Modelling and optimisation of Solid Polymer Fuel Cell (SPFC) systems for transportation and stationary applications

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MODELLING AND OPTIMISATION OF
SOLID POLYMER FUEL CELL (SPFC) SYSTEMS
FOR
TRANSPORTATION AND STATIONARY
APPLICATIONS

by

Maheboob. B. V. Virji
B.Eng. (Hons.), M.Sc. (Eng)

A Doctoral Thesis

Submitted in partial fulfilment of the requirement for the award of

Degree of Doctor of Philosophy of Loughborough University

August 2002

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ABSTRACT

Research and development of solid polymer fuel cell (SPFC) systems for the transportation and stationary power generation industries has evolved rapidly over the last decade. This growth has been due to the ever-increasing demand for a cleaner and more efficient technology in these industries. To compete with the existing technology, SPFC systems have to be highly efficient at both full and partial loads, environmentally friendly (in terms of emissions and noise) and competitively priced. For many applications, SPFCs have the potential to deliver a system that can fulfil these criteria. However, a number of system design issues have to be addressed in order to provide a well integrated and optimised system, which is a practical alternative to conventional modes of energy conversion.

A SPFC normally uses hydrogen as fuel and air as the oxidant. The hydrogen is supplied either in its pure form or as a hydrogen rich gas from a fuel processor. The air is usually supplied above ambient pressure via a compressor or air blower. The configuration and integration of the SPFC power system is greatly influenced by the choice of fuel. The overall performance of the system also depends critically on the thermal integration and operating conditions of individual components. A detailed and comprehensive analysis of three individual SPFC power systems has therefore been conducted with an aim to optimise the electrical and overall system efficiencies. Each particular system was characterised by the primary fuel utilised to produce a hydrogen rich gas, i.e. natural gas, methanol and diesel. All systems include a fuel processor, a compressor and an expander. Steady state and dynamic simulation tools were developed and employed to analyse these systems for stationary and transport applications.

A thermally integrated 40 kW<sub>e</sub> natural gas based SPFC combined heat and power (CHP) system achieved a predicted overall efficiency >80% and a heat to power ratio of 1.5. An optimised 50 kW<sub>e</sub> methanol fuelled SPFC vehicle system attained a high electrical (pre-drivetrain) efficiency >50% and superior vehicle system efficiency >45%. A dynamic simulation to study the component interactions between a 1.5 MW SPFC (marine) system, diesel fuel processor and 8448 kWh (C5 rate) battery pack
estimated an electrical system efficiency of 31% with the SPFC stack operating at a thermal efficiency of 58%. The performances of a 4.6 tonne SPFC powered van was compared with measured results from actual brass-board integration of a methanol reformer/SPFC/battery hybrid van system. The results for drive cycle simulation tests correlated to within 2-3% compared to results from the brass-board system.

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Finally and most importantly, I would like to thank my family for their support and love. A special thanks also goes to the Ismaili Community for providing financial support especially during early part of my education.
“Struggle is the meaning of life. Defeat or victory is in hands of god, but struggle itself is man's duty and should be his joy.”

Aga Khan III (1877-1957)
Dedicated to the loving memory of my
Mum and Dad
NOMENCLATURE

The symbols used in different sections of the thesis are listed below. SI units are used throughout.

Electrochemistry of the SPFC – (Thermodynamics & Electrode Kinetics)

\[ \Delta H^o \] - Enthalpy change for the reaction, kJ/mol
\[ \Delta G^o \] - Gibbs free energy change, kJ/mol
\[ \Delta S^o \] - Entropy change for the reaction, kJ/mol
\[ n \] - the number of moles of electrons transferred
\[ F \] - Faraday Constant, \( F = 9.64846 \times 10^4 \), C/mol
\[ L \] - Avogadro Constant, \( L = 6.02205 \times 10^{23} \), mol\(^{-1}\)
\[ e \] - Electron charge, \( e = 1.60219 \times 10^{-19} \), C
\[ E^o_{\text{rev}} \] - The standard theoretical reversible cell potential
\[ \eta_{\text{rev}} \] - Theoretical reversible efficiency, %
\[ Q_{\text{rev}} \] - Heat released from the fuel cell, kJ/mol
\[ W_{\text{elec}} \] - Electrical work output, kW
\[ I \] - Electrical current, Amps
\[ \dot{M}_{\text{H}_2} \] - Hydrogen molar flowrate, mol/s
\[ \dot{M}_{\text{O}_2} \] - Oxygen molar flowrate, mol/s
\[ \eta_{\text{Th}} \] - Thermal efficiency, %
\[ \eta_V \] - Voltage efficiency, %
\[ V \] - Fuel cell voltage, volts
\[ E \] - Thermodynamic equilibrium potential, volts
\[ \eta_{\text{act}} \] - Overvoltage due to activation loss, volts
\[ \eta_{\text{ohmic}} \] - Overvoltage due to ohmic resistance, volts
\[ E^0 \] - Standard state reference potential, V
\[ P_{\text{H}_2}, P_{\text{O}_2} \] - Partial pressure of components
\[ T, T_0 \] - Operating and datum temperature, K
\[ \xi_{1-4}, r_{1-3} \] - Estimated Parameters
Relative Humidity Calculations for SPFC

\( \phi \) - Relative humidity

\( P_a \) - Actual partial pressure of the vapour

\( P_s \) - Partial pressure of the vapour

\( T_{fc} \) - SPFC Operating temperature, K

\( P_{fc} \) - SPFC Operating Pressure, Bar

\( M_t \) - Total Molar flowrate of the Cathode, mol/s

\( M_w \) - Molar flowrate of water in cathode stream, mol/s

\( P_{ref} \) - Reference pressure = 1 atm = 1.01325 bar

\( T_{ref} \) - Reference temperature = Boiling point of water = 373.15 K

\( \Delta H_{vap} \) - Standard molar enthalpy of vaporisation = 40.62 kJ/mol

\( R \) - Gas Constant, \( R = 8.3145 \text{ J/molK} \)

\( \omega \) - Humidity ratio or specific humidity

\( m_a \) - Mass of the water vapour, kg

\( m_g \) - Mass of dry exhaust or feed gases, kg

\( V \) - Volume, m\(^3\)

\( P_g \) - Partial pressure of the dry cathode gases

\( M_{Wa} \) - Molecular weight of the actual water or vapour

\( M_{Wg} \) - Molecular weight of the dry cathode gases (O\(_2\), N\(_2\))

Chemical and Thermal Power Calculations

\( P_{Ch} \) - Chemical power of the working fluid, kW

\( \dot{M} \) - Molar flowrate of the working fluid in the stream, mol/s

\( P_{Th} \) - Thermal Power of the working fluid, kW

\( C_p \) - Molar heat capacity, kJ/mol K

\( T_1, T_2 \) - Absolute temperatures for operating condition 1 & 2, K

- VII -
> Condensing Economiser

\[ \begin{align*}
\text{P}_{\text{Cas}} & \quad \text{-Casing Losses, kW} \\
\text{T}_{W\text{.In}} & \quad \text{-Temperature of feed water, K} \\
\text{P}_{W\text{.In}} & \quad \text{-Thermal power of feed water, kW} \\
\text{T}_{W\text{.Out}} & \quad \text{-Temperature of hot water, K} \\
\text{P}_{W\text{.Out}} & \quad \text{-Thermal power of hot water, kW} \\
\text{T}_{\text{FG.In}} & \quad \text{-Flue gas inlet temperature, K} \\
\text{P}_{\text{FG.In}} & \quad \text{-Flue gas thermal power, kW} \\
\text{T}_{\text{FG.Out}} & \quad \text{-Flue gas outlet temperature, K} \\
\text{P}_{\text{FG.Out}} & \quad \text{-Flue gas outlet thermal power, kW} \\
\text{T}_{\text{Con}} & \quad \text{-Temperature of condensate, K} \\
\text{P}_{\text{Con}} & \quad \text{-Thermal power of condensate, kW} \\
\dot{M}_f & \quad \text{-Molar flowrate of gas, (mol/s)} \\
\text{Cp}_f & \quad \text{-Heat capacity of gas, kJ/mol K} \\
\text{T}_d & \quad \text{-Datum Temperature, } T_d = 298.15, \text{ K} \\
\text{T}_{\text{dew}} & \quad \text{-Dew point temperature of the water at its partial pressure, K} \\
\Delta \text{H}_{\text{vap}} & \quad \text{-Enthalpy of Evaporation at the dew point temperature, kJ/mol} \\
\text{Cp}(w), \text{Cp}(v) & \quad \text{-Heat capacity of water and vapour, kJ/mol K} \\
\eta_{\text{Ecn}} & \quad \text{-Condensing economiser efficiency, \%} 
\end{align*} \]

> Battery

\[ \begin{align*}
\text{R}_c & \quad \text{-Charge Resistance, ohms} \\
\text{R}_d & \quad \text{-Discharge Resistance, ohms} \\
\text{I} & \quad \text{-Battery Current, Amps} \\
\text{V}_B & \quad \text{-Battery Voltage, Volts} \\
\text{E}_C & \quad \text{-Cell Potential, Volts} \\
\text{P}_B & \quad \text{-Battery Power, kW} \\
\text{P}_{B\text{.Max}} & \quad \text{-Maximum Battery Power, kW} \\
\text{SoC} & \quad \text{-State of charge, \%} 
\end{align*} \]
Compressor & Expander

- Air inlet temperature, K
- Air outlet temperature, K
- Compressor isentropic efficiency, %
- Compressor outlet pressure, Bar
- Compressor air inlet pressure, Bar
- Ratio of specific heats, $C_p/C_v$, (1.4 for air, 1.33 for flue gases)
- Flue gas inlet temperature, K
- Flue gas outlet temperature, K
- Expander isentropic efficiency, %
- Expander outlet pressure, Bar
- Expander flue gases inlet pressure, Bar
- Mechanical transmission efficiency of the shaft, %

Efficiencies

- Reformer efficiency, %
- Power for the reformer reaction, kW
- Fuel processor efficiency, %
- Overall system efficiency, %
- Heat to power ratio
- Electrical system efficiency, %
- Heat system efficiency, %
- Overall drivetrain efficiency, %
- Ancillary system efficiency, %
- Vehicle efficiency, %
1. INTRODUCTION

A Solid polymer fuel cell (SPFC) or polymer electrolyte membrane (PEM) fuel cell is an electrochemical device which converts the chemical energy of a fuel, mainly hydrogen, into electrical and heat energy in the presence of an oxidant, usually oxygen from the atmospheric air. Unlike the conventional combustion of hydrogen and air, the SPFC prevents the direct chemical reaction of the reactants by means of a solid electrolyte and therefore, the overall reaction in a SPFC takes place at a much lower temperature and can be viewed as cold combustion. A SPFC power system is one in which the equipment for supplying the reactants to the cell at suitable operating condition and appliances for safely supplying the generated electrical power and removal of heat are present. A simple SPFC system may only consists of pressurised hydrogen and air tanks while a complex system may consists of a fuel processor (hydrogen rich gas generator) and a compressor/expander scheme. However, depending on the application of the SPFC power system some subsystems such as electrical vehicle traction system or a waste heat recovery scheme may also be included.

Since the resurgence of SPFCs in the early eighties, the SPFC performance has improved greatly and manufacturing costs have gradually fallen over the years. Today, the SPFC technology with its superior operational characteristics such as high efficiency, ultra-low emissions, part load characteristics and modularity, has emerged as one of the best fuel cell technologies to breakthrough into both the stationary and transportation market. However, the lack of hydrogen fuel supply infrastructure has hindered the further commercial success and mass-production of the SPFC power technology. Hydrogen storage, either as liquid or compressed gas, has its storage (low energy density) and handing (boiling point -253°C) problems. Chemical extraction of hydrogen from a hydrocarbon fuel with established supply infrastructure is becoming an attractive option, and is currently pursued strongly under research and development. However, the use of an on-board fuel processor makes the system design much more complex and introduces an inevitable loss in the overall system performance.
To penetrate the well-established and competitive power generating market, a practical SPFC power system with a fuel processor, for a given application, needs to be well designed and integrated and its performance optimised. To accomplish these objectives, an analysis is required, not only to understand the system requirements and integration issues, but to optimise the performance of individual component to achieve the best overall performance. However, to meet commercial cost targets, an economic appraisal should also be included in this study to make the necessary cost trade-offs over the various components, including SPFC stack.

1.1 OBJECTIVES AND OVERVIEW OF THE THESIS

The overall performance of a SPFC power system depends critically on the choice of fuel feedstock, fuel processing technology, air supply method and heat recovery scheme. Process variables critical to the performance of the individual components must also be determined to give rise to optimum system performance. Finally, the application of the SPFC power system has great influence on the system configuration and thermal integration.

Hence, the main objectives of this thesis are:

- To develop steady state models of a 40 kW\textsubscript{e} natural gas fuel processor/SPFC, a 50 kW\textsubscript{e} methanol fuel processor/SPFC and a 1.5 MW\textsubscript{e} Diesel fuel processor/SPFC system for cogeneration, transportation and marine applications respectively.

- To analyse each system’s performance as a function of operating conditions of the main components and to determine the optimal operating conditions to maximise the overall efficiency.

