

# The feasibility of a coal gasifier combined with a high-temperature fuel cell

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## Abstract

The purpose of the study presented in this paper was to find out the feasibility of integrating a 50 MW fuel cell system, fed by gas from a coal gasifier, with an existing network for distribution of heat and power. The work presented is the results of the technical evaluation of a 50 MW coal fired high-temperature fuel cell power plant. The overall system can be divided into four subsystems including: coal gasification, gas cleaning, power generation and heat recovery.

The final system, a entrained flow gasifier combined with standard low-temperature gas cleanup and SOFC, resulted in an overall electrical efficiency of about 47%, and an overall efficiency close to 85%.

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## 1. Introduction

The combination of a coal gasifier with a high-temperature fuel cell as an idea is far from new [1,2], but the recent development of such fuel cells makes it an even more viable option for coal-based power generation. The special issue that motivated the study presented in this paper was the advantages and disadvantages to meet a new need for energy production by integrating a fuel cell system fed by a coal gasifier with an existing network for distribution of heat and power.

### 1.1. Background

When considering the construction of a new production plant, no matter if it is for energy or more traditional consumer products, the different technical options available have to be established. Then, before a final decision is made, the economics of the most promising option, or options has

to be evaluated and compared. The first, technical evaluation, is often referred to as a technical feasibility study, which is a methodological and scientific way to determine the performance of a suggested system with relation to its capability to produce electricity and heat, and is often performed by simulations using chemical flowsheeting software.

In an effort to ensure an improved energy security with a durable and reliable energy service, the European Union has launched a number of non-nuclear research projects targeting the development of environmentally friendly, yet affordable, energy conversion techniques.

As part of this effort the European Commission decided to finance a project entitled: feasibility study of an urban fuel cell network with coal gasifier, within its JOULE III program.

One of the major advantages of the fuel cell, is its inherent high efficiency, which has the consequence that the amount of fuel needed per unit of electricity produced is lower than for traditional conversion options. Thus, the use of fuel cells are expected to result in lowered emissions than is the case for the heat engine-based systems. Furthermore, the fact that the impurities of the fuel to a large extent are removed prior to the fuel cell, i.e. before mixing the fuel with combustion

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air, means that a much lower gas quantity is treated in gas clean-up steps.

The participants of the study, which had the acronym Baraka, were:

- Bertin and Cie, acting as project co-ordinator;
- CERCHAR (Combustion Research and Development Centre of SNET);
- CdF INGENIERIE;
- Kungl Tekniska Högskolan (KTH);
- Netherlands Energy Research Foundation (ECN);
- Usine d'Électricité de Metz (UEM).

The study was to investigate the technical and economic feasibility for the integration of a high-temperature fuel cell (either molten carbonate fuel cell (MCFC) or solid oxide fuel cell (SOFC)) and a gas production unit based on coal gasification. One main issue of the investigation was to find out how a fuel cell-based system would perform both regarding electrical efficiency and environmental impact, compared to more traditional coal utilising power generation techniques. The overall fuel cell and coal gasifier system, with a thermal input of 50 MW, constitutes a combined heat and power (CHP) generation plant that can be integrated into the already existing networks for the distribution of power and heat in the city of Metz, France. This technical study was an integrated part of the overall BARAKA project [3] and was carried out using the state-of-the-art simulation software Aspen Plus<sup>TM</sup>. In all studied cases, it has been assumed that the cell-potential is the same. This implies that the cell design will change with the change of the system flow pattern.

The main characteristics of the Metz network are:

- electricity distribution to 135 000 customers;
- heat distribution to an equivalent of 25 000 households by hot water at 140–180 °C.

The system was required to have an overall efficiency for combined heat and power (CHP) of 80% or more on a LHV basis, while the project group itself added the requirement of an electrical efficiency exceeding 40% (LHV).

As already stated the system should also be environmentally benign, thus meeting the expected emission standards for Europe shown in Table 1 [4].

Other restrictions set upon the system in order to decrease the technical and economical risk were the criteria that only one process unit was allowed to be in a basic research state and two process units in a status of development. In addition

to this, only one unit was allowed to be of high complexity, one unit of high cost, two units of important complexity and two units of important cost.

## 2. The BARAKA process

As previously mentioned, the BARAKA process was to be a coal-fired CHP system with a thermal input of 50 MW. This system, the integration of a coal gasifier and fuel cells, can to some extent be divided into four subsystems. Each subsystem has its own purpose, and several different process routes might be taken to ensure the function of each subsystem. The four subsystems more or less coincide with the steps that have to be taken when converting the primary energy in coal into electricity and heat. The subsystems are as follows.

The gasification subsystem, where the solid fuel, coal, is converted into a gaseous syngas. The technology is rather mature, and the interest in it has been renewed as it has shown promise as a technique for increasing the efficiency when converting the energy in coal into electricity via combined cycles.

The gas cleanup subsystem is the part of the overall process where the syngas produced in the gasification subsystem is cleaned in order to meet the rather strict gas impurity limitations of high-temperature fuel cells, as may be seen in Table 2.

As the contaminant acceptance levels are considerably more investigated for MCFC than for SOFC, the acceptance levels for MCFC were used as a guideline in the selection of the processes for the gas treatment subsection.

Next comes the power generation subsystem, where the syngas that was produced and cleaned in the previous subsystems undergoes electrochemical conversion to electricity in the high-temperature fuel cells. In addition to the fuel cells, both gas turbines/expanders and a steam cycle are used for power generation.

The last subsection, which is quite closely integrated with the other three, is the heat recovery, where heat is recovered, and used for steam generation for the internal consumption of the process, as well as for transfer to the heat network in Metz. If desirable the electricity/heat-ratio can be increased by using some of the heat to generate steam that can be used in a steam turbine.

Within the study, four different flowsheet layouts were studied. These were the ones based on either solid oxide

Table 1  
Expected emission limits for various energy sources

	Future European rules for 50 MW power plant		Proposed for the BARAKA project
	Coal	Gas	
SO <sub>2</sub> (mg/N m <sup>3</sup> )	830	35	<35
NO <sub>x</sub> (mg/N m <sup>3</sup> )	400	100	<100
Dust (mg/N m <sup>3</sup> )	50	5	<5

Table 2  
Allowable gas impurity levels for MCFC [5]

Contaminant	Level	MCFC
NH <sub>3</sub>	ppm	<10000
H <sub>2</sub> S	ppm	<0.5
Particulates	g/l	<0.1
HCl	ppm	<10
Tar	ppm	<2000

