INVESTIGATION INTO THE GASIFICATION CHARACTERISTICS OF SOUTH AFRICAN POWER STATION COALS

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ABSTRACT

Electricity demand in South Africa is increasing at a rate of 1000 MW per year. Whilst there is increasing pressure to adopt non-fossil fuel electricity generating technologies, the abundant reserves and low cost of coal makes it the preferred energy source to meet increasing electricity demand for the foreseeable future. The challenge in the future is to enhance both the efficiency and environmental acceptability of coal use by adopting clean coal technologies (CCTs).

Integrated gasification combined cycle (IGCC) is a potential CCT that could be applied in South Africa to increase efficiency and reduce carbon dioxide emissions. IGCC also holds the advantage of reduced water consumption and the potential for co-production of liquid and gaseous fuels and chemicals.

Fine coal gasification is a key enabling technology for the implementation of IGCC plants. Fluidised bed gasification is being evaluated by the CSIR as a potential fine coal gasification process for incorporation into future IGCC plants.

A suite of four South African coals has been identified as being possible fuels for power stations which would operate for three or four decades, towards the middle of this century. This paper presents the results of coal characterisation, thermogravimetric analysis (TGA) and pilot plant gasification tests to ascertain the performance of the selected coals under fluidised bed gasification conditions.

Based on the experimental results a model is being developed for the fluidised bed coal gasification process. The use of the model to predict the performance of fluidised bed gasifiers is also described in the paper.

Key words: coal, gasification, fluidised bed, characterisation, combined cycle, modeling

1 Introduction

South Africa's primary energy supply is made up of the following components: coal 74.1%, oil 12%, renewable energy (hydro, biomass, solar and wind) 7.4%, nuclear 4.2% and gas 2.3% [1]. Due to the high cost and decreasing reserves of oil and gas, its contribution to the energy mix is expected to decrease. Since South Africa is a water scarce country the contribution of renewable energy such as hydro and biomass is not expected to increase significantly. The use of solar and wind power is also currently limited by its high cost. Safety and cost are issues that inhibit the increased use of nuclear energy. Abundant and cheap coal reserves will therefore almost certainly remain our most important energy resource for at least the next 75 years.

Based on scientific analysis it is generally accepted that a link exists between climate change and the use of fossil fuels such as coal. The development of CCTs has therefore received increased attention worldwide. CCTs are defined as "Technologies designed to enhance both the efficiency and the environmental acceptability of coal extraction, preparation and use" [1].

CCTs that are being developed for power generation include:

- Integrated gasification combined cycle technology (IGCC)
- Ultra supercritical pulverised coal combustion (SCPCC)
- Oxy-coal combustion
- Circulating fluidised bed combustion (CFBC)
- Post combustion capture

The CSIR has identified IGCC as a potential CCT that could be applied in South Africa to achieve near zero emissions of greenhouse gases which is likely to be a requirement for electricity producers towards the middle of the 21st century.

2 Integrated Gasification Combined Cycle Technology

The flowsheets for conventional and IGCC power generation cycles are given in Figure 1. In a conventional cycle all the energy in the coal is used to generate steam which is then exhausted through a steam turbine to generate electricity. The exhaust steam has to be recondensed and recycled to the boiler. Due to large energy losses during condensation the overall efficiency (coal to electrical power) of a conventional power station is between 33% and 38%. This can be raised to 45% - 47% by increasing the temperature and pressure of the steam (SCPCC). New high strength materials are being developed to achieve this target.

In an IGCC power station a coal gasifier is incorporated into the flowsheet. During gasification coal is reacted with oxygen/air and steam to produce a combustible gas (syngas). This gas stream has a low volume compared to flue gas resulting from conventional coal combustion, and therefore gas clean-up systems can be reduced in size. The cleaned gas is combusted in a gas turbine that produces electrical power while heat is recovered from the turbine exhaust gas by means of a conventional steam cycle. This configuration (IGCC) produces higher efficiencies (45% - 55%) and lower emissions than conventional power stations.

