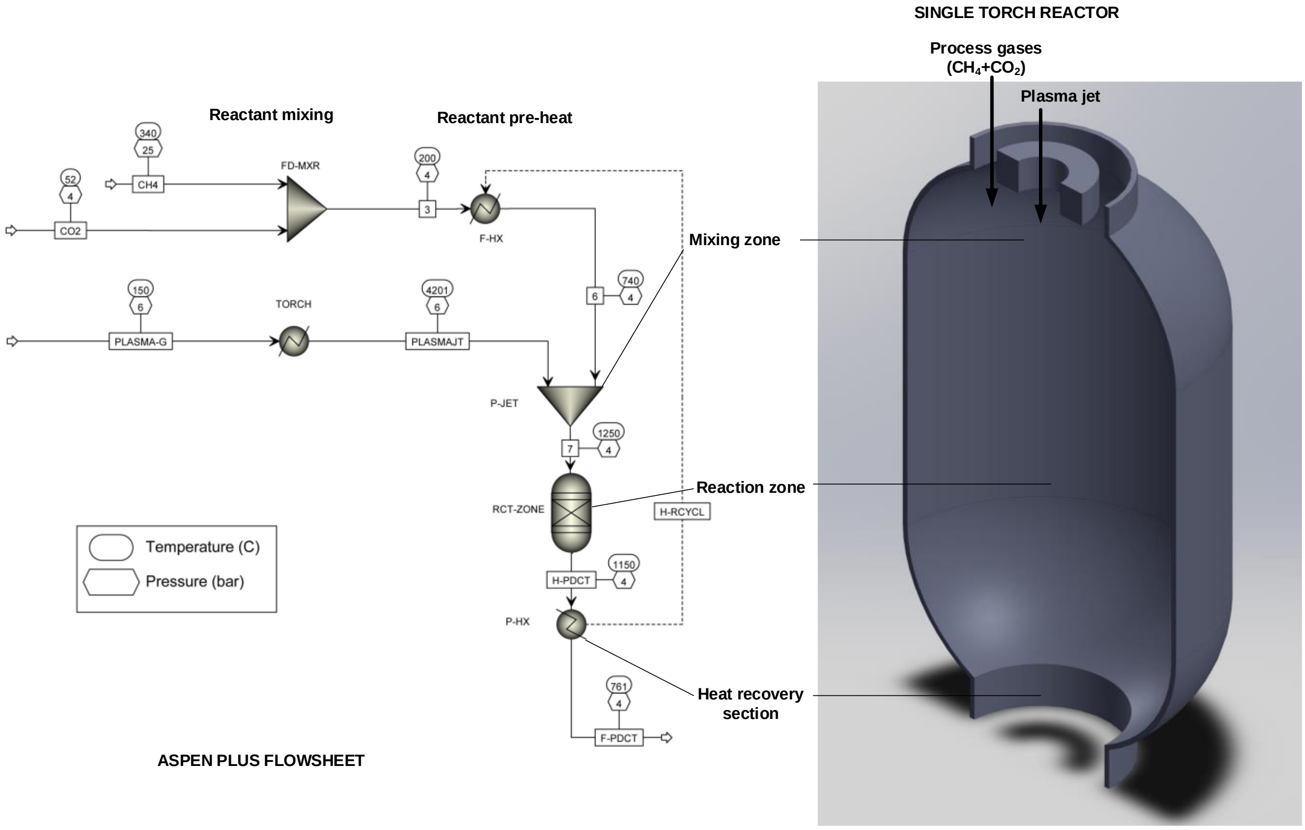


Fig. 3-4: Illustration of the simulation model of the plasma arc reformer used in the study

The flow sheet shown in **Fig. 3-4** was used to simulate the operation of the PAR in order to evaluate the different plasma systems. In the simulation study, methane and carbon dioxide were mixed in stoichiometric ratios (FD-MXR) and preheated in a heater block (FD-HX), which uses heat recovered from product quenching. After preheating, the mixed reagents were passed through the plasma jet and directed into the reactor. The plasma jet was produced by a plasma torch, modelled using a heater block (TORCH). The passing of reactants through the plasma jet was modelled as a mixing process (P-JET). The contacting of plasma jet with reactants results in direct heat transfer from the plasma gas to the reactants and some reactive plasma elements initiating the reforming reactions. Composition of products formed in the reaction was calculated by use of an equilibrium reactor (RCT-ZONE). Quenching of the products to preserve composition was represented by a heater block (P-HX) to deliver synthesis gas in stream F-PDCT.

3.4.1.4 Criteria used in technology selection

Technology selection was done by using the simulation model described in Section 3.4.1.3 to evaluate the performance of plasma reformers using air, nitrogen and carbon dioxide as plasma gas. Parameters for comparing performance were selected in accordance with cleaner production principles. According to cleaner production principles, production processes need to be resource and energy efficient in order for production to be sustainable (Fresner, 1998).

The measures used to assess the resource usage were reactant conversion and product selectivity. Conversion and selectivity were calculated using formulae shown in Eq.(3.2) to (3.4)

$$Conversion[\%] = \frac{(Reactant\ input - Reactant\ output)}{Reactant\ Input} \times 100\% \tag{3.2}$$

$$H_2\ Selectivity\ [\%] = \frac{moles\ of\ H_2 produced}{2 \times moles\ of\ CH_4 consumed} \times 100\% \tag{3.3}$$

$$CO\ selectivity\ [\%] = \frac{moles\ of\ CO\ produced}{(moles\ of\ CO_2 consumed\ +\ moles\ of\ CH_4\ consumed)} \times 100\% \tag{3.4}$$

The reformer yield of a product can be calculated by multiplying product selectivity by the conversion (Peacock and Richardson, 2012).

The following parameters were used to assess the energy performance of each PAR configuration: electrical duty [MW], and specific energy input, SEI [kJ/kg] and energy conversion efficiency (ECE). The electrical duty was a direct output of the simulation model, indicating required electricity supply.

Specific energy input is the energy input required to produce 1 mole of syngas. Specific energy input was calculated by Eq. (3.5) as defined by Tao et al. (2011);

$$SEI[kJ/mol] = \frac{Plasma\ energy\ input}{Product\ flow} \tag{3.5}$$

ECE is a measure of the efficiency of transfer of electrical energy supplied to the plasma reformer to chemical and sensible energy of products in the syngas. The ECE for each plasma reformer and was calculated by Eq.(3.6) as defined by Tao et al. (2011) ;

$$ECE[\%] = \left[\frac{(Product\ heating\ value)}{(Plasma\ power\ input\ +\ Reactant\ heating\ value)}\right] \times 100\% \tag{3.6}$$

3.4.2 Assessment of the impact of applying plasma arc reforming to coal to liquids

After selecting the most appropriate PAR technology for CTL, an assessment of the impact of integrating the PAR with CTL was done. To assess the impact of PAR application to CTL, the CTL flow sheet presented in Section 3.2 was modified as illustrated in **Fig. 3-5**.

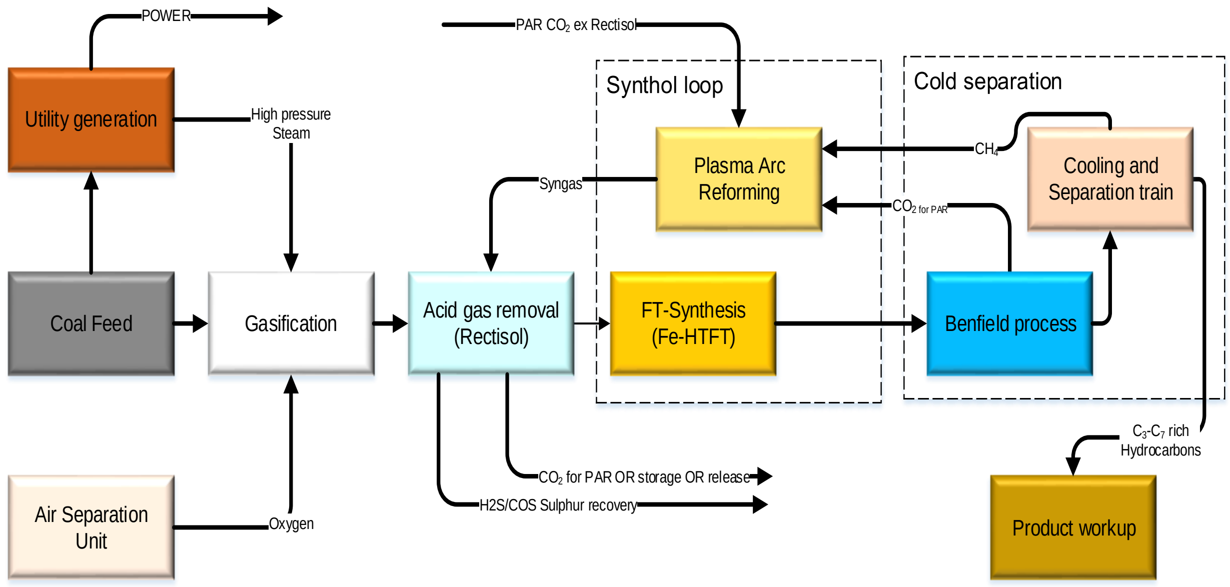


Fig. 3-5: A conceptual view of the proposed application of plasma arc reforming to CTL

In the block flow sheet **Fig. 3-5**, PAR replaces ATR that is used in the Sasol CTL. Feed carbon dioxide for the PAR is sourced from either the Benfield process and/or the Rectisol process.

To assess the impact of employing PAR in CTL, the conversion, selectivity and utility requirement characteristics of the chosen PAR technology were used to recalculate material and energy balances of CTL. The material balances of the Sasol process were developed on the basis of data reported by De Klerk and Furimsky (2010).

Carbon efficiency is a measure of how much of the carbon that is supplied into a process is converted to desirable product. For the CTL process, the coal feed is primarily carbonaceous hence carbon efficiency is a good indicator of the process productivity. The CTL carbon efficiency was calculated with Eq. (3.7).

$$Carbon\ Efficiency(\%) = \left(1 - \frac{net\ CO_2\ mol.emissions}{Carbon\ feed\ mol.}\right) \times 100\% \qquad (3.7)$$

The ratio adjusted carbon efficiency (RACE) represents a case where the ratio of hydrogen to carbon monoxide has been adjusted to the range most commonly used in fuel production, H_2: CO ratio of 1.7 to 2.1, by the use of tools like WGS reactors. For this study, the target syngas ratio of 2 was used for the adjustment. The calculated carbon efficiencies of the Sasol CTL and the PAR modified CTL processes were compared to highlight relative changes in carbon efficiency.

A high-level assessment of material and energy requirements of the PAR modified CTL process was carried out to highlight changes brought about by the modification.

3.4.3 Assessment of technology scalability and commercial readiness

After selecting the appropriate PAR system, a review of the considerations during scale up was done and then the technology readiness assessment was done. Section 3.4.3.1 presents the considerations during scale up and Section 3.4.3.2 presents the approach to assessment of technology readiness.

3.4.3.1 PAR scalability considerations

Increasing the capacity of PAR to industrial scale would involve increasing the capacity of the plasma source, volume of the reaction containment vessel and the capacity of the heat exchange equipment. Since the rules of scaling up reaction vessels and heat exchange equipment are well documented (Harmsen, 2013; Smith, 2005) , there is no need to discuss their scaling-up further as it is unlikely to be a source of risk. The focus of this section therefore is on scalability considerations of the plasma source for the PAR.

There are two approaches to scaling up thermal plasma equipment applied in a plasma arc reformer. The first is to increase the size of the plasma generator as throughput is increased and the second is combining a number of smaller units to achieve a higher rating as shown by Eq. (3.8).

Total reformer power rating,

$$P_{total} = \sum P_{torch} \tag{3.8}$$

Two factors favour use of torches over enlarging the plasma unit. The first factor is that enlarging the plasma unit presents higher technical risk as maintaining reactor stability with large arcs is not well understood for gas processing equipment (Roth, 1995). The second factor is that, plasma unit energy efficiency improves with increasing plasma gas flow (Fey et al., 1982). However, enthalpy of the plasma reduces as plasma gas flow increases (Fey et al., 1982) and a possibility of extinguishing the plasma arc increases with increasing gas flow (Solonenko, 2000). In applications where high energy densities are required such as chemical processing, torches are a flexible way of increasing capacity for the plasma reformer.

The number of torches used to provide the desired power rating needs to be optimised to meet design and operational objectives. A typical design objective could be to maintain a target system reliability. Taking into consideration that simpler technologies are less likely to fail (Stehlík, 2009) fewer torches per reforming vessel are desirable which makes a case for use of high power rating torches. If reliability is used as a design objective, the optimal distribution of torches per reformer can be derived using the reliability equations, Eq. (3.9) to (3.12).

Total number of torches in reformer section,

$$N_{PAR} = \sum (N_R \times N_{TPR}) = P_{total}/P_{torch} \tag{3.9}$$

Where P_{total} is the power requirement of the PAR system, P_{torch} is the power rating of an individual torch, N_R is number of reaction vessels in reformer section and N_{TPR} is the number of torches on a single reforming vessel.

If the non-maintenance related operational disturbances such as raw material outage, labour disagreements etc. are ignored, Eq. (3.10) to (3.12) can be used to solve for the optimal number of torches per reactor

$$R_{iR} = \prod_{j=1}^{N_{TPR}} (R_{ij}) = R_{ij}{}^{N_{TPR}} \tag{3.10}$$

$$R_{iT}=1 - \sum_{i=N_R-k+1}^{N_R} \left(\frac{N_R!}{k!\,(N_R - k)!} \times R_{iR}{}^{k} \times (1 - R_{iR})^{N_R-k} \right) \tag{3.11}$$

Where a single reforming reactor has n=N_{TPR} similar torches, zero redundancy is assumed and the single torch reliability, R_i is calculated by Eq. (3.12)

$$R_i = \frac{Mean\ time\ between\ failures}{Mean\ Time\ between\ failures + Maintenance\ time} \times 100\% \tag{3.12}$$

Using multiple torches could build some redundancy into the system. However, two practical issues would need to be considered in addition to reliability. The first issue pertains to safety in the event of failure of torches during operation. Failure of a torch on one side of the reforming vessel could result in unstable operation of the reactor. Given that plasma reactors will be operating at high temperature, cold spots in areas where torches have failed could raise chances of reactor metallurgical failure, which could lead to an explosion. However, application of multiple torches per vessels in closely related plasma gasification is an indication that the safety issues can be managed at industrial scale (Westinghouse Plasma Corporation, 2012). The second issue is that, installation of redundant torches would mean a higher capital investment hence, the level of redundancy required needs to be optimised.

3.4.3.2 Assessment of technological commercial readiness

Mature technology is generally presumed to present the minimum risk of failing to meet the performance requirements (Li et al., 2014). There are some exceptions where the risk of an immature technology is acceptable. In such exceptions, the technology can be deemed ready even though it is not yet mature (Smith, 2004). A technology readiness assessment presents a robust approach to minimising the risk of applying a new technology.

Researchers and systems engineering professionals have proposed a number of technology readiness metrics. Examples of such metrics include the technology readiness levels (TRL) initially proposed by NASA and subsequently modified by several other users such as the US-DoD, US-DoE (Mankins, 2009), whale diagrams which are also called maturity curves (Altunok and Cakmak, 2010; Nolte, 2008), DNV’s risk based technology qualification metric (Bakhtiary-Davijany and Myhrvold, 2013) among other tools. This study uses the TRL metric because of its widespread use and robustness. One of the key criticisms of TRL is that it does not consider integration with other components (Azizian et al., 2009). To overcome this shortcoming, the integration readiness level (IRL) metric was applied to assess the readiness of technologies for integration into the reactor system (Gove and Uzdzinski, 2013). Eq. (3.13) was then used to translate the TRL and the IRL metrics into a quantitative indicator , the system readiness level (SRL), which was calculated as outlined by Sauser et al. (2008). At a higher level, the SRL reported here corresponds to the technology readiness of the PAR reactor system.

$$SRL = \frac{(SRL_1/n + SRL_2/n + SRL_3/n + \cdots + SRL_n/n)}{n} \tag{3.13}$$

As current literature only describes laboratory plasma reformers it is clear that the PAR is a developing technology. To evaluate the technology development risks, two other metrics were borrowed from space and defence industry practice. These metrics are the Technology readiness and risk assessment (TRRA) (Mankins, 2009) and the research and development degree of difficulty (R&D^3) (Mankins, 1998) metrics. Finally, the manufacturing risks associated with PAR and supportability were evaluated by identifying possible component and parts manufacturers.

The potential barriers to implementation of PAR were identified by applying the TRL and IRL metric guidelines, supported by manufacturability and supportability assessment.

3.5 Results and Discussion

Results and discussion of the study are presented following the approach to the study. The results of technology selection, integration effects assessment and technology readiness are presented in Sections 3.5.1, 3.5.2 and 3.5.3 respectively.

3.5.1 Technology selection

A simulation model was used to compare the performance of three PAR configurations utilising common industrial scale torches. The results of the performance parameters used to compare the PAR configurations are summarised in **Table 3-1**.

Table 3-1: Summary of performance parameters used in technology selection

	Air	**Nitrogen**	**Carbon dioxide**
CH_4 Conversion (%)	99.7	99.7	99.8
CO_2 Conversion (%)	84.9	97.1	97.2
H_2 Selectivity (%)	85.9	100	100
CO Selectivity (%)	100	100	100
SEI (kJ/mol)	60.0	47.1	46.9
ECE (%)	73.1	87.9	88.0
Electrical Duty (MW)	381	337	334

From the simulation results in **Table 3-1**, it is deduced that nitrogen and carbon dioxide plasma systems offer superior performance for plasma arc reforming of methane with carbon dioxide. Air based plasma systems are disadvantaged by the introduction of oxygen into the reaction vessel, which results in conversion of hydrogen and carbon monoxide into less desirable products. Despite the similar performance of nitrogen and carbon dioxide systems, carbon dioxide is preferred for CTL as it introduces the least amount of inert gas into the synthol loop. The amount of inert gas in the synthol loop negatively affects the energy efficiency of the synthesis section. In addition to reducing efficiency, additional separation steps are required for the removal of inert gas from the synthol loop and that increases capital expenditure. As a result, the carbon dioxide plasma system was chosen for application to CTL.

3.5.2 Process impact of plasma arc reforming integration with coal to liquids

Carbon efficiency was used as the primary measure of the effect of applying plasma arc reforming to CTL. The rationale was that a higher carbon efficiency would imply that the application of PAR to CTL improves the carbon efficiency and reduces carbon emissions. The carbon efficiency of the baseline Sasol CTL, using ATR, was calculated to be 50.4%. The RACE for the CTL configurations is illustrated in **Fig. 3-6**.

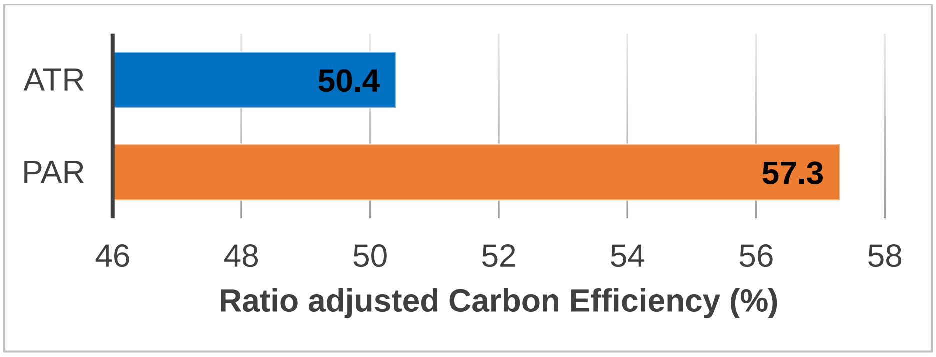


Fig. 3-6: Illustration of carbon efficiencies for the conventional and PAR modified CTL

Fig. 3-6 shows that there is an effective 14% improvement in RACE. This carbon efficiency improvement corresponds to a carbon dioxide emissions reduction of 12 million tons per annum reduction. The effective consumption of carbon was limited, in this case, by the amount of methane available for reforming, which was restricted to the internally generated methane. Where external sources of methane are available, it would be possible to recover all of the carbon from carbon dioxide resulting in a zero CO_2 emission. However, the economics would need to be considered to balance the benefits with costs of gas and required electricity.

Apart from the improvement in carbon efficiency, the replacement of ATR with PAR reduces the steam and oxygen requirements by 8% and 20% respectively. These reductions are due to PAR using carbon dioxide as an oxidant as opposed to ATR that requires oxygen and steam as oxidants. The improvement in carbon efficiency results in a 15% reduction in coal feed. This reduction is also connected to reductions in oxygen and steam to the gasification section resulting in an overall steam and oxygen reduction of 20% and 32% respectively. Reduction of oxygen requirements results in a smaller air separation plant being required in the syngas generation section of the CTL plant, which equates to a capital requirement reduction. The reduction in steam usage results in a lower water and carbon dioxide footprint of the CTL plant, which has benefits in water-constrained locations such as South Africa.

Use of plasma arc reforming requires electricity in the conversion of carbon dioxide to syngas and this represents an increase in the electrical energy requirements of the CTL plant. The sourcing of the electricity can result in a portion of the reduced direct emissions being externalised to a power plant. Using estimates based on emission factors for power generation (Letete et al., 2009), where electricity from a coal-fired power station is used an equivalent of 25% of recovered carbon dioxide would be externalised. However, use of nuclear or renewable electrical sources would result in negligible externalisation of emissions

3.5.3 Technology status

Technology status was evaluated along three dimensions, reactor readiness, component commercial availability and reactor supportability and barriers to implementation. The findings of the study are presented in 3.5.3.1 to 3.5.3.3.

3.5.3.1 Reactor readiness status

TRL and IRL assessments for the reactor components were done using the technology and integration readiness levels descriptors. Based on the level of development, the TRL levels for the torch, reactor shell and heat recovery quench system form a 3-row vector that was normalised and is shown in the relevant column in **Table 3-2**. The IRL metric was applied for the reactor system integrations and the corresponding normalised matrix for the different component integrations is shown in **Table 3-2**.

Table 3-2: Summary of the calculation of the system readiness level metric

Component coding	TRL	IRL	Product
Torch (1) Reactor (2) Heat recovery (3)	$\mathrm{TRL}=\begin{pmatrix}1\\0.6\\0.6\end{pmatrix}$	$\mathrm{IRL}=\begin{pmatrix}1 & 0.2 & 1\\0.2 & 1 & 0.1\\1 & 0.1 & 1\end{pmatrix}$	$\mathrm{IRL}\times\mathrm{TRL}=\begin{pmatrix}1.7\\0.8\\1.6\end{pmatrix}$

Applying Eq.(3.13), the system readiness level for the PAR reactor system

$$\mathrm{SRL}=\frac{(1.7/3+0.8/3+1.6/3)}{3}=\frac{(0.56+0.27+0.54)}{3}=0.45$$

The SRL indicates that some significant work needs to be put into developing the PAR system before it is ready for implementation in CTL without introducing significant technical risks. Using the R&D^3 metric, the degree of difficulty anticipated to develop the PAR to commercial readiness was determined to be at Level 2 difficulty. Level 2 degree of difficulty is consistent with programs that have 80 to 90% chance of achieving success in delivering a new capability. As alluded to previously, implementing PAR will require two technological refinements to deliver the envisaged requirements. The two refinements involve the kinetic data development for reaction containment and integration of reactor with a heat recovery or quenching technology capable of maintaining greater than 90% product profile integrity. By combining the SRL metric determined above and the research and development degree of difficulty in the TRRA metric, it was determined that the risk of development is moderate hence; the authors suggest that it would be possible to develop the PAR reactor system in the short to medium term.