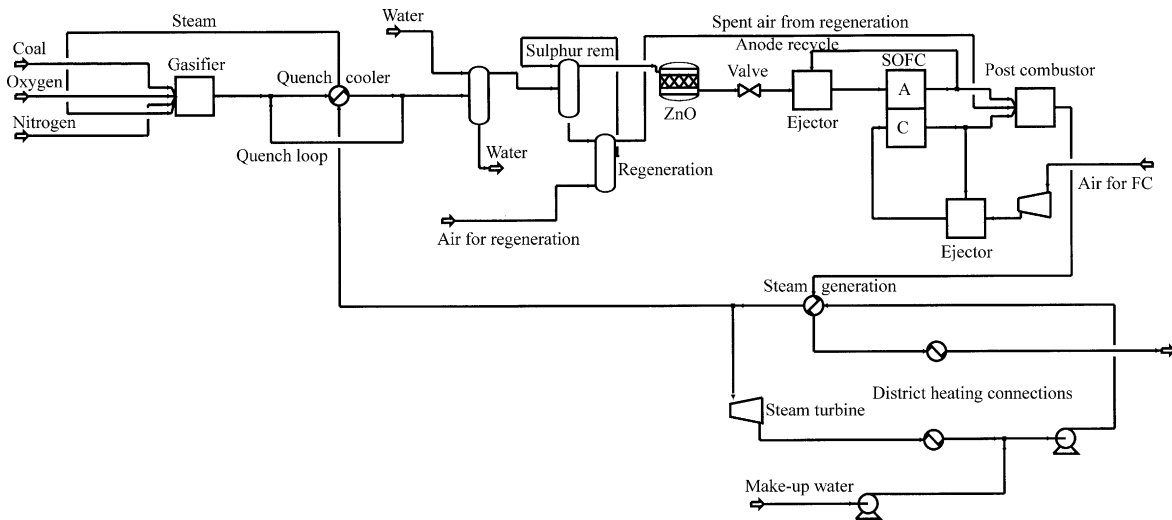


Fig. 1. SOFC system without anode off-gas recycle.

fuel cells or molten carbonate fuel cells. For each of the fuel cell options, layouts with and without, anode off-gas recycle were studied. The schematic flowsheets for the four options are shown in Figs. 1–4.

### 2.1. The gasification subsection

This is the first part of the overall process, where the primary fuel, coal, is converted into a gaseous product usually referred to as syngas.

Gasification is the term often used to describe the thermochemical processes between a solid fuel and a gaseous reacting medium, like air, oxygen or steam, resulting in the production of syngas.

The overall gasification process can be divided into four steps, resulting in a product mixture of gaseous, liquid and solid products.

The first step is drying, where the moisture of the coal fed to the gasifier evaporates. As the temperature increases above some 700 K, the second step, called pyrolysis, takes place. During this step volatile components of the coal evaporate forming a gaseous product mixture of hydrogen, carbon oxides, light hydrocarbons, tars, oils and phenols. During the pyrolysis step the initial weight of the coal is reduced by about 70% but the heating value of the gaseous, and at room temperature liquid, products is only about 50% of the initial heating value of the coal fed to the gasifier. The remaining 50% of the initial heating value is found in a solid residue called char.

The char mainly consists of the mineral content of the coal and the carbon left unconverted during pyrolysis. In addition to this, the char also contains heavier hydrocarbons that are formed by combinations and re-polymerisation taking place between the volatiles formed during pyrolysis. In order to

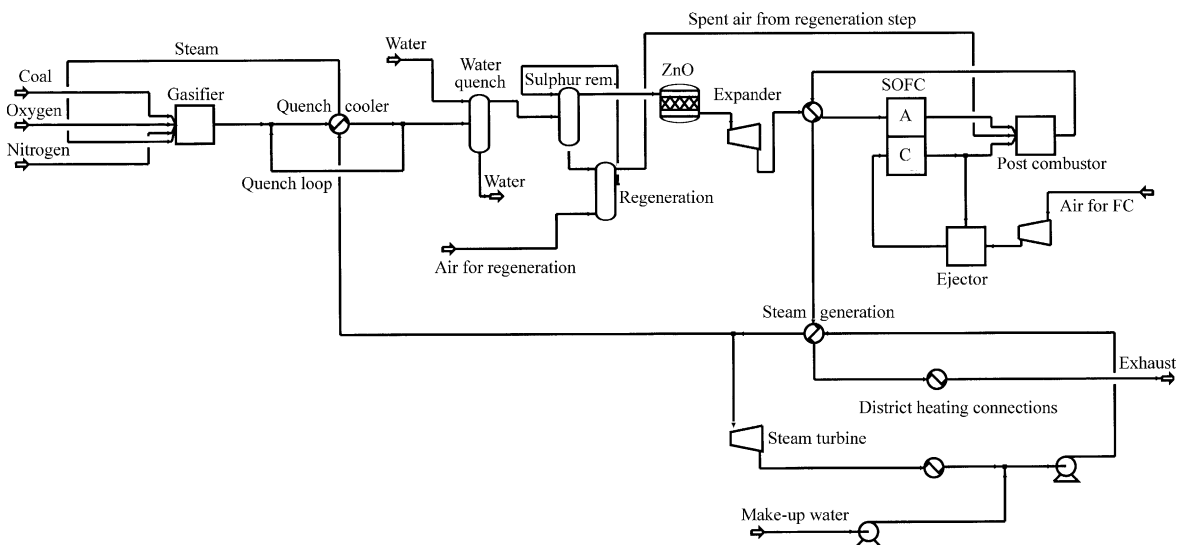


Fig. 2. SOFC system with anode off-gas recycle.

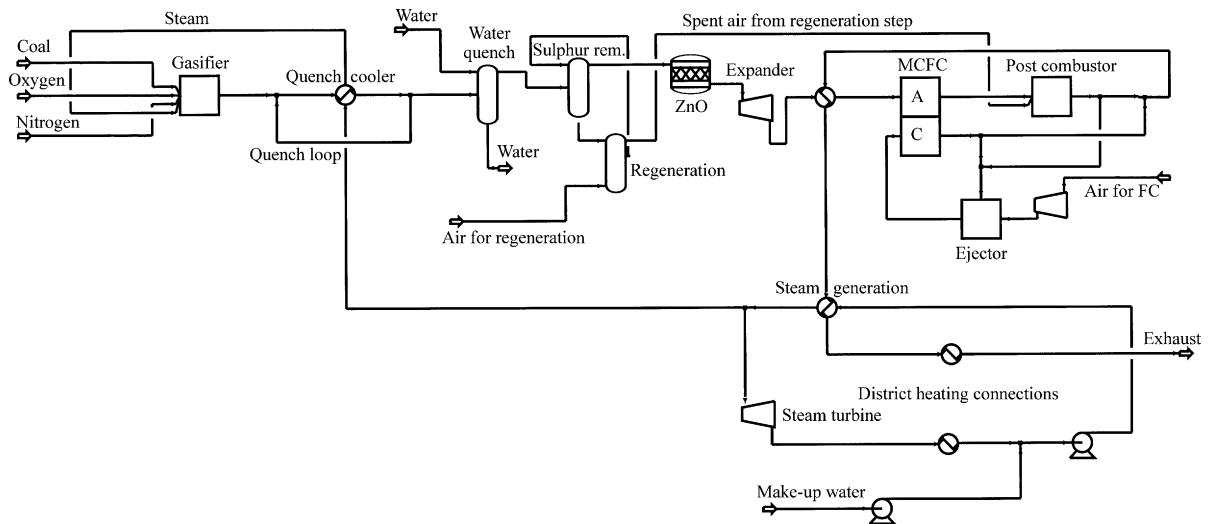


Fig. 3. MCFC system without anode off-gas recycle.

have an overall gasification process of a higher efficiency, the solid char has to undergo further conversion at temperatures exceeding 950 K in order to achieve the release of the fixed carbon and the higher molecular-weight compounds.