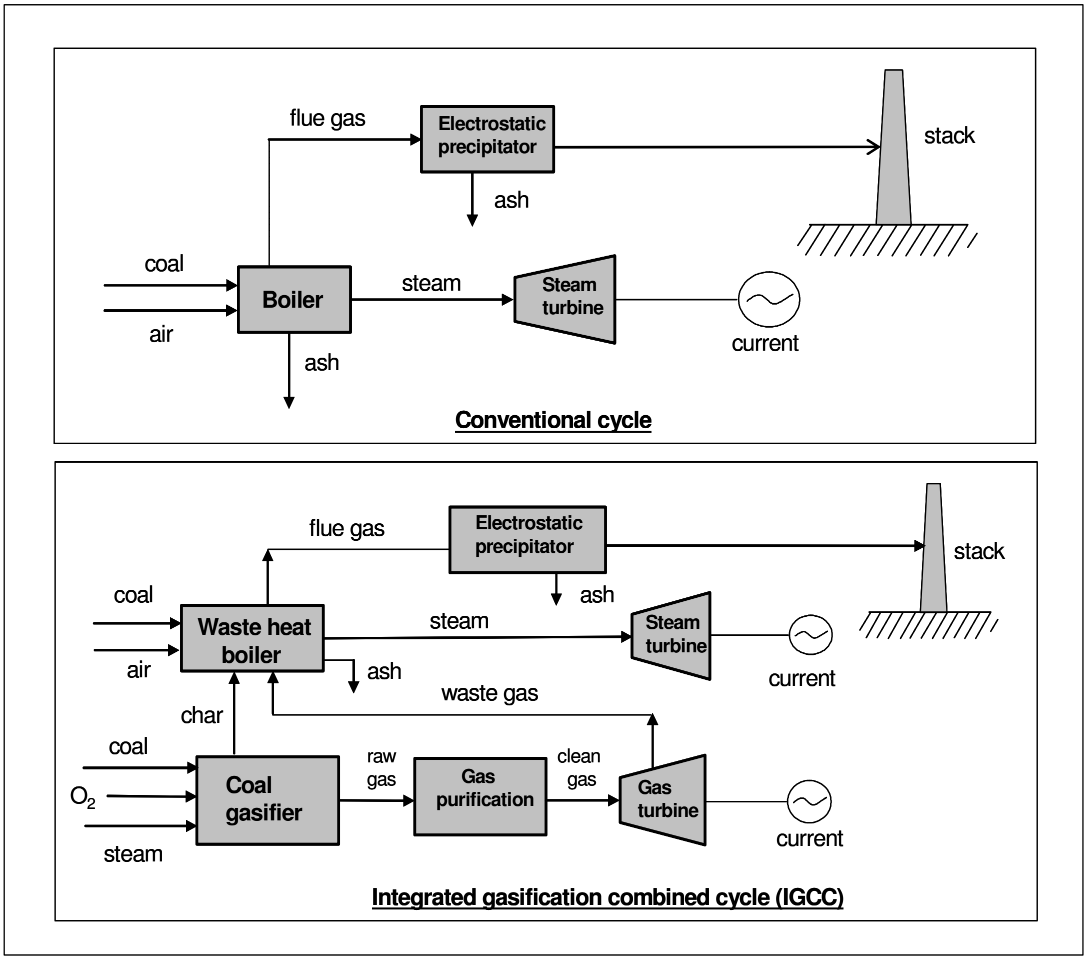

Figure 1. Conventional and IGCC power generation cycles.

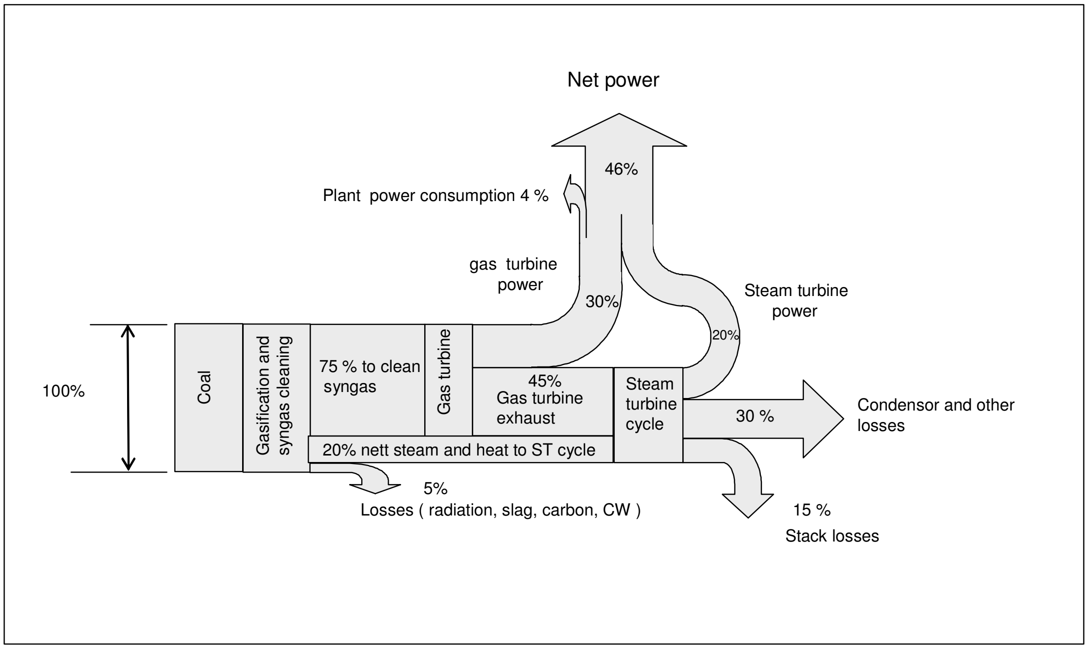

Figure 2. Energy flows in a IGCC power station.

The energy flows in an IGGC power station are given in Figure 2. The flow diagram shows that the coal to electric power efficiency of the power station is 46 %.

3 Coal gasification

Fine coal gasification is a key enabling technology for IGCC systems [2]. Fluidised bed and entrained flow gasifiers are examples of fine coal gasifiers that have been used commercially. These gasifiers are compared in Table 1 and Figure 3.

Table 1. Comparison of fluidised bed and entrained flow fine coal gasifiers.

	Fluidised bed	**Entrained flow**
Coal particle size	0.5 mm – 5 mm	0 – 0.5 mm
Coal moisture	Dry	Dry/slurry
Coal type	Non-caking coals	Low ash coals
Ash in coal	< 60%	< 30%
Gasification agents	Air/steam/oxygen	Steam/oxygen
Temperature	850℃ – 950℃	1300℃ – 1450℃
Pressure	0 - 10 bar	0 - 30 bar
Residence time	0.5 – 1.5 hrs	< 10 s
Carbon efficiency	65% - 85%	75% - 90%
Gasification efficiency	55% - 75%	55% - 70%
Commercial examples	High Temperature Winkler, Kellog Rust Westinghouse & U- Gas	Texaco, Prenflo, Shell & Koppers –Totzek