3.5.3.2 Component commercial availability and reactor supportability

The PAR reactor system can be manufactured using standard pressure vessel manufacturing processes and materials; hence, the manufacturability of the reactor system is not in question. Standard pressure vessels and heat exchangers or high temperature quench devices can be used effectively by design integration. Although application of industrial scale plasma torches is the most untested component in the PAR reactor system, a number of mature industrial scale torch manufacturers are in operation globally. The top four torch producers include Westinghouse Plasma Corporation, Euro plasma, Phoenix solutions and Tetronics that produce industrial torches of capacities ranging between 5 kW and 4000 kW. These torches have been applied for plasma gasification equipment in high temperature conditions similar to what would be required in a PAR reactor system (Dodge, 2008; Fabry et al., 2013). These and other manufacturers also produce spares and technical support which enable PAR equipment to be supported effectively (Europlasma Group, 2010; Westinghouse Plasma Corporation, 2012).

3.5.3.3 Barriers to industrial scale application

As can be expected with developing technologies, there are barriers that would impede full-scale commercial application of PAR reactors in CTL. These include:

- Kinetics data for high temperature plasma arc reforming is not readily available. The unavailability of the kinetic data presents a key technical challenge in the design and scale up of the reactor shell. To ensure that the technical risk is reduced to acceptable levels, kinetic characterisation of plasma reforming with thermal plasma contact would be essential.
- Energy consumption of plasma arc reforming remains a significant barrier to industrial scale implementation. Deployment of a plasma arc reforming system would raise the electricity consumption by up to 65%.
- The credibility of the benefits of deploying PAR for dry methane reforming into a CTL is not clear. This barrier can be overcome as the material benefits concerning improvement of carbon efficiency and reduction of oxygen requirements of the plant can be demonstrated. The electrical energy requirements challenge the credibility of benefits if the cost of electricity and associated footprint are high. With a futuristic perspective, sources of electricity such as renewable sources or nuclear are expected to improve the realisation of the benefits of using plasma arc reforming to create cleaner and more productive CTL plants.
- There is lack of clarity on the exact development needs of plasma reforming technology for operators of CTL plants and their technology providers. This barrier has been

partially addressed in this article as it gives suggestions on the areas PAR developers need to focus on in order to get PAR of methane deployable with minimum risk.

3.6 Conclusion

This paper presents the technology assessment of non-catalytic plasma arc reforming with the view of developing the technology to industrial scale. Findings support the proposition that non-catalytic PAR can be used to improve the carbon efficiency of CTL and reduce the greenhouse emissions at the same time. Besides the reduction of greenhouse gas emissions of CTL, reductions of oxygen requirements and direct steam usage can be realised. The application of PAR introduces additional electrical requirements, which may result in a portion of carbon dioxide being externalised to the power source.

Plasma arc reforming is not yet commercially ready and requires some development to minimise implementation risks. Two interventions were identified as critical to the sustainable delivery of results 1) development kinetics data to minimise technical risk on scale up, 2) sourcing of electricity requirements from low carbon sources such as nuclear and renewables.

Due to the use of an equilibrium-based model, the results presented may be optimistic. The results present a starting point for pursuing the opportunity to apply plasma arc reforming technology at industrial scale to develop cleaner and less resource intensive hydrocarbon synthesis processes. It is recommended that as future work, a more detailed process impact study and economic analysis of the plasma arc reforming integration with CTL processes be done to validate the costs and benefits of such an application.

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4 THE IMPACT OF DEPLOYING PLASMA ARC REFORMING ON PROCESS YIELD AND SUSTAINABILITY OF A COMMERCIAL COAL TO LIQUID

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Abstract

Plasma arc reforming has been proposed as a cleaner production intervention, which can improve the carbon efficiency and reduce the carbon intensity of a coal to liquids process. However, work done in this area so far does not adequately capture the operational implications of improving coal to liquid carbon efficiency. An incomplete understanding is a hurdle to the acceptance of plasma reforming as a way of achieving cleaner production in coal to liquid processes. This paper presents a system analysis of a coal to liquids process to evaluate the operational implications of introducing plasma arc reforming as a cleaner production initiative. The study serves two purposes 1) expand the understanding of the operational impact of deploying plasma reforming to a coal to liquid process and 2) provide a guide on requirements specifications for the plasma reforming system to be applied to coal to liquids. Analysis confirms the reduction of raw materials previously forecast and the degree of carbon efficiency improvement. In addition, plasma arc reforming also a marginal negative impact on product throughput for processes that use low temperature gasification, however, it represents an improvement in the mass of product per mass of raw material, which suggests an improvement in process productivity. The authors conclude that the application of plasma arc reforming to improve carbon efficiency of coal to liquids would create a cleaner and more productive process. The improvement of understanding of the impacts of plasma reforming will reduce anxiety around adoption of the technology as an option for creating cleaner coal to liquid processes in the future.

Keywords:

Process analysis, Plasma arc reforming, coal to liquids, technology impact, carbon reclamation

Highlights:

- Process impact of deploying plasma arc reforming to CTL is evaluated.
- Process productivity is improved and emissions reduced.
- Use of nuclear or renewables reduces externalised emissions.

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Abbreviations

ATR	Auto Thermal Reforming
CTL	Coal to Liquids
FT	Fischer-Tropsch
GHG	Green-house gases
HTFT	High Temperature Fischer-Tropsch
PAR	Plasma arc reforming

4.1 Introduction

Use of gas and coal as feedstock for synthetic oil is not currently considered competitive as the production costs are on the higher end of published cost curves (Aguilera, 2014; Reynolds, 2014). However, market developments prior to the 2014 crude oil price crash show that more expensive, unconventional resources will play a bigger role if the crude oil price ensures viable operation (Reynolds, 2014). As the cheaper crude oil resources are exhausted, overall crude oil prices will rise and the prospects of gas and coal as substitute oil sources will improve. Based on resource forecasts, coal resources will probably outlast gas and oil reserves (Aydin, 2014; Shafiee & Topal, 2009; Thielemann *et al.*, 2007) hence a long-term development strategy for coal to liquid production is advocated. Coal to liquids (CTL) processes enable the conversion of coal to synthetic crude for liquid fuel production along with other petrochemical-based products. These feedstocks can be used for production of commodities that are being produced from conventional crude oil (Dry, 1989; Dry, 2002; Zhou *et al.*, 2011).

CTL processes face a number of challenges that may reduce the near term viability for large-scale industrial application. Key challenges include high greenhouse gas (GHG) emissions(Li & Fan, 2008; Mantripragada & Rubin, 2013a), High capital costs (Ramage & Katzer, 2009; Steynberg & Nel, 2004) and lack of product price competitiveness versus conventional crude products (Dry, 1996; Mantripragada & Rubin, 2013b). To mitigate these challenges, several developments have been proposed. Some of the notable proposals include use of nuclear assisted CTL processes (Cherry & Wood, 2006; Chiuta & Blom, 2012; Harvego *et al.*, 2009), gas and coal hybrid feed processes (Sudiro & Bertucco, 2009) and CTL with carbon capture and storage(Knoope *et al.*, 2013; Mantripragada & Rubin, 2011; Mulder, 2009). Nuclear based solutions have not been favoured due to high capital cost of nuclear build and safety concerns (Huenteler *et al.*, 2012; Srinivasan & Gopi Rethinaraj, 2013). Adding carbon capture and storage will contain direct emission of GHGs into the atmosphere but will not add value with respect to the technical and economic performance of a CTL plant. Plasma arc reforming of methane with carbon dioxide is a potential way of improving carbon utilisation in CTL processes by recovery of carbon from the emitted carbon dioxide.

In a previous article (Mapamba *et al.*, 2015), demonstrated that the carbon efficiency of the CTL process can be improved by replacing Auto Thermal Reforming (ATR) with plasma arc reforming (PAR). In the same article, it was shown that an improvement of carbon efficiency results in a cleaner CTL process that requires less raw coal, water and oxygen. However, in the study there was no consideration of the effect of deploying plasma reforming on the products of the process. Acceptance for implementation will thus be affected leading to a missed opportunity. Additionally, without an understanding of the effect on the products, the benefits accrued cannot accurately determined, which can distort the determination of value added by such an initiative. Hence, a system analysis of the impact of PAR could lead to improved chances of success during approval stages and a better understanding of the impacts allows better conclusions of success or failure to be made in the evaluation stage.

The aim of this study was to improve the characterisation of the impact of deploying PAR as part of a cleaner production initiative in a commercial coal to liquid process. The Sasol Secunda synfuel plant was used as case to keep findings grounded in the reality of industrial practice. By clearly demonstrating that the application of PAR to CTL could provide a cleaner and more productive CTL process, anxiety around the value of developing the technology for future application can be reduced. This would create a foundation for the adoption of PAR in CTL as a tool for creating a cleaner process. Financial issues were excluded from the current study to focus the scope of the system analysis but will addressed in a future study.

4.2 Process description, modelling and simulation approach

In its simplest form, a Fischer Tropsch based coal to liquids plant consists of four steps. These are syngas generation, syngas cleaning and conditioning, and hydrocarbon synthesis and product workup. These four steps are common to almost all Fischer Tropsch processes that have been considered at industrial scale with the main differences being seen in the applied catalysts, the synthesis conditions and consequently the product profiles. This work uses the publicly available data on the Sasol coal to liquids process to evaluate the potential effects of applying PAR to improve carbon efficiency of CTL.

4.2.1 Baseline plant process

Section 4.2.1 gives brief description of the Sasol CTL process and the subsequent modelling and simulation approach used in this study.

4.2.1.1 Process description

The basic process overview of a high temperature Fischer-Tropsch (HTFT) process is shown in **Fig. 4-1**: Block flow diagram of baseline coal to liquids process. As shown in the block flow diagram, in the gasification step, coal is reacted with steam and oxygen at high temperature and pressure to form syngas. Syngas composition is influenced by pressure, temperature, coal quality, steam to coal ratio, oxygen to coal ratio and coal particle size (Higman & Van der Burgt, 2008). As a result, the choice of gasifier influences the composition of the syngas produced (Bell *et al.*, 2011; Van Dyk *et al.*, 2001). The Sasol plant used as a reference plant uses fixed bed dry bottom Sasol-Lurgi gasifiers (Martelli *et al.*, 2013).

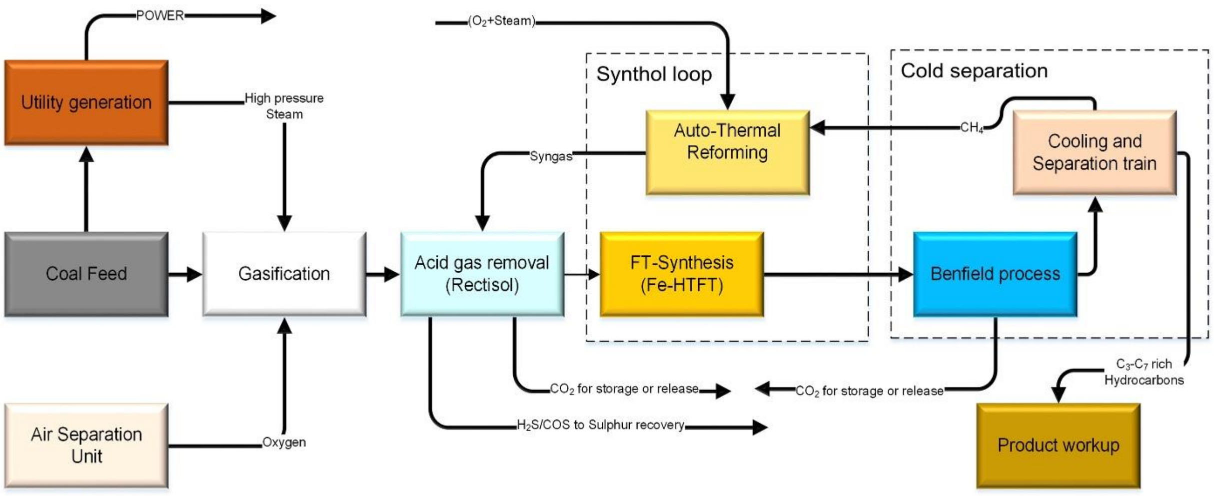

Fig. 4-1: Block flow diagram of baseline coal to liquids process

Syngas from the Sasol-Lurgi gasifiers contains tars, solid particulates such as residual ash, carbon dioxide and sulphur containing compounds (Kreutz *et al.*, 2008; Rumyantseva *et al.*, 2015). Tar and particulates can foul heat exchange equipment (Sharma *et al.*, 2008) and the sulphur is poisonous for catalyst in the synthesis step (De Klerk, 2011) hence they need to be removed from the raw gas stream before entering the synthesis process. Tar is removed by a water wash (Masuku, 2011). The carbon dioxide and sulphur containing compounds are removed using a rectisol process (Gatti *et al.*, 2014; Mohammed *et al.*, 2014) leaving pure syngas for hydrocarbon synthesis. If the ratio of hydrogen to carbon monoxide is not in the required ratio of about 2, ratio correction is done through the water gas shift (WGS) reaction (Gangadharan *et al.*, 2012; Nakhaei Pour *et al.*, 2011).

After cleaning and ratio correction, syngas is converted in a Fischer Tropsch synthesis reactor in the presence of an iron-based catalyst. The products of the synthesis step are diverse including alkanes, alkenes, alcohols, ethers, aldehydes, ketones, carboxylic acids and esters (De Klerk & Furimsky, 2010). Some of the general reactions that happen in the synthesis reactor are listed in Eq. (4.1)-(4.5) (De Klerk & Furimsky, 2010).

Alkanes: $(2n+1)H_2 + nCO \rightarrow C_nH_{2n+2} + nH_2O$ (4.1)

Alkenes: $2nH_2 + nCO \rightarrow C_nH_{2n} + nH_2O$ (4.2)

Alcohols and Ethers: $2nH_2 + nCO \rightarrow C_nH_{2n+2}O + (n-1)H_2O$ (4.3)

Aldehydes ad Ketones: $(2n-1)H_2 + nCO \rightarrow C_nH_{2n}O + (n-1)H_2O$ (4.4)

Carboxylic acids and Esters: $(2n-2)H_2 + nCO \rightarrow C_nH_{2n}O_2 + (n-2)H_2O$ (4.5)

The product workup process options are generally upgrading, partial refining and standalone refining (De Klerk, 2011). Upgrading produces a high quality syncrude while refining processes convert some or all of the syncrude into finished products such as liquid transportation fuels or commodity or specialty chemicals. These product-workup processes were excluded from the scope of the current study.

4.2.1.2 Modelling and Simulation of the baseline plant

This section describes the approach used to model the baseline plant. Section 4.2.1.2.1 discusses the scope of the study, Sections 4.2.1.2.2 to 4.2.1.2.4 discusses the model development and Section 4.2.1.2.5 describes the validation of the simulation model.

4.2.1.2.1 Simulation scope

Network interaction analysis was used to identify the areas that would be directly affected by the deployment of a plasma arc reformer to the CTL process. In building the Aspen model, only the process steps that account for the conversion of coal and movement of carbon-based materials that are converted to final synthesis products were included.

4.2.1.2.2 Components used in the simulation of the baseline plant

Most of the CTL reactants, intermediate products, products and by-products are standard conventional components in Aspen plus property databases. All primary syngas components, alkanes, alkenes, alcohols and acids in the C_1-C_{19} range were all readily available in the Aspen databases hence the supply of properties was not required. Since Fe-HTFT synthesis produces mostly lighter hydrocarbons, use of C_1-C_{19} molecules was considered adequate for this study. Tar is a complex mix of chemicals and based on work by Jiang *et al.* (2007), it was deemed that pyrene could adequately represent the average tar for assessing material flow impacts.

Two non-conventional components were used in the simulation, coal and coal ash. Coal and ash enthalpy and density were calculated using Aspen Plus standard methods HCOALGEN and DCOALIGT. The coal feed used was assumed to have the composition of a Twistdraai coal as shown in **Table 4-1**.

Table 4-1: Composition of coal used in the study (Source:(Govender, 2005))

Proximate analysis (% ad[4])		**Ultimate Analysis (% daf[5])**	
Moisture	4.6	Carbon	79.2
Fixed Carbon	47.0	Hydrogen	5.5
Volatile matter	19.4	Nitrogen	1.8
Ash	29.0	Sulphur	1.0
		Oxygen	12.5

4.2.1.2.3 Thermodynamic property selection

In this study the Peng-Robinson equation of state with the Boston Mathias mixing rules was selected as it provides good accuracy over the range of process conditions and hydrocarbons encountered in a Fe-HTFT CTL process (Twu *et al.*, 2002).

4.2.1.2.4 Flow sheet development

The flow sheet used in the simulation of the baseline plant was designed to model gasification, syngas cleaning and conditioning, Fischer-Tropsch synthesis, auto thermal reforming and part of the product workup process. **Table 4-2** shows a summary of the feed profile used in the base case simulation.

Table 4-2: Assumed feed profile for baseline plant simulation

Description	**Quantity**	**State (T [°C], P [MPa])**
Coal	1 442 tph	(25,0.1)
High pressure steam	2 095 tph	(420,4.2)
Oxygen	606 tph	(110,3.5)
Steam to Carbon Ratio	1.21	n.a
Oxygen to Carbon Ratio	0.34	n.a

The key flow sheet construction blocks, which consist of reactors and absorbers, are summarised in **Table 4-3**.

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[4] Air dried basis

[5] Dry ash free basis

Table 4-3: Summary of key flow sheet construction blocks

Process	**Model block**	**Block type**	**Function**
Gasification	DECOMP	RYield	Converts non-conventional coal into respective elements to enable participation in reactions
	PZLGG	RStoic	Reactor representing coal pyrolysis zone reactions
	GZLGG	RStoic	Reactor representing gasification zone reactions
	LGGIFP	Heater	Heat transfer block to capture energy exchange between coal and syngas in the gasifier
Syngas cleaning	RECTISL	SEP2	Separates the acid gases from syngas
FT synthesis	FTSYN	RStoic	Syngas reactor converting syngas to syncrude
Methane reforming	ATR	RGibbs	Reforming reactor converting recycled methane to syngas
Product workup	BENFLD	RStoic	Models absorption of carbon dioxide from synthesis tail gas in potassium carbonate (Benfield solution)
	REGEN	RStoic	Models regeneration of the Benfield solution to produce near pure CO_2 stream

When the heating, cooling blocks, stream mixers and separators are added to the flowsheet the resulting model for the baseline plant is shown in **Fig. 4-2**.

4.2.1.2.5 Validation of baseline plant model

The first check for model validity was to confirm that there was a good fit between the system to be modelled and the simulation package's capabilities. It was determined that the system has a good fit as evidenced by use of the package in similar simulation works such as those by Sudiro and Bertucco (2009) and Er-rbib *et al.* (2012). The second step was to validate if the model output correlated with an existing known industrial process. This was achieved by comparing the simulation model output versus the reported plant output for the Sasol Secunda plant. A targeted maximum variance of 10% between simulated results and existing plant output was used to calibrate the model using information by Sasol (Sasol Limited, 2012) and De Klerk (2011). The results of comparative outputs of the baseline plant simulation model and reported plant data is shown in **Fig. 4-3**.

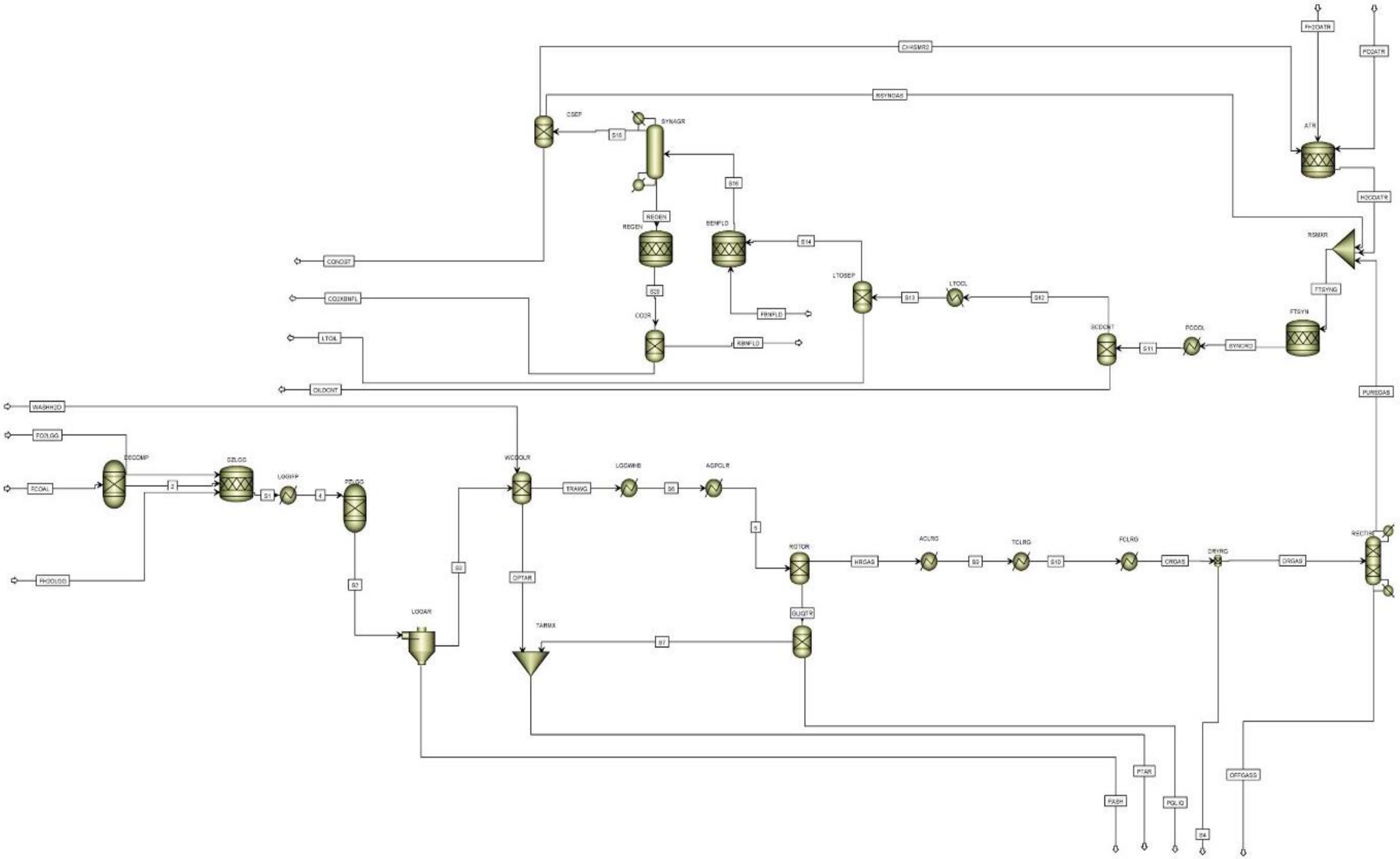

Fig. 4-2: Aspen Plus flow sheet of the baseline coal to liquids plant

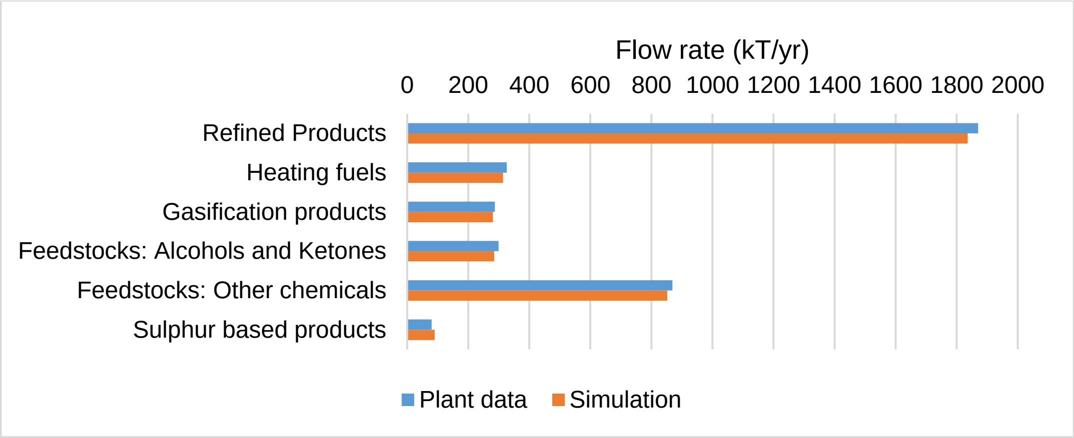

Fig. 4-3: Comparison of the baseline Aspen plus model output versus reported plant output[c]

[c] Based on Single train capacity of Sasol Secunda of 80000bpd, calculated as 2013 Sasol synfuel annual output x 0.5 (Sasol limited, 2014)

The product flows from the simulation model were 2-5% less than the reported plant output with the exception of the output of recovered sulphur. Sulphur based product flows from the simulation exceeded the reported sulphur flows by 12%. The deviation could be attributed to the difference in sulphur content of coal used in the simulation, the simulated coal had a slightly higher level of sulphur than the average coal used for the reported year. The overall correlation between plant product flows and simulation product flows was within an average deviation of 0.7%. The authors therefore concluded that the baseline plant model represented the plant adequately for the scope of the study.