As the conversion of char, gasification, is a considerably slower process than pyrolysis, it is the rate of the char gasification that to the largest extent will guide the sizing and design of the overall gasification reactor.

Even though the main overall reactions taking place during the overall gasification process are not very complicated and complex themselves, the difficult part is to establish the kinetic relations between the different species. The complete reaction mechanism is far more complex as it involves free radicals and a huge quantity of elementary reactions including the formation of phenols and higher hydrocarbons that form the tar.

The basic reactions involved in coal gasification are:

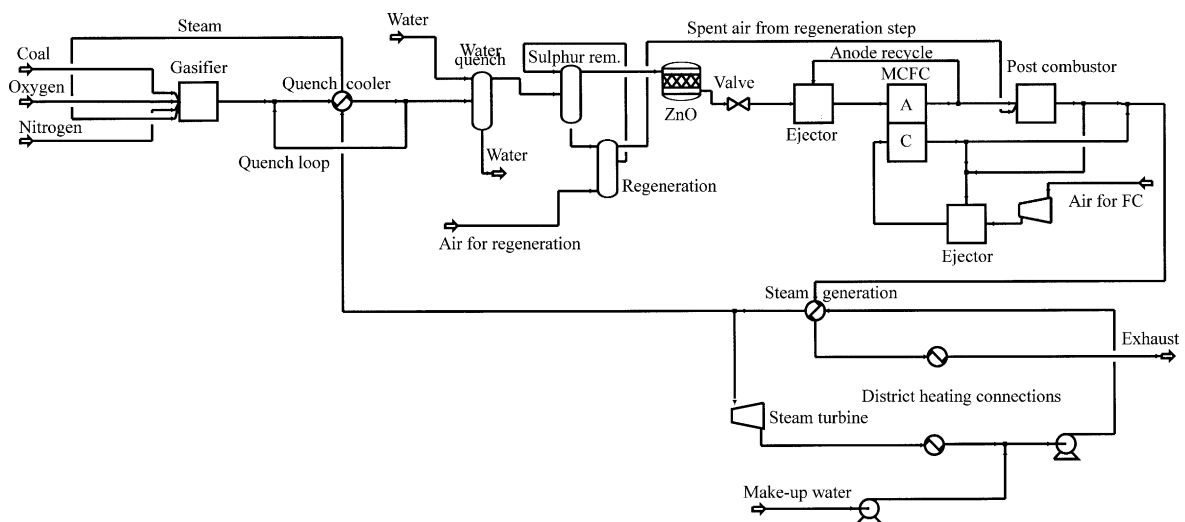
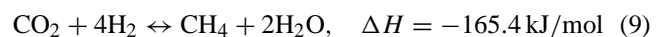
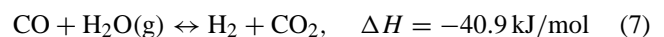
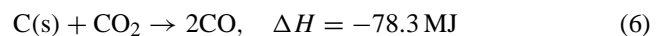
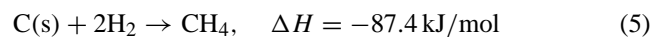
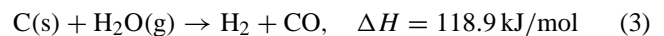
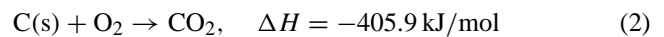
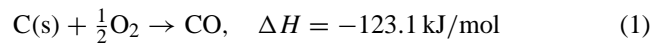


Fig. 4. MCFC system with anode off-gas recycle.

Some of the gasification reactions are highly endothermic, i.e. require heat to take place, and thus the heat balance is such that heat has to be supplied to the gasifier. The easiest way to do this is to combust a portion of the coal feed, according to reaction (2).

### 2.1.1. Choice of gasification medium, oxygen or air

In addition to heat, an oxygen source is necessary for accomplishing the gasification. The natural source is either oxygen or air, which is fed together with steam.

The factors guiding whether oxygen or air is to be used are commonly the operating temperature and pressure of the gasifier. Since air contains some 79% nitrogen, the use of air requires a larger portion of the coal to be combusted in order to maintain the gasifier temperature than when oxygen is used.

The use of oxygen rather than air may also be beneficial when operating the gasifier at an elevated pressure. The gases fed to the gasifier have to be compressed to the operating pressure of the reactor, and thus the nitrogen present in air would increase the work needed for compression.

### 2.1.2. Coal gasifiers

If neglecting more exotic gasification techniques such as the molten bath gasifier, the tumbling-bed gasifier and underground gasification, three basic techniques exist for coal gasification. These are the moving bed gasifier, the fluidised bed gasifier and the entrained flow gasifier as shown in Fig. 5.

The oldest, and probably least complex, gasifier is the moving bed gasifier which can handle lumps of non-caking coal in sizes of 5–80 mm. The gasifier is characterised by a rather linear temperature profile, from about 620 K at the product gas exit/coal inlet, up to about 1800 K in the combustion zone located in the lower part of the gasifier. The coal is fed at the top of the gasifier, contributing to the gasifier bed. By action of gravity the coal will move counter-currently downwards in the bed, undergoing drying, pyrolysis, gasification and combustion as the solid travels downwards through the gasifier. Since the volatiles liberated during pyrolysis and gasification come into contact with the fresh coal, no further thermal cracking of tars and phenols occur, which results in a product gas rich in these hydrocarbons, that have to be removed prior to any use in a fuel cell. Depending on the construction of the gasifier, the mineral-containing ash may be removed as a solid residue (dry ash) or as a slag.

The fluidised bed gasifier is characterised by an even temperature distribution in the gasifier bed as a result of the high degree of backmixing between freshly fed coal, ash and char. The crushed coal can be fed either at the top of the gasifier, or at the bottom together with the gasification and fluidisation media. In order to ensure that no ash melting occurs, the gasifier temperature has to be kept below the ash fusion temperature of about 1100 K. If the ash would melt, there is a high risk of ash agglomeration, resulting in the disruption of fluidisation. The low gasifier temperature results in

a lower carbon conversion than for a gasifier operating at a higher temperature, but the tar content in the product gas is lower than for the moving bed gasifier.

The entrained flow gasifier is characterised by a step-wise temperature increase from the coal inlet to the product gas outlet. As a result of this temperature increase which gives an outlet temperature of about 1500 K, most tars formed during pyrolysis are cracked during char gasification. The result is an almost tar-free product gas. The drawback of the high operating temperature is that it results in ash-melting, so that the ash has to be removed as a slag.

Depending on the design of the entrained-flow gasifier, the powdered coal is either fed as water slurry or entrained in an inert gas stream. This feed is fed co-currently together with the oxidising agents air/oxygen and steam. Depending on the feeding method, almost all coals can be gasified in an entrained flow gasifier, thus making it more fuel flexible.