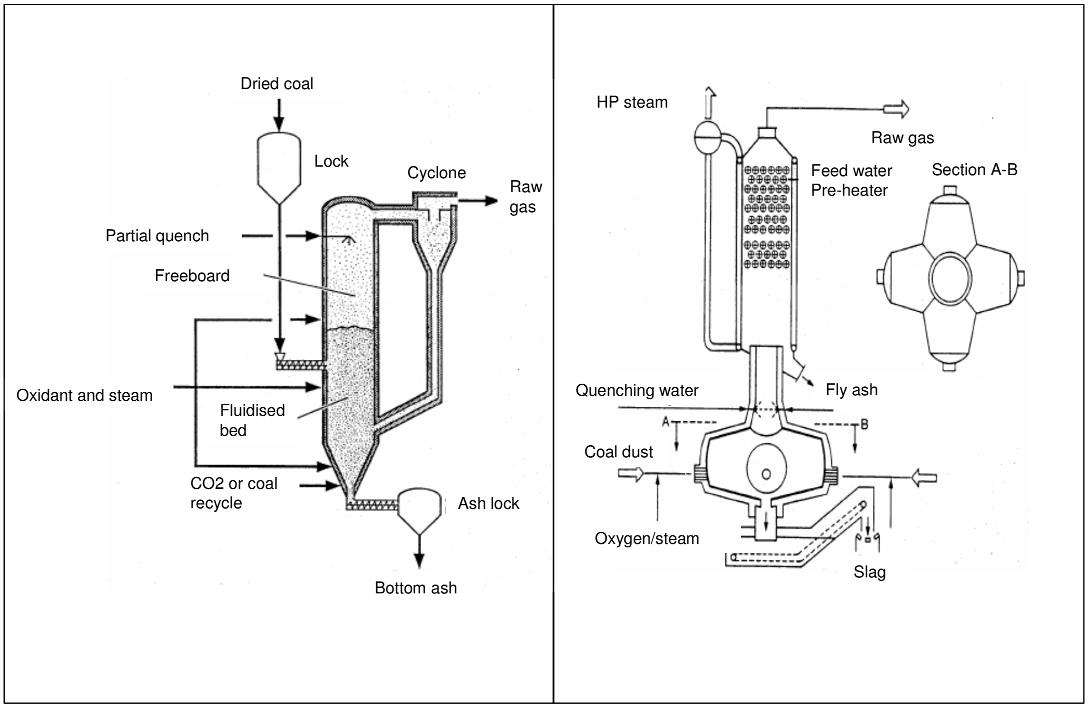

Figure 3. Fluidised bed and entrained flow gasifiers.

The only commercial example of fine coal gasification in South Africa is the 6 Koppers Totzek gasifiers which were operated by African Explosives and Chemical Industries (AECI) in Modderfontein for ammonia production. Gas production was ± 100000 Nm^3/h containing 60% CO. The fixed carbon conversion was between 70% and 80% and the gasification efficiency was between 60% and 70%. These gasifiers were operated from 1975 to 1992.

A pilot fluidised bed gasifier supplied by UHDE was operated by Highveld Steel and Vanadium in 1988. The objective of the project was to demonstrate fluidised bed gasification technology for the gasification of discard coal produced by the surrounding mines in the Witbank area. Problems experienced by the UHDE gasifier included low carbon conversion and clinkering of the coal at the oxygen and steam nozzles in the gasifier.

A better understanding of the gasification characteristics of South African coal is important for fine coal gasifier selection and development.

4 Coal selection and characterisation

A suite of four South African coals has been identified as being possible fuels for power stations which would operate for three or four decades, towards the middle of this century. The selected coals are currently used as fuel for the Lethabo (New Vaal coal), Matla, Matimba (Grootegeluk coal) and Duvha power stations and are typical of South African power station feed coal.

The coal characterisation tests done on the four selected coals are:

- Proximate analysis (Advanced coal technologies)
- Ultimate analysis (Advanced coal technologies)
- Petrographic analysis (SA Petrographics)
- BET surface area by N_2 adsorption (Protechnik laboratories)
- FSI and Roga index (Advanced coal technologies)

The laboratories that carried out the analysis are given in brackets. A summary of the analyses is given in Table 2.

Table 2. Coal characterisation parameters.

	New Vaal	Matla	Grootegeluk	Duvha
Calorific value (MJ/kg)	15.1	18.6	19.8	21.06
Ash content (%)	40.4	33.4	34.9	32.5
Carbon (%) (maf)*	79.10	80.2	81.8	89.3
Vitrinite reflectance (%)	0.53	0.64	0.68	0.75
Surface Area (m^2/g)$^+$	7.01	2.08	<1	< 1
Porosity (%)	3.2	1.3	1.5	1.1
Reactivity index (hr^{-1})	3.02	1.68	1.51	0.92
Free swelling index (FSI)	0	0	1	0
Roga index (RI)	0	0	10	0

* Moisture and ash free

$^+$ Particle size 1 mm

Due to the high ash content and low calorific value of the selected coals they are classified as low grade (D). The moisture and ash free (maf) carbon content and the vitrinite random reflectance are good indicators of coal rank. Table 2 shows that the selected coals are bituminous in rank since the carbon contents (maf) are between 75% and 85% and the vitrinite reflectance values are between 0.45 and 1.25. New Vaal coal has the lowest rank parameter being closer to the sub-bituminous coals and Duvha has the highest rank parameter being closer to the semi-anthracite coals. Approximately ninety percent of South African coals fall within the rank parameters given above.

The BET analysis measures the surface area and porosity of the coal by means of nitrogen adsorption. Due to more extensive coalification the older higher rank parameter coals have lower surface areas and porosities as reflected in Table 2.

Thermogravimetric analysis (TGA) is used to measure the reactivity index of coal. Carbon dioxide (CO_2) is reacted with a coal sample at 1000℃ and the weight loss is measured as a function of time. The reactivity index (Rs) is given by $Rs = 0.5/t_{0.5}$ with $t_{0.5}$ being the time required for 50% conversion of the fixed carbon. Table 2 shows that the reactivity index increases with increasing surface area and porosity. During the above reactivity test, CO_2 diffuses into the coal, adsorbs on the active sites within the coal and reacts by means of a surface reaction. The rate of the CO_2 gasification reaction would therefore be promoted by higher coal porosity and surface area resulting in a higher reactivity index. The reactivity index is also dependant on the surface chemistry and the catalytic effect of ash in the coal.

The Free Swelling Index (FSI) and Roga Index (RI) analyses are used to measure the caking and agglomerating nature (tendency to deform and stick together) of coal. The FSI is measured on a scale of 0 to 9 with 0 being the least swelling in nature and the RI is measured on a scale of 0 to 90 with 0 being the least sticky in nature. If the coals have caking and agglomerating properties this could potentially be problematic for fluidised bed operation since the coal particles will stick together, de-fluidised and clinkers will be formed in the bed possibly causing defluidisation. Of the selected coals only the Grootegeluk coal is expected to be weakly caking or agglomerating in nature as shown in Table 2.

5 Gasification kinetics

The gasification reactions (1 and 2) occur at a much lower rate (up to 1000 times slower) than the combustion reaction (3):

$$C + CO_2 \rightarrow 2CO \qquad (1)$$
$$C + H_2O \rightarrow CO + H_2 \qquad (2)$$
$$C + O_2 \rightarrow CO_2 \qquad (3)$$

The rate of the gasification reactions therefore has a major effect on the carbon conversion efficiency that can be achieved in a fluidised bed gasifier which operates at moderate temperatures (< 1000°C).