4.2.2 Plasma arc reforming modified plant process

After validating the baseline plant flow sheet, the aspen plus flow sheet was modified to incorporate the usage of a plasma arc reformer in the place of an auto thermal reformer. A block flowsheet of the plasma arc reforming modified CTL process is shown in **Fig. 4-4**.

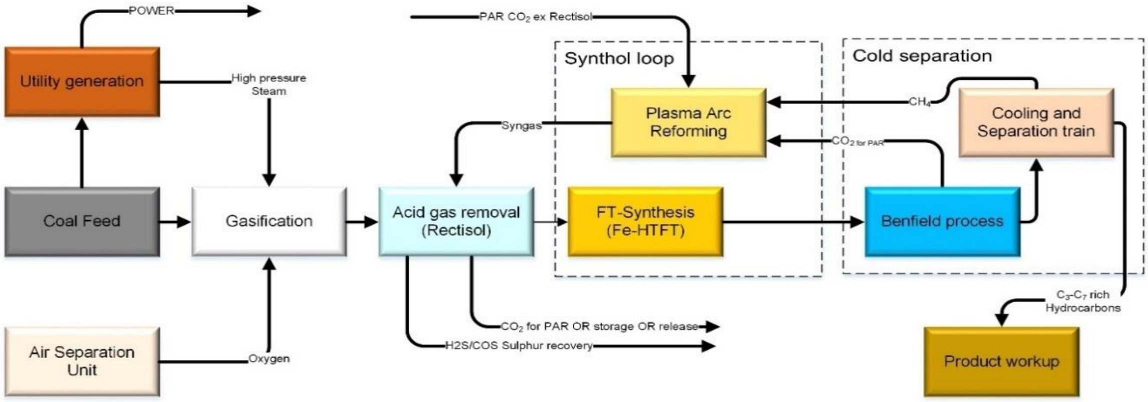

Fig. 4-4: Block flow diagram of the plasma reforming modified coal to liquids process

Fig. 4-4 shows that the steam and oxygen feeds that were connected to the ATR block have been replaced by a carbon dioxide stream that would have otherwise been released to the atmosphere. Section 4.2.2.1 presents a more detailed description of Plasma arc reforming.

4.2.2.1 Plasma arc reforming overview

Plasma is considered as the fourth state of matter and represents a highly ionised gas (Gallagher Jr & Fridman, 2011). When plasma is combined with other reagents it tends to create a highly reactive environment due to the presence of excited species and ions(Gallagher Jr & Fridman, 2011). In plasma arc reforming of methane with carbon dioxide (PAR), the process represents a series of reactions in which methane is converted to syngas with carbon dioxide as the oxidant. The overall reaction of dry reforming of methane is represented Eq. (4.6).

$$CH_{4(g)} + CO_{2(g)} \rightarrow 2CO_{(g)} + 2H_{2(g)} \ \Delta H = 247 kJ/mol \tag{4.6}$$

As shown in Eq.(4.6), the reaction is endothermic; as a result, heat supply is key to the completion of the desired reaction.

The plasma arc reactor comprises of 1) a plasma source 2) a reactor shell and 3) a heat recovery unit. Conceptually, the plasma source used in the reactor could be either a cold plasma (Aziznia et al., 2012; Tao et al., 2011) or a thermal plasma (Fauchais and Vardelle, 1997; Venkatramani, 2002). Cold plasmas are reported to have more species that are reactive (Fridman, 2008) but thermal plasmas are more effective for industrial chemical processing due to their providing higher reaction rates (Bosmans *et al.*, 2013). Therefore, the more effective thermal plasma source was chosen for this study.

4.2.2.2 Modelling and simulation of the plasma arc reforming modified plant

The flow sheet for the study of the PAR implementation case was similar to the baseline plant flowsheet with the exception of the replacement of the methane-reforming unit with the plasma arc reforming assembly. In the PAR modified CTL flowsheet, the function of the Aspen plus reactor block ATR was replaced by the assembly representing the PAR. The assembly consists of heaters (FP-HX, P-HX and TORCH), mixer blocks (R-MX and P-HX) and the Gibbs equilibrium reactor (RCT-ZONE), shown in **Fig. 4-5**. A water gas shift reactor unit (SPARSYN) was added to adjust the H_2: CO ratio of syngas from PAR from 0.95 to 2.7, which enabled the H_2: CO of syngas fed to the FT reactor to be adjusted to 2. To ensure comparability, the total syngas flow into the FT synthesis reactor was forced to be equal to the total syngas flow in the baseline plant. A feedback loop was used to adjust the feed-rate of coal and that allowed total syngas flow to be kept at baseline plant level. Oxygen and steam feed rates were simultaneously controlled by ratio ties to the coal flow rate. The PAR modified flow sheet is shown in **Fig. 4-5**.

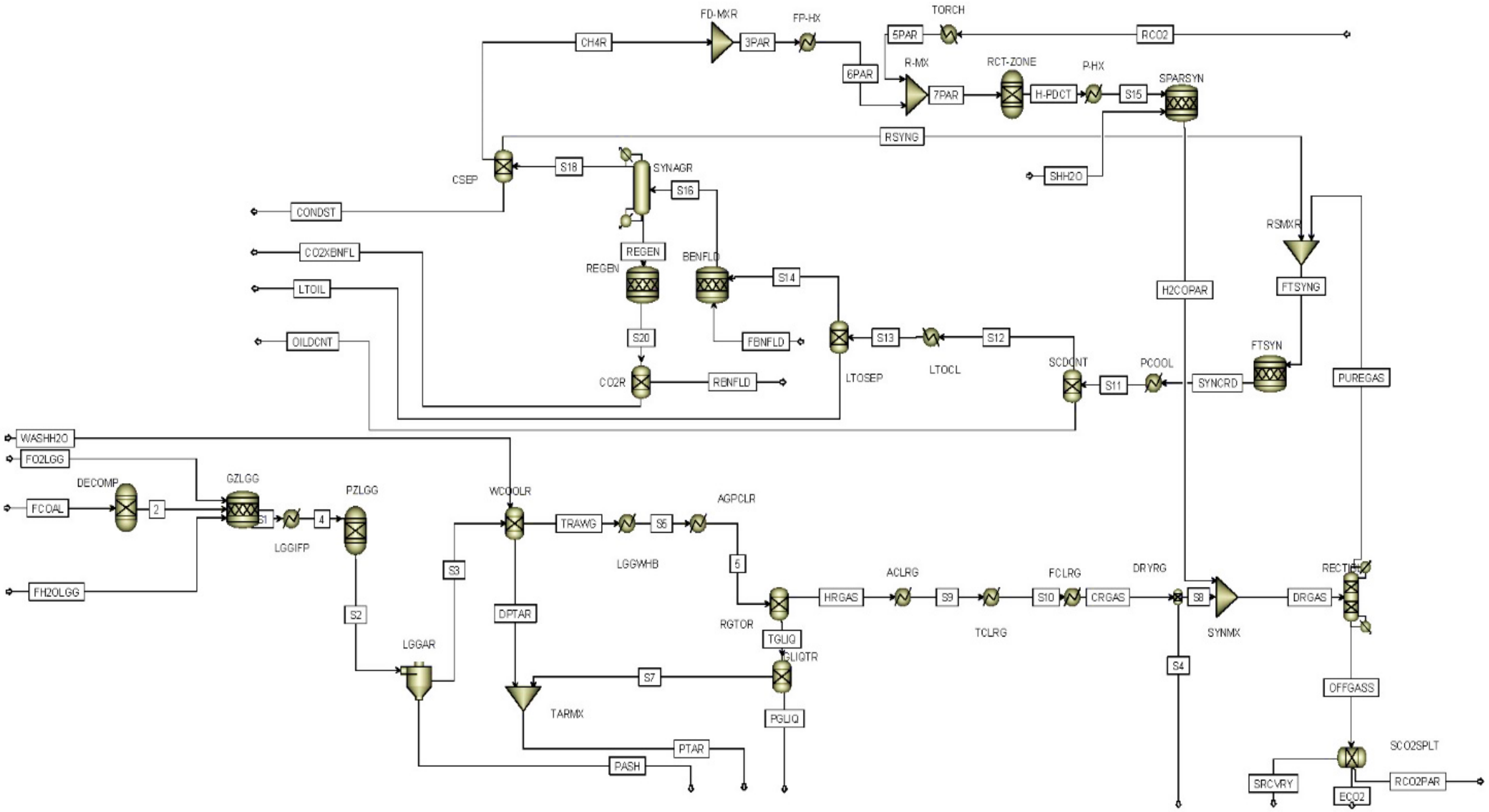

Fig. 4-5: Aspen flow sheet of the plasma arc reforming modified CTL

4.3 Results and Discussion

The systems analysis confirms that the application of plasma arc reforming to a CTL plant has an effect on the raw material requirements and environmental footprint. Additional detail of the effects on energy requirements and product throughput of the process were identified. A high-level view of the relative changes of the different parameters is presented in **Table 4-4** to give a quick view of the impacts. The discussion of the process changes then follows in Sections 4.3.1 to 4.3.4.

Table 4-4: A comparative summary of baseline CTL plant and PAR modified CTL processes

Raw materials		**Conventional**	**PAR modified**
	Coal	1	0.83
	Steam	1	0.80
	O_2	1	0.68
	Syngas fed to FT[6]	1	1
Energy requirements[7]			
	ASU	1	0.68
	Steam	1	0.80
	Overall external electricity supply	1	1.49
Products[8]			
	Sulphur based	1	0.84
	Other chemicals	1	1.02
	Alcohols & Ketones	1	1
	Gasification products	1	0.84
	Heating fuels	1	0.68
	Refined products	1	0.98
	Direct CO_2 emission	1	0.72
Ratios			
	Carbon efficiency	1	1.16

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[6] Flow of syngas fed to the FT reactor was kept constant, with an H_2: CO ratio of 2, in baseline and PAR modified process.

[7] Relative amounts based on normalised quantities.

[8] Relative quantity based on normalised quantities.

4.3.1 Impact of plasma arc reforming application on raw material requirements

When auto thermal reforming was replaced by plasma arc reforming in the CTL process, the coal required to generate the same amount of syngas as the baseline process was reduced by 16%. The coal requirement reduction is due to carbon being recovered from carbon dioxide. The reduction in coal feed to the gasifiers and replacement of ATR with PAR has the knock-on effect of an overall reduction of oxygen and steam requirements. Oxygen was reduced by 32% and steam by 20%, on a mass basis, when compared to the baseline CTL process. The reductions are because of the elimination of direct oxygen and steam requirement for reforming and the reduced requirement for coal gasification. However, the effective steam reduction is less than oxygen reduction due to an additional steam requirement for syngas ratio correction. Syngas ratio correction is done by the water gas shift reaction, which requires steam and produces carbon dioxide. Syngas ratio correction therefore reduces the net carbon dioxide consumption. Lower steam requirements have two implications 1) a lower water footprint and that reduces water concerns when applying CTL in water scarce regions and 2) a 20% reduction of coal fuel for steam generation, which has a further impact on reducing emissions. The indirect reduction of emissions from steam generation is important, in that carbon dioxide from steam generation tends to be dilute, due to use of air as oxidant, and would be expensive to remediate using sequestration and storage or any other means (Salkuyeh & Adams Ii, 2013). Overall, coal requirement for the CTL process was reduced by 17%.

4.3.2 Effect of PAR application on product throughput.

Changes in the gasification coal requirements affect the pyrolysis product output, recovered sulphur, ash output, methane available for reforming, and the emitted carbon dioxide.

Pyrolysis products (tar, phenol and ammonia), ash and recovered sulphur were reduced by 16%, which is the same proportion as the coal feed requirement reduction. A 16% reduction in recovered tar reduces the refined products output by 2.5% as the product from tar refining processes is blended with overall refined products. This impact is restricted to low temperature gasifiers only as high temperature gasification systems do not produce tars in syngas generation. The reduction in Ammonia and phenol output were reduced by 14%, which results in the products classified as gasification products being reduced by the same amount. The contribution of gasification products to overall valuable products is small hence; the impact on value of products is likely to be small. Reduction of ash produced could have a marginal impact on costs, as there is reduced solid waste to be managed.

The 16% reduction of gasification capacity results in a reduction of the net methane product since the methane produced by the CTL process is the sum of methane that is produced in gasification and FT synthesis. If the methane that is recycled to the PAR is the same quantity as supplied to ATR in the baseline plant, the methane that is available for external sales as a heating fuel is reduced by 32% in the PAR modified CTL. A summary of the changes in the product profile because of applying PAR to CTL are shown in **Fig. 4-6**.

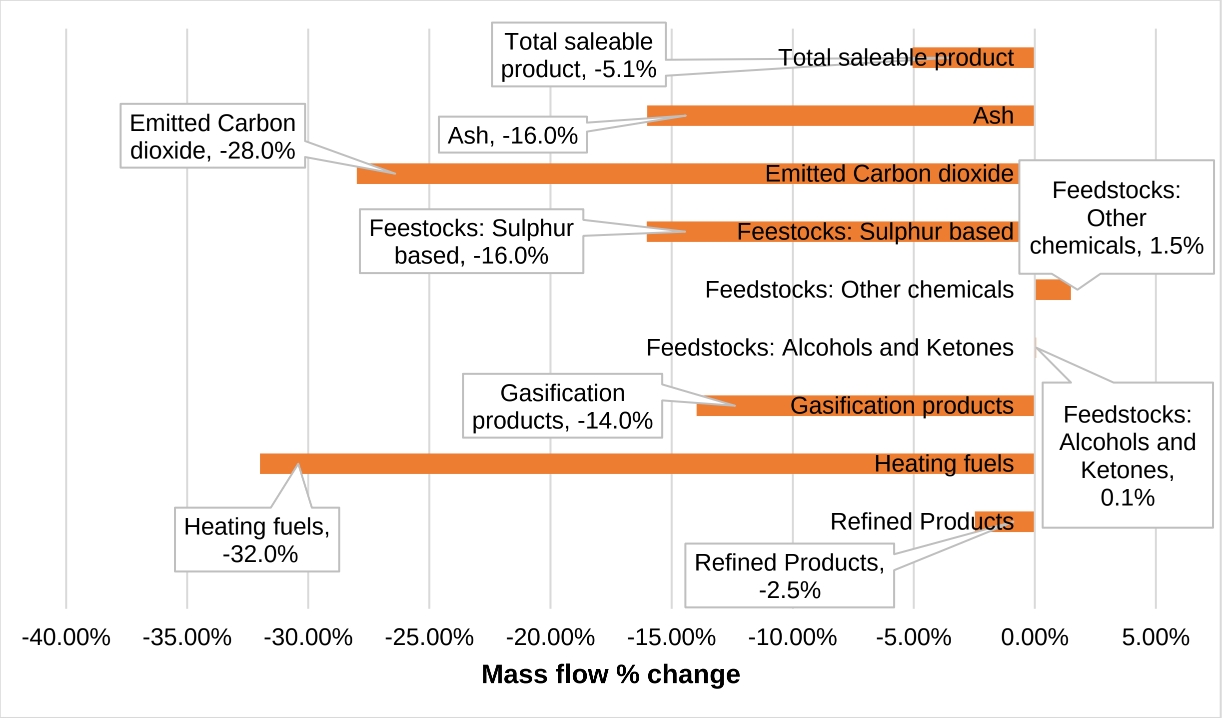

Fig. 4-6: Changes in product flow after applying plasma arc reforming to CTL

Fig. 4-6 shows the changes in the flows of the key product categories of CTL after application of PAR, including the flows of ash and emitted carbon dioxide, which are by-products of the CTL process. The ash and carbon dioxide were included as they represent waste flows that need to be managed and thus could have an effect on the operating costs.

Two important highlights from the evaluation of PAR application on product throughput are:

- The negative reduction of refined products due to tar reduction depends on the gasifier technology being used, with the negative impacts being more pronounced in low temperature technologies.
- Moreover, the proportion of affected products on the valuable products of CTL is on the low side, hence, the loss of value maybe negligible, but this would require confirmation through a financial analysis.

4.3.3 Effect of plasma arc reforming application on energy requirements

The energy consumption of plasma reactors has been cited as a potential hurdle for application at industrial scale (Tao *et al.*, 2011). In evaluating the application of plasma arc reforming technology, the impact on overall energy demand was considered. From the assessments, plasma arc reforming of methane requires 340 MW_e of electricity for the chosen study capacity. Since PAR was applied as a replacement for Auto Thermal reforming (ATR), which was electrical neutral, the electrical load of PAR represents an additional electrical load of the CTL plant.

Two supply cases can be considered in managing the added quantity electrical energy introduced by application of PAR to CTL. The first supply case would be to source the entire additional electrical load from an external supplier. An advantage of this scenario is that it creates an opportunity to purchase electricity from low-carbon sources such as renewable or nuclear power plants. Supply case two would be to maintain the size of the steam plant, as in the baseline plant, and use the excess steam for power generation. This supply scenario limits the opportunity to reduce the coal usage of the steam plant and the consequent emissions. In either case, the additional load is offset by the reduction of electricity requirements in the air separation section. The amount of electricity available for redirection from Air separation to PAR was calculated to be 62.8 MW_e. Based on the excess steam in the PAR modified process, there is an opportunity to generate 35 MW_e. As a result, the first power supply scenario requires 277 MW_e and the second requires 242 MW_e of external electricity supply. The net benefit of adopting each case would need to consider the trade-offs in cost of external supply, cost of emissions associated with internal power generation and the value of reduced dependency on external supply.

4.3.4 Effect of plasma arc reforming application on carbon efficiency and emissions

The carbon efficiency of the conventional CTL process was 50% before application of the PAR process. After application of PAR, the CTL carbon efficiency increased to 58%. The increase in carbon efficiency is due to carbon being recovered from waste carbon dioxide stream and being directed to the production of valuable products. The amount of carbon dioxide converted to syngas in the PAR influences the carbon efficiency increase, which raises the question of the minimum conversion required for there to be an improvement in CTL carbon efficiency. To answer that, an analysis of variation of carbon efficiency with carbon dioxide conversion in the PAR was done. The effect of carbon dioxide conversion in PAR on carbon efficiency is illustrated by **Fig. 4-7**.

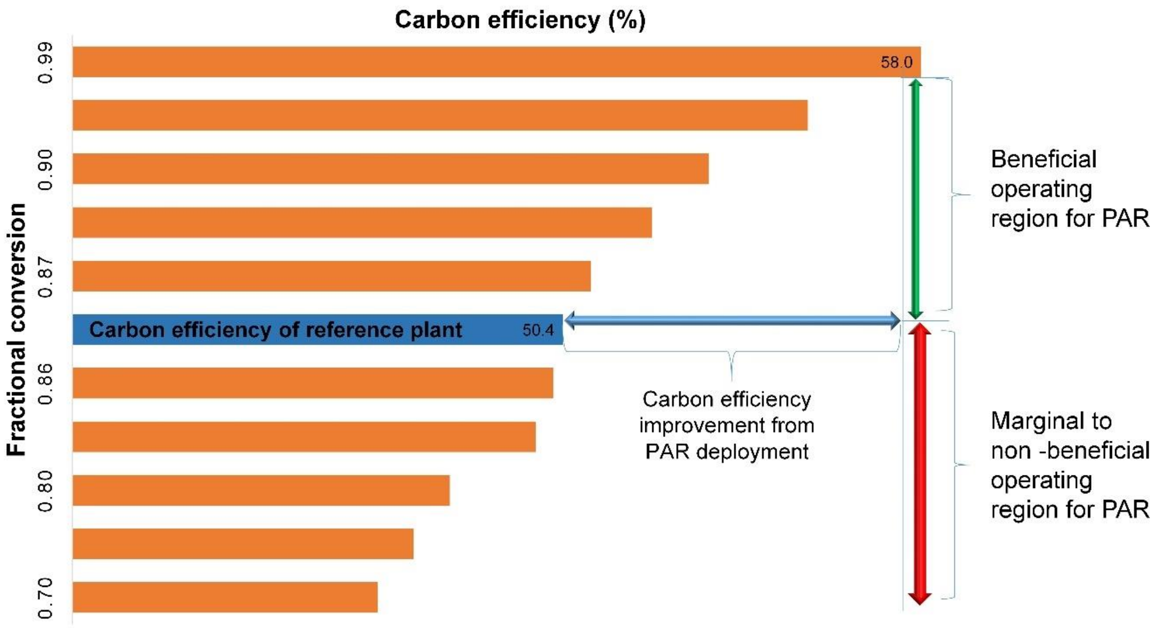

Fig. 4-7: Variation of carbon efficiency with carbon dioxide conversion in the PAR

The carbon efficiency value of the baseline plant was inserted into **Fig. 4-7** for comparison. **Fig. 4-7** shows that a methane conversion of at least 87% is necessary for there to be a carbon efficiency result that is better than the baseline CTL plant. If PAR achieves a methane conversion of less than 87%, then the application of PAR would not have a carbon efficiency advantage over baseline process. A high conversion is required in the PAR because of the relatively lower H_2: CO ratio of the syngas produced by PAR. Ratio correction to the required ratio for synthesis produces carbon dioxide, which limits the effectiveness of PAR. The implication is that for PAR to improve the carbon efficiency of a CTL process, an operational target of a conversion of above 87% is required for the plasma arc reformer. Tao *et al.* (2011) reports that a conversion of 90% has been achieved in laboratory plasma reactor, which suggests the target, may be achievable. However, the high conversion requirement limits the operational flexibility of the plasma reformer when applied to a commercial plant.

It is important to note that for this study, the recovery of carbon from carbon dioxide was limited by the amount of methane available to the plasma arc reforming process. If the methane availed for PAR is supplemented by methane from an external source, opportunity to achieve a higher improvement of carbon efficiency would be possible. However, considering that coal to liquids processes might only be attractive in a gas scarce environment, use of externally sourced methane might not be desirable. Economic evaluation of such a move would be necessary to assess feasibility.

4.4 Conclusions

The application of plasma arc reforming to a commercial CTL process affects material flows of feedstocks and products, increases carbon efficiency and increases energy requirements. After evaluating the changes in the operational requirements and performance, the authors conclude that the application of PAR results in a more efficient use of raw materials. This was demonstrated by a significant reduction of feedstock requirements being accompanied by a marginal reduction of valuable products. The increase in raw material utilisation was achieved by consumption of greenhouse gases and hence, direct emissions were reduced. Use of PAR in the synthol loop also reduced the steam requirement that lead to reduction of emissions from the steam plant and a lower water requirement. Hence, the PAR modified CTL is a cleaner and less resource intense process compared to the conventional process and that may make future application of CTL more sustainable.

Use of externally sourced electricity to supply the additional PAR electricity requirements could represent a transfer of a portion of direct emissions to indirect emissions. With greenhouse gas externalisation considered, application of PAR to CTL still represents a net improvement of raw material productivity and reduced emissions. However, further benefits could be obtained if low carbon electricity is used to supply the additional electrical requirements of PAR in the production of synthetic fuels. To minimise the externalised emissions, it is desirable to implement plasma modified CTL processes where nuclear or renewable electricity is available.

From the process analysis, the authors conclude that the application of PAR to CTL represents a positive operational improvement as it creates a cleaner and more productive CTL process. It is anticipated that the improved raw material utilisation efficiency and lower carbon intensity will positively influence economic performance of CTL by lowering feedstock and compliance costs. Detailed economic analysis to determine the significance of PAR impact on economic performance will be the subject a future study.