A summary of some of the features of the different gasifier types can be seen in Table 3. The reason for the intervals given is that each gasifier type covers several models, and also that such factors as the type of coal fed influence the product gas composition.

When comparing the three basic processes, it can be seen that the oxygen plus steam consumption is about the same for all of the processes. The differing aspects are the tar content of the product gas, as well as the coal conversion. The coal conversion is the fraction of the carbon present in the coal feed that is found in the product gas, i.e. a high coal conversion results in a higher fraction of the initial carbon being found in the product gas. Similarly the cold gas efficiency is a measure of the gasifier's efficiency to convert the solid coal into a gas with a high heating value. That

Table 3  
Characteristics of different types of coal gasifiers [6,7]

	Moving bed	Fluid bed	Entrained flow
Feed	Dry	Dry	Dry or slurry
Outlet temperature (K)	600–810	1200	1300–1700
Pressure (atm)	~28	~25	~25–42
Oxidant	Oxygen	Oxygen	Oxygen
O <sub>2</sub> /coal (kg/kg)	~0.5	~0.47	~0.55–0.78
H <sub>2</sub> O/coal (kg/kg)	~0.3	~0.27	~0–0.43
Carbon conversion (%)	~99	~96	~97–99
Cold gas efficiency (%)	~88	~70–85	~74–81
Product gas, HHV (MJ/m <sup>3</sup> )	~13	~11.5	~9.8–11.8
Gas composition (vol.%)			
H <sub>2</sub>	~26	~28	~26–30
CO	~46	~33	~29–63
CO <sub>2</sub>	~3	~15	~1.5–14.5
CH <sub>4</sub>	~4	~4.6	~0–0.6
C <sub>2</sub>	~0.1	–	–
H <sub>2</sub> S	~1.0	~0.2	~0.1–1.3
COS	~0.1	–	~0–0.1
N <sub>2</sub>	~2.7	~0.6	~0.5–4.3
Ar	~0.6	~0.7	~0.7–1.1
H <sub>2</sub> O	~16.3	~16.8	~2.0–25.8
NH <sub>3</sub> + HCN	~0.2	~0.1	~0–0.2
Tar content	High	Medium	Low

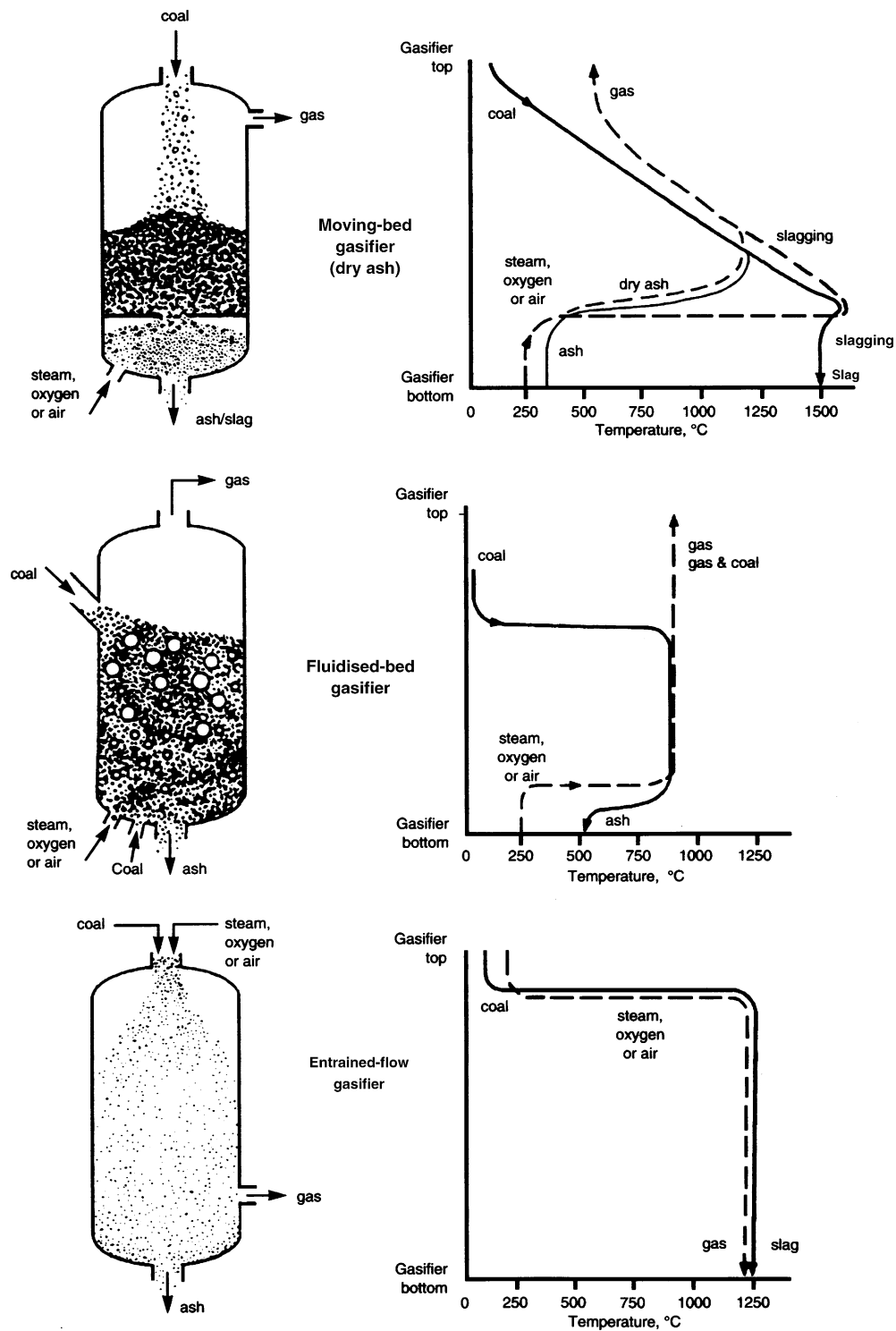


Fig. 5. Principles of different coal gasifiers [6].

is, the higher the cold gas efficiency, the less of the coal is combusted for gasifier heat generation instead of forming a high heating-value gas.

The tar content of the product gas will to a large extent influence the layout of the gas cleanup steps downstream of the gasifier. A high tar content will require a

more complex gas cleanup, thus making it less economically favourable.

With these factors in mind, and with state-of-the-art efficiency being a priority of the project, an entrained flow gasifier with dry feeding was selected. The Prenflo gasifier manufactured by Krupp Uhde [8] was selected. Another con-

tributing factor for this selection was that a full scale Prenflo gasifier is in operation in Europe [9], thus ensuring that the technique fulfils the requirement of proven technology for the different process steps.