The rate of char conversion is often expressed using the rate equation given below [3, 4].

$$\frac{dX}{dt} = K(1 - X)^{\beta} P_{CO_2}^{\ \alpha} \qquad (4)$$

X	-	Char conversion (-)
t	-	Time (min)
P_{CO_2}	-	Pressure of CO_2 (kPa)
β	-	Reaction order with respect to the solid phase
α	-	Reaction order with respect to the gas phase

$$K = k_0 \exp\left(\frac{-E}{RT}\right) \qquad (5)$$

k_0	-	Pre-exponential factor (min^{-1})
E	-	Arrhenius activation energy (J/mol)
R	-	Universal gas constant = 8.314 (J/mol.K)
T	-	Temperature (K)

The above rate equation is referred to as the grain model and is used to describe the effect of char conversion, CO_2 concentration and temperature on the gasification rate (dX/dt). Equation 4 shows that, as char conversion proceeds initially from X = 0 to X = 1, the gasification rate slows down. Increasing the temperature and CO_2 partial pressure speeds up the reaction rate.

Thermogravimetric analysis (TGA) is used to determine the parameters in the above model. A Bergbau – Forshung TGA at North West University was used to measure the kinetic parameters for each of the selected coals. The TGA experiments measure the weight loss against time of a pre-weighed sample. The data is converted to a conversion against time graph as shown in Figure 4 for Matla coal.

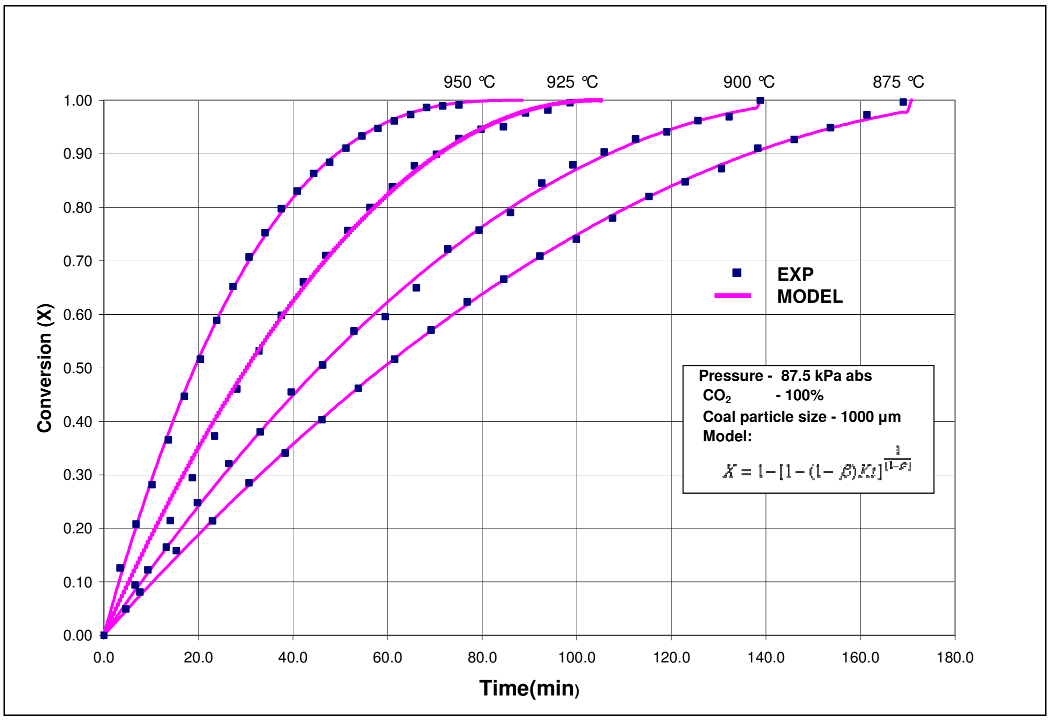

Figure 4. Conversion vs. time graph for Matla coal at four temperatures.

For the TGA tests the CO_2 pressure was maintained at 87.5 kPa. To model the experimental data equation 4 therefore reduces to:

$$\frac{dX}{dt} = K(1-X)^{\beta} \qquad (6)$$

Integration of equation 6 gives:

$$1-X = [1-(1-\beta)Kt]^{\frac{1}{(1-\beta)}} \qquad (7)$$

The model parameters β and K were fitted to the experimental data using least squares regression and are given in Table 3. Figure 4 shows that the model gives a satisfactory fit to the experimental data within the temperature range studied. The low value of β for the Grootegeluk test at 925°C could be due to caking of coal in the sample basket of the TGA.

Table 3. Grain model constants.

Coal / Temp (°C)	New Vaal		Matla		Grootegeluk	
	K (min^{-1})	β	K (min^{-1})	β	K (min^{-1})	β
875	0.050	0.76	0.010	0.49	0.004	1.09
900	0.110	0.99	0.013	0.51	0.009	1.11
925	0.138	1.03	0.019	0.51	0.018	0.38
950	0.195	1.05	0.032	0.64	0.028	0.86

The Arrhenius equation (5) can be used to describe the effect of temperature on the reaction rate constant. The Arrhenius equation can also be written as:

$$\ln(K) = (\frac{-E}{R})(\frac{1}{T}) + \ln(k_0) \qquad (8)$$

The parameters k_o (y-intercept) and $-E/R$ (gradient) are obtained by plotting ln (K) against $1/T$ as shown in Figure 5.