- To investigate the effect of thermal integration on the overall performance by maximising the use of waste heat energy and preheating reactants.
To investigate the effect of condensing or preheating SPFC stack anode and cathode (off-gases) exhaust gases on the performance of the system. The use of these exhaust gases in the burner/expander system is also analysed.

To develop a Methanol/SPFC hybrid vehicle simulation and study the performance of the hybrid vehicle under realistic drive patterns. The results of the simulation were compared with the results from an actual Methanol/SPFC hybrid vehicle drive train under the same realistic drive patterns.

To develop a dynamic Matlab/Simulink simulation of a 1.5 MW_e SPFC power system with a diesel fuel processor and to investigate the performance of this hybrid system under a marine load duty cycle.

To compare the results of the steady state analysis of the three different SPFC power generating systems.

This thesis consists of six chapters supplemented by an appendix. The thesis begins with a review of the SPFC technology (chapter 1) describing the initial pioneering work and continues on to the current status of technology. The review also highlights the successful performance of both SPFC and SPFC system achieved to date. Chapter 2 is an introduction to a generic fuel cell system and its major components. The chapter also includes the working aspects of a SPFC.

Chapters 3-5 focus extensively on three SPFC power systems for cogeneration, transport and marine applications respectively. Each chapter begins with an introduction, which gives the overview and review of the past and present status of both the fuel cell system and competing alternative technologies in that sector of the industry. Following the introduction, a steady state analysis (for each system) is carried out to find the optimal operating conditions and configuration to maximise the overall system performance. The results from these analyses are also discussed in these chapters. Chapter 4 and 5 also include the development of two SPFC hybrid systems simulation and the simulated results of these hybrid systems under a duty cycle.
Finally, the thesis finishes with chapter 6, which summaries the main findings of the three steady state analyses of SPFC power system for cogeneration, transportation and marine applications. Recommendations for possible future work are also provided.

1.2 REVIEW OF SPFC TECHNOLOGY

1.2.1 EARLY DEVELOPMENT OF SPFC (1889-1980)

Solid polymer fuel cells (SPFCs) were first developed and commercially used in the early 1960’s, nearly 120 years after Sir William Grove invented the fuel cell [1,2,3]. Although no commercial SPFC systems were develop prior to the 1960’s, there were attempts to develop laboratory practical systems. In 1889 Ludwig Mond and Charles Langer, who first named their apparatus fuel cell, developed a practical fuel cell which, for the first time, used a solid form of acid electrolyte, so called the matrix electrolyte. This fuel cell generated 1.5 W of electricity at 50% efficiency using impure hydrogen from coal and air instead of oxygen. The high cost of using platinum as the catalyst and the drop in the performance due to CO in the impure industrial gas, led to no further development of this fuel cell concept [2]. After 1889, the Mond and Langer fuel cell concept was further researched and coal fuelled fuel cells were develop by researchers like Jacques/Baur (1895), Haber/Brunner (1904) and Baur/Ehrenberg (1922), but without successful results due to unsuitable chemistry and inadequate engineering [4]. Eventually in 1959 Francis T Bacon combined the pioneering work of previous researchers to build the first practical fuel cell (H₂/O₂ alkaline electrolyte) system, capable of powering a small machine [2]. Subsequent use of this system in the NASA Apollo lunar project in 1960 resulted in rapid growth in fuel cell technology in both industries and research laboratories.

Following the success of fuel cell technology in the Apollo mission and the availability of Teflon led to the development of the SPFC by General Electric in early 1960 [4]. The fuel cell, then referred to as an ion-exchange membrane (IEM) cell, utilised a combined electrode-electrolyte assembly that consisted of a cationic membrane of sulfonated polystyrene resin. The electrolyte membrane structure made the SPFC simple, reliable and automatically water rejecting. However, the electrolyte
material restricted its operating temperature and hence its performance. These moderate power-delivering cells were used to build the first SPFC H₂/O₂ system for the Gemini Mission. The three SPFC stacks used in this system each consisted of 32 cells and delivered 1kWe of electric power [5]. These stacks were used in other Gemini missions between 1960 and 1965. Around 1968 DuPont manufactured an improved Nafion® membrane and this was used in the SPFC system to power the Biosatellite spacecraft in 1969. The new membrane significantly improved the power density of the SPFC from 538 W/m² to 969 W/m² and the operating lifetime of the SPFC by 500 h to 50 000-hrs [6]. Although the Nafion® membrane improved the performance of the SPFC, water management problem in the cell led to the membrane drying out which resulted in severe performance loss. Due to this problem, SPFCs achieved lower power densities compared to the Beacon alkaline fuel cells and hence were not selected for the Apollo program by NASA. This setback and the high cost of platinum as the electrocatalyst restricted the significant research advances and commercialisation of the SPFC technology until the 1980’s.

1.2.2 DEVELOPMENT OF THE SPFC AND SPFC SYSTEMS (1981-2001)

In the early 1980’s the defence industry recognised that SPFC technology could fulfil some of the growing military power needs and could be reengineered for terrestrial applications. In addition, a study conducted by General Electric (GE) concluded that an indirect methanol-air SPFC system had the potential of powering a small vehicle [6]. This interest by the defence sector and GE’s study initiated a resurgence in the SPFC research, after the initial set back in the 1960’s. To evaluate the SPFC’s potential in terrestrial applications, research work began in North America and Europe. In 1983 Siemens AG in Germany acquired knowledge from General Electric to develop a power source for an air independent submarine. Later in the same year Ballard Power systems also began developing SPFC technology with funding support from the Canadian Department of National Defence. The energy crisis in mid 1980 intensified the interest in fuel cell to provide an efficient and clean power source. Hence, by the late 1980’s many more companies, organisations and government energy departments were interested in conducting research work into SPFCs and developing environmentally friendly power sources, especially for transportation applications.
In 1989, Ballard Power Systems revealed at the first Grove Fuel Cell symposium in London that SPFC performance had improved by a factor of four and that the SPFC were ready for commercialisation. This improvement in the performance was due to a new ion-conducting membrane from Dow Chemical (Dow Membrane). This new membrane and electrode structure not only increased the performance, but also reduced the size, weight and cost of the cell. Compared to the Nafion® 117 membrane, the Dow membrane was thinner by around 75% and significantly flexible in the fabrication process which allowed performance optimisation and hence the improvement in the cell configurations. Ballard Power Systems also demonstrated the performance of their MK 4 single cell with Nafion® 117 membrane on air and reformed hydrogen fuels. There was a 30% drop in power at a given voltage using air as the oxidant. (The performance of MK 4 cells also decreased by 50% using 74.7% H₂, 25% CO₂ and 0.3% CO synthetic reformed gas). However, the performance was improved by 90% when the reformed gas was treated via a catalytic selective oxidation process [7].

SPFC commercialisation could be considered to have began with the MK 4 stack with Nafion® 117 membrane, which was delivered to Perry Energy Systems, to power an unmanned submersible. The performance of the MK 4 stack cells, with active electrode area of 50 cm², were improved by a factor of 5 by scaling up the electrode membrane assemblies from 12.7cm×12.7cm to 20.3cm×20.3cm and increasing the active area to 5232 cm². These new cells were used to build the MK 5 stack. In 1990, Ballard Power Systems were demonstrating their MK 5 SPFC system in a variety of applications in military, utility and motive areas. The MK 5 system was delivered to Perry Energy Systems and Daimler-Benz for evaluation purpose. Ballard also revealed that 10 kW H₂/air MK 5 system, using the Dow membrane, would also be delivered to Dow chlor-alkali plant and later to other companies in America, Canada, Europe and Japan for installation purposes [7, 8].

In Europe, Siemens AG were continuing with their three phase SPFC program, started in 1983 to develop a 34 kWe prototype unit. In 1990 they had completed the first phase of developing and evaluating a 5 kWe stack. The second phase, which was to build a 34 kWe laboratory type module, was under way and scheduled to be
completed in 1991 [9]. In the UK, Vickers Shipbuilding and Engineering Ltd and C.J.B developments Ltd were embarking on a project to develop a generic 20 kWe system demonstrator based on the Ballard SPFC stack and proposed a potential end use in either industrial or military market [10].

Research and development of the SPFC was continuing and was getting closer to commercialisation in both North America and Europe, as reported in the second Grove fuel cell symposium in late 1991. The US department of Energy had a SPFC propulsion system program for transport application. The program was divided into four phases, and the first phase of the program, to be completed in 1993 was to demonstrate a 10 kW breadboard system [11]. In Canada, Ballard Power Systems were focusing their attention on the development of the SPFC system and demonstration of the SPFC in practical applications. A hydrogen/air integrated fuel cell system was developed, based upon a stack with 32 cells and rated at 5 kW. In Europe, Siemens AG was continuing development of their laboratory 34 kW SPFC module and had only achieved 20 kW power (on pressurised hydrogen and oxygen) from a laboratory SPFC module consisting of 42 cells [12]. Vickers Shipbuilding and Engineering Ltd and C.J.B Developments Ltd (UK) were now focusing their effort on the development of support systems, such as a reformer, to be used in conjunction with the Ballard SPFC stack. Their current work was to produce a 20 kW methanol fuelled power generation system demonstrator [13].

At the 1992 Fuel Cell Seminar, Ballard Power Systems (BPS) reported the operation of a Methanol/Air SPFC system, which comprised a methanol reformer, selective oxidiser and a 10 kWe SPFC stack. The system was capable of load following operation to 3.5 kW for a duration of six hours. The prototype of this Methanol/Air SPFC system was schedule to be completed at the end of the year [14]. In addition to research and development of SPFC at BPS, an other notable SPFC research program was also underway at International Fuel Cells (I.F.C). During the late eighties research was carried out by I.F.C in order to develop SPFC systems as an alternative to battery technology. By the early nineties, I.F.C had successfully demonstrated a 10 kW prototype of a 20 kW SPFC plant (5 kW stacks with 80 cells each). The full-scale SPFC system was designed to replace existing Ag-Zn battery technology for an unmanned under water vehicle [15].
Between 1993 and 1996, substantial progress was made towards the commercialisation of SPFC. In Canada, Ballard Power System had announced the development of the third generation SPFC stack, MK 7. The MK 7 SPFC stack had at least five times greater power density than the MK 5, and consistent performance over a wide range of operating conditions. This performance was achieved in the MK 7 SPFC by use of bipolar plates, new membrane electrode assembly (MEA) design and better flow field design within the cells. A single cell and stack (10 cells) performance were tested for more than 2500 hours and the desired improvement in performance between MK 5 and MK 7 stacks was achieved. Table 1.1 summaries the performance and specification of the MK 5 and MK 7 stacks [16, 17].

Table 1.1 Performance and specification of Ballard MK 5 and MK 7 SPFC stacks

<table>
<thead>
<tr>
<th>SPECIFICATION</th>
<th>Mk 5</th>
<th>Mk 7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume (l)</td>
<td>32</td>
<td>32</td>
</tr>
<tr>
<td>Weight (kg)</td>
<td>40</td>
<td>40</td>
</tr>
<tr>
<td>No. of Cells</td>
<td>35</td>
<td>140</td>
</tr>
<tr>
<td>Power (kW)</td>
<td>5</td>
<td>32</td>
</tr>
<tr>
<td>Stack Efficiency (%)</td>
<td>47</td>
<td>55</td>
</tr>
<tr>
<td>Volumetric Power Density (W/l)</td>
<td>156</td>
<td>1000</td>
</tr>
<tr>
<td>Gravimetric Power Density (W/kg)</td>
<td>125</td>
<td>800</td>
</tr>
</tbody>
</table>

This third generation SPFC stack (MK 7) had exceed the power density target of 1000 W/l identified by PNGV (Partnership for a New Generation of Vehicles, US). Having attained the necessary power density, the emphasis of the development and commercialisation program was to retain this power density and concentrate on reducing the stack cost. This was to be achieved by lowering the platinum catalyst loading and manufacturing in volume at costs competitive with the internal combustion engine. Ballard had also reported that several organisations and companies where developing new, low cost, membrane electrolyte and flow field plates or bipolar plates which were either retaining or improving the current stack performance [16].
By 2001, the SPFC system was near commercialisation and the emphasis was on reducing the cost of manufacturing SPFC stacks. Many companies, government organisations and academic institutions were concentrating on developing high performance and low cost stack components like membrane electrode assemblies (MEAs), bi-polar plates and ancillary stack components (humidifiers, pumps, heat exchangers, condensers etc). By end of 2001, there were nearly 850 fuel cell related companies and organisations involved in development of fuel cell systems (SPFC, SOFC, AFC, PAFC & MCFC) and their components. This created competition and lowered costs via mass-production [18].

Although Ballard Power System were responsible for significant advances in commercialisation of SPFC technology between 1980 and 2001, there were many other companies, government organisations and academic institutions worldwide who were also pursuing vital research and development of the SPFC and SPFC system. The next two sections (1.2.3 & 1.2.4) highlight some achievements of this research and development of the SPFC systems for transport and stationary applications.