### 2.1.3. Gasifier simulation

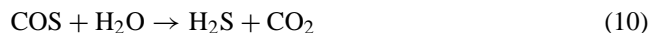
The modelling of the gasifier within Aspen Plus<sup>TM</sup> was based on the assumption that the gaseous products reach chemical equilibrium. The basis for this assumption is the high gasifier temperature, which results in high reaction rates [10]. Therefore, a reactor model based on the minimisation of Gibbs free energy was used. Furthermore the gasifier results of the calculations based on the Aspen Plus simulations were compared with the results obtained by an in-house model at CERCHAR and CdF INGENIERIE giving comparable results [11].

## 2.2. The gas cleanup subsection

### 2.2.1. Gas cleanup process selection

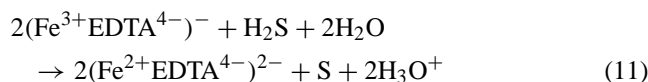
The raw syngas leaving the gasifier is far from clean. In addition to gaseous pollutants such as H<sub>2</sub>S, COS, HCN, and NH<sub>3</sub>, it also contains particulate matter carried from the gasifier by the gas stream. In order to be used in a fuel cell it has to undergo several steps of cleaning. The first part of the gas-cleaning subsection is the quench-cooler, where the hot raw syngas is mixed with a cooled and filtered syngas recycle stream. The slightly cooled stream is cooled further in steam-generating heat exchangers, before it is passed to bag filters removing particulates present in the gas. The particulate-free syngas is then slightly recompressed before being fed to the next process step, the COS hydrolysis. The particles trapped in the bag filters are mixed with the pulverised coal and returned to the gasifier.

During the COS hydrolysis, the COS is hydrolysed to H<sub>2</sub>S over a platinum-based catalyst according to reaction:



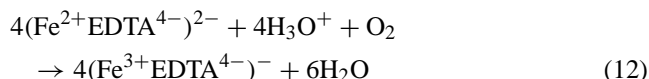
The hydrolysis step is followed by a water quench, where the temperature of the syngas is decreased by contact with water. This has a two-fold effect. The water will dissolve any HCl and NH<sub>3</sub> present in the syngas, and at the same time adjust the syngas temperature to the level of the subsequent sulphur removal process.

A traditional low-temperature process operating at 50 °C accomplishes the main part of the sulphur removal. The process syngas is contacted with an aqueous solution of a Fe<sup>3+</sup>/Fe<sup>2+</sup>-complex, resulting in the reduction of Fe<sup>3+</sup> into Fe<sup>2+</sup>, at the same time oxidising the sulphur present as H<sub>2</sub>S, producing elementary sulphur according to



The sulphur sludge is separated from the spent Fe<sup>2+</sup>-containing solution by filtration. The Fe<sup>2+</sup>-solution is regenerated

by contacting with air in a regeneration step, according to Eq. (12), prior to recycle back to the sulphur removal unit.



The conventional low-temperature sulphur removal step was chosen instead of a more efficient mid-temperature process relying on absorption and oxidation of H<sub>2</sub>S in a tin oxide bed at 400 °C. This would have resulted in a better temperature matching with the final polishing in a 400 °C ZnO-bed, thereby resulting in a gas purity meeting the sulphur levels tolerated by the fuel cell.

The reason for selecting the traditional low-temperature gas cleanup followed by subsequent re-heating before the ZnO-bed, was that the tin oxide process was judged to be on a development level, and thus could not fulfil the requirement of technical maturity.

### 2.2.2. Gas cleanup modelling

In the overall simulation model describing the whole system, the separator models present within Aspen Plus<sup>TM</sup> were used to describe the gas cleanup subsection. The separator models were assigned parameters obtained from the vendors of the different processes.

## 2.3. The fuel cell subsection

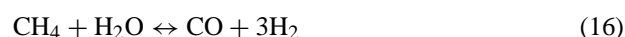
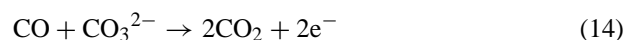
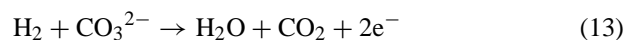
Following the gas cleanup is the fuel cell subsection, where the electrochemical conversion of the fuel species present in the syngas takes place.

As a result of the defined project objectives using high-temperature fuel cells, two types of fuel cells were initially considered for the electrochemical conversion. These were the molten carbonate fuel cell operating at an average temperature of 650 °C, and the solid oxide fuel cell with an average operating temperature of 900 °C.

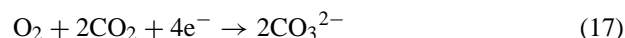
### 2.3.1. Molten carbonate fuel cell

The molten carbonate fuel cell consists of a nickel anode and a nickel oxide cathode, parted by a lithium–potassium carbonate melt acting as the electrolyte. In order to ensure that the electrolyte is kept as a melt, the typical operating temperature must be held in the range of 600–700 °C. The reactions taking place at the electrodes are:

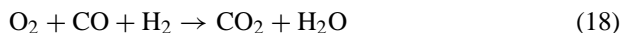
- *Anode:*



- *Cathode:*



- *Net reaction:*



The two first reactions taking place at the anode are the electrochemical conversions of hydrogen and carbon monoxide. In both these reactions carbon dioxide is one of the reaction products. The third reaction is the water-gas shift reaction, which forms additional hydrogen by the anode material-catalysed reaction between carbon monoxide and steam.

If a steam-reforming catalyst is placed in, or adjacent to, the anode compartment, it is possible to use the heat generated by the stack to carry out direct or indirect internal reforming, according to reaction (16). The advantage with this is that the endothermic steam-reforming reaction will assist in the cooling of the stack.

At the cathode side, oxygen is reduced and reacts with carbon dioxide forming a carbonate ion. This carbonate ion is then transported through the electrolyte to the anode, thus completing the net cell reaction (18).

As to the geometry of the MCFC, only planar configurations are developed. Different manufacturers/developers may use different flow configurations, i.e. co-flow, cross-flow or counter-current flow. Some of the companies that have been involved in MCFC development are Fuel Cell Energy (formerly Energy Research Corporation) [12] and M-C Power [13] in the USA, BCN [14], MTU [15] and Ansaldo [16] in Europe, as well as Hitachi [17], IHI [18] and Mitsubishi [19] in Japan.

As can be observed when looking at the electrochemical reactions above, the reactions at the anode produce carbon dioxide, whereas the reaction at the cathode consume carbon dioxide. Therefore, in order to accomplish a functioning system, an amount of carbon dioxide equivalent to that formed at the anode has to be supplied to the cathode inlet. Unless a direct source of CO<sub>2</sub> is present, systems with transfer of CO<sub>2</sub> from anode exit to cathode inlet tend to be more efficient, i.e. more efficient than by producing CO<sub>2</sub> from direct combustion of the primary fuel. The logic of this is that if the primary fuel were to be used as the CO<sub>2</sub> source, it would require the same amount of gas cleanup as the fuel stream fed to the anodes. This is because of the stringent impurity constraints set by the fuel cells. In addition to an additional gas cleanup section, an additional combustor would be required to oxidise the carbon content into carbon dioxide.

If, instead, the anode off-gas is used, the only additional item required to accomplish the CO<sub>2</sub> supply is a post-fuel cell combustor, where the non-utilised fuel components present in the anode off-gas are oxidised into carbon dioxide and water. Because of emission issues, the anode off-gas cannot be emitted to the surroundings without the post-oxidation step, consequently it cannot really be considered as an additional subsection, but simply as an original part of the fuel cell subsection.