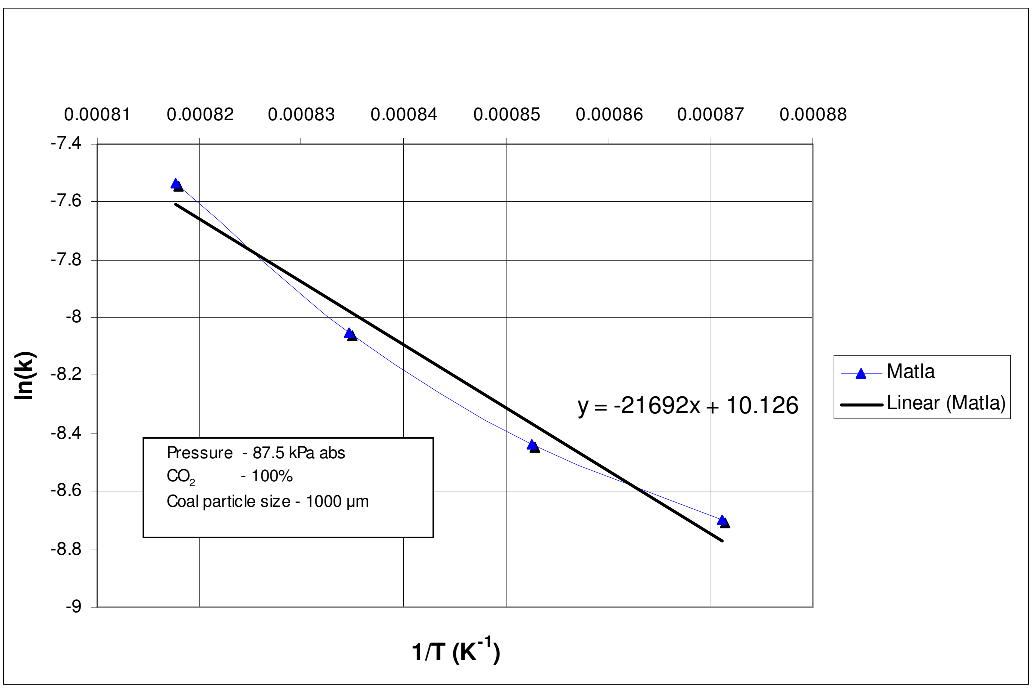

Figure 5. Arrhenius plot for Matla coal.

The Arrhenius constants and pre-exponential factors are given in Table 4.

Table 4. Arrhenius constants.

	New Vaal	Matla	Grootegeluk
k_o (s^{-1})	1.49×10^6	2.50×10^4	5.74×10^9
E (kJ/mol)	202	180	305

The reaction rate parameters given in Tables 3 and 4 can be used to plot the gasification rate as conversion proceeds as shown in Figure 6.

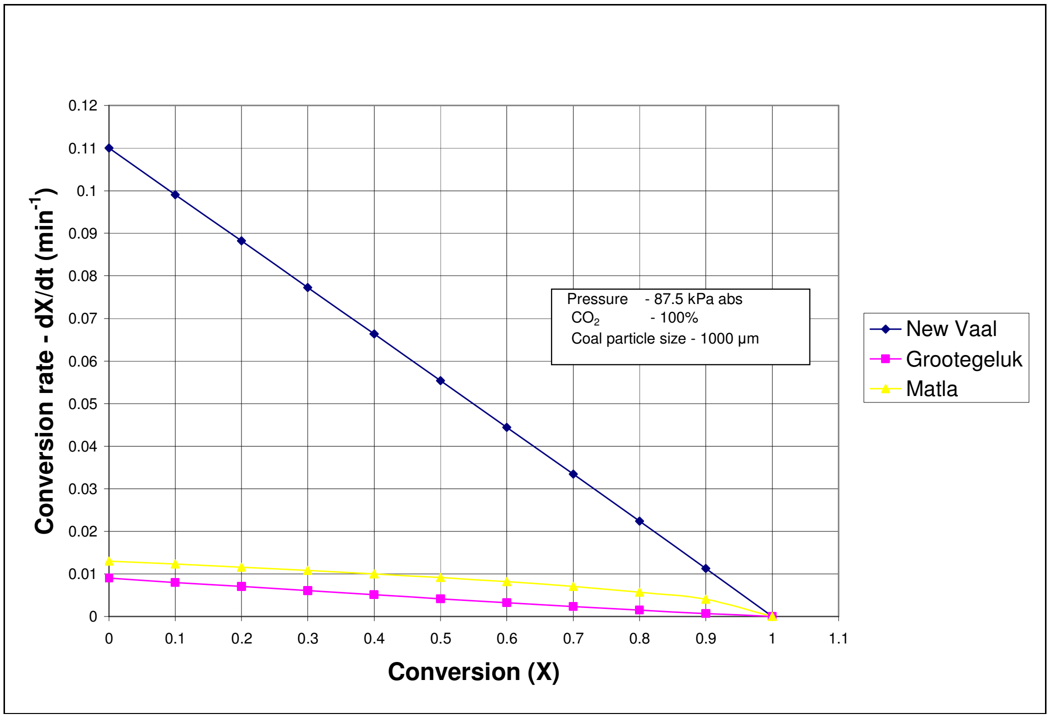

Figure 6. Conversion rate vs. conversion.

Figure 6 shows that at 90% conversion the gasification rates (dX/dt) are 11%, 31% and 8% of the initial rate for the New Vaal, Matla and Grootegeluk coals. Due do the large decrease in gasification rate at high conversions it is difficult to achieve conversions over 90% in a fluidised bed gasifier.

Two special cases of the grain model are the shrinking core model (β = 2/3) and the homogenous model (β =1) (also referred to as the volumetric model). The shrinking core model assumes that the reaction occurs at the external surface of the particle and gradually moves to the middle of the particle leaving an ash layer behind. The homogenous model assumes that the reaction takes place uniformly throughout the whole volume of the particle. The actual reaction normally takes place simultaneously via both of the above models. A lower value of β indicates that the shrinking core model is the dominant mechanism [3, 4]. The data in Table 3 suggests that, for the Matla coal, the shrinking core model is the dominant mechanism and for the New Vaal coal the Homogenous model is dominant.

The random pore model (RPM) developed by Bhatia and Perlmutter [5] is used to predict the char conversion rate if the rate increases from the initial rate to a maximum at conversions of between 10% and 30% and then decreases to zero. This model is expressed as:

$$F(X) = (1 - X)\sqrt{1 - \Psi \ln(1 - X)} \quad (9)$$

$$\Psi = \frac{4\pi L_0 (1-\varepsilon_0)}{S_0^2} \quad (10)$$

In the above equation Ψ is referred to as the structural factor. S_o, L_o and ε_0 represent the initial surface area, pore length and porosity of the particles.

The RPM was not applied for analysis of our TGA data since only the Matla coal showed a slight increase in the reaction rate (12%) at a conversion of 10%.

6 Pilot scale gasification tests

Pilot scale gasification tests were carried out on the four selected coals using an atmospheric pressure air-blown bubbling fluidised bed gasifier.

A flow diagram and specifications of the CSIR pilot fluidised bed gasifier are given in Figure 7 and Table 5.