1.2.3 DEVELOPMENT OF SPFC SYSTEM FOR TRANSPORT APPLICATION (1981-2001)

In 1989 all major types of fuel cells were evaluated for use in transportation applications. SPFCs were found to fulfil most of the stringent requirements such as high power density, rapid start-up, toleration to CO₂ and being sufficiently inexpensive to compete with internal combustion engines. Hence, the U.S. Department of Energy endorsed SPFCs as the leading contender for passenger vehicles [19]. However, before the SPFC system could be used to power these vehicles, a great deal of research and development work was still required in order to optimise the performance of the fuel cells and the integration of the system into the vehicles.

Research and development in fuel cell system and fuel processing system grew rapidly as the demand for an efficient and clean technology intensified in the early 1990’s. In North America, especially in California State, the focus was on finding an alternative technology to replace conventional engines. In 1990, General Motors
Corporation conducted a simulation study of a methanol fuelled fuel cell/battery hybrid vehicle which showed that SPFC had similar power density to spark ignition engines, high part load efficiency and 90% reduction in regulated emission, with 40% reduction in CO₂. They also revealed a 4 phase, six and half-year programme in conjunction with US Department of Energy (DOE), Los Alamos National Laboratory, Dow Chemical Company and Ballard Power Systems, to build, test and install in a vehicle a 80 kWe methanol fuelled SPFC/battery hybrid power source [20]. In Canada, they were also involved in a methanol reformer program and a 100 kW unit for a Canadian bus program with various Canadian authorities and Government department [8].

The renewed interest in the fuel cell technology (for transport application) was sparked off by the new Clean Air Act passed by US congress and made law by the president of the USA in late 1990. The law mandated a nation wide reduction in SO₂, NOₓ, ozone emissions and the control of CO₂ emissions by enforcing a carbon tax. This law put a real ‘cleaning’ cost on existing technologies and justified the price of developing fuel cell technology. This renewed interest in fuel cell technology further boosted the fuel cell commercialisation programs not only in America, but also worldwide [21]. Furthermore, the call by the California Air Resources Board (CARB) for a mandatory 2% sale of Zero-emission vehicles (ZEV) by 1992 (10% in 2003), had initiated the South Coast Air Quality Management District (SCAQMD) to devote similar resources to fuel cell development as to battery development, and promised great strides in technology improvement for the electric vehicle, with a view to improve the air quality in major urban areas of the world [22].

In 1991 Ballard Power Systems were embarking on a SPFC bus demonstration program. The first phase of this program was the demonstration of a commercial transit bus, fully powered by SPFCs and fuelled by on-board compressed hydrogen tanks. The bus was to achieve a range of at least 150 km and accelerate 1-50 kph in 20 seconds. The first phase of the program was to be completed in March 1993 [23]. Beside the research and development of the SPFC and SPFC system for transportation application, Lucas Automotive Ltd [24] and Loughborough University [25], in UK, were also conducting feasibility and simulation studies of SPFC hybrid electric vehicle.
Ballard Power Systems reported in 1992 that the fuel cell bus power plant was built and successfully tested. It consisted of 24 of Ballard’s first generation MK 5 fuel cell stacks, an air supply subsystem, fuel supply sub system, cooling subsystem, plant and traction motor controls [14]. General motors co-operation also stated in 1992 that with the current development of the SPFC system and its components at Los Alamos National Laboratories, the Dow Chemical Co. and Ballard Power Systems, SPFC technology had the potential to become competitive with future internal combustion engines and were envisioning a multiphase program leading to proof of concept testing of a fuel cell/hybrid vehicle [26].

In order to successfully commercialise and to compete with conventional technology, the fuel cell technology required major investment and sustained commitment from both government and industry. This aspiration was achieved in September 1993 in America, when a historic partnership between the US government and the automobile industry was announced. The partnership was called the Partnership for a New Generation of Vehicles (PNGV). The initiation of the PNGV further enhanced the fuel cell commercialisation program, especially for transportation applications. The PNGV’s aim was to strengthen US competitiveness by developing technologies for new generation of energy efficient and environmental friendly vehicles [27].

One of the goals of the PNGV was to develop a vehicle that could achieve up to three times the fuel efficiency of comparable 1994 American family sedans. The aim was produce a prototype vehicle by 2004, which would have a fuel consumption of 80 miles/gallon or 34 km/l and meet the safety and emission requirements. To achieve this goal, in 1994 the US Department of Energy (DOE) had awarded cost-shared, competitive contracts to teams led by General Motors (GM) Corporation, Ford Research Laboratory and Chrysler, to develop SPFC technologies for light duty vehicle. The GM team was to develop a SPFC based 60 kW brassboard system with on-board methanol reformer, while both the Ford and Chrysler teams were to develop 30–50 kW SPFC brassboard system using hydrogen fuel stored directly on-board the vehicle. These programs would also evaluate hydrogen storage, safety and infrastructure issues [27].
The Ballard's four phase bus program had completed the first phase in 1992 and successfully demonstrated that a SPFC system was capable of providing the entire power requirement for a bus. The second phase of the program, which involved the development of an engineering prototype for a commercial bus engine and the demonstration of a full size transit bus, powered by such an engine, was also completed by 1995. The 40 ft commercial transit bus engine consisted of 20 second generation (MK 513) SPFC stacks and produced a total of 200 kW (275 hp), the same power as the diesel engine typically installed in this bus. With the gaseous hydrogen fuel stored at a pressure of just above 200 bar (3000 psi), the bus had a range of 400 km (250 miles). The third phase of the program involved production of two or three small fleets for testing by transit companies in routine operations, and the final phase, to be completed in 1998, was to commercialise the buses. The final commercial bus was to be based upon the third generation of the SPFC stack (MK 7 - 32 kW per stack) and the bus would incorporate an energy recovery system for regenerative breaking, which would increase the bus range to 560 km [16].

In Europe by 1995, many organisations and companies were also involved in the development of SPFC stacks and programs to develop SPFC systems for transport application. Siemens (Germany) [28] and De Nora (Italy) [29] were involved in developing SPFC stacks for automobile and naval applications respectively. The fuel cell group at Loughborough University (UK) had developed their first 1 kW stack as a research tool and were also involved in the European "BrassBoard Project" to develop a traction system for a 5 tonne vehicle [30,31,32].

By 1996, the application of the SPFC stack in a small passenger vehicle had been successful demonstrated by a joint program (started in 1993) led by Daimler-Benz and Ballard Power Systems (BPS). The aim of the joint program was to develop a high power density SPFC stack and to demonstrate it in a 6-passenger Minivan. The first phase of the program was to use the MK 5 SPFC stack and integrate it into a commercially available Mercedes MB 180 BZ Minivan. This phase was successfully completed in 1994 and the Minivan was given the name NECAR I (New Electric Car). The purpose of the NECAR I was to provide insight into the operation of a motive SPFC plant and to learn about the requirements for technology advancement [17]. A second SPFC powered vehicle (second phase), based on the Mercedes V-
Class Minivan, was also built (unveiled in 1996) and given the name NECAR II. The motive fuel cell power system used in the NECAR II was built around two MK 7 stacks, which provided the same power as the 12 Mk 5 stacks in NECAR I. The NECAR II exhibited an increased range of around 100 km and a maximum speed of 110 km/h (90 km/h for NECAR I). Compared to an IC engine van, the NECAR II averaged fuel efficiency of up to 40% (15-25% for IC engine), similar derivability and zero emissions [17].

Other SPFC vehicle development in America was also being carried out at Energy Partners, Inc. In 1996 they revealed the development of a Gator™ SPFC powered utility vehicle. The utility vehicle was powered by a 10 kW SPFC stack and used pressurised hydrogen as fuel. The vehicle achieved a maximum speed of 23 mph, and at maximum power the SPFC stack generated 9 kW, of which, around 3 kW was used to operate air compressor and ancillary equipment. At low loads, the vehicle did achieve high efficiency and operated for more than 4 hours [33].

In Europe, many companies such as Ansaldo and De Nore and other organisation were involved in utilising SPFC systems in both surface and marine vehicles. The EQHHPP FC BUS and BOAT programs were currently in their final stages, with testing due in 1997, while the FC-BUS and HYDRO-GEN (Joule III) programs were just starting in 1996. The European Commission Joule II project, FEVER (Fuel Cell Electric Vehicle for Efficiency and Range), which started in 1994, was aiming to develop a high efficiency passenger car (Renault LAGUNA) and achieve a range of about 500 km. The testing of this vehicle was due to start in spring 1997 [35].

In 1997, the first fuel cell vehicle to run on liquid fuel, NECAR III, was unveiled at the International Auto Show in Frankfurt. The NECAR III was a 50 kW experimental vehicle operating with a methanol reformer and having a long range up to 400 km [35]. In addition, in 1997, DaimlerChrysler also revealed the NeBus, a fully functioning city transit bus with a 250 kW fuel cell system (10 stacks) and on-board hydrogen tanks.

In Japan, Toyota had developed and introduced a SPFC electric vehicle using hydrogen as fuel in 1996. The SPFC system was installed under the floor of RAV4L,
sport utility vehicle, along with a metal hydride tank and synchronous permanent-magnet motor. The Toyota FCEV had a 20 kW_e SPFC stack and a range of 250 km per hydrogen hydride tank charge and maximum speed of 100 km/h. A methanol fuelled FCEV, based on hydrogen FCEV, was also developed and introduced in 1997. The methanol fuelled FCEV traction system had a 25 kW_e SPFC stack, a 50 kW motor, battery and a methanol tank. The methanol fuelled FCEV achieved a range of 500 km on a full methanol tank and a maximum speed of 125 km/hr. The performance of the SPFC stack used in the methanol fuelled FCEV was hindered by the presence of CO, CO₂ and methanol in the anode fuel stream. Toyota were addressing this problem of performance deterioration by the use of a CO selective oxidiser and an alloy electrocatalyst (Pt-Ru) in the fuel cell which would be tolerant to a mixture of gases and methanol in the anode fuel stream [36].

The PNGV program was focusing on increasing the performance and reducing the size of the SPFC and fuel processor system. The DOE-industry R&D program was supporting SPFC development by various fuel cell suppliers in America including Energy Partners, International Fuel Cells, Mechanical Technology, Inc., Analytic Power, Delphi Automotive and AlliedSignal [37]. By 1997 International Fuel Cells had built a high efficiency 50 (2 × 25 kW_e) SPFC stack that operated on hydrogen and ambient pressure air. It was believed that this SPFC stack would meet the PNGV performance target with low parasitic load (0.5 kW at 20% rated power and 3 kW at 100% rated power) [38]. With support from DOE, the fuel processing development for the PNGV program was being carried out at Arthur D. Little and Argonne National Laboratory (ANL), while a gas cleanup reactor (PROX technology – preferential oxidation) was developed at Los Alamos National Laboratory (LANL). Arthur D. Little had completed over 3000 hrs of testing on a 50 kW_e laboratory prototype of a fuel-flexible POX fuel processor, achieving 78% and 84% efficiency with gasoline and ethanol respectively. Furthermore, Arthur D. Little’s gasoline fuel processor was also integrated with 10 kW PROX unit (from LANL) to reduce CO levels from 8000 to 50 ppm. The next phase of the program was to integrate and test the fuel processor and gas clean unit with the SPFC stack [38].
In April 1999, a public/private California Fuel Cell Partnership (CaFCP) was formed to prepare fuel cell vehicles for the commercial introduction in California by 2003-04. The partnership expects to place up to 60 fuel cell passenger cars and fuel cell buses on the road between 2000 and 2003. In addition to testing the fuel cell vehicles, the partnership is also examining fuel infrastructure issues and beginning to prepare the California market for this new technology. The CaFCP currently consists of nineteen full members and nine associate members. The partnership includes companies like DaimlerChrysler, Ford, General Motors, Honda, Hyundai, Nissan, Toyota, Volkswagen and Ballard Power Systems, The UTC Fuel Cells, BP, ExxonMobil, Shell Hydrogen and Chevron Texaco. The CaFCP also includes organisations like the California Air Resources Board, the California Energy Commission, the South Coast Air Quality Management District, the U.S. Department of Energy and the U.S. Department of Transportation [39].

By 2000, the use of the SPFC power system with hydrogen as the fuel was well established, proven and demonstrated in many transport applications. Many of the SPFC transport application R&D projects or programs were either completed or in their final phase of development. The PNGV program was still pursuing the third objective of their program, which was to develop a prototype of an 80 miles/gal or 34 km/l family sedan that would meet customers' needs for quality and performance by 2004. To achieve this third goal of the program, the DOE was encouraging and supporting R&D of SPFC stacks, stack components (MEA, bipolar etc) and fuel processors. Epyx had developed a 50 kW_e partial oxidation fuel flexible processor, which could operate on methanol, gasoline and methane. The processor operated for more than 300 hrs and an achieved efficiency of > 70%. Argonne National Laboratory (ANL) had demonstrated a 3 kW_e fuel flexible autothermal reformer on gasoline and achieved a hydrogen outlet concentration of 38%. Los Alamos National Laboratory (LANL) had developed and tested the first 50 kW_e PROX CO clean-up system and the PROX system was installed in Energy Partners' natural gas SPFC system. PROX was capable of maintaining an outlet CO concentration of below 50 ppm at varying inlet CO concentration [40].