4.5 Acknowledgements

The authors are grateful to the North West University School of Chemical and Minerals engineering for access to facilities and process evaluation tools and to THRIP for funding parts of the project as Waste to Energy project, TP: 12083011540. The assistance of Frikkie Conradie in review of early versions is also acknowledged and appreciated.

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5 IMPACT OF PLASMA ARC REFORMING DEPLOYMENT ON ECONOMIC PERFORMANCE OF A COMMERCIAL COAL TO LIQUIDS PROCESS

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Abstract

Coal remains integral to the supply of energy in many parts of the world with negative effects on the environment. Plasma arc reforming has the potential of making coal to liquids processes cleaner by recycling greenhouse gases. Since the economic performance of the overall plant is a key consideration in the adoption of a new technological option, this paper evaluates the economics of the use of PAR in coal to liquids. Financial models were built using an existing commercial coal to liquids process as a reference case. Economic analyses were done to evaluate the impact of deploying a plasma arc reformer and the introduction of carbon tax on financial performance of a coal to liquids process. Results show that deploying plasma arc reforming reduces the oil price required for break-even from $89/ bbl. to $82/ bbl., adds at least $400 million to the project NPV and improves the IRR from 10.32 % to 12.23 %. In the process, it reduces vulnerability to introduction of carbon tax. While a requirement for extra low carbon electricity can be a hurdle, a sufficiently long term view of electrical plant investment makes the risk acceptable to independent providers. Overall, it was concluded that the deployment of plasma arc reforming to coal to liquids processes is value adding. The project demonstrates that it is possible to reduce environmental impact of coal to liquids with plasma arc reforming as a cleaner production initiative without significantly losing shareholder value.

Keywords

Economic analysis, Plasma arc reforming, coal to liquids, carbon reclamation

Highlights:

- Financial model is developed to evaluate plasma reforming in coal to liquids.
- Break-even price for modified plant is lower than of conventional plants.
- Deployment of plasma arc reforming is value adding to coal to liquids.

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Abbreviations

ATR	Auto thermal reforming
CAPEX	Capital expenditure
CEPCI	Chemical equipment Plant Cost Index
CTL	Coal to liquids
HTFT	High temperature Fischer-Tropsch
IRR	Internal rate of return
NPV	Net present value
OPEX	Operating expenditure
PAR	Plasma arc reforming
PAT	Profit after Tax
SARS	South African Revenue Services
USD	United States Dollar
WACC	Weighted average cost of capital
WGS	Water gas Shift
ZAR	South African Rand

5.1 Introduction

South Africa meets up to 30% of its fuel requirements through the use of coal derived liquid fuels and petrochemicals produced by a coal-to-liquid (CTL) plant. The coal to liquids plant is sustained by the availability of cheap and abundant coal resources (Dry, 2002). Replacing this supply source with a cleaner alternative at which gives the same level of economic benefit is difficult because of the scale of the coal to liquid contribution. The coal derived fuels sector contributes significantly through provision of jobs and tax revenue (Nkomo, 2009). In terms of making use of local resources to provide energy security, South Africa’s success is exemplary (Goldstein *et al.*, 2006; Qi *et al.*, 2012). Hence, it presents an important case for the evaluation of the impact of applying cleaner production.

Conventional CTL plants are some of the biggest point source emitters of carbon dioxide (Stoker & Conradie, 2015). Increased use of CTL would result in significant growth of greenhouse gas emissions, which would defeat climate change mitigation goals. However, given the significance of CTL contribution where it is being used, it is necessary to make existing and planned plants greener. The introduction of plasma arc reforming (PAR) technology into the CTL process has the potential of reducing coal usage, water requirements and greenhouse gas emissions from CTL pants thus reducing the environmental impact of CTL(Mapamba *et al.*, 2015). While it is acknowledged that lowering the carbon footprint is not an ideal solution, it is a potentially helpful transitory solution. Transitory because it would serve to bridge the current scenario where the sectors are fully on fossil fuels and petrochemicals and the ideal scenario where decarbonisation has reached full extent. However, this impact can only be realised if CTL operators adopt PAR modified plants.

PAR modified plants can only be adopted if it can be demonstrated that they meet technical and economic criteria of CTL operators. Mapamba *et al.* (2015) showed that when developed fully, PAR could meet the key technical criteria for integration in a CTL plant. However, whether a PAR modified plant could meet economic expectations of a CTL operator has not been evaluated yet. This paper seeks to reduce this knowledge gap by evaluating impact of PAR on CTL economic performance with the hope of addressing potential operator concerns that might stand in the way of PAR adoption. As a starting point, the authors focus on addressing three issues: 1) Evaluating how the economic performance of a PAR modified CTL plant compares to the performance of a conventional CTL plant? 2) Identifying conditions where the performance of a PAR modified plant is more attractive to a CTL operator? 3) Estimating how likely these conditions are?

Improving the understanding of the impact of PAR on economic performance of a CTL plant is important for two reasons. The first is that it provides a guide to PAR developers on performance targets that would give CTL operators an economic incentive to adopt PAR. CTL operators tend to be cost sensitive, as is common for commodity chemical producers, and are more likely to adopt technologies that help improve economic performance. This is supported by data from conventional oil producers who preferentially deploy lower cost rigs (Baker Hughes, 2015; Williams, 2015). Since CTL operations are on the high cost end of oil production infrastructure spectrum, economic performance is a high priority for CTL operators (Aguilera, 2014). The second reason is that economic performance is an important aspect of sustainability. Understanding the economic performance of a PAR modified CTL plant gives an indication of the sustainability of use, which helps developers make configuration decisions that improve adoption of the PAR modification of CTL as a cleaner production initiative.

The remainder of this article presents an overview of the plant configurations in Section 5.2.1, financial modelling and economic analyses in Sections 5.2.2 and 5.2.3. Finally, Sections 0 and 5.4 present the results, discussion and conclusions of the study.

5.2 Approach

Using a South African CTL plant as a case study, a comparative approach was used in this study to evaluate the impact of deploying PAR on CTL economic performance. The economic data of a commercial CTL plant was used as the baseline and configuration changes were made to the baseline model to predict the performance of a PAR modified plant. Financial models of the conventional and PAR modified plants were used to evaluate the impact of deploying PAR to CTL. **Fig. 5-1** shows the anatomy of the evaluation process used in the study.

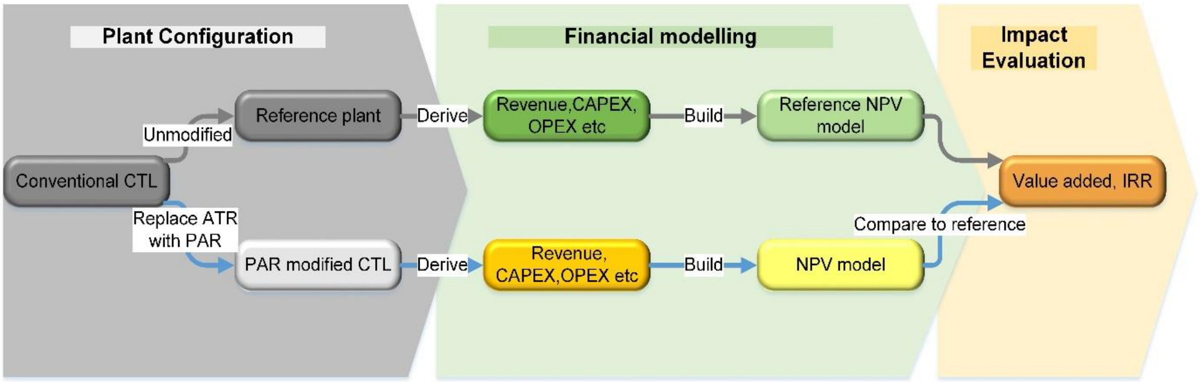

Fig. 5-1: Schematic of the approach to the evaluation of impact of PAR on CTL economic performance

As shown in **Fig. 5-1**, the study has three aspects; 1) Definition of plant configurations, 2) financial modelling and 3) economic impact evaluation. Plant configuration is discussed briefly in Section 5.2.1, financial modelling in Section 5.2.2 and the approach to economic impact analysis in Section 5.2.3.

5.2.1 Configuration of coal to liquids simulation model

Two plant configurations were modelled to evaluate the effect of PAR on CTL. A model of the Sasol Secunda plant was used as a representative conventional commercial CTL plant. The same model was modified to introduce PAR and that model was the technical basis of the plasma arc modified CTL plant. Brief descriptions of both plant configurations follow.

5.2.1.1 Conventional coal to liquids plant

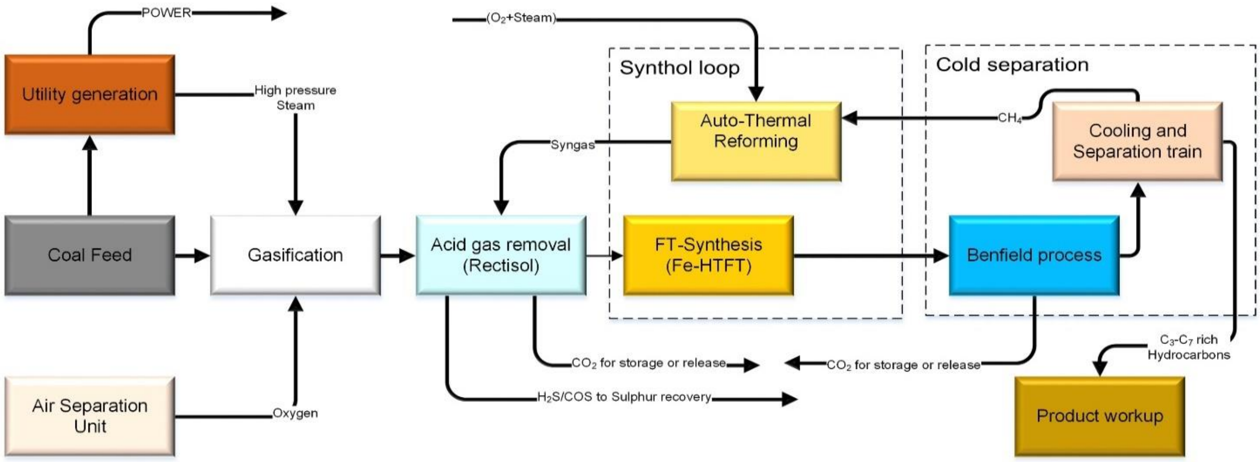

Fig. 5-2: Block flow diagram of a conventional CTL process

Fig. 5-2 illustrates a simplified block flow diagram of a conventional CTL process. In the process, Coal is prepared to a size range that is suitable for gasification taking into consideration the gasifier type being used (Bell *et al.*, 2011b). The gasifier uses oxygen and steam under high temperature and pressure to convert coal to synthesis gas (Zennaro *et al.*, 2013). The specific conditions in the gasifier influence the amount of CO_2 present in the raw synthesis gas stream (Bell *et al.*, 2011a). If necessary, the ratio of hydrogen to carbon monoxide in the syngas is adjusted through the water gas shift (WGS) (Zennaro *et al.*, 2013). The use of the WGS to produce hydrogen comes at the cost of producing carbon dioxide, which reduces the net benefit associated with the use of PAR. As part of the conditioning process, syngas, sulphur based compounds and carbon dioxide are removed by the rectisol process (Sun & Smith, 2013) or selexol process (Mohammed *et al.*, 2014). Purified syngas is then used to produce synthetic hydrocarbons, which are also known as syncrude, under high pressure with the help of a cobalt or iron catalyst (De Klerk, 2011). The syncrude is processed in the product work-up section in preparation for refining, upgrading or shipping to different product markets (De Klerk, 2011). Methane produced in gasification and Fischer-Tropsch synthesis is recovered in cold separation and recycled to produce more syngas by auto thermal reforming (ATR) (De Klerk, 2008).

5.2.1.2 PAR modified coal to liquid plant

The plasma modified CTL plant is similar to the conventional plant in many respects with the exception that the ATR in the synthol loop was replaced by a PAR system as shown in **Fig. 5-3**.

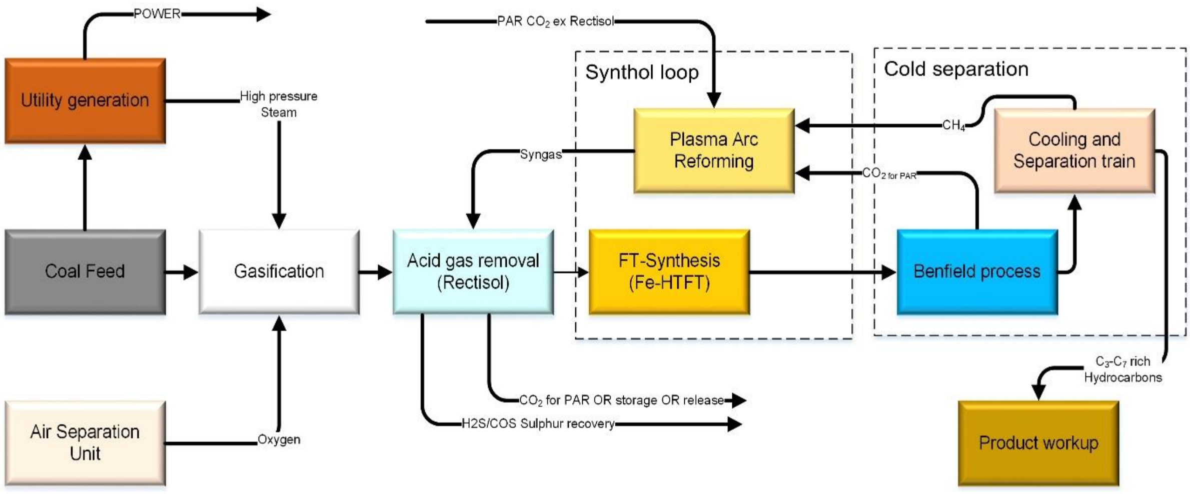

Fig. 5-3: Block flow diagram of a plasma reforming modified coal to liquids process

The process redesign, in **Fig. 5-3**, enables some of the carbon dioxide to be utilised within the process by introducing the dry reforming reaction, Eq.(5.1).

$$CH_{4(g)} + CO_{2(g)} \rightarrow\ 2CO_{(g)} + 2H_{2(g)}\ \ \Delta H =\ 247kJ/mol \tag{5.1}$$

As can be seen from Eq.(5.1), the process of using PAR to create a carbon dioxide sink is an endothermic process. PAR technology makes use of electricity to create plasma, which supplies the energy and catalytic effect required for the dry reforming reaction to proceed. To retain focus on the current research problems, plasma technology has not been discussed in this paper, however, works by Solonenko (2000) and Tao *et al.* (2011) could be enlightening for the curious reader. Details of the design of plasma system used in this paper were discussed in a previous article by the authors (Mapamba *et al.*, 2015).

It is important to note that the use of electricity would be beneficial if sourced from a low carbon source such as renewable energy and nuclear. Such use of electricity in the PAR has cost implications attached to it. However, if it is correctly viewed as a trade-off between additional input costs and potential savings from avoided emissions penalties, it becomes more acceptable. The quantification of whether this trade-off yields a net benefit or not will be presented in sections that follow.

On a technical level, the deployment of a PAR modified CTL process promises to be of benefit over a conventional CTL process. A summary of some of the key process changes is presented in **Table 5-1**. Based on these changes, a change in economic performance is expected.

Table 5-1: Impact of plasma arc reforming on CTL process parameters in relative terms

		Reference CTL	**PAR modified**
Raw materials	Coal	1	0.86
	Steam	1	0.82
	O_2	1	0.69
	Syngas fed to FT	1	1.02
Energy requirements	Air Separation Unit (ASU)	1	0.69
	Steam	1	0.82
	External electricity supply	1	1.52
Products	Sulphur based	1	0.86
	Other chemicals	1	1.04
	Alcohols & Ketones	1	1.02
	Gasification products	1	0.86
	Heating fuels	1	0.69
	Refined products	1	1.00
	Direct CO_2 emission	1	0.73
Ratios	Carbon efficiency	1	1.18

Source: (Mapamba & Fick, 2015)

5.2.1.3 Naming of scenarios

For traceability of results, the reference plant (a conventional plant) configuration was treated as configuration 1 (C1) and the PAR modified plant configuration 2 (C2). Further, a scenario that assumed no carbon tax was classified as an A scenario and one that assumed presence of carbon tax a B scenario. Hence, a reference plant evaluated with an assumption of no carbon tax was named C1A. Using this system, the names of the four plant scenarios that were evaluated is listed in **Table 5-2**.

Table 5-2: Naming of scenarios and the corresponding configuration

Scenario	Configuration	Carbon tax included.
C1A	Conventional	No
C1B	Conventional	Yes
C2A	PAR modified	No
C2B	PAR modified	Yes

5.2.2 Financial modelling and economic evaluation

Several measures of economic performance were considered in selecting appropriate measures for comparing the performance of a PAR modified plant to the performance of a conventional CTL plant. The net present value (NPV) model was eventually selected as it can provide several economic parameters that are used in evaluating energy projects, including NPV, internal rate of return (IRR) and payback price (Short *et al.*, 1995).

The remainder of this section presents the development of an NPV model in deterministic and stochastic forms so as to build in a mechanism for evaluating uncertainty.

5.2.2.1 Overview of the financial model

NPVs of PAR modified CTL and conventional CTL configurations were compared to evaluate the impact of deploying PAR to a CTL plant. The formula for evaluating NPV is given by Eq.(5.2).

$$NPV = -I_T + \sum_{t=1}^{N} \frac{CF_t}{(1+r)^t} = -I_T + \frac{CF_1}{(1+r)^1} + \frac{CF_2}{(1+r)^2} + \cdots + \frac{CF_n}{(1+r)^N} \tag{5.2}$$

Where:

I_T - Total investment cost. Negative sign is due to the initial capital being a negative cash flow on the project

r - Discount rate (Equated to the Sasol weighted average cost of capital, WACC)

t – time period of evaluation. Such that N is the effective project life for investment evaluation

CF_t - Net annual cash flow after tax, which can be written as Eq. (5.3).

$$CF_t = PAT_t + Depreciation_t \tag{5.3}$$

The profit after tax, PAT_t is calculated by Eq. (5.4)

$$PAT_t = (1 - Tax\ rate) \cdot (Revenue_t - Costs_t - Depreciation_t) \tag{5.4}$$

Substituting expressions for PAT_t and CF_t into the NPV expression, Eq. (5.2) becomes

$$NPV = -I_T + \sum_{t=1}^{N} \frac{(1 - Tax\ rate) \cdot (Revenue_t - Costs_t - Depreciation_t) + Depreciation_t}{(1+r)^t} \tag{5.5}$$

In addition to the NPV, the IRR of the CTL plants were evaluated as part of project acceptance testing. Since IRR is the discount rate that makes the NPV = 0, IRR was calculated by solving for the discount rate (r), when Eq. (5.5) is equal to zero.

A description of the assumptions and derivation of the model components is presented in Sections 5.2.2.2 to 5.2.2.5 and the description of the economic analyses follows in Section 5.2.3

5.2.2.2 Assumptions used in financial modelling

The assumptions used in the creation of the financial model used in this paper are:

- Exchange rate of 10.09 ZAR/USD was used to convert costs in ZAR to USD based on the average exchange rate used by Sasol in their financial report for 2014 (Sasol limited, 2015)
- Project economic life assumed to be 25 years (Towler & Sinnott, 2013)
- South African tax regime was assumed for analysis so effective tax rate of 28% was used (South African Revenue Service, 2015)
- Construction period of 48 months was assumed, with equal disbursement of capital. This is based on reported standard times for similar chemical plant (Towler & Sinnott, 2013).
- A 10 year straight line depreciation schedule was used as per SARS tax guidelines (South African Revenue Service, 2012)
- A carbon tax rate of \$12/ ton CO_2 with an effective 60% tax-free base was assumed in line with the draft carbon tax policy for South Africa was used (South Africa National Treasury, 2013)
- The carbon pricing policy was assumed to remain constant over the life of the project.

5.2.2.3 Estimation capital costs

The authors used publicly reported economic data to estimate capital costs. This was done to avoid the restrictions that accompany disclosure of actual detailed capital costs. Capital costs of conventional CTL plant were sourced from reports by Rahmim (2008) and (Kreutz *et al.*, 2008) and PAR capital costs were obtained from vendor estimates. Data for conventional was checked against data reported by De Klerk (2011), who had an insider view of actual commercial CTL operations. The authors took a conservative view of the costs and as such used the higher cost values in calculations.

Investment costs of the CTL plant configuration were calculated for an 80000 bpd plant. Data from literature was capital corrected for capacity and basis year using the six-tenths cost curve shown in Eq.(5.6)

$$C_T = C_B \times \left(\frac{CEPCI_{2014}}{CEPCI_{Base\ year}}\right) \times \left(\frac{Q_T}{Q_B}\right)^n \tag{5.6}$$

Where;

C_T - Cost of equipment at new capacity in year 2014

C_B - Cost of reference equipment in the base year

$CEPCI_{2014}$ - Chemical engineering plant cost index for 2014

$CEPCI_{Base\ year}$ - Chemical engineering plant cost index in the base year

Q_T - Capacity of plant in the year being evaluated

Q_B - Capacity of the plant being used as the reference for costing

n – Size exponent, 0.67 was used (Kreutz *et al.*, 2008)

5.2.2.4 Estimation of operating costs

Operating costs of the conventional plant were based on operating costs reported by Sasol for the Secunda synfuel plant in their Analyst booklet (Sasol limited, 2014). Costs of feedstocks, labour and general and administration costs are presented in the report. Electricity and general energy costs were determined using Eskom tariff guides (Eskom, 2013) and engineering judgement based on requirements presented in the Sasol analyst reports. The forecast process impact was used to calculate operating costs for the plasma reforming modified plant using operating costs of a conventional plant.

Carbon tax was not included in the operating costs derived from the Sasol analyst book excluded carbon tax, which is reflective of the current policy. However, for futuristic analysis carbon tax was added to the operating costs at different levels to evaluate the effect of carbon pricing on the economic performance of the different CTL configurations. Guidance on the relevant carbon pricing regimes was derived from papers by Alton *et al.* (2014) and South Africa National Treasury (2013).

5.2.2.5 Estimation of revenues

The sale of refined products as syncrude was used as the basis for revenue calculation. Since the study excludes refining of syncrude into final products, the price of crude oil was considered as a fair basis for estimation of revenues. Hence, revenues for the CTL configurations studied were estimated based on anticipated crude oil prices and syncrude product quantities for the plant capacity of 80000 bpd of crude equivalent product. To ensure that the model could be verified, the prevailing product price used by Sasol for revenue calculation in the 2014 Analyst book (Sasol limited, 2014) to provide an initial basis for comparison. Further exploration of other crude price scenarios was done to check if the economic performance is persistent in different economic scenarios.

5.2.3 Economic analyses

Two phases of economic analyses were done. The first phase of analysis sought to compare the basic performance of a conventional plant to the performance of a plasma-modified plant. The second phase of analysis evaluated the quality of the results taking into consideration the uncertainty in the financial model inputs. Monte-Carlo analysis was chosen to factor in the uncertainty into the analysis due to its ability to factor in uncertainty in multiple model inputs in the analysis (Khindanova, 2013; Vithayasrichareon & MacGill, 2012).

5.2.3.1 Economic performance of plant

The effect of deploying PAR was firstly measured by the break-even price. Given that the primary products of CTL plants are commodity chemicals, which are bought on a cost competitiveness basis (Smith, 2005), lower break-even price corresponds with higher probability of project success. The value was determined using a deterministic NPV model and simple WHAT-IF analysis in Microsoft Excel®. Break-even prices were evaluated for the process scenarios discussed in Section 5.2.1.3.

A comparison of the NPV of the reference plant scenario and the PAR modified plant scenario was done to determine the value added by the deployment of PAR, the difference being an indication of the value added by PAR.

IRR was used to test whether the financial performance of each plant scenario met the acceptance criteria used for similar commercial plants. The Sasol hurdle rate was used as a standard of the minimum acceptable project IRR. Hence, for a project to be acceptable, CTL a project has to deliver a minimum return of 1.3 times the weighted average cost of capital (WACC) of the company (Sasol limited, 2014). For Sasol, the hurdle rate for 2014 translates to 8.84% on a real basis.