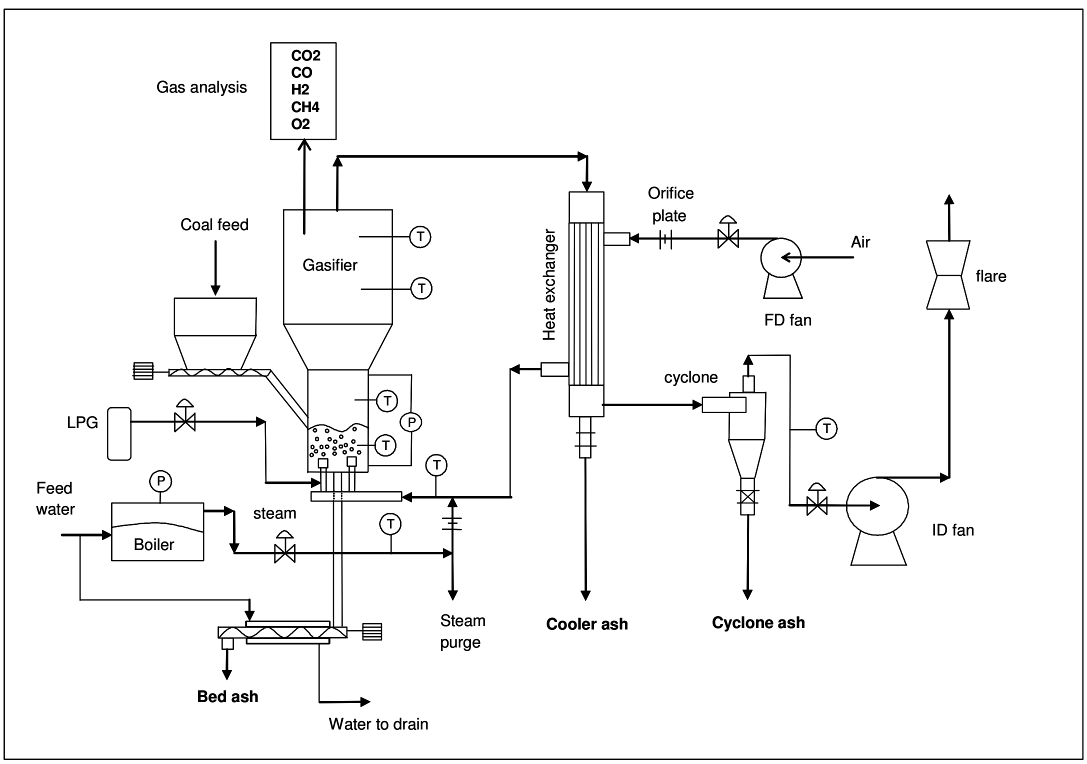

Figure 7. Flow diagram of the pilot fluidised bed gasifier.

Features of the pilot plant include:

- A screw feeder is used to feed coal into the gasifier above the bed
- A water-cooled screw is used to remove coarse ash from the bed
- A cyclone is used to removed fly ash from the gas
- The gasification air is preheated by means of a gas-to-gas heat-exchanger
- The area of the freeboard is 7.5 times the area of the bed to increase freeboard residence time
- Online gas analysers are used for gas analysis
- LPG is used for start-up.

Table 5. Specifications of the CSIR pilot fluidised bed gasifier.

Bed dimensions (m)	0.2 × 0.2
Bed area (m^2)	0.04
Freeboard dimensions (m)	0.55 × 0.55
Freeboard area (m^2)	0.3025
Furnace height (m)	4 (2m bed & 2m freeboard)
Fluidised bed height (m)	< 0.6
Coal feed rate (kg/h)	20 to 30
Coal particle size (mm)	< 5
Coal CV (MJ/kg)	15 to 25
Air flow rate (Nm^3/h)	40 to 60
Steam flow rate (kg/h)	7 to 13
Bed temperature (℃)	900 to 950
Air temperature (℃)	160 to 210
Fluidising velocity (m/s)	1.5 to 2.5
Gas CV (MJ/Nm^3)	2.5 to 3.5
Pressure	Atmospheric
Operating mode	Combustion and gasification
Gas cleaning	Cyclone

Plant start-up and operation consists of the following steps:

- LPG heating for two hours to reach a bed temperature of 650℃
- Coal addition is started at 650℃ and the temperature is increased to 925℃
- LPG is switched off and the bed temperature is controlled at 925℃ with coal addition only
- Operate the fluidised bed for 6 hours in combustion mode at 925℃ with coal addition to allow for thermal soaking of the refractories
- Switch over to gasification mode (reducing conditions) by increasing the coal flow rate
- Set the coal/air ratio and control the bed temperature at the required value with steam addition
- Operate for 6 hours in gasification mode to allow the bed carbon content and freeboard temperature to stabilise
- Operate for a further 3 hours at stable conditions during which time plant operating data and samples are collected.

Results of the pilot plant tests at 925°C and 950°C are given in Tables 6 and 7 respectively.

Table 6. Pilot plant test results at 925°C.

Plant parameters	Tests at 925°C			
	New Vaal	Matla	Groote-geluk	Duvha
Coal feed rate (kg/h)	28.7	27.0	23.0	26.4
Airflow (Nm^3/h)	52.2	50.6	50.3	47.5
Steam flow (kg/h)	9.1	8.5	10.2	10.9
Air and steam temp (ºC)	204	190	173	176
Coal particle size - d_{50} (mm)	2.4	1.6	1.9	1.7
Bed temperature (ºC)	925	925	927	927
FB exit temperature (ºC)	750	752	742	761
Dry gas composition				
CO (%)	-	10.8	9.7	8.8
H_2 (%)	-	10.0	9.4	8.5
CH_4 (%)	-	0.8	1.1	0.8
CO_2 (%)	-	15.5	15.0	15.3
H_2S (%)		0.2	0.4	0.3
N_2 (%)	-	62.8	62.6	66.3
Gross calorific value (MJ/Nm^3)	-	3.0	3.0	2.6
Bed height (mm)	540	520	520	510
Coal residence time (min)	37.0	37.4	45.1	35.7
Carbon in bed ash (%)	2.8	24.3	26.8	38.6
Carbon in fly ash (%)	19.5	32.3	31.0	41.6
Ash elutriated from furnace (%)	61.3	53.8	51.3	57.0
Carbon in total ash (%)	14.4	28.6	29.0	40.2
Total carbon conversion (%)	86.0	73.8	72.6	61.2
Fixed carbon conversion (%)	82.7	68.2	63.2	52.0
Gasification efficiency (%)	-	43.6	43.0	37.35

Table7. Pilot plant test results at 950°C.