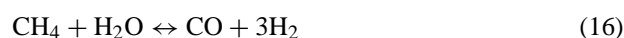
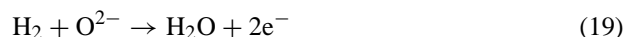
Thus, the use of external fuel to generate the carbon dioxide needed for the functioning of the cathode is less advan-

tageous than using the anode off-gas as the carbon dioxide source.

### 2.3.2. Solid oxide fuel cell

The solid oxide fuel cell has ceramic electrodes separated by a solid oxide electrolyte. In order to achieve a high enough conductivity of the cell components, the operating temperature traditionally has to be kept in the range of 800–1000 °C. The reactions taking place in the fuel cell are as follows:

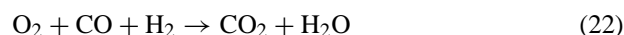
- *Anode:*



- *Cathode:*



- *Net reaction:*



The first two reactions are the electrochemical conversions of hydrogen and carbon monoxide together with the oxide-ion into water and carbon dioxide. The third reaction is again the water-gas shift reaction converting carbon monoxide and water into carbon dioxide and hydrogen. The fourth reaction is steam reforming, the catalytic conversion of methane and steam into carbon monoxide and hydrogen. Because of the high operating temperature the anode consisting of a porous Ni/ZrO<sub>2</sub> cermet has a high enough activity to catalyse the steam reforming reaction (16). An advantage with this is that if methane is present in the syngas, the endothermic nature of the methane steam reforming reaction will assist in the cooling of the fuel cell stacks.

As to the geometry of the fuel cells there are two basic configurations, the tubular and the planar stack assembly.

The tubular configuration, which is the most developed so far, is the geometry suggested and developed primarily by what used to be Westinghouse [20], now known as Siemens–Westinghouse [21]. The advantages of the tubular cell are that it does not require any gas seals between individual cells, and that the tubular shape can handle the thermal expansion of the cells.

The planar cell geometry is a shape that is pursued by companies such as SOFCo, Ztek and Allied Signal in the USA [22], Fuji [23], Mitsubishi [24] and Sanyo [25] in Japan, and companies such as Sulzer Hexis [26] and ECN [27] in Europe. Before the Siemens and Westinghouse merger, Siemens used to be a major planar SOFC player in Europe [28]. The reason for pursuing a planar geometry is the expectation that such a configuration will enable a higher current density and an overall better cell performance than the tubular geometry. Also the manufacturing of the



planar SOFC is expected to be easier and less expensive than the manufacturing of the tubular geometry.

Drawbacks with the planar geometry are associated with the high operating temperature of the fuel cell. Thus, mismatching thermal expansions of the cell components as well as problems with gas tight sealing are major obstacles that have to be overcome before the planar SOFC can be considered fully developed.

A new trend regarding SOFC is the so-called intermediate temperature SOFC (IT-SOFC) where the adoption of new materials enable the operating temperature to be decreased to about  $\sim 600\text{--}700^\circ\text{C}$ . The decrease in operating temperature is hoped to allow the use of less costly materials, thus improving the economics of the fuel cells. The reduced temperature is, however, not only an improvement. As a result of the lower operating temperature, an external steam reformer may be necessary to avoid carbon deposition in the fuel cell [29], and to enable the use of  $\text{CH}_4$  as a fuel [30]. Since the IT-SOFC technique was considered even less developed than the traditional SOFC, it was ruled out as a realistic alternative for this study.

### 2.3.3. Selection of fuel cell type for the BARAKA system

When comparing the MCFC and SOFC technologies, it was considered that a system based on SOFC might be less complex as no  $\text{CO}_2$  transfer from the anode outlet to the cathode inlet has to take place. Also, the allowable temperature increase is  $200^\circ\text{C}$  for the SOFC, which is twice the allowable temperature increase of the MCFC, indicating that the cooling need and thus the needed flow of air through the cathode should be lower for the SOFC. Since the air passing through the cathode has to be compressed to the pressure level of the fuel cell, a higher airflow means higher energy consumption to compress the air. Another feature that favours the SOFC is the fact that since the electrolyte in the SOFC is a solid, it allows for deviating pressure levels between anode and cathode. The MCFC, on the other hand, has an electrolyte melt as the electrolyte, and if operating with different pressures at anode and cathode, could cause a fateful gas crossover.

When looking at the cost for the fuel cell, the least developed unit of equipment in the system, the data are scarce. For the MCFC there are a few cost predictions [31–33], ranging from US\$ 1000–2000  $\text{kW}_e$  for the stack only. Similar predictions regarding the SOFC [20,22,34,35], indicate stack costs up to US\$ 1000  $\text{kW}_e$ .

Based on these factors, the SOFC was selected as the primary fuel cell of choice to investigate with respect to both technical and economical feasibility, whereas the technical feasibility of an MCFC option was also investigated.

### 2.3.4. Other types of equipment included in the fuel cell subsection

In addition to the fuel cells, other items of process equipment are included to make the fuel cells work and to complete the overall power generation subsection.

In order to provide the compressed air needed to feed the cathode, a multi-stage air compressor is used. This air is compressed to a higher pressure than the cathode inlet pressure, and is used as the driving medium of the ejector, which is used to recycle the cathode outlet gas.

The same type of equipment was also selected to accomplish an anode off-gas recycle. The use of an anode recycle eliminated the need for an expensive heat exchanger to pre-heat the desulphurised syngas prior to anode entry.

After passage through the fuel cells, the recycle streams were extracted, and then anode off-gas and cathode off-gas were contacted in a post-oxidation unit. Here the remainders of the combustibles in the anode off-gas were combusted with the oxygen remaining in the cathode off-gas. This made it possible for the off-gas to meet the required CO concentration limits. The hot combustion off-gas was then expanded in an expansion turbine in order to regain part of the compressor work of the system. Heat still present in the stream was used for steam generation, followed by generation of district heat. The generated steam was further superheated in various parts of the system, and finally expanded through a steam turbine.

## 3. The fuel cell model used in the study

The fuel cell model used in the Aspen Plus<sup>TM</sup> studies is a one-point model, using Faraday's law (23) to calculate the power generation by the fuel cells. To some extent the reasoning in the construction of the model resemble the basis for the so-called KTH-model, which have been described in more detail elsewhere [36–38]:

$$P_{\text{el,dc}} = \left( \sum n_i y_i \right) U_{\text{fuel}} \dot{N}_{\text{anode}} F E_{\text{stack}} \quad (23)$$

where  $P_{\text{el,dc}}$  is the electrical power produced by the fuel cell stacks (W),  $y_i$  the mole fraction of fuel species  $i$  in the anode gas,  $n_i$  the number of electrons transferred during the electrochemical conversion of  $i$  to carbon dioxide and water (this number equals 2 for hydrogen and carbon monoxide),  $U_{\text{fuel}}$  the average fuel utilisation,  $\dot{N}$  the reactant flow to the anode (kmol/s),  $F$  the Faraday's constant (A s/kmol), and  $E_{\text{stack}}$  is the average cell voltage (V).