5.2.3.2 Effect of uncertainty on economic performance

Researchers adopting an overly optimistic sometimes compromise the quality of output from an economic model or pessimistic position is selecting input parameters. Monte Carlo analysis was used to assess and mitigate the effect of bias in the researcher's perspective.

Crystal Ball® was used to execute the Monte-Carlo analysis. To enable this, the deterministic model in Section 5.2.2.1 was converted to a stochastic model by replacing the single value inputs with input probability distributions (Khindanova, 2013). Crystal Ball then uses the input probability distribution models to compute the distribution of output values e.g. the NPV or IRR. The choice of probability distribution of each input is discussed in **Table 5-3**.

Table 5-3: Distributions of financial model inputs

Input	Distribution	Range	Notes
Crude oil price	Custom Scenarios	\$100/bbl. and \$123.50/bbl.	The effect of price changes was evaluated for 2 price cases. 123.5 \$/bbl. was effective product price in 2014 (Sasol limited, 2014)
Carbon emissions	Triangular	Maximum: 30246 ktpa CO_2 Probable: 23921 ktpa CO_2 Minimum: 22976 ktpa CO_2	The range factors in the uncertainty in performance of PAR.
Carbon tax	Triangular	Maximum: 30 \$/ton CO_2 Probable: 12 \$/ton CO_2 Minimum: 4 \$/ton CO_2	Conservative range adopted and influenced by the tax deliberations
Electricity cost	Triangular	Maximum: 133 \$/MWh Probable: 108 \$/MWh Minimum: 91 \$/MWh	Based on probable Nuclear electricity costs (Stoker & Fick, 2012)
Coal cost	Logistic	32 \$/ton ± 30%	Price based on Sasol supplied cost (Sasol limited, 2014) and range based on historical data.
Water cost	Logistic	1.49 \$/m^3 ± 10%	Based on historical cost data

Input	Distribution	Range	Notes
Capital requirement	Triangular	Total capital ± 30%	Range based on accuracy of level 4 capital requirements estimates for process plants (Towler & Sinnott, 2013).
Discount rate	Triangular	6.8% ± 1.5%	Based on Sasol real WACC

5.3 Results and discussion

Results were presented and discussed in three sections, Sections 5.3.1 and 5.3.2 covers the impact of PAR deployment on the capital requirements and financial performance of CTL respectively based on the deterministic model. Section 5.3.3 presents the evaluation of the effects of uncertainty on the results by factoring in the input and output variability through use of the stochastic model.

5.3.1 Impact of PAR deployment on CTL Capital requirements

The total capital investment for the reference plant, with a capacity of 80000bpd, was estimated to be $ 7.4 billion in 2014 dollars, which translates to 92540 $/bpd. A summary of the breakdown of the capital cost is presented in **Table 5-4** and an extension of the calculations is provided in Appendix A.4. The total capital requirement for the PAR modified plant was determined to be $6.9 billion in 2014 dollars and that translates to a specific capital cost of 86250 $/bpd. This estimate excludes the cost of building a power plant to supply additional electricity requirements. The authors assumed that a low carbon power plant is available to supply any additional electricity requirements at a market related cost. While this approach increases the exposure to external electricity supply forces, it allocates the risks associated with investing in a power plant in the hands of those best equipped to do so, such as an independent power producer. The specific capital cost for the modified CTL plant is comparable to 87500 $/bpd reported for a commercial CTL plant that uses nuclear hydrogen Stoker and Conradie (2015).

Table 5-4: Summary of capital contribution by plant section

Section	Conventional plant		PAR modified plant	
	($ m)	**%**	**($m)**	**%**
Coal preparation and gasification	2329	30	2071	30
Syngas cleaning	1232	17	1233	18
Air Separation	1232	17	952	14
Utilities	1305	18	1124	16
FT, gas recovery, refining	1201	16	1201	17
Reforming[10]	104	1.4	300[11]	4
Total	**7403**		**6881**	

These figures seem achievable considering that they are on the lower end of the range for conventional commercial CTL plants as reported by De Klerk *et al.* (2013). For the plasma modified CTL, the lower capital cost is consistent with the reduction in coal processing and air separation plant sizes. However, given the ± 20% inaccuracy of the method used in the estimations, the 7% difference in capital of the conventional and PAR modified CTL plants was not practically significant. For practical purposes, the deployment of PAR has no real advantage or disadvantage with respect to capital requirements.

5.3.2 Impact of PAR deployment on economic performance of CTL

Three measures of economic performance were used to evaluate if the deployment of plasma arc reforming could positively influence the performance of a commercial CTL, break-even price, NPV and IRR. A comparison of the break-even prices of the CTL scenarios is presented below in the waterfall diagram shown in **Fig. 5-4**.

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[10] Reforming technology is changed from ATR in the reference plant to PAR in the modified plant

[11] Based on quotes to supply components of reformer and adjusted to factor in EPC costs

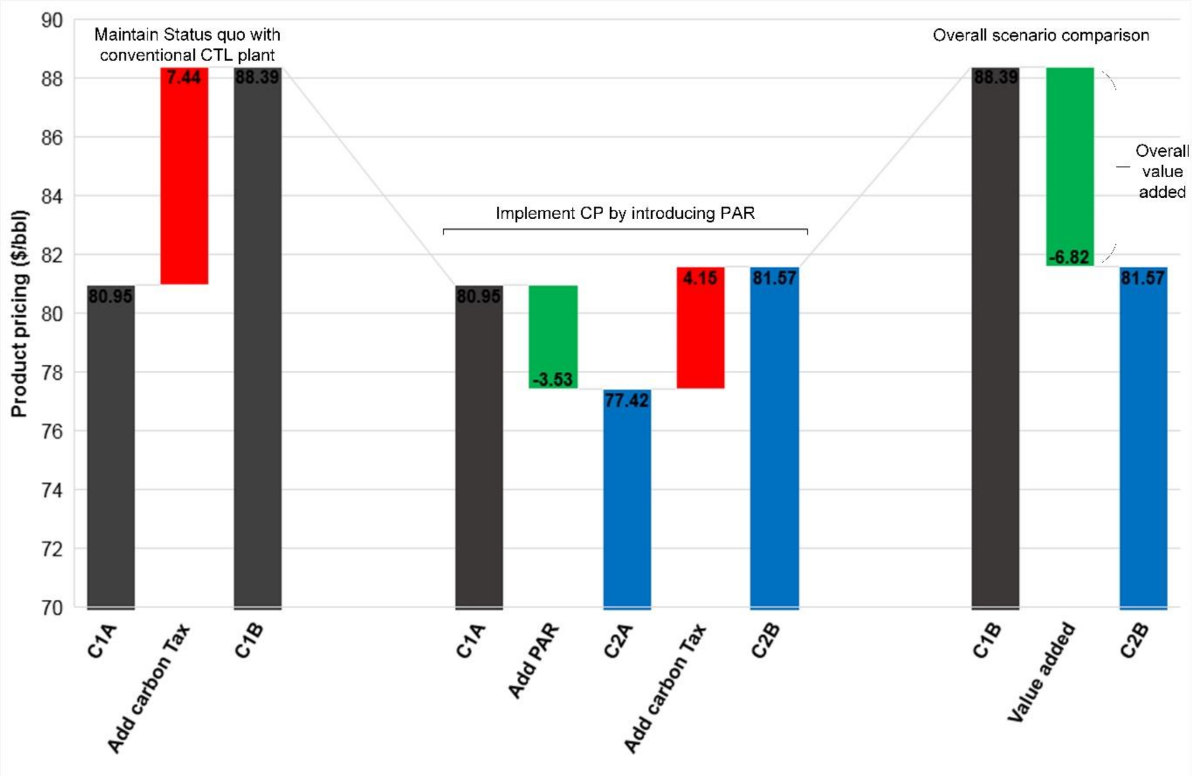

Fig. 5-4: Comparison of break-even prices of the plant scenarios

Fig. 5-4 shows a plot of the breakeven prices for the different CTL configurations versus the actions applied to achieve them. For a conventional CTL plant (C1A), the introduction of carbon tax would raise the breakeven price by $7.44/bbl. However, if PAR is introduced first before the introduction of carbon tax, the introduction of PAR improves productivity, which lowers the breakeven price by $3.53/bbl. When carbon tax is introduced, the concomitant increase in breakeven price would be $4.15, which is much less than the $7.44/bbl. encountered in a conventional CTL plant. Overall, the model used by the authors predicts that the benefit accruing from the deployment of PAR would amount to a $6.82/bbl. reduction of the breakeven price.

An examination of the NPV and IRR results obtained from the deterministic model also followed the same trends shown by break even prices. This logically follows from the fact that carbon tax adds to the operating costs, which reduces the net cash flow. The introduction of PAR mitigates the effect of carbon tax resulting in an increase in cash flows, adding an average project value of $1.5 billion for the oil price range considered in the study. However, carbon tax erodes some of the value added with the net value added by deployment of PAR being $ 400 million. The project value added stems from potential savings in capital and operating expenditure. All process scenarios also exceeded the hurdle rate acceptance criteria, with the PAR modified scenarios performing better than the conventional configurations. The extent to which the scenarios exceeded the desired hurdle rate followed the trend seen in break-even price and NPV as shown in **Fig. 5-5**. While the trends in **Fig. 5-4** and **Fig. 5-5** assumed higher oil prices, an assessment at lower prices showed that the trend remains intact with PAR scenarios maintaining the lead. Hence, the deterministic model suggests that the deployment of plasma arc reforming positively influences CTL economic performance.

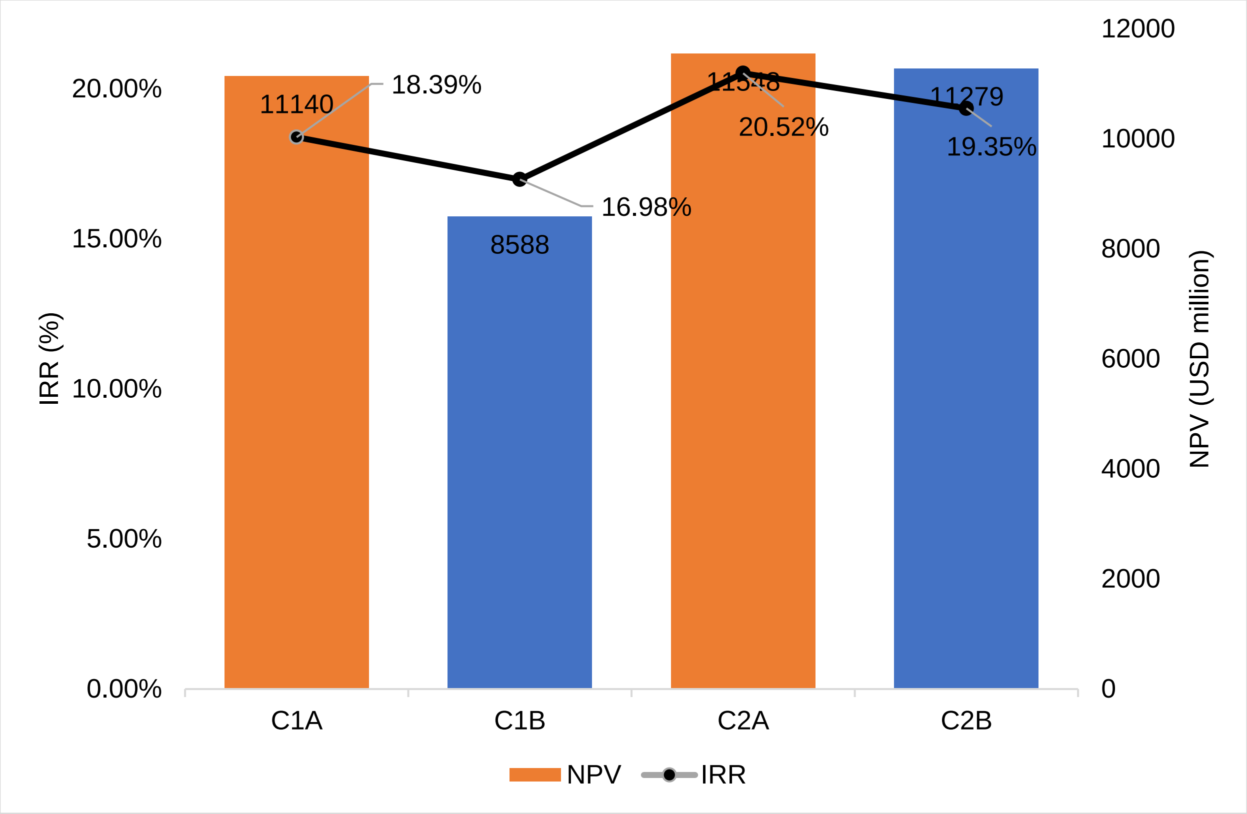

Fig. 5-5: NPV and IRR from deterministic model for process scenarios.

5.3.3 Effect of uncertainty on economic performance

Considering that the combination of PAR and CTL has not been tried commercially, it was essential to evaluate the effect of uncertainty on forecast economic performance. This was done by using a stochastic model in the place of the deterministic model. The results from the stochastic and deterministic models were compared to see if the trends hold when variability in inputs was factored into the model calculations. Results obtained suggest that the deterministic model produces optimistic results as they were almost double the mean values obtained from the stochastic model. A summary of the comparisons of NPV and IRR for the CTL process scenario is presented in **Fig. 5-6** and **Fig. 5-7**.

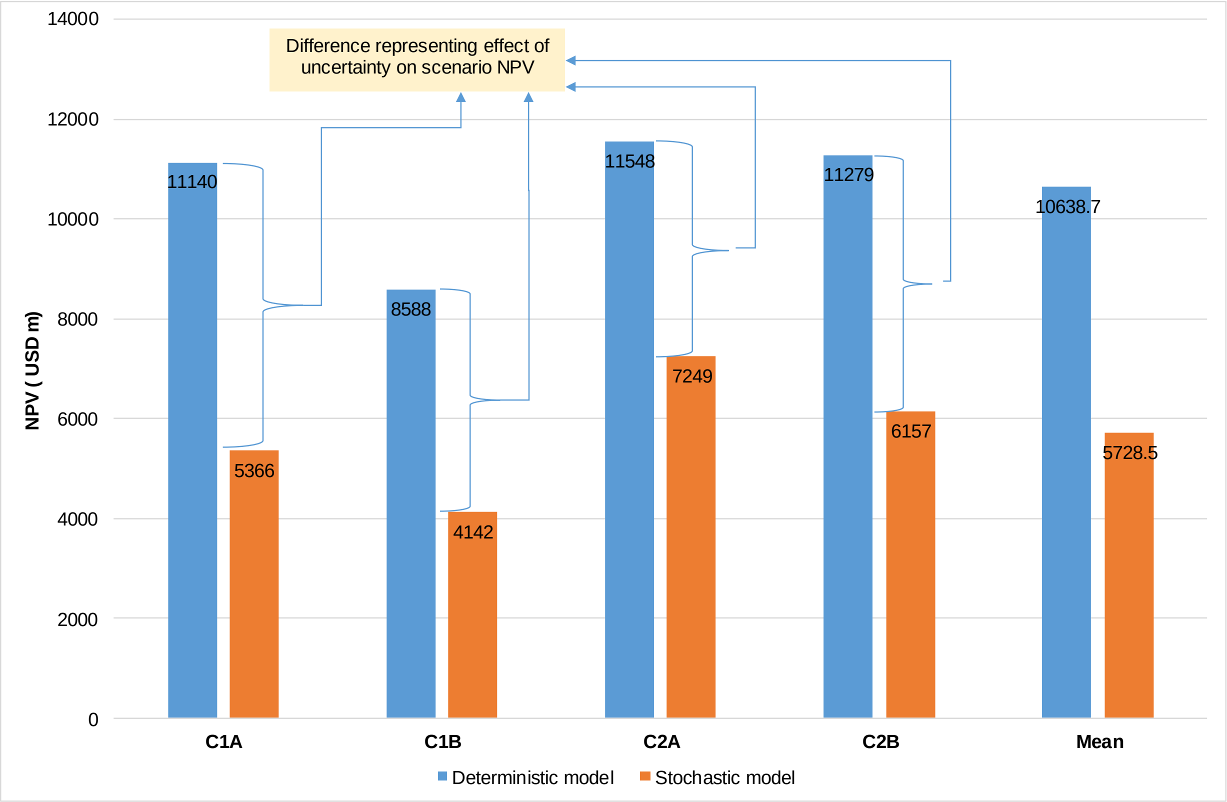

Fig. 5-6: Summary of NPV comparisons for the CTL process scenarios

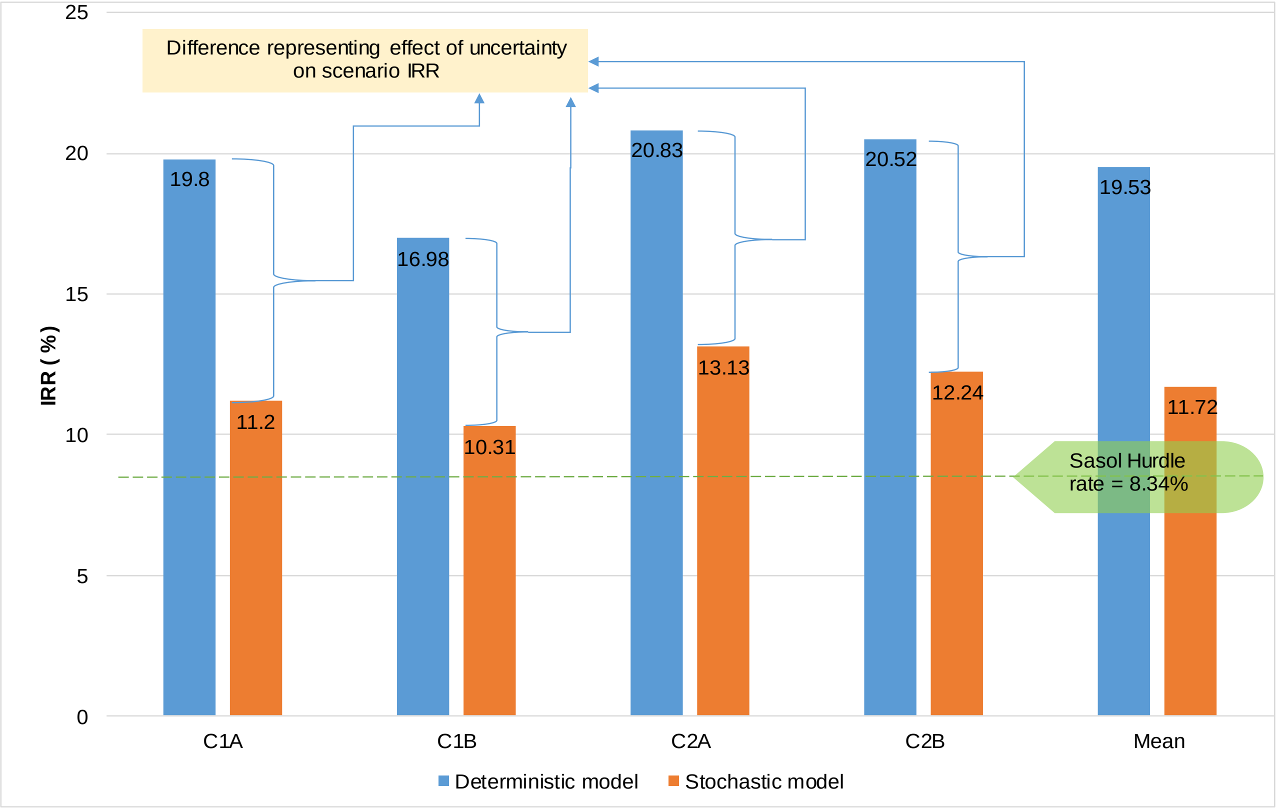

Fig. 5-7: Summary of IRR comparisons for the CTL process scenarios

Fig. 5-6 and **Fig. 5-7** show that the deterministic model predicted higher NPVs and IRRs than the stochastic model predictions for the same parameters. However, despite the differences in the absolute values, the trend of NPV and IRR values was consistent between the models. Overall, the PAR modified plant scenarios had better results than conventional plants under the same market conditions. The difference in absolute values for the models was attributed to the contribution of uncertainty arising from market conditions and technology performance.

To understand the significance of the impact of market conditions further, sensitivity analyses were done to determine the contribution of different model inputs to the observed output variability. A summary of the analyses is presented in **Fig. 5-8** as a contribution to variance chart.

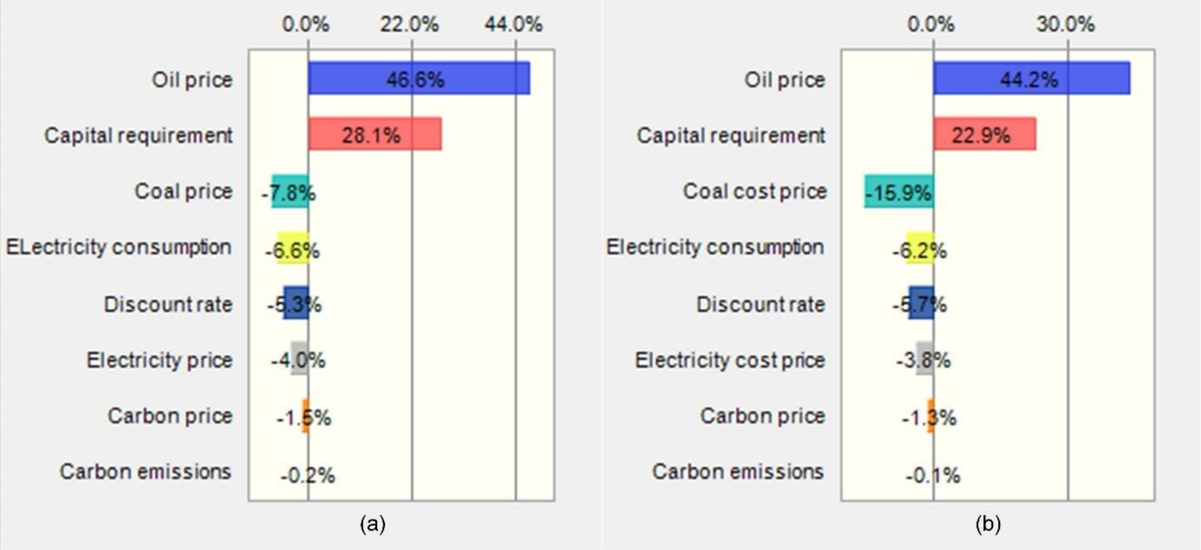

Fig. 5-8: Sensitivity analyses for plant scenarios (a) represents analysis for C1B and (b) is analysis for C2B

The charts in **Fig. 5-8** show that significance of inputs to observed variability is similar for both the conventional (C1B) and plasma modified (C2B) plants. The results of sensitivity analysis show that crude oil price, capital requirements, coal price and discount rate have a significant effect on NPV and IRR. However, two conditions that were seen to favour the PAR modified process scenarios are 1) Cheap low carbon electricity and 2) High carbon tax prices for both the NPV and IRR analyses. The other subtle differences seen in the results are attributable to the different cost bases where, the PAR modified scenario has a lower capital cost and a higher overall cash flow.

5.4 Conclusions

This paper evaluated the economic performance of a PAR modified CTL in comparison with the economic performance of a conventional CTL process. The evaluation challenged the assumption that a PAR modified CTL would not be viable due to its electrical requirements. Overall, the results showed that the PAR modified CTL exceeded the economic performance of a conventional plant in all three measures that were used to compare the plants. Hence, it can be concluded that, though the electricity cost of PAR may be high, it makes more economic sense to use PAR to create a lower footprint CTL regardless of the carbon pricing regime in the market. Since economic performance of a process is often a high priority in the consideration for adoption or rejection of a new technology or process, it is reasonable to conclude that PAR has a good chance of adoption in the CTL application.

Fundamentally, embarking on a new build program of a CTL plants of any configuration may not be desirable or sustainable in the long term. However, considering the rate of demand side transformation of the areas currently being served by CTL plants, from fossil energy to low carbon energy, it is necessary to develop transitory solutions like a PAR modified CTL. In view of this, retrofitting existing CTL plants with PAR technology may be a more desirable option. In the long term view, the additional low carbon electrical capacity developed to enable PAR in the transition term, would still be useful in the decarbonised economies. Hence, a sufficiently long term scope for supply of low carbon electricity would help overcome some of the key limitations with PAR use in CTL.