Plant Parameters	Temperature 950°C		
	Matla	Groote-geluk	Duvha
Coal feed rate (kg/h)	24.3	23.0	26.4
Airflow (Nm^3/h)	50.9	47.8	47.8
Steam flow (kg/h)	8.5	10.0	9.0
Air and steam temp (ºC)	185	178	186
Coal particle size - d_{50} (mm)	1.6	1.9	1.7
Bed temperature (ºC)	949	953	949
FB exit temperature (ºC)	756	764	773
Dry gas composition:			
CO (%)	11.6	10.2	9.9
H_2 (%)	9.6	9.5	9.3
CH_4 (%)	0.65	1.1	0.7
CO_2 (%)	14.6	14.9	15.0
H_2S (%)	0.2	0.4	0.3
N_2 (%)	63.4	63.9	64.8
Gross calorific value (MJ/Nm^3)	3.0	3.0	2.8
Bed height (mm)	480	523	510
Coal residence time (min)	37.6	45.1	35.7
Carbon in bed ash (%)	20.8	26.4	33.9
Carbon in fly ash (%)	27.8	27.0	43.2
Ash elutriated from furnace (%)	55.7	49.3	60.2
Carbon in total ash (%)	24.7	26.7	39.2
Total carbon conversion (%)	78.4	75.5	62.6
Fixed carbon conversion (%)	74.0	67.0	53.7
Gasification efficiency (%)	44.3	48.0	41.6

The results show that:

- A gas calorific value of between 2.6 MJ/Nm^3 and 3.0 MJ/Nm^3 was obtained
- The gasification efficiency varied between 37% and 48%
- The fixed carbon conversion varied between 52.4% and 82.7%
- Increasing the temperature from 925°C to 950°C improved the carbon conversion
- The carbon conversion increased with decrease in the rank parameter (vitrinite reflectance) as shown in Figure 8.

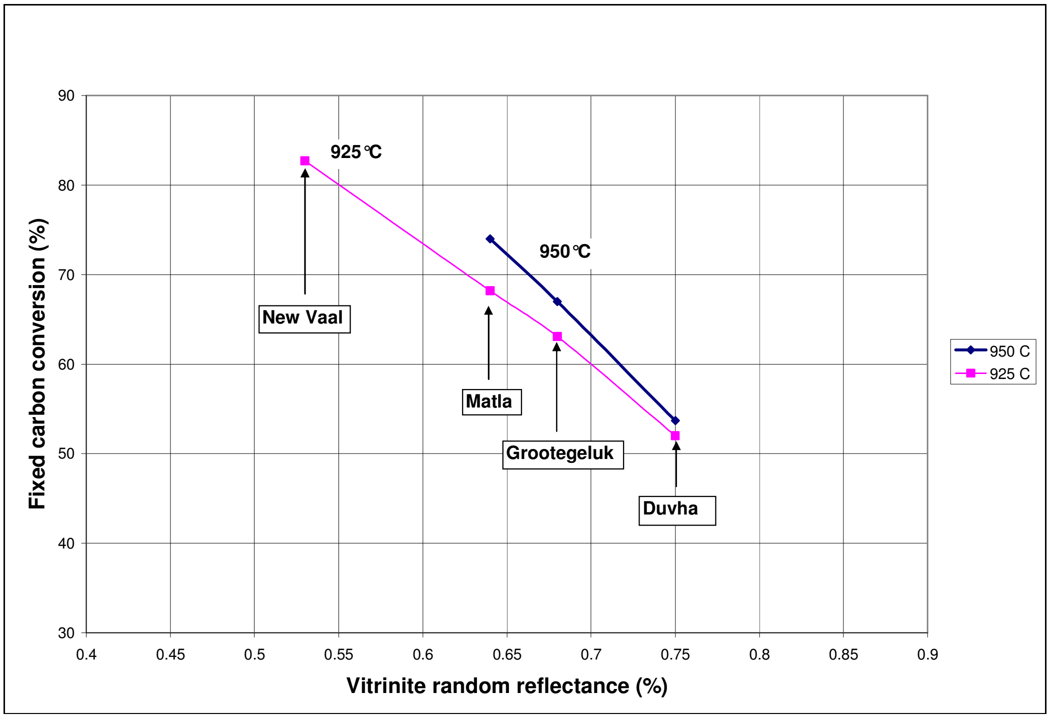

Figure 8. Relationship between fixed carbon conversion and vitrinite reflectance at 925℃ and 950℃.

Other investigators [6] have also found that carbon conversion decreases with increase in coal rank.

The carbon conversion and gas quality of a large scale fluidised bed gasifier can be improved by:

- Increasing the height of the furnace
- Increasing the freeboard temperature
- Increasing the fluidised bed height
- Increasing the air and steam preheat temperatures.

During the tests it was observed that the temperature above the distributor (30 mm above) was higher (up to 100℃) than the temperature in the middle of the bed. This is due to the partial combustion reaction ($C + O_2 \rightarrow CO + CO_2$) occurring in the bottom 10% of the bed. The average bed temperature therefore has to be maintained well below the ash fusion temperature of the coal to prevent clinkering and agglomeration of the bed

7 Modeling of fluidised bed coal gasifiers

7.1 Overview of models

The objective of fluidised bed gasifier modeling is to predict the performance of the gasifier based on given input conditions.

The input conditions include:

- Coal feed rate and analysis
- Air flow rate and temperature
- Oxygen flow rate and temperature
- Steam flow rate and temperature
- Bed height
- Furnace dimensions
- Heat losses

The performance parameters include:

- Gasifier temperature
- Gas flow rate and composition
- Carbon conversion
- Temperature and concentration profiles inside the gasifier

Models that have been developed generally belong to one of the following categories:

- Kinetic [7-9]
- Equilibrium [10-12]

Kinetic models require kinetic data for the individual gasification reactions occurring in the gasifier. A hydrodynamic model is also required to describe the mixing in the bed [7]. The two phase theory of fluidisation developed by Davidson *et al* [15] and Kunii *et al* [16] is used to describe the bed hydrodynamics. It assumes that the bed consists of two phases; a bubble phase and an emulsion phase. Kinetic models are a very complex to set up and solve. They consist of several differential and linear equations that have to be solved simultaneously. Kinetic models however still require the combustion product distribution coefficient (φ) and the relative reactivity factor (f_o) to be adjusted to fit experimental data. This is because there are processes such as coal devolatilisation and coal shattering and attrition that are not taken into account in these models.