The authors are well aware of the fact that the use of a one-point model has its limitations, but so does the use of a rigorous and complex model in the context of system simulations. The use of the more detailed model carries the risk of resulting in extensive calculation times and a overall model of great complexity. The selection of using a one-point model can be considered a trade off made between the two alternative approaches.

## 4. Inputs for the technical analysis

The coal selected as feedstock for the study was a Pittsburgh No. 8 coal, which was finely ground prior to feeding

Table 4  
Data for Pittsburgh No. 8 coal

Ultimate analysis (%)	
Carbon	74.9
Hydrogen	5.1
Oxygen	5.2
Nitrogen	1.5
Sulphur	2.4
Chlorine	0.09
Fluorine	0.009
Ash	10.8
Proximate analysis (%)	
Moisture	1.0
Ash	9.0
Fixed carbon	52.3
Volatile matter	37.7
Lower heating value (MJ/kg (mf))	30.4
Higher heating value (MJ/kg (mf))	31.5

mf: moist free.

Table 5  
Data for the Prenflo gasifier

Gasifier outlet temperature (°C)	1450
Gasifier pressure (bar)	20
Coal feed (including 1% moisture) (kg/h)	5986
Oxygen feed (99% purity) (kg/h)	5722
Nitrogen feed (carrier gas and purge) (kg/h)	526
Steam feed (kg/h)	571

into the Prenflo gasifier. The composition of the coal [11] is given in Table 4.

The data given in Table 5 were used to describe the Prenflo gasifier [11]. The operating parameters established for the fuel cell stacks are given in Table 6. The characteristics for rotating equipment and inverter acquired from different vendors are summarised in Table 7.

In the SOFC cases the air compressor is mounted on the same shaft as the post-fuel cell expansion turbine, and thus no electrical drive is necessary. As will be discussed later, the situation in the MCFC cases is somewhat different, and the air compressor electrical efficiency is expected to be 96%.

Table 6  
Data for the SOFC and MCFC stacks, used in the simulations

	SOFC	MCFC
Inlet temperature (°C)	800	600
Outlet temperature (°C)	1000	700
Operating pressure (absolute) (bar)	8.0	3.0
Pressure loss, cathode (bar)	0.5	0.5
Pressure loss, anode (bar)	0.5	0.5
Average cell voltage (V)	0.725	0.750
Fuel utilisation (%)	85	80
Heat loss to the surroundings (%)	2.5	2.5

Table 7  
Characteristics of rotating equipment and inverter

Equipment	Isentropic efficiency (%)	Mechanical efficiency (%)	Electrical efficiency (%)
Post-fuel cell expander	87	96	96
Steam turbine	88	96	96
Air compressor	88 (each step)	93	–
			(SOFC), 96 (MCFC)
Hot gas quench blower	20	91	88
Sulphur recovery blower	83	87	92
Inverter	–	–	98

## 5. Results and discussion of the technical study

Table 8 shows the gas composition and mass-flow leaving the gasifier, based on the calculations carried out in the Aspen Plus<sup>TM</sup> simulation software.

The four different flowsheet options that were evaluated were SOFC and MCFC alternatives with and without an anode off-gas recycle. As will be discussed below, the introduction of an anode off-gas recycle can have opposite effects depending on which type of fuel cell, MCFC or SOFC, is used.

One result that can be seen directly is that only the SOFC cases meet the requirement of an overall efficiency of 80% or above, while at the same time fulfilling the added constraint of an electrical efficiency exceeding 40%.

### 5.1. SOFC cases with and without anode off-gas recycle

When comparing the two SOFC options, as shown in Table 9, it can be seen that the introduction of the anode off-gas recycle results in a 12% increase of the power output from the fuel cells. This is the direct result of the 9.9% increase in overall fuel cell fuel utilisation resulting from the introduction of an anode recycle loop. This can be seen

Table 8  
Gas compositions obtained from the gasifier, prior to gas cleanup

Gasifier outlet temperature (°C)	1500
Gasifier pressure (bar)	20
Gasifier outlet flow (kg/h)	12446
Mole fractions (%)	
CH <sub>4</sub> (ppm)	20
H <sub>2</sub>	26.3
CO	59.6
CO <sub>2</sub>	3.4
H <sub>2</sub> O	5.7
N <sub>2</sub>	4.2
H <sub>2</sub> S	0.6
COS	0.05
HCl (ppm)	256
NH <sub>3</sub> (ppm)	16.7
Cl <sub>2</sub> (ppm)	5.4
HF (ppm)	49
Ash	0.15

Table 9  
A summary of the obtained results

Case	Case I	Case II	Case III	Case IV
Fuel cell type	SOFC	SOFC	MCFC	MCFC
Anode recycle	Yes	No	Yes	No
Fuel cell fuel utilisation				
Single pass (%)	85.0	85.0	80.0	80.0
With anode recycle (%)	93.4	–	90.7	–
Flow at cathode inlet (kg/h)	200971	238669	418568	399800
Cathode recycle ratio (%)	70	75	44	54
Flow at anode inlet (kg/h)	35259	11326	38007	11326
Anode recycle ratio (%)	56	–	54	–
Thermal input (LHV-kW)	50000	50000	50000	50000
Thermal input (HHV-kW)	51854	51854	51854	51854
Power output fuel cells (kW <sub>e</sub> )	17616	15724	17585	15700
Steam turbine (kW <sub>e</sub> )	3629	3747	3320	3320
Anode expander (kW <sub>e</sub> )	0	348	0	863
Post-fuel cell expander (kW <sub>e</sub> )	10010	10780	9401	9339
Gross power (kW <sub>e</sub> )	31255	30599	30306	29222
FC air compressor (kW <sub>e</sub> )	–6800	–7870	–19505	–18140
Hot gas quench blower (kW <sub>e</sub> )	–118	–118	–118	–118
Sulphur recovery blowers (kW <sub>e</sub> )	–885	–885	–885	–885
Pumps (kW <sub>e</sub> )	–70	–73	–72	–72
Net consumption	–7873	–8946	–20580	–19215
District heat (kW)	19036	20074	29045	28908
Net power (kW <sub>e</sub> )	23382	21653	9726	10007
Power efficiency (% LHV)	46.7	43.3	19.4	20.0
Overall efficiency (% LHV)	84.8	83.1	77.5	77.8

as the “best case” scenario, but in reality the increase in fuel cell power production is likely to be less than 12%. This is because the one-point model used in the simulations does not account for the influence of increased gas flow or changes in gas composition on the average cell voltage. As the anode recycle is introduced, the concentration of the reacting species, i.e. H<sub>2</sub> and CO, will decrease, thus lowering the average cell voltage.

As the anode recycle is introduced, the expansion step, which in the case without recycle is used to expand the high-pressure syngas to the inlet pressure of the anodes, has to be removed. This piece of equipment is replaced by an ejector, which increases the pressure of the anode off-gas recycle flow, using the high-pressure syngas stream as the driving stream.