In November 2000, BPS in conjunction with DaimlerChrysler also unveiled the NECAR 5 (Methanol fuelled, 75 kW) prototype automobile in Berlin, Germany. The
NECAR 5 utilised methanol as a fuel with an advanced Ballard fuel processor and system developed to supply hydrogen to a Ballard fuel cell power train. Furthermore, BPS had also formed many sister companies to develop SPFC systems for different applications, while BPS would concentrate on commercialisation of SPFC stacks [41].

In October 2001, Ballard Power Systems announced that the ZEbus (Zero Emission Bus) had successfully completed its fuel cell bus demonstration program with SunLine Transit Agency (leader in alternate fuels research) in Thousand Palms, California and had produced exceptional performance results. The objective of the program was to educate the public on the safety and reliability of fuel cell vehicles. The ZEbus provided officials and riders alike with an opportunity to experience the pollution-free transportation technology of the future [39]. Furthermore, Ballard Power Systems (BPS) had completed (by 2001) its SPFC bus (P3 Bus - 205 kW, Hydrogen fuelled) demonstration program. Three local buses in Chicago, USA and three in Vancouver, Canada were used to prove SPFC engine efficiency in everyday operation during two separate two-year test programs. Collectively, these six buses travelled over 118,000 km (73,000 miles) in revenue service and over 200,000 passengers had an opportunity to experience the benefits of fuel cell technology.

By the end of 2001, many SPFC vehicles were built and demonstrated in North America, Europe and Japan. These vehicles were developed as part of joint programs or project between the SPFC system developers and major automobile manufactures with major investments and sustained commitment coming from the American and Japanese governments, the European Union and industry. The following is a list of some of these SPFC vehicles with selected details of the SPFC vehicle system specification and performance:

**North America:**

**Ford Motor Company:** passenger car P2000 FC EV presented in January 1999 at the Detroit Auto Show. This was believed to be the world’s first full size, full performance, five passenger car powered by SPFC. The engine consisted of $3 \times 25$ kW SPFC stacks from Ballard (Mark 700, 381 cells), 67 kW traction drive from
Ecostar (peak efficiency 91%) and a service battery pack. The car used pressurised hydrogen from two carbon fibre wrapped tanks from Dynatek. Each tank had a capacity of 41 l at 21°C, and a maximum operating pressure of 24.8 MPa. The car had a range and top speed of 160 km and 145 km/hr respectively. The car had successfully demonstrated that SPFC technology could power a vehicle that was emission free, fuel efficient, and competitive with IC engine vehicle performance [42].

**General Motors “Precept”** presented in January 2000 at the North American International Auto Show in Detroit, USA. The vehicle had 100 kW SPFC (400 cells, 260 - 340 V, 105 kW peak, 75 kW continuous) developed by GM with a compact design (1.0 kW/l, 1.0 kW/kg), 85 kW (peak, 35 kW continuous) elector motor (liquid-cooled) and two interchangeable battery packs. The hydrogen fuel was stored in a specially formulated "chemical Hydride" material (120 kg, 100 l total, 4.9 kg hydrogen storage) and the refuelling time was five minutes. The vehicle had a range of 800 km and a top speed of 190 km/hr [42].

**Ford Th!nk FC5 (Demo Ila vehicle)** was presented in September 2000 and the vehicle had 80 kW of SPFC stacks. The vehicle used compressed hydrogen as its fuel (2 kg at 35 MPa) and had a range and top speed of 160 km and 80 mph respectively. As part of the CaFCP, the vehicle was demonstrated in Californian cities and up to fifteen more vehicles were planed for 2001/2002 [42].

**Daimler-Chrysler "Sprinter”,** presented in 2001. The vehicle had 75 kW SPFC stacks and a 55 kW e-motor. The fuel used in the vehicle was hydrogen from 3 compressed hydrogen tanks (100 litres at 25 MPa). The vehicle had a range of > 150 km and top speed of 120 km/hr [42].

**GM/Chevrolet** presented in September 2001 and their vehicle engine had 25 kW SPFC stacks with gasoline reformer. The reformer had a hydrogen production rate of 70 kW, which could supply a fuel cell up to 35 kW [42].

**DaimlerChrysler Jeep Commander 2 (demonstrated vehicle),** presented in October 2001, the engine had 2 electric motors for permanent 4 wheel drive, SPFC
stacks, methanol reformer and nickel-metal-hydride battery. The vehicle ran on methanol [42].

**Europe:**

**Neoplan: Midi FC Bus** was presented in October 1999 and the bus project involved many partners such as Gottlob Auwärter GmbH & Co KG (Neoplan, Stuttgart) as project leader, bus manufacturer Deutsches Zentrum für Luft- und Raumfahrt e.V. (Stuttgart), De Nora as the supplier of the fuel cell stacks and many other Germany companies responsible for system integration, system control, propulsion and power electronics, project monitoring, technical vehicle maintenance etc. The bus engine had three SPFC stacks with net power of 40 kW, 14 modules of nickel metal hybrid batteries (21 kWh, max. 100 kW) and a water-cooled tandem asynchronous electric motor of 45 kW. The bus used four lightweight carbon fibre pressurised hydrogen tanks (250 MPa) as fuel and it had a range of 600 km and a top speed of 30-50 km/hr [42].

**Proton Motors: Bayern-Bus II** was presented in May 2000 at the fuel cell day in Munich. The bus engine had 80 kW SPFC stacks, four 70 kW electric motors with regenerative braking and energy storage system. The bus used pressurised hydrogen and achieved a range of 150-250 km. The bus also achieved a tank–wheel efficiency of 40%-45%. The project partners included Proton Motors PM (SPFC stack), Neoplan and Magnet Motor [42].

**PSA Peugeot Citroen: Hydro-Gen** was presented in June 2000 and was developed under the "HYDRO-GEN" project, funded by the European Commission (now the European Union) (JOULE III programme (reference number JOE-CT-95-013)). The project partners included Air Liquide, CEA, Nuvera (Fuel Cell), Ansaldo Ricerche Srl., Renault and Solvay S.A. (Belgium). The bus engine included a 30 kW SPFC stack, an electric motor (20 kW nominal, 33 kW max), storage battery and used pressurised hydrogen as fuel. The main objective of the project was the development of an innovative fuel cell system based on a SPFC stack with emphasis placed on cost reduction for on board application in electric vehicles [42, 43].
**CHAPTER I - INTRODUCTION**

**MAN: Fuel Cell City Bus** presented in May 2000 at the fuel cell day in Munich. The bus project was also supported by the European Union (EU) JOULE-THERMIE demonstration program. The project partners involved were L-B-Sytemtechnik GmbH (project coordination), MAN Nutzfahrzeuge AG (vehicle), MAN Technologie AG (storage system), Siemens AG Energieerzeugung KWU (SPFC stacks & drive system) and Linde AG (filling and periphery). The engine consisted of an ELFA drive system of 2 asynchronous motors, model 1 PV5135 (max. output 2 x 75 kW) and four SPFC modules with output of 120 kW. The bus was fuelled by hydrogen from nine pressurised tanks, with maximum filling pressure of 25 MPa. The bus range was more than 250 km and its top speed was 80 km/hr [42, 43].

**Volkswagen AG: CAPRI** completed by the end of May 2000. The project was supported by the EU JOULE III (Ref. JOE3950039) with approx. 2 million Euro. The partners involved in this project were Volkswagen AG (administrator, technical co-ordinator and tester of the demonstrator vehicle), Johnson Matthey Technology Centre, UK (catalytic technology and fuel processing unit), ECN, Energy Research Foundation NL (Electro-Chemical engine), AB Volvo Technological Development (compressor-expander unit, DC/DC converter and simulation work). The hybrid engine included an SPFC stack from Ballard, a traction battery and a methanol autothermal reformer [42, 43].

**Opel/GM: passenger car HydroGen 1** was presented in March 2000 at the Geneva and June 2000 Brussels motor shows. The car was a joint development between Opel and GM in the GAPC (Global Alternative Propulsion Centre). The car was powered by a 75 kW SPFC (GM) and a 55 kW three phase current motor. The fuel used was liquid hydrogen from a 75-litre tank and the car achieved a range of 400 km and a top speed of 140 km/hr. The car will be ready for market by 2004 [42].

**MAN: low floor bus with FC and LH2** will be ready sometime in 2001/02. This second bus under the same MAN project, under different contract, JOULE-THERMIE (Ref. TR-93-1998-DE, NNE5-1999-312), was to run on liquid hydrogen (350 litres). The bus engine has three SPFC stacks (40 kW) developed by De Nora. Other partners include Air Liquide and Siemens AG (electric drive). The bus range is
300 km and its top speed is 75 km/hr. The bus was to be demonstrated in Berlin, Copenhagen and Lisbon in year 2001-2002 [42, 43].

**Fiat Seicento Elettra H2 Fuel Cell** presented in February 2001. The Seicento Elettra project was the result of a co-operation between Fiat Auto and the Italian Ministry for Environmental Affairs and was developed by Fiat's Research Centre (Centro Ricerche Fiat). The prototype vehicle had 7 kW SPFC stack, battery pack and asynchronous three-phase AC electric motor (max. output: 30kW). The car runs on pure hydrogen from six pressurised tanks (200 bar). The range on hydrogen was 100 km and 140 km with battery. The top speed was 100 km/hr [42].

**Japan:**

**Honda Motor Company:** FCX-V1 was presented in November 1999 at the Tokyo Motor Show. The prototype vehicle used 60 kW Ballard SPFC stacks and hydrogen as fuel from metal hydride storage system. Three hundred cars are to be introduced into the market in 2003 [42].

**Mazda:** small passenger car was presented in November 1999 at the Tokyo Motor Show. The car was developed in an alliance with Ford, DaimlerChrysler and Ballard Power Systems and the aim was to test drive the car in Japan. The car engine included 50 kW SPFC stacks and a newly developed SPFC drive system. The car used hydrogen as fuel from a metal hydride storage system [42].

**Nissan:** passenger car was presented in May 1999. The car engine included 10 kW Ballard Stacks, lithium ion battery, synchronous motor (permanent magnet) and a methanol reformer. The car had top speed of 70 km/hr. The future targets were to use bigger SPFC stack (50-80 kW) and achieve a top speed of 120 km/h and a range 1.5 time better than the gasoline version with comparable consumption. Commercialisation was planed for 2003 or 2004 [42].

**Honda Motor Company:** passenger car was presented in November 1999 at the Tokyo Motor Show. The car was developed in co-operation with three companies, but the reformer and fuel cell stack were developed exclusively by Honda. The prototype
CHAPTER I - INTRODUCTION

car had 60 kW SPFC stacks and methanol reformer. The car is to be introduced into the market in 2003 [42].

Mazda Premacy FC-EV was presented in 2001. The car was powered by a Ballard fuel cell power train using methanol as the fuel. The Premacy is currently being road-tested in Japan [41, 42].

Hyundai "Santa FE" was presented in March 2001. The demonstration car was develop as part of CaFCP and powered by 75 kW SPFC by IFC. The car was fuelled by pure hydrogen from pressurised tanks and had a range of 160 km [42].

Toyota / Hino Fuel Cell Bus was presented in June 2001. The prototype bus had a hybrid engine with 90 kW SPFC stacks, Ni MH battery and a permanent magnet electric motor (max. output-2x80kW). The bus was fuelled by pressurised hydrogen from storage tanks (25 MPa, 250 bar). The bus had a range and top speed of over 300 km and 80 km/h respectively [42].

Toyota FCHV-4 was presented in June 2001. The prototype vehicle had a hybrid engine (similar to the Toyota Prius) with 90 kW of SPFC stacks, battery and electric motor (80 kW). The car had a range of 300 km on pure hydrogen (hydrogen absorbing alloy) and a top speed of 150 km/hr [42].

Honda FCX-V4 was presented in September 2001. The car was powered by 78 kW of Ballard SPFC stacks and compressed hydrogen (35 MPa). The car had a range of 300 km and a top speed of 140 km/hr. It has had been road tested in Japan and California and is marked for production in 2003 [42].

1.2.4 DEVELOPMENT OF SPFC SYSTEM FOR STATIONARY APPLICATION (1993-2001)

The major development activity in the SPFC stationary application between 1993–95 was mainly conducted by Ballard Power System, who were in the midst of a four phase program to commercialise a stationary SPFC power plant. Phase 1, completed in 1993, involved developing a subscale 22 kW natural gas power plant based on the
MK 5 stack. The system used four 106 cell stacks, which provided the power plant voltage of 320 V d.c and produced a peak power output of 40 kW. The next phase was to use the second generation of the stack and develop a 280 kW natural gas power plant for demonstration purposes by 1999 [16]. Interest in developing a residential fuel cell system by other SPFC system developers was also starting in both America and Japan around this period.

The demand for environmentally clean power sources for small decentralised cogeneration power plants was growing and SPFC technology was one of the ideal candidates for stationary application after its successful demonstration in transportation applications. At the fifth Grove fuel cell symposium (1997), many papers were presented regarding the opportunities and technical challenges forced by fuel technology in the power generation industry. In the symposium, Ballard Power System announced the formation of Sister Company Ballard Generation System (BGS), a venture between Ballard Power System and GPU International. BGS revealed their significant achievement of the world's largest natural gas fuelled SPFC stationary power plant. The unit had a peak power output of 213 kW and an electrical efficiency of 34% (LHV). The stack used in the power plant unit incorporated the use of plastic components, which significantly reduced its cost and showing a clear path to reaching cost targets for commercial production and sales. The future objectives of the company were to enter exciting markets around the globe and build its business around emerging market opportunities [44].