Overall, considering the projected value added by the deployment of plasma arc reforming, the authors conclude that deployment of plasma arc reforming would be beneficial and it is worthwhile to develop plasma arc reforming technology for commercial scale application in the long term.

5.5 Acknowledgements

The authors are grateful to the North West University School of Chemical and Minerals engineering for access to facilities and process evaluation tools and to THRIP for partially funding the project as Waste to Energy project, TP: 12083011540.

5.6 References

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6 CONCLUSIONS AND RECOMMENDATIONS

"To be suspicious is not a fault. To be suspicious all the time without coming to a conclusion is the defect.*"- Lu Xun*

6.1 Introduction

The coal to liquid process has contributed significantly to the economy of South Africa in the form of contributing to fuel supply security (Nkomo, 2009), creation of jobs, tax revenue and petrochemical products (Mangena, 2012). However, changing operating landscape and policy pressures are threatening the continued use of CTL. This is sad considering that coal reserves will continue to be a primary energy source for longer than oil and gas (Shafiee & Topal, 2009).

Literature has shown that production costs of CTL are escalated by three issues, high capital cost (De Klerk *et al.*, 2013; Zennaro, 2013), low carbon efficiency (Maitlis & de Klerk, 2013) and high greenhouse gas emissions (Miglio *et al.*, 2013). These issues make CTL uncompetitive. Policy driven costs such as carbon tax, while noble, threaten the competitiveness of CTL further by adding to the production costs. Considering the nature of the challenges CTL faces and their relationship, CTL can benefit from the application of cleaner production initiatives.

Plasma arc reforming was proposed on suspicion that it could be a feasible and viable solution to CTL challenges. This suspicion was tested within the CTL context as part of evidence gathering. The argument pursued in the testing was that it is feasible to deploy plasma arc reforming to a commercial scale process and it could be viable to operate a PAR modified CTL plant in the near future. This argument was split into two sub hypotheses to separate the issues. The sub hypotheses are:

- It is feasible to deploy plasma arc reforming to a commercial coal to liquid process, which corresponds to the research question "Is it technically feasible to deploy plasma arc reforming to a commercial coal to liquid process?"
- Deploying plasma arc reforming in a commercial coal to liquid process could be viable in the future, corresponding to the question "Could the deployment of plasma arc reforming to a commercial coal to liquid process be economically viable in the future?"

In this chapter, a reflection of the research carried out in this study is presented. In the reflection, a discussion of the lessons learnt from the reviewing the evidence against the initial objectives is presented in Section 6.2 and a discussion the implications of the lessons is presented in Section 6.2.3. The limitations of the research are presented in Section 6.4 and suggestions for future work on deploying PAR to commercial CTL are presented in Section 6.6.

6.2 What was achieved in this study?

Some challenges with CTL were identified and PAR was proposed as a solution in Chapters 1 and 2. Methods to test PAR as a solution, analysis and results of the testing were presented as articles in Chapters 3, 4 and 5, with conclusions being made in each chapter.

In this section, highlights of the key findings and contributions in testing the main hypothesis are presented. The highlights were grouped by sub-hypotheses with the findings pertaining to technical feasibility being discussed in Section 6.2.1 and findings relating to economic viability being presented in Section 6.2.2. The contribution of each achievement to the body of knowledge is discussed along with the relevant findings. Section 6.2.3 presents a brief discussion of the validity of the findings as a quality assurance check.

6.2.1 Is it feasible to deploy plasma arc reforming to commercial scale?

Most of the work done in this area is presented in Chapter 3, which was published in the Journal of Cleaner Production (Mapamba *et al.*, 2015). Other aspects of the work will be published in a bridging article presented in Chapter 4, also submitted to the Journal of Cleaner Production. Highlights of the achievements in line with the assessment of feasibility are given in bullet point below:

- It was concluded that it is feasible to deploy plasma arc reforming to commercial scale using existing components. An exploration of whether the technology can be scaled up to the required scale using existing industrial torches was documented in Chapter 3. In the process, it was found that the thermodynamic limit of improving carbon efficiency by deploying plasma reforming was determined to be 15%, assuming only internally generated methane is reformed with carbon dioxide in a PAR. These findings address research questions 2 and 3 in Chapter 1.
- In Chapter 4, it was found that for plasma arc reforming to improve the carbon efficiency of CTL, it has to achieve a minimum conversion of 87%, which is a high target that puts pressure on designers and imposes a narrow operational limits for the reactor.
- Taking a system view of CTL allowed the author to translate what an improvement in carbon efficiency means in practical terms and this was used to address research question 4. Findings show that improving carbon efficiency translates to a lower requirement of coal, process steam and oxygen, which is associated with capital and operating cost reductions.
- If PAR is used to achieve the improvement, it comes with a higher electrical requirement and that has an additional cost element. This electrical requirement creates an opportunity to use low carbon energy for production of petrochemicals, which can lower their carbon footprint of commercial CTL.

- In deploying plasma arc reforming to CTL, use of carbon dioxide as plasma gas presents the most compatible configuration as it has the best balance between performance and negative downstream effects. This addresses research question 1, which queries the PAR configuration most compatible with CTL.
- Using existing components to scale-up plasma arc reforming is desirable, as it has established manufacturing methods for components and spares. Currently, manufacturers of plasma torch components are concentrated in North America and Europe but there is growth in Asia. As the manufacturing network grows, the costs of using plasma torches for PAR at industrial scale should decrease.

6.2.2 Is the deployment of plasma arc reforming viable in the future?

The financial modelling and analytical work that was used in testing this hypothesis is presented in Chapter 5, which was submitted to the Journal of Cleaner Production as a full research article. The key takeaways from the economic analysis were:

- In the absence of a carbon tax, the deployment of plasma arc reforming to CTL adds significant value by reducing capital costs and feedstock costs, which reduces the break-even price required by a commercial plant.
- In the context of a carbon priced environment, the deployment of plasma arc reforming absorbs the additional costs by reducing tax obligations. Instead of a \$6.82/bbl. being added to the break-even price, a marginal cost addition of \$0.62/bbl. results.
- By comparing the breakeven prices with forecast oil prices, it is seen that it may be viable to operate plasma modified CTL plants from \$82, which may be achieved from as early as 2019 (IEA, 2015).
- High carbon tax and use expensive coal increases the benefit accruing from avoided compliance and feedstock costs.

6.2.3 Validity of findings

Verification and validation (V&V) were done as part of quality assurance. According to the Faculty of engineering guidelines, verification ensures that the study is designed properly and validation ensures that the study is relevant to the intentions (Faculty of Engineering, 2013). Because the thesis is presented in article format, very little V&V data and discussion could not be included in in Chapters 3, 4 and 5 due to journal limitations. This section gives a primer to the philosophy applied in checking the validity of findings presented in this thesis. An expanded discussion of the validation and verification process is presented in Appendix A.1.

Aspen Plus models were used in the evaluation of the technical feasibility aspects of the study. Since the underlying execution logic for the models was similar for both the plasma arc reforming models and the coal to liquid process, the V&V activities were similar. Since Aspen plus uses rigorously validated data in its property databases, the reliability of property data in models was deemed not to be an issue. As a result, the focus of verification was on ensuring that states and methods were 1) obtained from credible sources, 2) compatible with the relevant system components and 3) methods are sufficiently robust under the range of operational conditions. For the remaining technical feasibility assessments, the frameworks were verified against manuals such as those provided by the US Department of Energy (2010). The PAR simulation results compared favourably with experimental results reported by (Tao *et al.*, 2011), hence the model was deemed valid. The CTL model of the reference plant was validated by comparing plant output with reported Sasol output and the overall results were within a 5% deviation. Hence, the CTL model was also considered valid. By combining a valid PAR model with a valid CTL model, the resulting plasma arc reforming plant was considered valid. Further confidence was derived from analytical results comparing well with the simulation results.

A financial model was built in Microsoft Excel to evaluate the economic viability. The focus of verification was on using data from credible sources. Part of validating the financial model was to use product throughput from validated process models as that influences the revenue aspect of the model. In addition to using validated process models as a revenue basis, the remaining cost and input probability distributions were obtained from credible sources. The comparability of the reference plant financial model was done by comparing the profitability with published data on the Sasol Secunda synfuel business (Sasol limited, 2014). The average profit of the financial model was within a 10% margin.

Since the overall results produced by the models used in the evaluations were within 10% of published data, the findings produced by the use of the models were deemed valid.

6.3 Implications of the findings

The study confirmed what was theorised about the use of plasma arc reforming, in that it improves the carbon efficiency of the CTL process. It then goes on to expand what was known, to highlight that the benefits of plasma arc reforming do not require entirely new technologies or methods to deploy to commercial scale. However, some practical issues need to be managed in the deployment process for the application to be successful.

Key among the issues is the characterisation of plasma reforming kinetics data, which will be useful in reducing technology risk by improving accuracy of reactor design and configuration. Second, in the deployment, the risk allocation in the assumption of capital expenditure for developing plasma arc reforming modified CTL plants makes a significant difference in the break-even price required. In the study, the avoidance of assuming the cost of a nuclear power plant and a nuclear hydrogen plant provides sufficient evidence to suggest it may be viable to operate a plasma reforming modified CTL plant at commercial scale.

6.4 Limitations

This study was primarily limited by three issues, 1) a dependency on information in the public domain and 2) the use of simulation models for process evaluation and 3) the improvement scope was limited to using methane being generated by the system. An additional limitation that was considered is the philosophy around whether it is reasonable to use low carbon energy to produce a fossil fuel that will produce greenhouse gases when in use. While not a real limitation to the study it has potential to limit acceptance of the findings presented here.

The dependency on data in the public domain means that the quality of information from models was only as good as the quality of the CTL information in the public domain. The quality of information on the CTL greenhouse gas emissions was of particular concern in this regard considering that accuracy of emissions reports by commercial organisations is un-corroborated. A review of related literature shows consistency in reported data. The accuracy of the data in relation to actual operational data could not be ascertained. However, consistent use of the same basis for the reference and modified plants means that the impact observed takes into account the inaccuracies in the raw information and would be repeatable with data that are more accurate.

Simulations enable the evaluation of processes at low cost and with relatively, short turnaround time. Use of simulation sometimes fails to capture unexpected behaviour when the system in question is configured differently. The result is that the opportunity to capture unexpected behaviour that could be discovered in an experimental setting could be missed. However, the missed opportunities do not undermine the value of the results obtained in the study.

The reclamation of carbon from waste carbon dioxide streams was limited by the amount of methane available within the CTL system for dry reforming in the plasma arc reformer. If external methane is available for completely converting the waste carbon dioxide stream into syngas, further improvements in the carbon efficiency could be possible. While it limits understanding the full extent of the opportunity of improvement possible, not introducing external gas avoids economic disturbances introduced by gas market events.

The final limitation presented as an important consideration, could undermine the acceptance of the findings and recommendations of this study. The issue of whether it is reasonable to use low carbon electricity for CTL versus using investing in cleaner alternatives has to be viewed in the long term context for it to make sense. Firstly, PAR modification of CTL is not proposed as a permanent solution as that would not be sustainable from an environmental perspective. Hence, PAR modified CTL is proposed as an interim or transitional measure to lower the environmental footprint of the energy supply side while the consumer side of the market transforms sufficiently to make low carbon supply options sustainable. Second, taking the South African case as an example, the capital required to transform the demand side of the market into a low carbon system is prohibitive. This would result in progress towards decarbonisation being severely limited by financial constraints. Hence, recognising PAR modified CTL as a transit solution, it stands a better chance of overcoming resistance when it comes to implementation.

6.5 Final conclusion

After considering the evidence gathered during the development of this thesis, it is feasible to deploy plasma arc reforming to a commercial CTL plant. For the technology risk to be managed effectively, it is necessary to characterise the kinetics of plasma arc reforming of methane with carbon dioxide. The results also suggest that it will be viable to operate a PAR modified CTL plant at commercial scale in the near future. All things being equal the PAR modified plant will be more competitive than a conventional CTL plant.

6.6 Recommendations for future work

The findings of this study could be valuable in altering the fate of CTL in the future. Findings in this report mainly represent big picture information about deploying plasma arc reforming to CTL. To improve the chances of application, further research is necessary to improve the precision of information on the performance of PAR within the CTL context. Some of the recommended issues for future research include:

- It is essential to characterise plasma reforming kinetics under CTL conditions. This would facilitate a more accurate design of PAR reactors and allow a more accurate determination of performance parameters, which would reduce the technical risk in deploying a plasma arc reformer at a commercial scale.
- Determination of the optimal coal-methane hybridisation mix for maximising carbon utilisation in plasma arc reforming synthetic oil production processes.
- The identification of higher performing electrode materials for plasma equipment to improve lifespan may be desirable. Higher performing electrodes would lower the costs incurred in operating plasma reformers and minimise maintenance stoppage time.
- A computational fluid dynamics (CFD) study of the plasma reactors is recommended to identify optimal torch configuration and reactant distribution within the reactor system. Such a study could also be instrumental in assessing metallurgical failure risks because of torch configuration.
- Evaluation of control system options for safe and optimal operation of a high temperature plasma arc reformer

- Finally, it will be necessary to design and construct a demonstration unit to evaluate the actual system behaviour in a controlled environment, which will enable to an evaluation of the practical operability limits to be done.

6.7 References

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APPENDICES

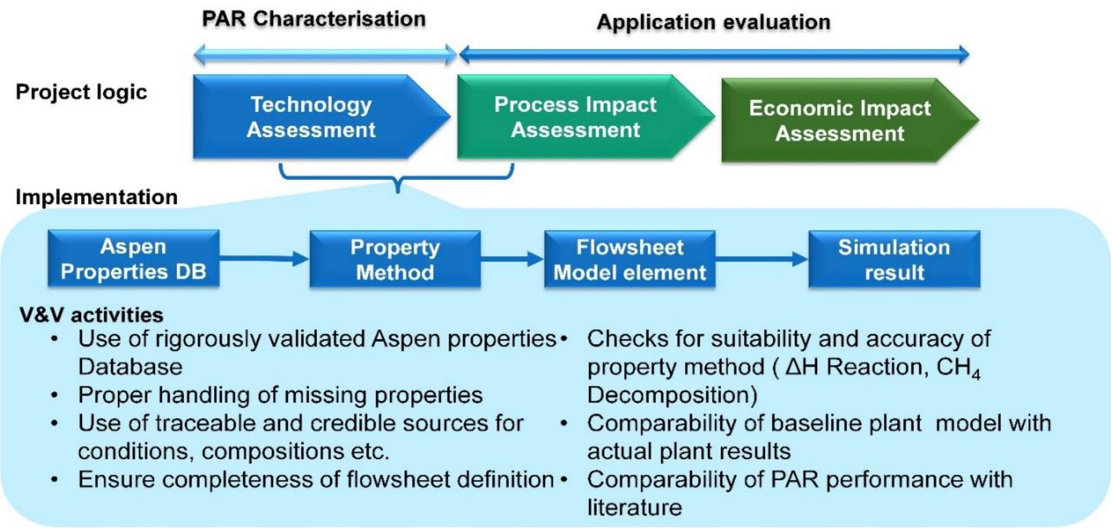
A.1 Validation and verification

A.1.1 Introduction

Verification and validation (V&V) were done as part of quality assurance. According to the Faculty of engineering guidelines, verification ensures that the study is designed properly and validation ensures that the study is relevant to the intentions (Faculty of Engineering, 2013). The V&V activities done during this study were based on this understanding. Since the thesis is presented in article format, some of the V&V activities are included in Chapters 3, 4 and 5. However, the scope of discussion was limited by journal requirements. The verification and validation activities were separated into technical feasibility related V&V and economic viability related V&V activities.

A.1.2 Validation and verification of technical models

Aspen Plus models were used in the evaluation of the technical feasibility aspects of the study. Since the underlying execution logic for the models was similar for both the plasma arc reforming models and the coal to liquid process, the V&V activities were similar. Since Aspen plus uses rigorously validated data in its property databases, the reliability of property data in models was deemed not to be an issue. As a result, the focus of verification was on ensuring that properties were complete and methods were compatible with the relevant system. For the remaining technical feasibility assessments, the frameworks were verified against manuals such as those provided by the US Department of Energy (US DOE). Validation for the PAR was done by comparing the experimental results reported by (Tao et al., 2011).



- Use of rigorously validated Aspen properties Database
- Proper handling of missing properties
- Use of traceable and credible sources for conditions, compositions etc.
- Ensure completeness of flowsheet definition
- Checks for suitability and accuracy of property method (ΔH Reaction, CH_4 Decomposition)
- Comparability of baseline plant model with actual plant results
- Comparability of PAR performance with literature

Fig. 0-1: Summary of verification and validation strategy for technical feasibility evaluation

Completeness of data input

The simulation model for the screening of plasma arc reformers was simple with gaseous reactants that are conventional components in the Aspen properties database. The use of thermodynamics made it unnecessary to cater for intermediate free radicals, as thermodynamics is evaluates the overall changes without accounting for the pathway taken (Smith et al., 2001). Hence, the inbuilt properties for were complete for the evaluation of PAR.

For the CTL process, most of the CTL reactants, intermediate products, products and by-products are standard conventional components in Aspen plus property databases. All primary syngas components, alkanes, alkenes, alcohols and acids in the C_1-C_{22} range were all readily available in the Aspen databases hence the supply of properties was not required. Since Fe-HTFT synthesis produces mostly lighter hydrocarbons, use of C_1-C_{22} molecules was considered adequate for this study, which is consistent of the syncrude composition presented by De Klerk (2011). However, the inbuilt properties database up to C_{36}, which leaves room for experimentation with heavier hydrocarbons (Sudiro and Bertucco, 2009). Tar is a complex mix of chemicals and based on work by Jiang et al. (2007), it was deemed that pyrene could adequately represent the average tar for assessing material flow impacts.

Two non-conventional components were used in the simulation, coal and coal ash. Coal and ash enthalpy and density were calculated using Aspen Plus standard methods HCOALGEN and DCOALIGT as per the guidelines given by Aspen Technology (Aspen Technology, 2010).

Suitability of property method

The thermodynamic property package of a simulator contains properties and rules for computing chemical interactions of materials in a reactive process. The extent to which method is suitable for a particular application depends on the components of the system and the conditions in the system. The Carlson algorithm (Carlson, 1996) for property selection was used to ensure the selection of an appropriate property model. Using the algorithm, the recommended property method for dry reforming is the Peng Robinson method (Peng and Robinson, 1976). Use of the Peng-Robinson method, or derivatives of it, for modelling dry reforming of methane was corroborated by other researchers such as Øi (2007) and Özkara-Aydınoğlu (2010). Er-rbib et al. (2012) used the Peng Robinson with the Boston Mathias mixing rules and obtained equally satisfactory thermodynamic property predictions.

A.1.3 Validation and verification of the financial models

The challenge with verifying the financial model was the unavailability of some data in publicly available data. However, the combined use of financial reports and analyst reports allows for the estimation of missing data. One of the focus areas in the validation of financial model was to ensure that the data and methods used in the estimation of costs and revenues were realistic.

Hence, the issue of credible and reliable sources of data was instrumental. All due care taken, the estimation of costs in operational plants if full of uncertainty and unpredictability hence, understanding the effect of uncertainty on the accuracy of predictions from the financial model was important. Monte Carlo simulation was used to quantify the effects of uncertainty on the precision of financial model results.

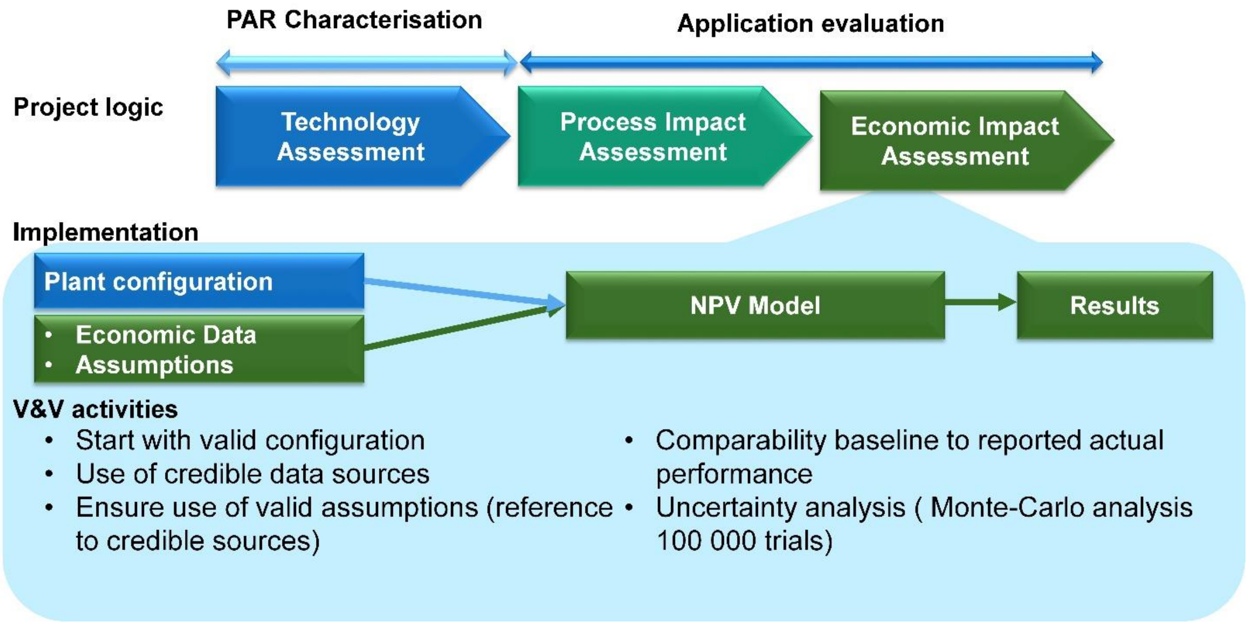


Fig. 0-2: Summary of verification and verification strategy for economic viability evaluation

A.1.4 Conclusion

Generally conceptual studies are expected to be ± 50% accurate in whatever predictions they make (Towler and Sinnott, 2013). A comparison of the models used in this study yielded results that were 10-20% of operational and experimental published data. As a result, the outcome of the model validation process and the evaluations gave significant confidence of the validity of the overall findings of the study.