Equilibrium models are developed by firstly setting up mass and energy balance equations for the system. The equations are solved by assuming that the water gas shift reaction ($CO + H_2O \rightarrow CO_2 + H_2$) and the hydro-gasification reaction ($C + 2H_2 \rightarrow CH_4$) are in equilibrium [6].

Furusawa *et al* [11] and Kovacik *et al* [12] concluded that good predictions of the gas yield and product gas composition can be obtained using equilibrium models. The bed temperature is predicted by means of an overall energy balance. Equilibrium models however cannot predict carbon conversion and profiles (temperature and gas concentration) inside the gasifier.

7.2 CSIR model

An equilibrium model was developed by the CSIR based on mass balances, energy balances, water gas shift equilibrium and hydro-gasification equilibrium.

A method was developed to predict the fixed carbon conversion in the gasifier based on the vitrinite random reflectance. This method was used since the pilot plant results show a good correlation between vitrinite random reflectance and fixed carbon conversion.

For the above model (method) it is assumed that the fixed carbon conversion can be described by equation 11. Other workers [13] found that equation 11 gives a good estimation of fixed carbon conversions for conversions up to 85%.

$$\frac{dX}{dt} = K(1 - X) \qquad (11)$$

X	-	Fractional conversion of char (-)
t	-	Residence time in the gasifier (min)
K	-	Reaction rate constant (min^{-1})

Other assumptions of the model are:

- Perfect mixing in the gasifier
- Bed temperature range : 900℃ to 975℃
- Freeboard top temperature : 740℃ to 780℃
- Residence time : 30 - 50 min
- Carbon conversion : 40% to 85%
- Vitrinite random reflectance : 0.53% to 0.75%
- The Arrhenius equation can be use to describe the effect of temperature on conversion.

Integration of equation 11 gives:

$$X = 1 - e^{-Kt} \qquad (12)$$

and rearranging gives:

$$K = \frac{-\ln(1 - X)}{t} \qquad (13)$$

The conversion and residence time data obtained during the pilot plant tests (Tables 6 and 7) were substituted into equation 13 to obtain the reaction rate constants (*K*) given in Table 8.

Table 8. Reaction rate constants (min^{-1}) derived from the pilot plant data.

	Temperature (℃)	
	925	950
Matla	0.0306	0.0358
Grootegeluk	0.0221	0.0246
Duvha	0.0206	0.0216

The reaction rate constant given in Table 8 is a lumped parameter and includes the contribution of:

- CO_2 gasification (equation 1)
- H_2O gasification (equation 2)
- O_2 combustion (equation 3)
- Inhibiting effects of CO and H_2 on gasification reactions

The temperature variation of the reaction rate constant given in equation 12 is usually described by the Arrhenuis equation (5):

$$K = k_0 \exp(\frac{-E}{RT}) \qquad (5)$$

Using the values of K in Table 8 values of E and k_o were calculated for each coal and are given in Table 9 together with their vitrinite random reflectance values.

Table 9. Arrhenius constants.

	E (kJ/mol)	ln(k_o)	k_o (min^{-1})	Vitrinite reflectance (%)
Matla	76.3	0.08	65.0	0.64
Grootegeluk	51.7	-2.71	4.0	0.68
Duvha	23.4	-5.63	0.21	0.75

Using the values in Table 9 empirical formulas were developed for E and k_o as a function of vitrinite reflectance (vr):

$$k_0 = f_1(vr) \qquad (14)$$

$$E = f_2(vr) \qquad (15)$$

Substituting equation 14 and 15 into equation 11 gives:

$$K = f_1(vr).\exp(\frac{-f_2(vr)}{RT}) \qquad (16)$$

Substituting equation 16 into equation 12 allows the carbon conversion to be calculated for values of vitrinite reflectance (vr), temperature (T) and residence time (t) in the ranges:

- $0.53 < vr < 0.75$
- $900 < T < 975$
- $30 < t < 50$

The carbon version calculated above is used in the mass balance of the equilibrium model. The extent of the water gas shift reaction ($CO + H_2O \rightarrow CO_2 + H_2$) and the hydro-gasification reaction ($C + 2H_2 \rightarrow CH_4$) were varied to minimise the combined least squares fit between the measured and calculated gas compositions.

Table 10. Comparison of measured and predicted gas analysis.

Gases	Matla - 925°C		Grootegeluk - 925°C		Duvha – 925°C	
	measured	predicted	measured	predicted	measured	predicted
CO_2(%)	15.5	14.7	15.0	14.9	15.3	13.9
CO(%)	10.8	11.4	9.7	9.8	8.8	9.0
H_2(%)	10.0	13.8	9.4	14.9	8.5	11.3
CH_4(%)	0.8	1.8	1.1	2.0	0.8	1.0

The results in Table 10 were obtained by assuming that the hydro-gasification reaction ($C + 2H_2 \rightarrow CH_4$) proceeds to 55% of the equilibrium value and the water gas shift reaction ($CO + H_2O \rightarrow CO_2 + H_2$) is at or near equilibrium.

Other investigators [14] also found that the above equilibrium assumptions provide a good correlation for steady-state fluidised bed gasifier data.

The model can be used to predict the performance of the pilot gasifier using different coals and operating conditions than used during the pilot plant tests.

8 Conclusions and recommendations

- Electricity demand in South Africa is increasing at a rate of 1000 MW per year
- Coal generation is likely to provide 80 – 90% of the increased capacity
- New coal power stations need to incorporate clean coal technology (CCT)
- IGCC is a potential CCT that can be applied in South Africa
- Fine coal gasification is a key enabling technology for an IGCC power station
- Fluidised bed gasifiers can utilise high ash South African coals and therefore are a potential candidate technology for IGCC power stations
- The vitrinite random reflectance of bituminous coal is a good indicator of the carbon conversion that can be achieved in a fluidised bed gasifier

- An equilibrium model using the rank parameter (*vr*) to calculate the carbon conversion gives a satisfactory simulation of gasifier performance

- Due to the relatively low reactivity of South African bituminous coals a secondary combustion stage may be required after the fluidised bed gasifier to convert the residual carbon in ash.

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