As a result, the power from the pre-anode expansion is no longer available in the anode recycle case. Furthermore, the introduction of the anode recycle stream, results in an increased gas flow through the anodes, which will give a higher contribution to the cooling of the fuel cells. The effect of this contribution can be seen in the fact that the non-anode recycle case has a 19% higher inlet flow to the cathodes than does the case with anode recycle.

However, this effect of decreased cathode inlet flow is not entirely beneficial. As a result of both decreased cathode throughput, and anode recycle, the mass flow through the post-fuel cell expander will decrease, decreasing the power produced by this unit by 7%. Similarly the amount of steam that can be raised by the expansion step effluent

stream will decrease, thus lowering the power output of the steam turbine by 3%. As a result the net power production will increase by 8%.

A consequence of the increased fuel utilisation resulting from the introduction of the anode recycle is that the design of the fuel cell stack has to be changed compared to the stack used in the cases without a anode recycle. The reason is that if the same stack, with a constant current density were to be used, the increased fuel utilisation would result in a decrease in average cell voltage. In order to avoid this drop in cell voltage the current density has to be decreased. In order to maintain the same power production, or even increase it, the cell area has to be increased. Therefore, another stack design will be required.

## 5.2. MCFC cases with and without anode off-gas recycle

When comparing the MCFC cases in a similar way as the SOFC cases earlier, it can be noticed that even though the introduction of an anode off-gas recycle results in an increase in the power produced by the fuel cell by 12.6%, the overall power produced by the system is slightly lower. This is quite the opposite from the SOFC case where the introduction of an anode off-gas recycle increased the overall power produced.

So, what may be the cause for this completely different behaviour?

To start with, the increase in overall fuel utilisation by 13% does result in a similar 12% increase in the power

Table 10  
Comparison of different power generation techniques

Case	BARAKA	IGCC [39]	PFBC [40]
Unit size (MW <sub>e</sub> )	23.4	262	70
Electrical efficiency (% HHV)	45.1	39.7	33.2
SO <sub>2</sub> (g/MWh)	0.7	612.4	774.5
NO <sub>x</sub> (g/MWh)	133.6	494.4	288.0

produced by the fuel cells as in the SOFC case. But here the similarities end. In the SOFC case the introduction resulted in a flow increase through the anode, which could balance the increase in cooling need, resulting from a higher fuel utilisation. In the case of the MCFC, however, the increase in anode flow is not high enough to remove the extra heat resulting from a higher fuel utilisation, and thus the cathode flow has to be increased by 4.6%. This results in a 0.8% increase in the fresh airflow and an increase of almost 13% in the pressure to which this stream has to be compressed. As a result the power consumption of the fuel cell air compressor will increase by 7.5%.

The slight increase in power production by the post-fuel cell expander is not able to make up for the increased work consumed by the air compressor, and as a consequence the overall power production will decrease by about 3%.

As in the case with, and without anode recycle in the SOFC cases, different stack designs have to be used in the non-anode recycle and anode recycle cases.

### 5.3. Efficiency and environmental issues compared to existing technique

As mentioned, one issue to investigate was how the BARAKA-system would perform compared to systems based on more traditional power generation techniques.

In Table 10, below, the characteristics of different techniques for power generation from coal are presented. The techniques that were compared were integrated gasification combined cycle (IGCC) and pressurised fluidised bed combustion (PFBC).

As can be clearly seen, the BARAKA system is able to compete, and actually outrun the existing techniques, both regarding electrical efficiency, as well as emissions.

### 5.4. General discussion

When comparing the different options, MCFC and SOFC, it is obvious that in this application the SOFC seems to be superior to the MCFC option. It is not possible in the MCFC cases to mount the fuel cell air compressor on the same shaft as the post-fuel cell expander. Therefore, the air compressor has to be powered individually, introducing an electrical efficiency into the calculations.

An additional factor that may influence the result in an unfavourable direction for the MCFC is the fact of the more

Table 11  
Gas compositions obtained after gas cleanup

Gas outlet temperature (°C)	400
Outlet pressure (bar)	19.25
Purification outlet flow (kg/h)	11325
Mole fractions (%)	
CH <sub>4</sub> (ppm)	20
H <sub>2</sub>	27.9
CO	63.3
CO <sub>2</sub>	3.7
H <sub>2</sub> O	0.5
N <sub>2</sub>	4.5
H <sub>2</sub> S	1
COS (ppm)	0

complex flowsheet resulting from the need to transfer the CO<sub>2</sub> produced at the anodes to the inlet of the cathodes.

The introduction of the anode recycle has a different effect on the overall electrical efficiency for the SOFC and MCFC cases. In the SOFC case, the recycle increases the overall electrical efficiency, but lowers it for the MCFC option. One explanation is different operation windows regarding the operational temperature. The SOFC has an 800–1000 °C temperature window of operation, compared to the 600–700 °C window of the MCFC. As a result, the increased anode flow through the SOFC anodes resulting from the anode recycle is able to remove the additional heat generated by the increase in fuel utilisation. In the MCFC case, however, the smaller allowable temperature increase has the consequence that the increased anode flow itself does not provide sufficient heat removal, and the airflow through the cathode has to be increased.

Regarding the environmental merits of the system, it was noted that as a result of the extensive gas cleaning needed prior to the fuel cell, the level of impurities after gas clean up is low. As seen in Table 11, the levels of H<sub>2</sub>S after the gas clean up is in the range of 1 ppm. As a result of the dilution taking place during the post-fuel cell combustion, the concentration drops further down to 0.08 ppm on a volume basis.

The advantage regarding gas clean up that a fuel cell system has compared to the combustion of the gasifier gas in a gas turbine is easy to realise when comparing the gas flows to be treated.

The NO<sub>x</sub> formed in the combustion step of a traditional combustion process makes it necessary to put the gas cleaning step after the combustion step, resulting in high volume gas flows to be treated. The absence of processes producing harmful substances in the fuel cell makes it possible to place the gas clean up prior to the fuel cells, where only the anode feed has to be treated.

Calculations show that the mass flow leaving a gas turbine fed with the same amount of fuel as a fuel cell is about 12.5 times greater than the flow leaving the gas clean up in the fuel cell case. If the volumetric flows at different pressures are compared, the difference is even greater.

## 6. Conclusions

As has been shown in this study, it should be possible to convert coal into electricity via coal gasification and high-temperature fuel cells with an electrical efficiency exceeding 40%.

The performance of the combined system of coal gasification and fuel cells are able to compete with, and outperform, existing techniques regarding efficiency and emission levels.

In order to achieve an overall efficiency exceeding 80%, the power system must be included as part of a network for the distribution of district heat.

In order to do so, the best option is found to be solid oxide fuel cells, with both an anode and cathode off-gas recycle for fuel cell stack cooling.

As somewhat of a surprise it is found that in the case of molten carbonate fuel cells, the behaviour is different, i.e. the introduction of both anode and cathode off-gas recycles actually results in a slight decrease both in the electrical efficiency and overall efficiency of the system.

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