By the late nineties, American companies like Analytic Power Corporation, Energy Partners, Plug Power, H-Power and Northwest Power System were also developing and demonstrating stationary SPFC systems ranging from 0.05-1kW for portable applications, to 3-20 kW for residential applications. In 1998, Analytic Power Corporation had developed a 10 kW (peak power) residential power generator (RPG) that operated on hydrocarbon fuels (natural gas). The power plant was demonstrated for power levels from zero to 10 kW and an average efficiency of about 38% was achieved [45]. Also, in 1998, Energy Partners developed and demonstrated a 10 kW (3 modules) Alpha prototype natural gas SPFC system. The company was developing a 1 kW AC power output methanol SPFC system to be completed in year 2000 and a
3 kW natural gas powered Beta prototype to be completed for field testing by early 2001[46].

Interest in Combined Heat and Power (CHP) was growing rapidly throughout many European Union (EU) member countries by the late nineties. In Germany, the first 250 kW SPFC plant started up in Berlin at end of year 1999. The natural gas SPFC system, developed by a newly formed European company ALSTOM BALLARD GmbH, was installed by a group of Germany companies who aimed to introduce the fuel cell technology to the European power economy and route the SPFC technology towards commercialisation [47].

Also, by the late nineties, many utility and gas companies in Japan and Korea had developed SPFC stacks and were either embarking or continuing on many different projects to develop prototype SPFC system for either residential or co-generation applications. In Japan, companies like Toshiba (30 kW) and Sanyo (2-3 kW) were developing cogeneration systems using natural gas for small building and residential use respectively, under the NEDO New Sunshine R&D program [48]. Other companies developing SPFC system for residential application in Japan were Osaka Gas Co. (1 kW on methane [49]), Matsushita Electric Industrial Co. Ltd, Tokyo Gas Co. (1 kW System [50]) and Fuji Electric Co. Ltd (1 kW System on city gas [51]). A prototype of a residential natural gas cogeneration system, developed by Matsushita Electric Industrial Co. Ltd, included a 1.5 kW SPFC stack, a natural gas fuel processor, an inverter and a hot water tank. The system provided 1.5 kW of electric power and 2 kW heat, as hot water. The system was also able to cope with different load levels and connect to the commercial power grid. Test runs to evaluate the system’s energy efficiency and durability were scheduled to be carried out in 2000-2001 [52].

In 2000, Ballard Power Systems Inc. disclosed the development of a high performance Mk 6000 SPFC stack (62% efficiency) for use in the natural gas SPFC power plant. The Mk 6000 was tested for 8000 hours of continues operation without much cell voltage decay and the field experience in BGS natural gas SPFC plants would develop the stack’s proficiency and commercial potential [53]. Analytic Power Corporation merged with Dais Corporation to form a new company Dais-Analytic
Corporation (DAC). DAC had received support from the Electric Power Research Institute and a consortium of 16 utility companies to further develop their RPG technology (alpha test program) and use the test results and experience from this alpha test program in a beta prototype program due to start in 2001[54]. By 2000, Energy Partners had also completed their 1 kW methanol SPFC system with AC power output. Energy Partners along with Honeywell were also involved in designing a 50 kW\textsubscript{e} natural gas, high temperature SPFC (>100°C), co-generation plant for buildings. The project, supported by the DOE (USA), was in its initial stage of system study at the end of year 2000 [55].

1.2.5 CLOSING REMARKS

From this review of SPFC technology, it is evident that SPFC technology had matured and been successfully demonstrated in both transport and stationary applications. Besides the drive to lower the manufacturing cost of the SPFC stack, the emphasis has also been on reducing the size and weight of the SPFC system (maximising the gravimetric and volumetric power densities). This improvement in the power density of the SPFC system is currently being addressed by development of compacted multiple fuel processors and smaller and efficient ancillary components. Although, SPFC vehicles have been built and demonstrated, the important questions of what fuel to use and its supply (i.e. fuel infrastructure) still need to be answered. Many government departments around the world are currently addressing these questions along with fuel cell heath and safety standards.
1.3 REFERENCES


2. FUEL CELL SYSTEM

2.1 INTRODUCTION

In principle, a fuel cell power system consists of a fuel cell stack, a fuel supplying subsystem, an oxidant supplying subsystem and a power conditioner. Hydrogen is the most common fuel for use in fuel cell stack and is either supplied from a storage tanks (gaseous or cryogenic) or a hydrocarbon fuel processor. The oxidant usually used in the fuel cell is oxygen, which is economically available from air via a blower (atmospheric system) or air compressor (pressurised system). Depending upon the end use of the system, a fuel cell power system may also require an energy storage subsystem, a waste heat recovery subsystem and a control subsystem. Figure 2.1 shows a representation of a generic fuel cell power system. The objective of this chapter is to give a general overview of major components of the fuel cell power system and the different types and operating conditions of these components.

2.2 COMPONENTS OF FUEL CELL POWER SYSTEM

The fuel cell power system comprises of the following subsystems and their components:

> Fuel cell system: Fuel cell and stack
> Fuel supply: Hydrocarbon fuel processors, hydrogen storage system and electrolysis of water.
> Oxidant supply: Storage tanks, electrolysis of water, blowers and compressors.
> Electrical storage systems: Battery, fly wheel and ultracapacitors.
> Power conditioner equipment: Converters and inverters.
> Ancillary equipment: Pumps, motors, humidifiers and pressure valves etc.
Figure 2.1: Schematic representation of a generic fuel cell power system
2.2.1 Fuel Cell System

2.2.1.1 Fuel Cell and Types of Fuel Cells

A fuel cell is an electrochemical device that converts the chemical energy of the fuel and oxidant into direct current (d.c) electricity. Unlike the primary or secondary battery, where the chemical energy is stored and consumed within a sealed container, the fuel cell operate for as long as the cell is fed with appropriate fuel and oxidant and the reaction products removed. The fuel and the oxidant are thus stored external to the fuel cell and the operational period of the cell depends upon the size of the storage tanks [1,2].

A fuel cell consists of an anode, a cathode and an electrolyte. The anode and cathode electrodes are connected electrically through a load via an external circuit. The external circuit transports the electric current or flow of electrons and the resultant ions are transported via the electrolyte. There are number of types of fuel cells with each type generally characterised by the electrolyte used within it. Based on the electrolyte type, the fuel cell operating conditions, principles of operation and the cell material are determined. Table 2.1 describes the characteristic of the five most advanced fuel cells types, which are currently being developed, demonstrated and commercialised [2,3,4,5].

The principle of operation of a fuel cell will be illustrated using a SPFC operating on hydrogen and air. Hydrogen enters a fuel cell at the anode is electrocatalytically reduced to produce hydrogen ions (protons) and electrons. The electrons flow via the external circuit to the cathode, where they combine with incoming oxygen gas and the protons, which have migrated from the anode through the electrolyte to the cathode, to produce water. The overall reaction which takes place within the fuel cell may be viewed as the cold combustion of hydrogen fuel with oxygen to produce water. (The anode, cathode and the overall reactions which takes place within the hydrogen/oxygen fuel cell are shown in table 2.1). However, depending on the type of fuel cell, the electrolytes and ionic carriers may be different, e.g., hydroxyl ion (OH⁻) in alkaline electrolytes or carbonate ion (CO₃²⁻) in molten carbonate electrolytes.
(Table 2.1). Figure 2.2 shows the schematic representation of a solid polymer fuel cell and the fundamental operation, which takes place within the cell.

In a SPFC, the total energy of the hydrogen reacted ($\Delta H$) is converted into electrical (free energy, $\Delta G$) and heat energy at the fuel cell operating temperature. The heat energy released at the fuel cell temperature is the difference between the heat of reaction ($\Delta H$) and the available free energy ($\Delta G$). Usually excess fuel and oxidant are fed into the fuel and the unreacted reactants are removed through the anode and cathode exhausts. A cooling system is usually required to remove the heat energy and this maintain a constant fuel cell temperature. The cooling system is a prominent feature of a fuel cell stack. The individual cells are assembled in series to produce the fuel cell stack. Parallel arrangement of the stacks can then facilitate the desired voltage and current requirements.
<table>
<thead>
<tr>
<th>Type of Fuel</th>
<th>Solid Polymer</th>
<th>Alkaline</th>
<th>Phosphoric Acid</th>
<th>Molten Carbonate</th>
<th>Solid Oxide</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrolyte</td>
<td>Perfluorosulphonic acid polymer (Solid)</td>
<td>KOH (30%) (liquid)</td>
<td>$\text{H}_3\text{PO}_4$ (liquid retained in microporous matrix)</td>
<td>Potassium &amp; Lithium carbonate mixture</td>
<td>Ytrria stabilised zirconia ($\text{ZrO}_2$)</td>
</tr>
<tr>
<td>Temperature</td>
<td>60–90 °C</td>
<td>60–100 °C</td>
<td>180–200 °C</td>
<td>600–700 °C</td>
<td>900–1000 °C</td>
</tr>
<tr>
<td>Anode Materials</td>
<td>Platinum Supported upon P.T.F.E bound carbon</td>
<td>Raney nickel catalyst</td>
<td>Platinum Supported upon P.T.F.E bound carbon in contact with layer of carbonate zirconia ($\text{ZrO}_2$)</td>
<td>Nickel &amp; Chromium</td>
<td>Nickel-Zirconia Cermet</td>
</tr>
<tr>
<td>Cathode Materials</td>
<td>Same as Anode</td>
<td>Silver catalyst</td>
<td>Platinum &amp; Lithium carbonate mixture</td>
<td>Lithiated nickel</td>
<td>Strontium doped Lanthanum Manganite</td>
</tr>
<tr>
<td>Anode Reaction</td>
<td>$2\text{H}_2 \rightarrow 4\text{H}^+ + 4e^-$</td>
<td>$2\text{H}_2 + 4\text{OH}^- \rightarrow 4\text{H}_2\text{O} + 4e^-$</td>
<td>$2\text{H}_2 \rightarrow 4\text{H}^+ + 4e^-$</td>
<td>$2\text{H}_2 + 2\text{CO}_3^{2-} \rightarrow 2\text{CO}_2 + 2\text{H}_2\text{O} + 4e^-$</td>
<td>$2\text{H}_2 + 2\text{O}^{2-} \rightarrow 2\text{H}_2\text{O} + 4e^-$</td>
</tr>
<tr>
<td>Cathode Reaction</td>
<td>$\text{O}_2 + 4\text{H}^+ + 4e^- \rightarrow 2\text{H}_2\text{O}$</td>
<td>$\text{O}_2 + 2\text{H}_2\text{O} + 4e^- \rightarrow 4\text{OH}^-$</td>
<td>$\text{O}_2 + 4\text{H}^+ + 4e^- \rightarrow 2\text{H}_2\text{O}$</td>
<td>$\text{O}_2 + 2\text{CO}_2 + 4e^- \rightarrow 2\text{CO}_3^{2-}$</td>
<td>$\text{O}_2 + 4e^- \rightarrow 2\text{O}^{2-}$</td>
</tr>
<tr>
<td>Advantages</td>
<td>Low temp operation</td>
<td>Highest operating efficiency</td>
<td>High grade heat available</td>
<td>No noble metal required</td>
<td>CO tolerant</td>
</tr>
<tr>
<td></td>
<td>Non-corrosion electrolyte</td>
<td></td>
<td>CO$_2$ tolerant</td>
<td>Fuel flexibility &amp; internal reforming</td>
<td>High grade heat available</td>
</tr>
<tr>
<td></td>
<td>Rapid start-up</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>High power density</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Disadvantages</td>
<td>CO electrode poisoning</td>
<td>CO$_2$ free reactants to avoid carbonate formation</td>
<td>CO electrode poisoning</td>
<td>Material corrosion problems</td>
<td>High temp material problem</td>
</tr>
<tr>
<td></td>
<td>Low grade heat available</td>
<td></td>
<td>Noble metal catalysts</td>
<td>CO$_2$ required for cathode</td>
<td>High electrolyte resistivity</td>
</tr>
<tr>
<td></td>
<td>Noble metal catalysts</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
The performance of a SPFC is conventionally illustrated by a polarisation curve, which is a plot of cell (or stack) potential versus current (or current density). The cell voltage decreases from the open circuit voltage or the reversible thermodynamic \( E_r \), when a current is drawn. This drop in cell voltage is due to electrode kinetics effects, which leads to cell polarisation within the cell. Figure 2.3 depicts the effects of cell polarisation on the performance of the SPFC. Cell polarisation, as seen from figure 2.3, can be divided into three distinctive types, the activation, ohmic and concentration polarisations [5,6].

Activation polarisation is a result of slow charge transfer reaction across the electrode-electrolyte interface. Activation polarisation occurs at both electrodes. For the \( \text{H}_2/\text{air} \) fuel cell, the polarisation effect at the cathode electrode is the most significant due to the slower rate of oxygen reduction and lower electrocatalytic activity. The oxygen reduction reaction is \( \approx 1 \times 10^6 \) slower than \( \text{H}_2 \) oxidation. The effects of the activation polarisation may be reduced by choosing appropriate
operating conditions such as temperature and pressure and increasing the active surface area of the electrode and electrocatalyst activity [5,6].