A.2 Additional technical analysis for chapter 3

The additional information used to decide on reactor temperature and feed ratio for article 1 in Chapter 3 is presented in this section

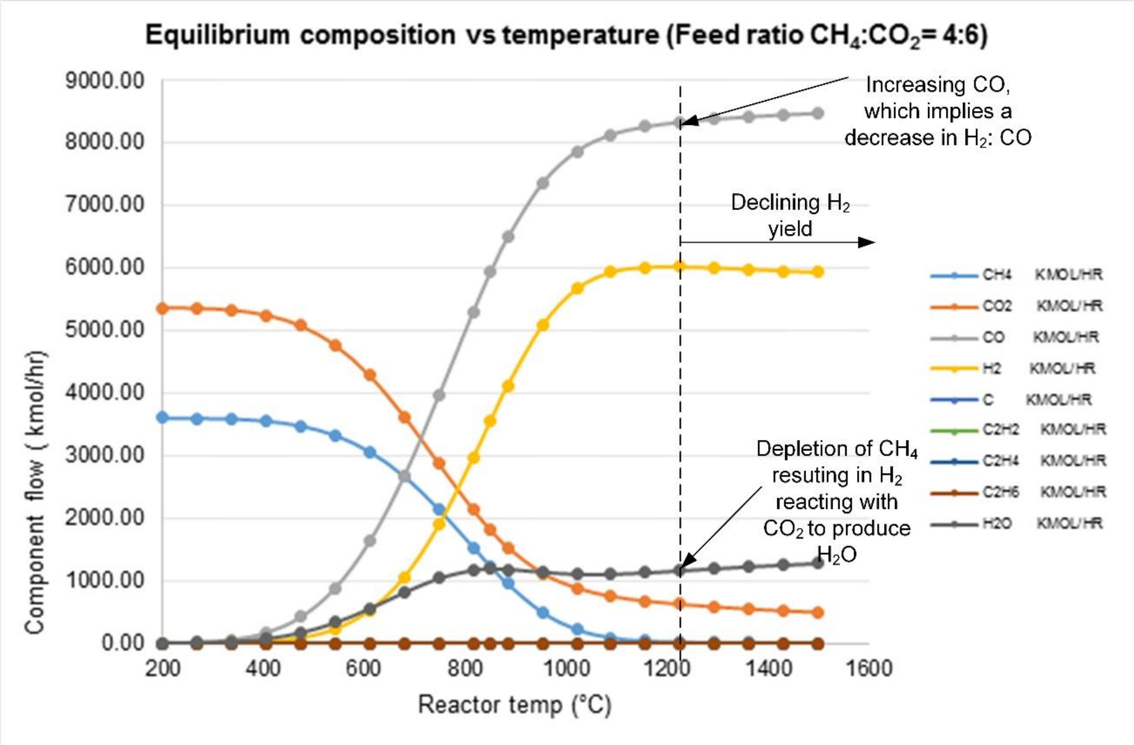


Fig. 0-3: Composition of reactor exit vs reactor equilibrium temperature (FR= 4:6)

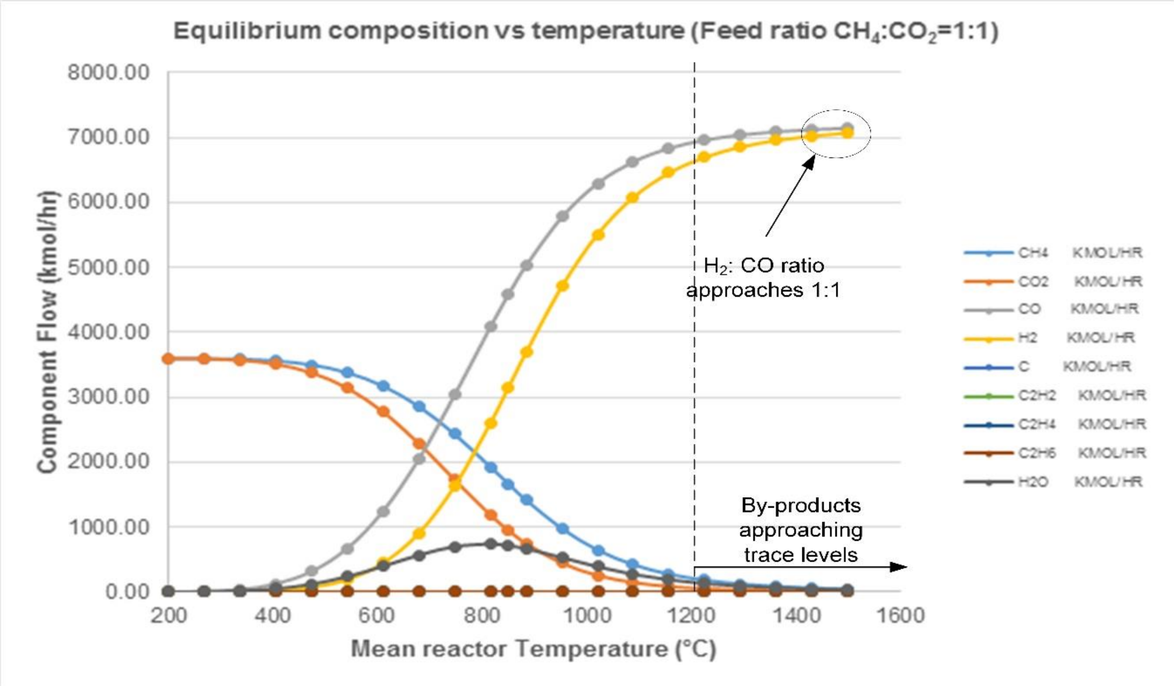


Fig. 0-4: Composition of reactor exit vs reactor equilibrium temperature (FR=1:1)

In deciding to recover heat or not the impact on SEI and ECE were used as decision criteria

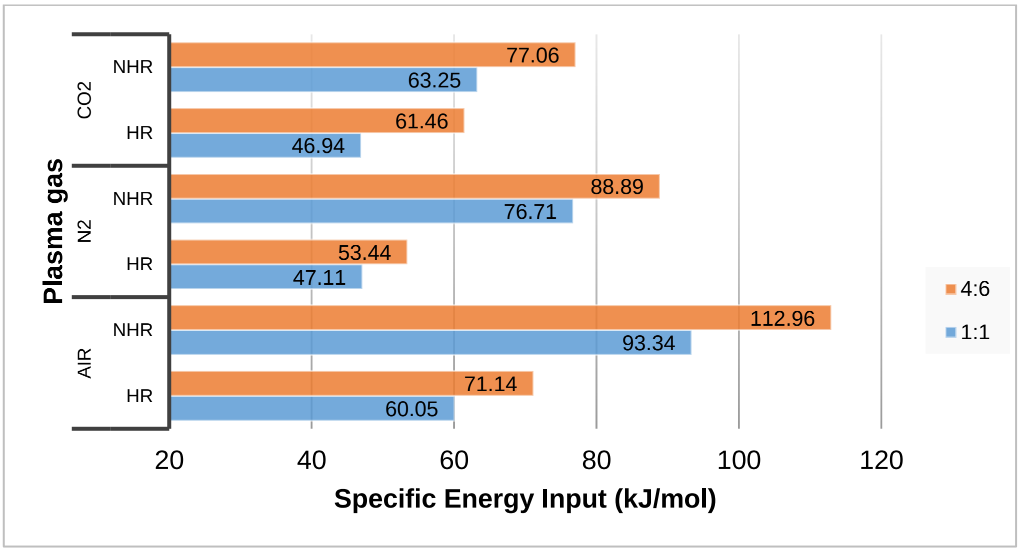


Fig. 0-5: SEI variation by configuration

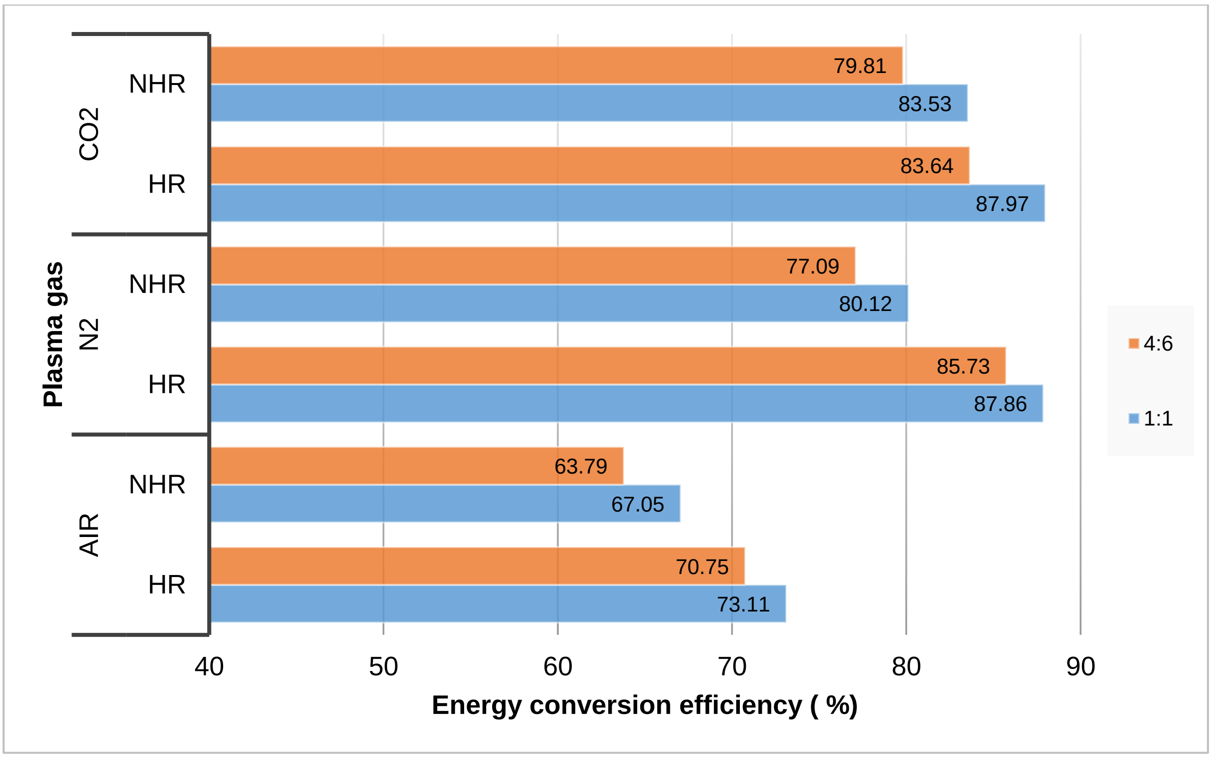


Fig. 0-6: ECE variation by configuration

A.3 Material balances for plasma modified coal to liquid plant flowsheet

(see overleaf for the relevant attachment)

		FCOAL	FH$_2$OLGG	FO$_2$LGG	WASHH$_2$O	PASH	PGLIQ	PTAR	SRCVRY	ECO$_2$	RCO$_2$PAR	FTSYNG	SYNCRD	OILDCNT	LTOIL	CONDST	FBNFLD	CO$_2$XBNFL	RCO2	RBNFLD	S4	SHH$_2$O
Temperature	C	25	420	110	90	500	160	86	159	159	159	156	340	120	50	40	-193	80	35	80	35	360
Pressure	BAR	1	42	35	1	29	29	1	25	25	25	25	30	29	29	25	25	6	29	6	29	6
Component Mass Flow																						
H_2O	KG/HR	0	1457939	0	3699992	10	934714	3738892	0	38686	0	0	392375	0	353137	0	47978	872	0	86343	9	197023
N_2	KG/HR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6681	0
O_2	KG/HR	0	0	407048	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NO_2	KG/HR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
NO	KG/HR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
S	KG/HR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SO_2	KG/HR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
SO3	KG/HR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H_2	KG/HR	0	0	0	0	1	0	0	0	0	467	123703	26373	0	1319	20391	0	0	397	0	0	0
CL_2	KG/HR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HCL	KG/HR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C	KG/HR	0	0	0	0	682	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CO	KG/HR	0	0	0	0	6	0	0	0	0	5201	863397	234791	0	11740	215229	0	0	3970	0	0	0
CO_2	KG/HR	0	0	0	0	9	0	0	0	847350	453596	32046	32046	0	0	0	0	32045	453596	0	0	0
CH_4	KG/HR	0	0	0	0	1	0	0	0	0	0	141096	176936	0	0	10636	0	0	0	0	0	0
C_6H_6	KG/HR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
C_7H_8	KG/HR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
CH_3OH	KG/HR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H_2S	KG/HR	0	0	0	0	0	0	0	8563	0	0	0	0	0	0	0	0	0	0	0	0	0
ETHENE	KG/HR	0	0	0	0	0	0	0	0	25	0	0	22845	0	228	22617	0	0	0	0	0	0
C_2H_6	KG/HR	0	0	0	0	0	0	0	0	0	3156	5378	30091	0	150	29941	0	0	3644	0	0	0
ETHACD	KG/HR	0	0	0	0	0	0	0	0	0	0	0	3260	0	3260	0	0	0	0	0	0	0
PROPENE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	42035	0	420	41615	0	0	0	0	0	0
PROPANE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	6098	0	183	5915	0	0	0	0	0	0
ACETONE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	8018	0	8017	1	0	0	0	0	0	0
1-PRPNL	KG/HR	0	0	0	0	0	0	0	0	0	0	0	3208	0	3205	3	0	0	0	0	0	0
1-BUTENE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	40117	0	401	39716	0	0	0	0	0	0
N-BUTANE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	14333	0	143	14190	0	0	0	0	0	0
MEK	KG/HR	0	0	0	0	0	0	0	0	0	0	0	3849	0	3849	0	0	0	0	0	0	0
1-PENTEN	KG/HR	0	0	0	0	0	0	0	0	0	0	0	21820	0	21798	22	0	0	0	0	0	0
N-PENTN	KG/HR	0	0	0	0	0	0	0	0	0	0	0	7274	0	7267	7	0	0	0	0	0	0
1-HEXENE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	17007	0	16990	17	0	0	0	0	0	0
HEXENE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
HEXANE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	5670	0	5670	0	0	0	0	0	0	0
1-HEPTN	KG/HR	0	0	0	0	0	0	0	0	0	0	0	11231	0	11230	1	0	0	0	0	0	0
N-HPTNE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	3744	0	3744	0	0	0	0	0	0	0
1-OCTENE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	7701	7700	1	0	0	0	0	0	0	0
N-OCTANE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	2567	2565	3	0	0	0	0	0	0	0
1-OCTNOL	KG/HR	0	0	0	0	0	0	0	0	0	0	0	1283	13	1270	0	0	0	0	0	0	0
1-OCTANL	KG/HR	0	0	0	0	0	0	0	0	0	0	0	1283	13	1270	0	0	0	0	0	0	0
1-NONENE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	7059	7052	7	0	0	0	0	0	0	0
N-NONANE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	2353	2351	2	0	0	0	0	0	0	0
1-NONNL	KG/HR	0	0	0	0	0	0	0	0	0	0	0	1176	12	1165	0	0	0	0	0	0	0
1-NONNAL	KG/HR	0	0	0	0	0	0	0	0	0	0	0	1176	12	1165	0	0	0	0	0	0	0
1-DECENE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	6147	6141	6	0	0	0	0	0	0	0
N-DECANE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	1537	1537	0	0	0	0	0	0	0	0
1-UNDENE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	4348	4348	0	0	0	0	0	0	0	0
N-UNDANE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	1087	1087	0	0	0	0	0	0	0	0
1-DODENE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	3050	3050	0	0	0	0	0	0	0	0
N-DODANE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	762	762	0	0	0	0	0	0	0	0
1-TRIENE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	2124	2124	0	0	0	0	0	0	0	0
N-TRIANE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	531	531	0	0	0	0	0	0	0	0
1-TETENE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	1471	1471	0	0	0	0	0	0	0	0
N-TETANE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	368	368	0	0	0	0	0	0	0	0
1-PENENE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	1014	1014	0	0	0	0	0	0	0	0
N-PENANE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	253	253	0	0	0	0	0	0	0	0
1-HXDENE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	695	695	0	0	0	0	0	0	0	0
N-HXDANE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	174	174	0	0	0	0	0	0	0	0
1-HPDENE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	475	475	0	0	0	0	0	0	0	0
N-HPDANE	KG/HR	0	0	0	0	0	0	0	0	0	0	0	119	119	0	0	0	0	0	0	0	0
1-OCTDEN	KG/HR	0	0	0	0	0	0	0	0	0	0	0	964	964	0	0	0	0	0	0	0	0
N-OCTDAN	KG/HR	0	0	0	0	0	0	0	0	0	0	0	241	241	0	0	0	0	0	0	0	0
ETHANOL	KG/HR	0	0	0	0	0	0	0	0	0	0	0	12538	13	12526	0	0	0	0	0	0	0
TAR	KG/HR	0	0	0	0	0	0	30423	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PHENOL	KG/HR	0	0	0	0	0	12125	5196	0	0	0	0	0	0	0	0	0	0	0	0	0	0
AMMONIA	KG/HR	0	0	0	0	0	7048	3021	0	0	0	0	0	0	0	0	0	0	0	0	0	0
K_2CO_3	KG/HR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	368400	0	0	368400	0	0
$KHCO_3$	KG/HR	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
COAL	KG/HR	1208972	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
ASH	KG/HR	0	0	0	0	349886	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Mass Flow	KG/HR	1208972	1457939	407048	3699992	350595	953887	3777532	8563	886060	462420	1165619	1165619	45084	470164	400303	416378	32918	461607	454744	6690	197023

A.4 Additional information for chapter 5

This section provides additional information that could not be included in the main body of article 3 presented in Chapter 5. The calculation of cost of equipment is presented in Section A.4.1 and condensed financial models for the scenarios considered in the economic evaluation are presented in Section A.4.3.

A.4.1 Calculation of cost of equipment

Investment cost of the reference plant was calculated for the capacity of 80000 bpd and then adjusted for basis year using capital cost curve in Eq.(5.6)

$$C_T = C_B \times \left(\frac{CEPCI_{2014}}{CEPCI_{Base\ year}}\right) \times \left(\frac{Q_T}{Q_B}\right)^n \tag{5.7}$$

Where;

C_T - Cost of equipment at new capacity in year 2014

C_B - Cost of reference equipment in the base year

$CEPCI_{2014}$ - Chemical engineering plant cost index for 2014

$CEPCI_{Base\ year}$ - Chemical engineering plant cost index in the base year

Q_T - Capacity of plant in the year being evaluated

Q_B - Capacity of the plant being used as the reference for costing

n - Scaling exponent for the type of equipment being costed

Using a specific capital cost of 98000$/bpd (De Klerk et al., 2013), the total capital of an 50000bpd coal to liquid plant would have been **$4.9 billion** in 2007.

To get the cost of the reference plant, the capital was adjusted for scale (from 50000bpd to 80000bpd) and the time value of money (2007 to 2014) by using the Eq. 5.7 with relevant Chemical engineering plant cost indices (CEPCI).

The capital cost for the reference coal to liquids plant was calculated as:

$$C_T = C_B \times \left(\frac{CEPCI_{2014}}{CEPCI_{Base\ year}}\right) \times \left(\frac{Q_T}{Q_B}\right)^n = \$4.9\ billion \times \left(\frac{567.5}{525.4}\right) \times \left(\frac{80000}{50000}\right)^{0.67} = \$7.4\ billion$$

The capital cost of the plasma reforming modified CTL was calculated in three steps:

i. the capital cost of the reference plant was broken down into sectional costs as detailed by Kreutz et al. (2008) and reported by De Klerk et al. (2013)
ii. the cost of Auto thermal reformer was replaced by cost of plasma arc reforming and
iii. Escalation factors were applied to adjust the sectional cost.

A summary of Sectional costs with the relevant scaling factors is presented in **Table 0-1**.

Table 0-1: Summary of capital cost contribution of PAR modified CTL plant

Section	Scaling factor	Cost contribution
Coal preparation and gasification	0.84	2 070 589 282
Syngas cleaning and conditioning	1	1 232 767 531
Air Separation	0.68	952 055 264
Heat recovery and Utilities	0.8	1 124 022 649
FT, gas recovery-ATR	1	1 240 019 104
PAR	1	300 000 000
Refining	1	65 264 163
Total estimated capital in 2014 $		**6 984 717 993**

The calculation of capital requirements for the PAR system were based on equipment cost estimates supplied by Westinghouse Plasma Corporation and the equipment and EPC items are shown in **Table 0-2** and **Table 0-3**.

Table 0-2: Equipment items used in calculation of capital requirements

Item description	Qty	Cost
Plasma Torch @ 8MW each	48	102 000 000
Local control and Ethernet connectivity	48	12 750 000
Arc ignitors	48	12 750 000
Electrode cooling system	8	38 250 000
Additional air system capacity	6	25 500 000
Vessel shell, lining and fittings	1	47 000 000
Start-up spares		16 750 000
Total		**255 000 000**

Table 0-3: EPC items used in the capital requirements of PAR

Item description	Cost
Engineering Design	16 000 000
Shipping	3 500 000
Installation	12 000 000
On sites: (Connection, Training, Commissioning and Start-up)	13 500 000
Total cost	**45 000 000**

A.4.2 Evaluation of retrofit economics

The economic evaluation carried out in this study assumed a new build and as such the models were built around evaluating the economic performance of a new build program. However, PAR can also be deployed as a retrofit than as a new build as that would allow for a quicker deployment than a new build program. This section provides a description of how to adapt the new build economics to evaluate the retrofit economics.

As with the new build case, NPV and IRR can be used as measures for project acceptance and validation criteria. For the calculations, a modification of the model inputs is necessary.

$$NPV = -I_{TPAR} + \sum_{i=1}^{N} \frac{(B_i - C_i)}{(1+r)^i} = -I_{TPAR} + \frac{(B_1 - C_1)}{(1+r)^1} + \frac{(B_2 - C_2)}{(1+r)^2} + \cdots + \frac{(B_N - C_N)}{(1+r)^N}$$

Where, $B_i$and B_{Tn} represent the benefits accrued in year i of the retrofit project and the cumulative benefits respectively. In the PAR context, the benefits considered include Feedstock cost savings, avoided carbon tax and additional saleable products. Hence, as the tax rate increases and coal price becomes higher, the net cash flow increases increasing NPV.

And, $C_i$and C_{Tn} represent the costs accrued in year i of the retrofit project and the cumulative costs over the project life respectively. The costs considered in the PAR retrofit evaluation would include: additional electricity costs and reduced by-product sales.

The initial project investment would be calculated as the sum of Total investment costs of PAR (I_{TPAR}) and the cost of decommissioning ATR. In the Sasol context it would be beneficial to use the decommissioned ATR to add capacity to a GTL plant.