The ohmic polarisation is due to electrical resistance losses within the cell. These losses arise from the ionic resistances of both the electrolyte and electrode, the electronic resistance of the electrodes and the contact resistance of the electrical connectors. The ohmic losses can be minimised by using thin electrolyte layers with good ionic conductivity and low resistance electrodes.

The concentration polarisation arises due to mass transport limitations i.e. the availability of the electroactive species in the vicinity of the electrode-electrolyte interface. To sustain the flow of electric current, the electrode reaction requires a constant supply of reactant species. When these species are not available due to diffusion or convection limitations concentration gradients arise. These concentration gradients result in a reduction of electrode activity, leading to drop in cell voltage. One way to reduce or avoid concentration gradients is to introduce forced convection of reactants [5,6].

The performance of the fuel cell is also affected by the operating conditions such as temperature, pressure and reactant stoichiometries. The effects of these particular operating condition are discussed with respect to SPFC in chapter 3, section 3.2.2.

2.2.1.2 Solid Polymer Fuel Cell (SPFC)

A SPFC is characterised by its use of a solid polymer membrane as its electrolyte. The solid polymer membrane consists of a cross-linked organic perfluorinated sulfonic acid polymer. The membrane has a high capacity for proton conduction. The membrane electrode assembly (MEA), which forms the core part of the fuel cell, is a sandwich of the polymer membrane between two platinum impregnated porous carbon based electrodes. Due the solid nature of the electrolyte, the SPFC can be constructed to be very compact and lightweight [7]. The other fuel cell characteristics, which are also intrinsic of the materials used, are low operational temperature, high
power density, low corrosion, minimal maintenance and longer cell life [7]. Table 2.1 describes other SPFC characteristics.

Since the renaissance of interest in the SPFC in early eighties, the performance of the fuel cell has significantly improved due to substantial investment in research and development of both the components of the cell and stack. State of art components include thinner MEA's (membrane electrode assembly), high activity catalyst materials and bipolar plates are being designed primarily to reduce the inefficiency of fuel cell operation (activation, ohmic and concentration polarisations) [7]. The most favourable operating conditions for the SPFC used today are pressure of 3 bar(a) and temperature of 80°C, However, in the future, these operating conditions may be improved with improvement in the MEA material and better water management within the cell [8,9]. A future SPFC stack may operate at an atmospheric pressure and temperature of 60°C.

2.2.2 Fuel Supply

Pure hydrogen is attractive for fuel cell applications because of its relatively high electrochemical reactivity, its low environmental impact (water as a combustion product) and its high gravimetric energy density (table 2.2). Although hydrogen is the most abundant element in the universe, it is not directly available in nature and hence hydrogen has to be produced from primary and secondary energy sources. Unfortunately, storing and handling of hydrogen (gaseous or liquid) fuel remains a major challenge due to its low density (0.09 kg/m³ @ STP) and boiling point (-253°C). Alternatively, hydrogen can be produced via a suitable process on site and supplied directly to the fuel cell system or plant [10].
Table 2.2: Comparison of Fuels for Fuel Cell Applications

<table>
<thead>
<tr>
<th>Fuels</th>
<th>Gravimetric Energy Density (LHV) (MJ/kg)</th>
<th>Volumetric Energy Density (LHV) (MJ/l)</th>
<th>Gravimetric Energy Density (LHV) (kWh/kg)</th>
<th>Volumetric Energy Density (LHV) (kWh/l)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen (g) (300 bar) +</td>
<td>120.00</td>
<td>2.703</td>
<td>33.33</td>
<td>0.751</td>
</tr>
<tr>
<td>Natural Gas (0°C, 1 bar)</td>
<td>47.70</td>
<td>0.040</td>
<td>13.25</td>
<td>0.011</td>
</tr>
<tr>
<td>Hydrogen (l) (-162°C) +</td>
<td>119.88</td>
<td>8.50</td>
<td>33.30</td>
<td>2.36</td>
</tr>
<tr>
<td>Metal Hydrides (Fe-Ti) *</td>
<td>2.70</td>
<td>17.56</td>
<td>0.75</td>
<td>4.88</td>
</tr>
<tr>
<td>Regular Gasoline</td>
<td>42.70</td>
<td>30.74</td>
<td>11.86</td>
<td>8.54</td>
</tr>
<tr>
<td>LPG (Propane) +</td>
<td>46.30</td>
<td>26.92</td>
<td>12.86</td>
<td>7.48</td>
</tr>
<tr>
<td>Methanol</td>
<td>19.70</td>
<td>15.56</td>
<td>5.47</td>
<td>4.32</td>
</tr>
<tr>
<td>Diesel</td>
<td>42.50</td>
<td>34.85</td>
<td>11.81</td>
<td>9.68</td>
</tr>
</tbody>
</table>


Hydrogen can be readily produced from the electrolysis of water as long as a suitable electrical power source and water are available. The ideal source of this electrical power would be via geological energy resources such as wind, solar, hydro and geothermal power, which offer great environmental benefit. However, these energy resources or the power generation technology accompanying them remain restricted by either unavailability of technical development or high capital cost. Hydrogen can also be produced via a chemical process from fossil fuels (primary energy sources - coal, oil or natural gas) and derived hydrocarbon fuels (secondary energy sources - diesel, gasoline, LPG, methanol etc). Processing of hydrocarbon fuels for production of pure hydrogen or hydrogen rich gas is a well established process in industry today. However, nearly 90% of the hydrogen produced in the industry is consumed in the refining and petrochemical industries rather than sold as a commercial fuel [12,13].

Hydrogen fuel can be supplied to a fuel cell system via three different ways, the hydrocarbon fuel processor, hydrogen storage system (tanks, metal hydride) and electrolysis of water.
2.2.2.1 Hydrocarbon Fuel Processors

Fuel processing of hydrocarbon fuels to produce hydrogen rich gas for consumption in a fuel cell system involves a chain of reactors. These reactors are responsible for the production of hydrogen rich gas and purification of the gas to a particular standard depending on the requirement of the fuel cell system. There are three main processes by which hydrocarbon fuels can be processed to produce hydrogen, namely steam reforming, partial oxidation and autothermal reforming. Following the production of the hydrogen rich gas, the purification stage, depending on the type of hydrocarbon fuel and fuel cell used, may include a high temperature shift reactor, a low temperature shift reactor, preferential oxidation (selective oxidation) reactor and a membrane separator unit. However, there are other impurities such as sulphur compounds, that may degrade fuel cell system performance and require additional stages of removal either from the reactants or processed gas stream. These impurities and techniques to remove these impurities are not considered in this section [14].

2.2.2.1.1 Catalytic Steam Reforming

Steam reforming is the most commonly used and well established method of producing hydrogen rich gas from hydrocarbon fuels in industry today. The objective of the catalytic steam reforming process is to extract the maximum quantity of hydrogen held in the water and hydrocarbon feedstock. Steam reforming is the endothermic reaction of hydrocarbon with steam. However, the process of the steam reforming is best suited for lighter hydrocarbon fuels or low molecular weight such as saturated hydrocarbon with general formula $\text{C}_n\text{H}_{2n+2}$. Although efforts are being continuously made to extend it to higher fractions [14,15,16].

The steam reforming reaction for saturated hydrocarbon can be represented as

$$\text{C}_n\text{H}_{2n+2} + n\text{H}_2\text{O} \leftrightarrow (2n+1)\text{H}_2 + n\text{CO} \quad ... (2.1)$$

and water gas reaction
CO + H₂O → H₂ + CO₂  ...(2.2)

Since CO will reversibly poison the noble metal catalysts used in the SPFC at ≤ 80°C, the CO is encouraged to further react with excess steam via the water gas shift reaction. This reduces CO concentration and also increases hydrogen yield [16]. The hydrogen yield is highly dependent on the operating conditions of the reactor, steam to carbon molar ratio and the type of catalyst used in the reactor.

From the thermodynamic study of the steam reforming process, it is evident that high temperature (800-1000°C), low pressures and S:C stoichiometric ratio favour steam reforming process of light hydrocarbon fuels. However, for a practical reactor, an excess steam (S:C ratio of between 1.5-3.5) is favoured to avoid carbon formation. The operating pressure is also usually fixed by end use of the product gas (usually 3-5 bar for fuel cell applications). Nickel metal or nickel based compounds have been recognised as the most suitable catalyst for steam reforming of light hydrocarbon fuels such as natural gas [16]. Steam reforming of natural gas or methane is the best and common example of hydrocarbon steam reforming and is discussed in detail in chapter 3, section 3.2.1.

For fuel cell transport applications, methanol has become an important energy carrier and steam reforming of methanol has become a valuable source of hydrogen rich gas on board a vehicle. Steam reforming of methanol takes place at much lower temperature (200-250°C) compared to hydrocarbon steam reforming and therefore the construction of the reactor is much simpler, compact and high fuel conversion. Steam reforming of methanol is discussed in great detail in chapter 4, section 4.2.1.1.

2.2.2.1.2 Partial Oxidation

Partial oxidation process involves the incomplete combustion of the hydrocarbon or alcohol fuel, to produce hydrogen rich gas. The O:C ratio is controlled in the high temperature process to achieve maximum hydrogen yield with reasonable reactor efficiency. For some applications of partial oxidation, steam is also supplied to encourage water shift reaction (2.2). Commercially, the non catalytic partial oxidation
reactors are mostly preferred for heavier hydrocarbon fuels at higher temperatures. However, catalytic reactors are currently being developed to enable lower temperature and better reaction control operation.

Partial oxidation process has the following advantages over steam reforming [14,17]:

- The process allows the use of liquid fuels from naphtha to heavy fuel oils due to lower tendency of carbon formation.
- The high temperature reactors can tolerate the presence of many impurities, including sulphur.
- The reactor is more compact (if water is not used), allows rapid start-up and fast response.

However, a major disadvantage of the partial oxidation fuel cell system is that the reactor can not make use of any waste heat or fuel cell exhausts. An additional disadvantage is that less hydrogen is produced compared to steam reforming and hence, high and low shift reactors are required.

In general the partial oxidation reaction for a hydrocarbon fuel can be chemically represented as

\[ C_nH_m + (0.5n) (O_2 + 3.76 N_2) \rightarrow nCO + (0.5m)H_2 + (1.88n) N_2 \]  \( \ldots (2.3) \)

However, if water is also added to the reactor then some of the CO will react to give the following overall reaction:

\[ C_nH_m + (0.5n)(O_2 + 3.76 N_2) + nH_2O \rightarrow nCO_2 + (n+0.5m)H_2 + (1.88n) N_2 \]  \( \ldots (2.4) \)

From equations 2.3 and 2.4 it is evident that the molar ratio of O:C and S:C are critical parameters in determining the performance of the partial oxidation reactor. The non-catalytic or thermal partial oxidation reactor typically operate in the temperature range of 800-1400°C and pressure range of 5-100 bar. O:C and S:C molar ratios of between 1-2 and 0.5-1 respectively are usually employed [17]. The
thermal partial oxidation of diesel fuel is discussed in detail in chapter 5, section 5.2.1.

2.2.2.1.3 Autothermal Reforming

Autothermal reforming combines both features of steam reforming and partial oxidation. The autothermal reforming utilises the exothermic heat of reaction of the partial oxidation process to promote the endothermic process of the steam reforming. An example of autothermal reforming is the Johnson Matthey HotSpot™ technology, which was invented in the mid 1980s [18]. The HotSpot™ reactor can be started from cold by partial oxidation, which generates enough heat for the endothermic steam reforming process. Since both these chemical reactions and heat transfer occur within the same reactor, the reactor is compact and avoids complex heat exchanger engineering.

Today, the HotSpot™ technology is designed with the objective to be integrated into a fuel cell vehicle drivetrain. Therefor, the technology is designed not only to achieve nearly 100% conversion, but also integrate within the reactor a gas clean up section and use of fuel cell exhaust gases. Furthermore, the HotSpot™ technology today is also designed to use conventional fuels, such as natural gas, LPG or gasoline and applicable for many fuel cell applications [19]. Some of the characteristics of the HotSpot™ technology today are [19]:

- The overall reaction rate is fast and hence the catalyst bed is small.
- High production of hydrogen rich gas since the hydrogen is generated from both the water and fuel i.e. steam reforming and partial oxidation.
- The reactor is compact, fast start-up and rapid response.
- Incorporates a Demonox™ system which reduces CO levels from over 3% to < 5 ppm over a range of throughputs.
- Incorporates an anode exhaust gas catalytic burner.
2.2.2.1.4 Hydrogen Purification and Enrichment

Depending on the fuel feedstock, reactors are required for both hydrogen purification and enrichment. The choice of the method of purification and enrichment also depends on the operating conditions of the steam reforming or partial oxidation reactors. For example, a partial oxidation (PoX) of diesel fuel (for SPFC stack) would require both high and low temperature water shift reactors and a gas clean up unit to produce a high yield hydrogen rich gas with minimum CO concentration. Furthermore, a fuel cell type also imposes its own requirements, for example, a alkaline fuel cells are sensitive to CO\(_2\) in the feed gas and require complete CO\(_2\) removal. On the contrary, SPFC are insensitive to CO\(_2\), but require low concentration of CO (ppm levels) in their feed gas.

The CO concentration from some (i.e. natural gas steam reforming or diesel PoX) of the fuel processor are usually high (5%-20%) and need reducing down to part per million (ppm) level. The first stage of achieving this lower level of CO concentration is to use high and low temperature shift reactor, which not only lower the CO concentration, but also increase the hydrogen concentration in the gas stream.

The high and low shift reactors are usually used in conjunction with high temperature steam reforming or partial oxidation processes, since these processes produce relatively lower and higher concentrations of H\(_2\) and CO respectively compared to lower temperature steam reforming. The water shift reaction (2.2) is encouraged to produce hydrogen from available CO by introducing more steam into the reactors and forcing the equilibrium reaction (2.2) towards the right. Beside reactant concentrations in the reactor, optimum operating conditions and a suitable catalyst are also required to favour H\(_2\) production.

The HTS reactor is usually operated at a temperature of 400\(^\circ\)C and typically reduces CO concentrations in the gas stream down to 2-4% from 10-15%. The LTS reactor is operated at a lower temperature of approximately 200\(^\circ\)C and can reduce CO concentrations further down to 0.3% [20]. Other reactions are also favourable within these temperature ranges. The methanation reactions are very thermodynamically favourable at this temperature as seen from reaction (2.5) and (2.6) [20].
These reactions if allowed to take place in the reactor would consume most of the hydrogen and reverse the reforming process. To avoid the methanation reactions, suitable catalysts have to be used in the reactors whose selectivity favours water shift reactions rather than the methanation reactions. In industrial reactors, chromia-supported iron based catalysts are used in the HTS reactor while copper and zinc oxide catalysts are used in the LTS reactor \[20\].

In addition to the shift reactors, further purification stages are required depending on the type of the fuel cell. The electrode catalyst of an acidic electrolyte fuel cell (SPFC or PAFC) can only tolerate very low levels of CO (ppm level), while in an alkaline fuel cell (AFC), the electrolyte will not tolerate \( \text{CO}_2 \) in both anode and cathode feed streams. However, the high temperature fuel cells (MCFC or SOFC) will accept hydrogen rich gas directly from a fuel processor. The final stage purification methods discussed in this section are the ones which are associated with the SPFC technology.

A catalytic selective oxidation reactor (gas clean-up unit) is a common method and used for reducing the CO level from 1-0.3% down to ppm levels. The advantages of a catalytic selective oxidation reactor over other methods (palladium membranes, methanation and pressure swing adsorption) are that the reactor offers fast reaction kinetics, low pressure drop and relatively low temperature operation \[21,22\]. Physically the reactor can be compact and lightweight unit, and thus ideally suited for some fuel cell transportation application.

The catalytic selective oxidation reactor preferentially oxidises the CO to \( \text{CO}_2 \) over a heterogeneous catalyst via the chemical equation (2.7):

\[
\text{CO} + \frac{1}{2} \text{O}_2 \leftrightarrow \text{CO}_2
\]

\[\text{(2.7)}\]
The optimal performance of the selective oxidation reactor (GCU unit) is highly dependant on a suitable catalyst and operating conditions of the reactor. A GCU unit developed by the Fuel Cell Group at Loughborough University achieved its optimal performance at a temperature range of between 120°C-200°C, an $O_2:CO$ molar ratio of between 1-4 and using a Platinum Ruthenium (Pt-Ru) based catalyst, applied directly to high surface area aluminium heat exchanger. With Pt-Ru based catalyst and these operating conditions, the GCU unit was capable of reducing CO level to less than 15 ppm (<5ppm on dry basis). This GCU unit scaled for a 20 kW$_e$ fuel cell stack was 3.7 litres in volume and had a mass of 4.9 kg [21,22].

Alternatively, CO concentrations in the hydrogen rich gas stream can be reduced using palladium membrane technology. The palladium (Pd) membrane is a well established technology and used extensively in the petrochemical industry today to achieve very high purity hydrogen gas. The hydrogen molecule is allowed to diffuse through the membrane and ionised into protons and electrons. These atomic components migrate across the membrane and recombine on the downstream side of the membrane. The other impurities present in the gas stream do not migrate through the membrane and are removed via different exit.

The performance of the palladium (Pd) membrane unit depends on membrane surface area and thickness, operating temperature and differential membrane pressure. The hydrogen recovery from a reformed gas feed is enhanced by increasing the rate of diffusion across the membrane. The rate of diffusion across the membrane can be improved with greater differential pressure, higher membrane temperature, bigger surface area and smaller membrane thickness [23,24]. At present commercially available Pd or Pd based alloy membranes are investigated together with various fuel processors for fuel cell applications. A Pd-40Cu alloy membrane unit was tested with a methanol reformer and the membrane unit produced 99.9999% pure hydrogen with trace of CO (1 ppm). The differential pressure and temperature of the unit were 9 bars and 300°C respectively. The hydrogen recovery by the membrane was 75% [25].

Although attractive in terms of H$_2$ purity, the technology is characterised by the large differential pressure requirements to obtain sufficient recovery of hydrogen, the relatively high operating temperature and the high price of the Pd metal. Beside these
drawbacks, there are other problems associated with stability of the membrane and the leakage caused by thermal expansion and contraction of the Pd metal [24].

2.2.2.2 Hydrogen Storage Systems

Hydrogen can be supplied to the fuel cell system from a high pressure (compressed gas) tanks or metal hydride system. However, the hydrogen for these storage systems has to be produced using a primary energy source and hence, the energy losses for hydrogen production and compression also need to be accounted for when considering these storage systems. Hydrogen is normally compressed to between 200 and 250 bar for storage in cylindrical tanks of up to 50 litres. These tanks may be made from aluminium or carbon/graphite compounds and can be used for either small industrial projects or transportation. However, for some fuel cell application ultra high pressure storage tanks (400-600 bar) can be used for a much compact storage system. Compared to a metal hydride storage system, the compressed hydrogen storage is much lighter, simpler to use and relatively easy to refuel [26].

Metal hydride storage system is favoured method of supplying hydrogen for small scale or portable fuel cell applications. Metal hydrides possess the unique ability to reversibly absorb hydrogen either at room temperature or via heating of the storage tank. The total amount of hydrogen absorbed is generally 1% - 2% of the total weight of the tank. Some metal hydrides are capable of storing 5% - 7% of their own weight, but only when heated to temperatures of 250°C or higher. The percentage of gas absorbed to volume of the metal is still relatively low, but hydrides offer a valuable solution to hydrogen storage. The metals used are various compounds of titanium, iron, manganese and other metals [26,27].

Although metal hydride storage offer a safe and compact (60% more hydrogen by volume as compared to liquid storage) way of storing hydrogen, it has many disadvantages which make it unattractive for some fuel cell applications. Some of these disadvantages are that metal hydrides requires high pressure (≈10 bar) and high purified hydrogen to charge them, have reasonably longer refuelling time and the hydride packs are usually bulky and relatively very heavy [27].
2.2.2.3 Electrolysis of Water

Electrolysis of water can provide hydrogen and oxygen for a small scale or portable fuel cell system as long as an electric power source and water is available. Electrolysis of water is the reverse operation of the hydrogen/oxygen fuel cell, where electricity is provided to decompose water into hydrogen and oxygen. Potassium hydroxide (KOH) solution is usually used as the electrolyte, to improve the conductivity of the ions. If the electricity is produced via a renewable source of energy or geological energy resources such as wind, solar or hydro then the electrolysis of water can be a viable source of hydrogen and oxygen. A typical industrial scale plants operate at about 67% at higher current density. The electrolysis of water also require a hydrogen and oxygen purifiers and storage tanks [28].

2.2.3 Oxidant Supplying System

All fuel cells need oxygen for operation. The oxygen supply system (either pure or from the atmosphere) is an important and integral part of the fuel cell system. Air is obviously the most favourable source of oxygen for most fuel cell system, even though the performance of the fuel cell is best on pure oxygen. This loss of performance due to the use of air instead of oxygen is usually acceptable and a compromise for the cost, weight and system complexity (storage or purification) associated with use and supply of pure oxygen either from a pressurised tank or electrolysis of water (2.2.2.3).

For an alkaline fuel cell, a CO₂ free air supply is required while for the acidic fuel cell the filtration of the atmospheric air is sufficient. The performance of the fuel cell is enhanced with use of pressurised air. However, some compression process may introduce further impurities such as oil, which gradually decreases the fuel cell performance. Therefore, the use of efficient oil free compressor is desired for SPFC application.

In most fuel cell systems, the power required to drive the compressor corresponds to a parasitic load of approximately 20-25% of the fuel cells stack power [29,30]. The parasitic load depends on both the fuel cell stack operating conditions e.g. pressure
and cathode stoichiometry, and the efficiency of the compressor. Ideally, the compressor (for fuel cell application) should have the capability to handle changes in the airflow at approximately constant pressure ratio and deliver uncontaminated air in one stage compression. Although current commercial compressors are not suitable to supply oil free air to the fuel cell efficiently, efforts are being made to design and develop small efficient compressors such as the sliding vane [31] and screw-type [30] for fuel cell applications.

2.2.4 Energy Storage Systems

For some fuel cell applications, an additional energy storage system is required for the starting up process, peak sharing and for storing excess power generated by the system. The most common, well established and practical energy storage device used is the rechargeable battery. However, there are other energy storage devices such as flywheels and super- or ultra-capacitors, which can also be utilised.

2.2.4.1 Rechargeable Batteries

A battery is very similar to a fuel cell in its principle of operation (section 2.2.1.1), but compared to a fuel cell, a battery stores within its container the chemical energy that is converted to electrical power and heat. For this reason, a battery is a compact, sealed and convenient source of limited power. Batteries have been used for approximately 200 years and their performance (energy density) has tremendously improved over this period. Rechargeable batteries or secondary battery development began in the early 1900’s, when practical generators and chargers became available. Secondary batteries such as lead acid, nickel cadmium cells, which can be recharged and reused, are mostly used in industrial and automotive applications [32]. In this section a general overview of only the rechargeable batteries will be discussed.
<table>
<thead>
<tr>
<th>Type of Energy Storage System</th>
<th>Gravimetric Energy Density (Wh/kg)</th>
<th>Volumetric Energy Density (Wh/l)</th>
<th>Specific Power (W/kg)</th>
<th>Energy Efficiency (%)</th>
<th>Life Duration in cycles</th>
<th>Operating Temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lead Acid (sealed)</td>
<td>35</td>
<td>95</td>
<td>80</td>
<td>75</td>
<td>800-1000</td>
<td>-65...+65 (2)</td>
</tr>
<tr>
<td>Lead Acid (Flooded)</td>
<td>40</td>
<td>85</td>
<td>80</td>
<td>75</td>
<td>800-1000</td>
<td>-30...+65 (2)</td>
</tr>
<tr>
<td>Lead Acid (Bipolar)</td>
<td>55</td>
<td>110</td>
<td>100</td>
<td>-</td>
<td>800</td>
<td>-</td>
</tr>
<tr>
<td>Ni-Cadmium (Sealed)</td>
<td>42</td>
<td>100</td>
<td>100</td>
<td>60</td>
<td>1000</td>
<td>-30...+70</td>
</tr>
<tr>
<td>Ni-Cadmium (Flooded)</td>
<td>48</td>
<td>100</td>
<td>120</td>
<td>60</td>
<td>1200</td>
<td>-</td>
</tr>
<tr>
<td>Ni-Cadmium (SHFT) (3)</td>
<td>60</td>
<td>115</td>
<td>225</td>
<td>74</td>
<td>2500</td>
<td>-40...+80</td>
</tr>
<tr>
<td>Ni-Metal Hydride (Sealed)</td>
<td>55</td>
<td>120</td>
<td>100</td>
<td>50</td>
<td>1000</td>
<td>-20...+60</td>
</tr>
<tr>
<td>Na-Sulphide</td>
<td>100</td>
<td>150</td>
<td>150</td>
<td>88</td>
<td>600</td>
<td>+300...+380</td>
</tr>
<tr>
<td>Air-Zinc</td>
<td>150</td>
<td>160</td>
<td>80</td>
<td>-</td>
<td>500</td>
<td>-</td>
</tr>
<tr>
<td>Lithium Polymer</td>
<td>120</td>
<td>250</td>
<td>160</td>
<td>-</td>
<td>600</td>
<td>+60...+100</td>
</tr>
<tr>
<td>USABC (Mid term) (3)</td>
<td>80</td>
<td>135</td>
<td>150</td>
<td>75</td>
<td>600</td>
<td>-30...+65</td>
</tr>
<tr>
<td>USABC (long term) (3)</td>
<td>200</td>
<td>300</td>
<td>400</td>
<td>75</td>
<td>1000</td>
<td>-40...+85</td>
</tr>
<tr>
<td>Flywheel (4)</td>
<td>14</td>
<td>-</td>
<td>800</td>
<td>-</td>
<td>300000</td>
<td>-</td>
</tr>
<tr>
<td>Ultracapacitor (5)</td>
<td>7</td>
<td>9</td>
<td>2000</td>
<td>85</td>
<td>3000</td>
<td>-20...+60</td>
</tr>
</tbody>
</table>

Notes: USABC – United States Advance Battery Consortium (Battery Goals)

(1) Data from reference [33], (2) Data from reference [32], (3) Data from reference [34],
(4) Data from reference [35], (5) Data from reference [36] and rest of data from reference [37].
The two most common and commercial rechargeable batteries used in industrial and transportation applications are the lead acid and nickel cadmium batteries. As these batteries have evolved over a period of nearly a century, their performance has improved and manufacturing cost reduced as demand for portable power and clean source of power for automobiles grew during this period. Today, the lead acid, nickel cadmium and many other types of rechargeable batteries continue to be improved in order to meet the ever demanding battery performance requirements e.g. those set out by the United States Advanced Battery consortium (USABC). Some of the USABC’s battery goals are shown in Table 2.3 and these performance goals are also compared to some of current leading rechargeable batteries.