A.4.3 Financial model data summaries

For the relevant attachments of financial model summaries see overleaf **A.1.3.1- A.1.3.4**

Year	**Units**	**-3 to 0**	**1**	**3**	**5**	**7**	**9**	**10**	**12**	**14**	**20**	**21**	**22**	**23**	**24**	**25**
Revenue		**CONSTRUCTION**														
Crude oil price	$/bbl		123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50
Capacity factor			0.50	1	1	1	1	1	1	1	1	1	1	1	1	1
Annual production capacity	bbl/yr		14 600 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000
Total revenue	***$/yr***		1 803 100 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00
Cost of sales																
Coal price	$/ton		31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29
Annual coal requirement	tons/yr		18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83
Water price	$/m^3		1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49
Water requirements	m^3/yr		50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83
Feedstock costs	*$/yr*		668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63
Electricy price	$/MWh		79.00	79.00	79.00	79.00	79.00	79.00	79.00	79.00	79.00	79.00	79.00	79.00	79.00	79.00
Electricity requirements	MWh/yr		4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00
Electricy costs	*$/yr*		387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00
Gross Income			746 816 361.37	2 549 916 361.37	2 549 916 361.37	2 549 916 361.37	2 549 916 361.37	2 549 916 361.37	2 549 916 361.37	2 549 916 361.37	2 549 916 361.37	2 549 916 361.37	2 549 916 361.37	2 549 916 361.37	2 549 916 361.37	2 549 916 361.37
Maintenance	*$/yr*		60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59
Catalysts and Chemicals	*$/yr*		150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48
Operations insurance	*$/yr*		34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91
Direct labour	*$/yr*		81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66
General and Admin	*$/yr*		42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14
Miscellaneous	*$/yr*		17 157 806.45	19 024 730.22	21 094 792.09	23 390 095.32	25 935 148.20	27 309 711.06	30 281 253.41	33 576 126.31	45 772 097.79	48 198 018.97	50 752 513.97	53 442 397.21	56 274 844.27	59 257 411.01
Health and Safety	*$/yr*		42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14
Depreciation	*$/yr*		740 713 420.14	740 713 420.14	740 713 420.14	740 713 420.14	740 713 420.14	740 713 420.14	740 713 420.14	740 713 420.14						
Annual CO_2 emission	tons/yr		30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00
Carbon Tax price	$/ton		-	-	-	-	-	-	-	-	-	-	-	-	-	-
Carbon Tax	*$/yr*		-	-	-	-	-	-	-	-	-	-	-	-	-	-
Total operating expenses	$/yr		1 169 658 581.51	1 171 525 505.28	1 173 595 567.15	1 175 890 870.38	1 178 435 923.26	1 179 810 486.12	1 182 782 028.47	1 186 076 901.37	457 559 452.70	459 985 373.89	462 539 868.89	465 229 752.13	468 062 199.19	471 044 765.93
EBIT			-422 842 220.14	1 378 390 856.10	1 376 320 794.23	1 374 025 490.99	1 371 480 438.11	1 370 105 875.26	1 367 134 332.91	1 363 839 460.01	2 092 356 908.67	2 089 930 987.49	2 087 376 492.48	2 084 686 609.24	2 081 854 162.19	2 078 871 595.44
Tax	$		-	385 949 439.71	385 369 822.38	384 727 137.48	384 014 522.67	383 629 645.07	382 797 613.21	381 875 048.80	585 859 934.43	585 180 676.50	584 465 417.89	583 712 250.59	582 919 165.41	582 084 046.72
PAT		$ -7 403 264 793.12	317 871 200.00	1 733 154 836.53	1 731 664 391.98	1 730 011 773.66	1 728 179 335.58	1 727 189 650.33	1 725 050 139.83	1 722 677 831.34	1 506 496 974.24	1 504 750 310.99	1 502 911 074.59	1 500 974 358.65	1 498 934 996.78	1 496 787 548.72
NPV		$ 11 140 026 474.60														
IRR		19.80%														

Year	**Units**	**-3 to 0**	**1**	**3**	**5**	**7**	**9**	**10**	**12**	**14**	**20**	**21**	**22**	**23**	**24**	**25**
Revenue		**CONSTRUCTION**														
Crude oil price	$/bbl		123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50
Capacity factor			0.50	1	1	1	1	1	1	1	1	1	1	1	1	1
Annual production capacity	bbl/yr		14 600 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000
Total revenue	***$/yr***		1 803 100 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00
Cost of sales																
Coal price	$/ton		31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29
Annual coal requirement	tons/yr		15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82
Water price	$/m^3		1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49
Water requirements	m^3/yr		42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11
Feedstock costs	*$/yr*		555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06
Electricy price	$/MWh		108.67	108.67	108.67	108.67	108.67	108.67	108.67	108.67	108.67	108.67	108.67	108.67	108.67	108.67
Annual energy requirements	MWh/yr		4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	7 309 344.00	7 309 344.00	7 309 344.00	7 309 344.00	7 309 344.00	7 309 344.00	7 309 344.00	7 309 344.00	7 309 344.00	7 309 344.00
Electricy costs	*$/yr*		533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00
Gross Income			714 953 219.94	2 518 053 219.94	2 518 053 219.94	2 518 053 219.94	2 518 053 219.94	2 518 053 219.94	2 518 053 219.94	2 518 053 219.94	2 518 053 219.94	2 518 053 219.94	2 518 053 219.94	2 518 053 219.94	2 518 053 219.94	2 518 053 219.94
Maintenance	*$/yr*		60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59
Catalysts and Chemicals	*$/yr*		150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48
Operations insurance	*$/yr*		34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91
Direct labour	*$/yr*		81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66
General and Admin	*$/yr*		42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14
Miscellaneous	*$/yr*		17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45
Health and Safety	*$/yr*		42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14
Depreciation	*$/yr*		698 471 799.00	698 471 799.00	698 471 799.00	698 471 799.00	698 471 799.00	698 471 799.00	698 471 799.00	698 471 799.00	-	-	-	-	-	-
Annual CO_2 emission	tons/yr		23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00
Carbon Tax price	$/ton		-	-	-	-	-	-	-	-	-	-	-	-	-	-
Carbon Tax	*$/yr*		-	-	-	-	-	-	-	-	-	-	-	-	-	-
Total operating expenses	$/yr		1 127 416 960.37	1 127 416 960.37	1 127 416 960.37	1 127 416 960.37	1 127 416 960.37	1 127 416 960.37	1 127 416 960.37	1 127 416 960.37	428 945 161.37	428 945 161.37	428 945 161.37	428 945 161.37	428 945 161.37	428 945 161.37
EBIT			-412 463 740.43	1 390 636 259.57	1 390 636 259.57	1 390 636 259.57	1 390 636 259.57	1 390 636 259.57	1 390 636 259.57	1 390 636 259.57	2 089 108 058.57	2 089 108 058.57	2 089 108 058.57	2 089 108 058.57	2 089 108 058.57	2 089 108 058.57
Tax	$		-	389 378 152.68	389 378 152.68	389 378 152.68	389 378 152.68	389 378 152.68	389 378 152.68	389 378 152.68	584 950 256.40	584 950 256.40	584 950 256.40	584 950 256.40	584 950 256.40	584 950 256.40
PAT		$ -6 984 717 993.19	286 008 058.57	1 699 729 905.89	1 699 729 905.89	1 699 729 905.89	1 699 729 905.89	1 699 729 905.89	1 699 729 905.89	1 699 729 905.89	1 504 157 802.17	1 504 157 802.17	1 504 157 802.17	1 504 157 802.17	1 504 157 802.17	1 504 157 802.17
NPV		$ 11 279 306 868.95														
IRR		20.52%														
Discount rate	6.8%	(Sasol Limited, 2014)														
Tax rate	28	(SARS,2014)														

Year	**Units**	**-3 to 0**	**1**	**3**	**5**	**7**	**9**	**10**	**12**	**14**	**20**	**21**	**22**	**23**	**24**	**25**
Revenue		**CONSTRUCTION**														
Crude oil price	$/bbl		123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50
Capacity factor			0.50	1	1	1	1	1	1	1	1	1	1	1	1	1
Annual production capacity	bbl/yr		14 600 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000
Total revenue	***$/yr***		1 803 100 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00
Cost of sales																
Coal price	$/ton		31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29
Annual coal requirement	tons/yr		18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83	18 950 111.83
Water price	$/m^3		1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49
Water requirements	m^3/yr		50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83	50 867 274.83
Feedstock costs	*$/yr*		668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63	668 741 238.63
Electricy price	$/MWh		108.67	108.67	108.67	108.67	108.67	108.67	108.67	108.67	108.67	108.67	108.67	108.67	108.67	108.67
Electricity requirements	MWh/yr		4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00
Electricy costs	$/yr		533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00	533 091 552.00
Gross Income			601 267 209.37	2 404 367 209.37	2 404 367 209.37	2 404 367 209.37	2 404 367 209.37	2 404 367 209.37	2 404 367 209.37	2 404 367 209.37	2 404 367 209.37	2 404 367 209.37	2 404 367 209.37	2 404 367 209.37	2 404 367 209.37	2 404 367 209.37
Maintenance	*$/yr*		60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59
Catalysts and Chemicals	*$/yr*		150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48
Operations insurance	*$/yr*		34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91
Direct labour	*$/yr*		81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66
General and Admin	$/yr		42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14
Miscellaneous	*$/yr*		17 157 806.45	19 024 730.22	21 094 792.09	23 390 095.32	25 935 148.20	27 309 711.06	30 281 253.41	33 576 126.31	45 772 097.79	48 198 018.97	50 752 513.97	53 442 397.21	56 274 844.27	59 257 411.01
Health and Safety	*$/yr*		42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14
Depreciation	*$/yr*		740 713 420.14	740 713 420.14	740 713 420.14	740 713 420.14	740 713 420.14	740 713 420.14	740 713 420.14	740 713 420.14						
Annual CO_2 emission	tons/yr		30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00	30 246 000.00
Carbon Tax price	$/ton		12.00	12.00	12.00	12.00	12.00	12.00	12.00	12.00	12.00	12.00	12.00	12.00	12.00	12.00
Carbon Tax	*$/yr*		145 180 800.00	145 180 800.00	145 180 800.00	145 180 800.00	145 180 800.00	145 180 800.00	145 180 800.00	145 180 800.00	145 180 800.00	145 180 800.00	145 180 800.00	145 180 800.00	145 180 800.00	145 180 800.00
Total operating expenses	$/yr		1 314 839 381.51	1 316 706 305.28	1 318 776 367.15	1 321 071 670.38	1 323 616 723.26	1 324 991 286.12	1 327 962 828.47	1 331 257 701.37	602 740 252.70	605 166 173.89	607 720 668.89	610 410 552.13	613 242 999.19	616 225 565.93
EBIT			-713 572 172.14	1 087 660 904.10	1 085 590 842.23	1 083 295 538.99	1 080 750 486.11	1 079 375 923.26	1 076 404 380.91	1 073 109 508.01	1 801 626 956.67	1 799 201 035.49	1 796 646 540.48	1 793 956 657.24	1 791 124 210.19	1 788 141 643.44
Tax	$		-	304 545 053.15	303 965 435.82	303 322 750.92	302 610 136.11	302 225 258.51	301 393 226.65	300 470 662.24	504 455 547.87	503 776 289.94	503 061 031.33	502 307 864.03	501 514 778.85	500 679 660.16
PAT		$ -7 403 264 793.12	27 141 248.00	1 523 829 271.09	1 522 338 826.54	1 520 686 208.22	1 518 853 770.14	1 517 864 084.89	1 515 724 574.39	1 513 352 265.90	1 297 171 408.80	1 295 424 745.55	1 293 585 509.15	1 291 648 793.21	1 289 609 431.34	1 287 461 983.28
NPV		$ 8 588 421 972.20														
IRR		16.98%														
Discount rate	6.8%	(Sasol Limited, 2014)														
Tax rate	28	(SARS,2014)														

Year	**Units**	**-3 to 0**	**1**	**3**	**5**	**7**	**9**	**10**	**12**	**14**	**20**	**21**	**22**	**23**	**24**	**25**
Revenue		**CONSTRUCTION**														
Crude oil price	$/bbl		123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50	123.50
Capacity factor			0.50	1	1	1	1	1	1	1	1	1	1	1	1	1
Annual production capacity	bbl/yr		14 600 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000	29 200 000
Total revenue	***$/yr***		1 803 100 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00	3 606 200 000.00
Cost of sales																
Coal price	$/ton		31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29	31.29
Annual coal requirement	tons/yr		15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82	15 728 592.82
Water price	$/m^3		1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49	1.49
Water requirements	m^3/yr		42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11	42 219 838.11
Feedstock costs	*$/yr*		555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06	555 055 228.06
Electricy price	$/MWh		79.00	79.00	79.00	79.00	79.00	79.00	79.00	79.00	79.00	79.00	79.00	79.00	79.00	79.00
Annual energy requirements	MWh/yr		4 905 600.00	4 905 600.00	4 905 600.00	4 905 600.00	7 309 344.00	7 309 344.00	7 309 344.00	7 309 344.00	7 309 344.00	7 309 344.00	7 309 344.00	7 309 344.00	7 309 344.00	7 309 344.00
Electricy costs	*$/yr*		387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00	387 542 400.00
Gross Income			860 502 371.94	2 663 602 371.94	2 663 602 371.94	2 663 602 371.94	2 663 602 371.94	2 663 602 371.94	2 663 602 371.94	2 663 602 371.94	2 663 602 371.94	2 663 602 371.94	2 663 602 371.94	2 663 602 371.94	2 663 602 371.94	2 663 602 371.94
Maintenance	*$/yr*		60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59	60 052 322.59
Catalysts and Chemicals	*$/yr*		150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48	150 130 806.48
Operations insurance	*$/yr*		34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91	34 315 612.91
Direct labour	*$/yr*		81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66	81 499 580.66
General and Admin	$/yr		42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14
Miscellaneous	*$/yr*		17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45	17 157 806.45
Health and Safety	*$/yr*		42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14	42 894 516.14
Depreciation	*$/yr*		698 471 799.00	698 471 799.00	698 471 799.00	698 471 799.00	698 471 799.00	698 471 799.00	698 471 799.00	698 471 799.00	-	-	-	-	-	-
Annual CO_2 emission	tons/yr		23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00	23 921 000.00
Carbon Tax price	$/ton		12.00	12.00	12.00	12.00	12.00	12.00	12.00	12.00	12.00	12.00	12.00	12.00	12.00	12.00
Carbon Tax	*$/yr*		114 820 800.00	114 820 800.00	114 820 800.00	114 820 800.00	114 820 800.00	114 820 800.00	114 820 800.00	114 820 800.00	114 820 800.00	114 820 800.00	114 820 800.00	114 820 800.00	114 820 800.00	114 820 800.00
Total operating expenses	$/yr		1 242 237 760.37	1 242 237 760.37	1 242 237 760.37	1 242 237 760.37	1 242 237 760.37	1 242 237 760.37	1 242 237 760.37	1 242 237 760.37	543 765 961.37	543 765 961.37	543 765 961.37	543 765 961.37	543 765 961.37	543 765 961.37
EBIT			-381 735 388.43	1 421 364 611.57	1 421 364 611.57	1 421 364 611.57	1 421 364 611.57	1 421 364 611.57	1 421 364 611.57	1 421 364 611.57	2 119 836 410.57	2 119 836 410.57	2 119 836 410.57	2 119 836 410.57	2 119 836 410.57	2 119 836 410.57
Tax	$		-	397 982 091.24	397 982 091.24	397 982 091.24	397 982 091.24	397 982 091.24	397 982 091.24	397 982 091.24	593 554 194.96	593 554 194.96	593 554 194.96	593 554 194.96	593 554 194.96	593 554 194.96
PAT		$ -6 984 717 993.19	316 736 410.57	1 721 854 319.33	1 721 854 319.33	1 721 854 319.33	1 721 854 319.33	1 721 854 319.33	1 721 854 319.33	1 721 854 319.33	1 526 282 215.61	1 526 282 215.61	1 526 282 215.61	1 526 282 215.61	1 526 282 215.61	1 526 282 215.61
NPV		$ 11 548 995 632.61														
IRR		20.83%														
Discount rate	6.8%	(Sasol Limited, 2014)														
Tax rate	28	(SARS,2014)														

A.4.4 Summary of stochastic analysis data

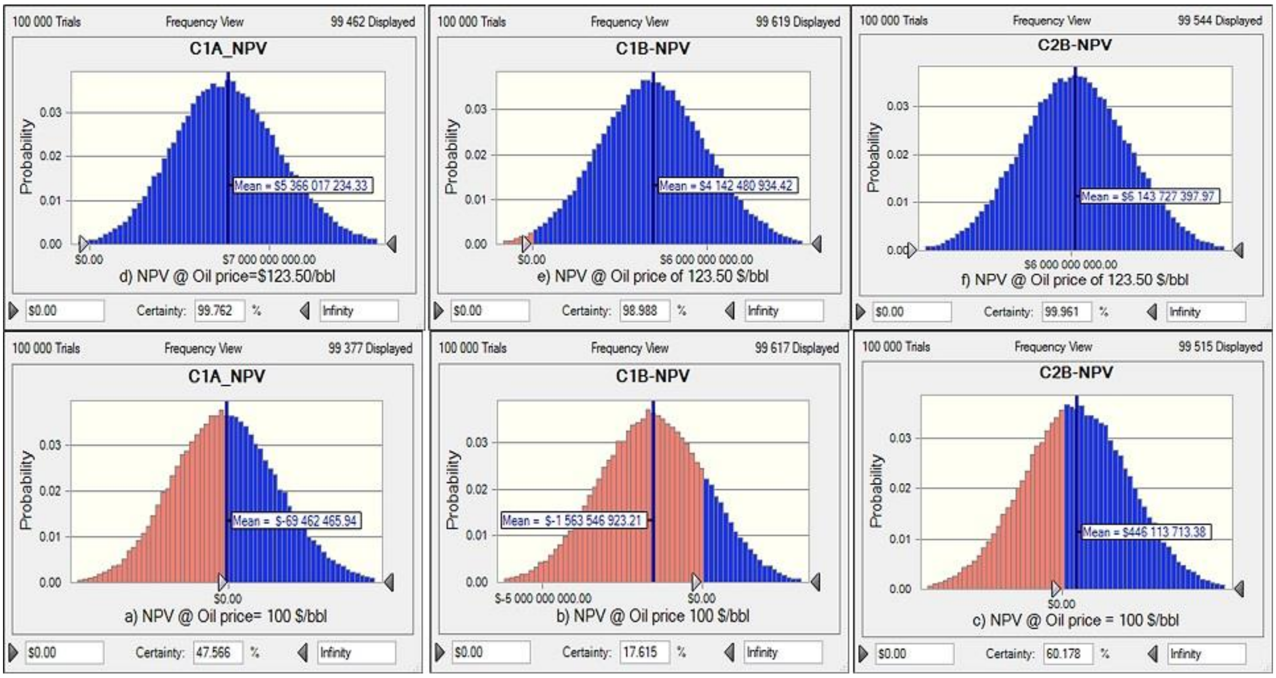


Fig. 0-7: Summary of NPV calculations for Oil price scenarios P=USD 100/bbl. (a-c) and P=123.50 (d-f)

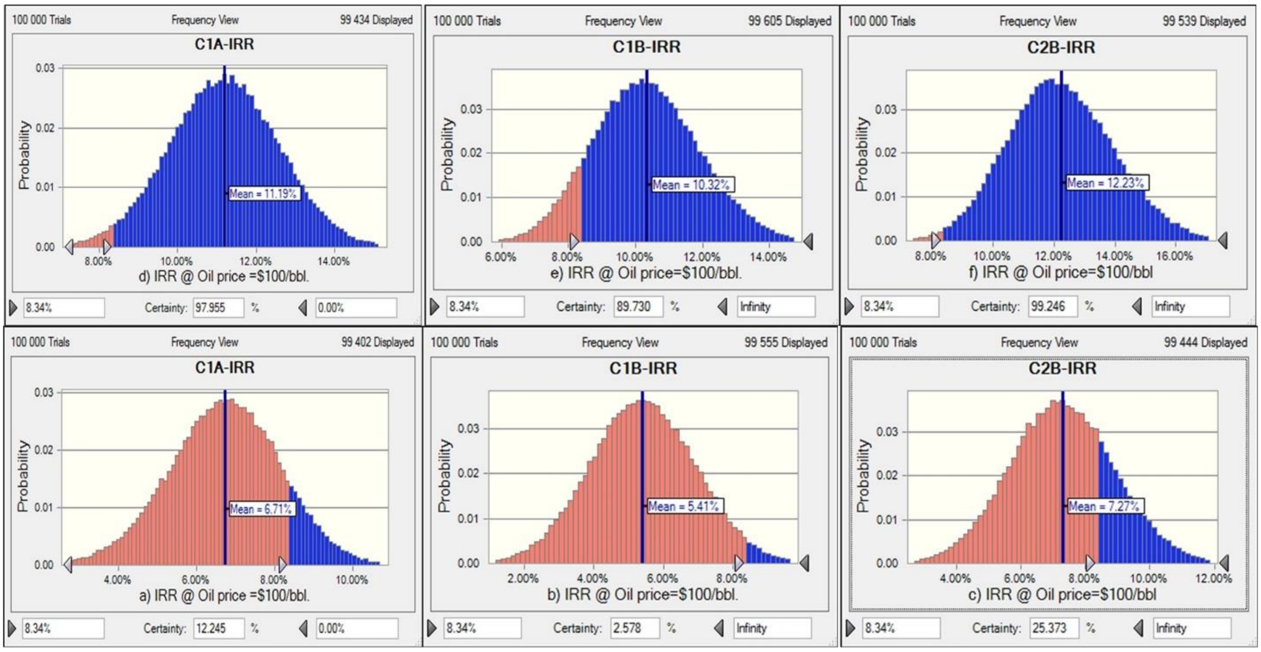


Fig. 0-8: Summary of IRR calculations for Oil price scenarios P=USD 100/bbl. (a-c) and P=123.50 (d-f)

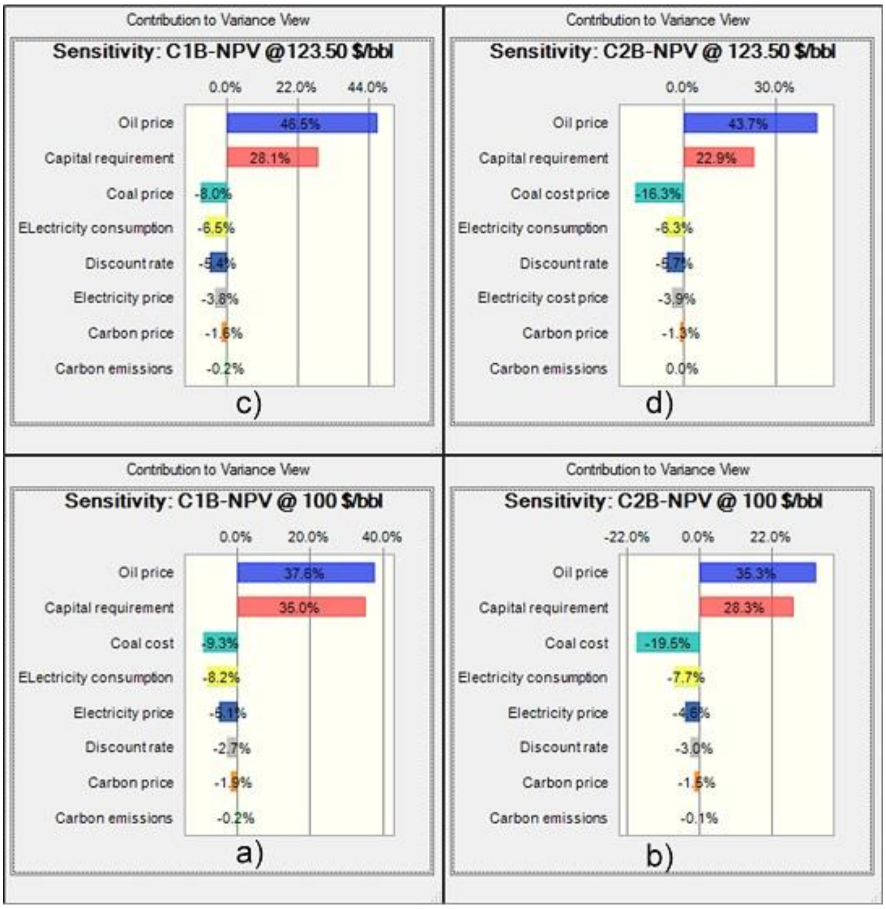


Fig. 0-9: Summary of sensitivity analyses for Carbon priced scenarios at price = USD 100/bbl. (a-c) and Prices = USD123.50/bbl.

A.5 Journal of Cleaner Production Author’s guidelines

(NOTE: GUIDELINES PRESENTED AS IS WITH MINOR FORMATTING CHANGES)

JOURNAL OF CLEANER PRODUCTION

AUTHOR INFORMATION PACK

ISSN: 0959-6526

Description

Audience

Abstracting and Indexing

Editorial Board

Guide for Authors

DESCRIPTION

The Journal of Cleaner Production serves as a transdisciplinary, international forum for the exchange of information and research concepts, policies, and technologies designed to help ensure progress towards making societies and regions more sustainable. It aims to encourage innovation and creativity, new and improved products, and the implementation of new, cleaner structures, systems, processes, products and services. It is also designed to stimulate the development and implementation of prevention oriented governmental policies and educational programmes.

Cleaner production is a concept that goes beyond simple **pollution control**. It involves active research and development into new structures, systems, processes, materials and products that are more resource and energy efficient, whilst engaging and empowering people. Such approaches have become necessary for businesses, institutions, governments, and civil society to ensure ecologically, socially,and economically sustainable, consumption production and service strategies. These involve educational, training, management, and technical assistance programs, which are needed to accelerate the adoption of cleaner production and sustainability by industries, governments and universities.

Authors are invited to submit papers from the following areas: Industrial Applications including:

Toxics use reduction in product design, process development and in the usage and end-of-life

management phases of products

New and novel uses of materials and technologies

Improved processes through development and usage of "environmentally friendlier" technologies

Advances in Green Chemistry, Green Engineering and Green Architecture

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Environmental Management Initiatives:

Improvements in the integration of environmental management systems

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Improved life cycle management of products and services

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Improvements in environmental reviewing, auditing and reporting

Advances in life cycle assessment and life cycle management

Advances in risk reduction

Advances in reduction of the life cycle usage of energy, water and other materials

Advances in applications of renewable energy and other low-carbon technologies and products

Improvements in corporate social responsibility

Advances in corporate sustainability reporting

Advances in Industrial Ecology and Regional Sustainable Development

Legislation, Policy and Regulations:

Improved regulatory and policy initiatives designed to promote implementation of proactive and preventive approaches throughout society

Advanced governmental policies and programmes to promote the transition to sustainable societies

Education, Training and Learning:

Improved educational & training initiatives on values, paradigms, concepts and tools to help societies make the transition to sustainable societies.

AUDIENCE

a. Managers, engineers, designers in all the process and service industries;

b. Academic and research scientists specializing in cleaner production, regional sustainability, and education for sustainable development;

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