It can be observed from Table 2.3, that none of the current rechargeable batteries are capable of meeting all of the long term criteria, or even the more practical mid-term goals. The gravimetric or volumetric energy density of current battery technology (which determines the driving range of an electric vehicle between recharges) are relatively lower compared to the values established by the USABC. The values of gravimetric or volumetric energy density established by the USABC are very similar to those for refuelling of a gasoline powered vehicle [34]. However, when these batteries are used in hybrid configuration with fuel cell technology (specific power 300 W/kg) then the combined power of the fuel cell and battery in the hybrid electric vehicle can compete with the current internal combustion engine vehicles. Hence, the batteries in a hybrid fuel cell system would provide the peak power demand (acceleration) and storage facility, while the fuel cell would provide the necessary power for an adequate range. The range limiting depends on the size of the fuel tank, rather than the energy in the battery container.

2.2.4.2 Flywheel and Ultracapacitor

A flywheel stores its energy in a rotating mass of composite material connected to a motor/generator. The flywheel can increase or decrease its energy storage capacity by changing the rotating structure. The energy stored in the rotor depends on the strength of the composite fibres, mass density, height, speed and outer diameter of the rotor. Although the interest in flywheel technology started in 1970s, the current resurgence
in the technology has been influenced by both advances in efficient bearing systems and stronger composite material. Today, flywheel units are being designed for motive, electric utility storage and power quality applications. Table 2.3 shows the current performance of a flywheel. Although the specific power (W/kg) is much superior, the gravimetric energy density (Wh/kg) compared to the USABC’s battery goals is poor. However, the prediction is to double this value to 30 Wh/kg by 2004 [34].

An ultracapacitor or electrochemical capacitor stores its energy in a polarised liquid layer which forms when an electrical potential is created between two electrodes in an electrolyte. Unlike batteries, the capacitor stores energy by charge separation within the micro-pores of high surface area electrode materials and these materials do not undergo chemical changes. In early 1990s, the US Department of Energy established a program to develop and evaluate ultracapacitors as an enabling electric/hybrid vehicle technology. Table 2.3 shows the performance of prototype ultracapacitors. Both the gravimetric and volumetric energy densities are very poor and therefore the ultracapacitors are used as an auxiliary power source either in electric vehicle to load level and extend vehicle range or in a fuel cell system to provide power for start up process and supplementary power supply [38].

2.2.5 Waste Heat Recovery System

The waste heat recovery system is a significant part of any power generating system, since it maximises the overall system efficiency. A waste heat recovery system may include simple recovery methods such as insulation through to complex methods such as heat pumps, recuperative (waste heat boilers & shell-and-tube) and regenerative (thermal wheel) heat exchangers and heat pipes. The choice of recovery method or methods depends on the quality of the thermal energy and the end use of the recovered thermal energy. However, in some cases a feasibility study and financial analysis (such as pinch technology) must be undertaken before the choice is made [40]. The end use of recovered thermal energy depends on the application of the overall system. For an industrial application, the thermal energy could be used to raise steam (high grade heat) while in a domestic or commercial sector application the
thermal energy would be used in space heating and hot water supply (high & low
grade heat respectively).

The design choice of waste heat recovery system depends on the temperature of the
working fluid, either in the whole system or in a particular component of the system
or plant. The higher the temperature of the fluid going to waste, the more obvious is
the desirability of recovering some of the thermal energy. For fuel cell applications,
the type of recovery method will depend on both the type of fuel cell (i.e. high or low
temperature fuel cell) and fuel supply system. For example, in the case of a low
temperature fuel cell such as the SPFC, if hydrogen tanks are used to supply the fuel
to the cell or stack, then the highest temperature of the working fluid would be
between 80-90°C and the best method to recover heat energy from this working fluid
would be a common heat exchanger design e.g. shell and tube or plate-fin. However,
if a fuel processor is used to generate the hydrogen rich gas, where the temperature of
the working fluid may be as high as 800-1200°C, then technologies such as
expanders, economisers, waste heat boilers or condensing boilers could also be used
together with the common heat exchangers, for heat recovery.

2.2.5.1 Heat Exchangers

The most applicable heat recovery technology for a fuel cell application is the heat
exchanger. The most common type of heat exchanger used is the recuperative type. A
recuperative heat exchanger e.g. shell-and-tube design, is characterised by the two
fluids being separated at all times by a solid barrier. The fluids can flow in the
counter-flow, in parallel-flow, in cross-flow, or combination of these. The
performance of these heat exchangers depend on the flow rates of the two fluids (cold
& hot), the area of the wall separating the two fluids, the temperature difference (or
the logarithmic mean temperature difference (LMTD)) and the overall heat transfer
coefficient. The heat loss to the atmosphere is negligible compared with the heat
transferred between the two fluids [40]. The performance of the heat exchanger is
sometimes quoted by its effectiveness, which is defined as the ratio of the actual heat
transferred compared to the maximum possible heat transfer available.
2.2.5.2 Flue Gas Expander

The thermal energy in the pressurised exhaust gas or flue gas from a burner can be recovered via a expander. In a low temperature fuel cell system, a burner can either be introduced to combust the fuel cell stack exhaust (anode and cathode) gases. Alternatively, presence of a fuel processor, where a burner is usually an integral part of the fuel processor, the burner can also burn the stack exhaust gases and fuel feed to provide the energy for the fuel processor. Similar to the compressor, the flue gas expander is currently being developed for fuel cell application, especially for low temperature and pressure of the flue gas. The expander performance depends on the pressure ratio, flowrate and temperature of the working fluid and isentropic efficiency. Since no manufacturing data are available to date [41], a constant isentropic efficiency of 80% is used in various fuel cell system analyses, the working properties of the flue gases is determined by the fuel cell system design. However, the isentropic efficiencies of both the expander and compressor are varied to investigate the effect on the overall system efficiency (section 3.4.4).

2.2.5.3 Boilers

Further thermal energy from the flue gas, especially the latent heat of condensation of the water vapour present in this flue gas, can be recovered via a condenser or waste heat boiler. This technology is mostly utilised when the fuel cell technology is applied in a total energy scheme or combined heat and power (CHP) scheme. A CHP scheme is one in which a plant’s energy requirements in the form of power and heat are provided from a supply of primary fuel and the energy wastage is reduced to a minimum. Hence, to maximise the total energy recovery from flue gas for a fuel cell system, a condenser boiler can be applied to utilise the thermal energy of the flue gas energy, including the latent heat of the water vapour.

A condensing boiler has potentially the highest efficiency both at part and full load. A boiler efficiency as high as 95% can be obtained if the water vapour in the flue gas is condensed by cooling the vapour below its dew point and the heat rejected (which is equivalent to the enthalpy of the evaporation of the water vapour at its partial
pressure) is recovered. The high efficiency performance of the boiler is very much dependable upon the control of inlet water temperature to the secondary heat exchanger, which is used for condensing purpose, and type of primary fuel used. The feed water (to the secondary heat exchanger) or the water returning from a heating system has to be controlled to a certain temperature, usually between 30-50°C, to achieve higher efficiency than conventional boilers. To avoid any corrosion problems in the boiler due to the acidic condensate, either a low sulphur or sulphur free fuel has to be used with a condenser boiler. (However, for the fuel cell application, the sulphur will be removed before the fuel cell stack). The boiler has to also be manufactured from suitable materials to which is resistance to corrosion (such as stainless steel or aluminium). Beside the extra secondary heat exchanger, the boiler also requires a condensate draining system and a fan to ensure adequate dispersal of the rest of the flue gas due to low flue gas exit temperature of about 40°C. These addition requirements make the condensing boiler much more expensive than conventional boiler. However, with the improvement in efficiency which would led to fuel saving, the boiler would therefore pay for itself in the long term [42].

2.2.6 Power Conditioner Equipment

The fuel cell system usually requires a power conditioning unit to either match the dc power of the fuel cell stack to a dc link voltage or to convert the fuel cell stack dc power to quality ac power, which is then supplied to the necessary system load. The two state of the art power conditioners used today with the fuel cell system are the DC/DC converter and DC/AC inverter. A DC/DC converter converts the fuel cell stack voltage into a regulated voltage corresponding to either a battery voltage or dc link voltage. This process includes a small power loss, which is usually between 1-2% i.e. 99%-98% efficient [43]. The role of the inverter is to convert dc power to ac power and is the interface between the fuel cell stack and the system load. The modern power electronics in the inverter offer high efficiency of > 97% [43].
2.2.7 Ancillary Equipments

Every fuel cell system requires ancillary equipments such as pumps, motors, humidifiers, pressure control valves etc for control and monitoring purposes, for start-up processes and above all to satisfy the number of safety requirements. The power for these ancillary equipments has to be provided at all times either from a battery or a small electrical generator or external electrical supply. The performance and power demand of the ancillary equipments used in the study of the fuel cell systems will be stated and detailed where there are used in the analyses.
2.3 REFERENCES


3. ANALYSIS AND OPTIMISATION OF A 40 kW_e NATURAL GAS SPFC COMBINED HEAT AND POWER SYSTEM

3.1 INTRODUCTION

A cogeneration or combined heat and power (CHP) scheme is one in which electrical power generation is combined with utilising waste heat for space-heating and/or specific industrial processes. A Solid Polymer Fuel Cell (SPFC) system which includes a fuel processor can be configured into a CHP scheme, producing both the high and low grade heat in addition to the electrical output. High efficiency, fast load following and environmentally "friendliness" can make the SPFC system a more attractive CHP plant than those based on the internal combustion engine or gas turbines.

A typical conventional power plant has a cycle efficiency of between 23% (Gas turbine)-38% (Steam turbine), while a CHP plant utilising the waste heat, will increase this efficiency to around 80%-85% (power & heat) [1-5]. Subsequent to the 1983 Energy Act, which obliged the Electricity supply industry to allow private generating plants to connect their equipment to the grid network, there has been a rapid growth in the use of small scale CHP in the service industry sector [4]. However, the small-scale CHP plant (< 50 kWe) using conventional prime movers such as the reciprocating engine were usually unacceptable in this market sector since the CHP scheme was noisy, inefficient and expensive to maintain [2]. Additional problems with CHP schemes also include higher capital and installation costs and common to all plants, is the need to meet the ever increasingly stringent demands of environmental legislation, relating to noise and air pollution [1]. However, the advantage the fuel cell technology will have over present CHP schemes is its low noise operation, extremely low air pollutant emissions, higher fuel conversion efficiency and ability to be modular in various sizes and power ranges [2]. These advantages make fuel cells particularly attractive for the small scale CHP market in the service industry sector, such as hospitals, leisure centres and hotels.

System efficiency analysis of projected SPFC systems in transportation and stationary applications indicate that a system efficiency (electrical) of 52% can be obtained
when using pressurised H₂ from on-board tanks, while an efficiency of between 35%-45% can be obtained when using a hydrocarbon fuel processor as a source of H₂ [6]. However, the system efficiency depends significantly upon the operating conditions of the fuel cell, H₂ and oxidant utilisation in the fuel cell, type of fuel and choice of reforming technology. It has been reported that a methanol (Steam Reformer) fuelled SPFC system can achieve a system efficiency of 42% with the fuel cell efficiency of 55% [7], while a gasoline (Partial Oxidation Reformer) based system with fuel cell operating at 0.685 volts and 85% fuel utilisation can achieve an efficiency of around 35% [8]. An investigation of a SPFC Diesel system for marine application showed that an efficiency of 26% (LHV) could be achieved at 0.66 volts and 67% H₂ utilisation [9]. Previous studies have shown the effect of pressure on the system efficiency i.e. a 40-kWe methane-fuelled SPFC system achieved 33% and 25% efficiency at 4 bar (a) and 1.5 bar (a) respectively [10]. Table 3.1 details estimated efficiencies for various operating conditions of the fuel cell, utilising a variety of fuels and fuel processor technologies.

Many of the systems calculations reported are for a particular application and end use of the electrical power. For a transport application system, the aim is to achieve maximum electrical efficiency with high volumetric and gravimetric power densities i.e. kW/l & kW/kg and minimum fuel consumption. For a stationary application, the system characteristics are highly dependent upon the operating criteria of the system. A system for power generation purposes will require different design and system targets compared to a system designed for CHP and remote or portable purposes. The design targets of the industrial scaled fuel cell CHP system should essentially be to achieve overall efficiency of greater than 80% and heat to power ratio of approximately 1 in order to compete with conventional form of CHP system [16]. Table 3.2 shows values of efficiency and heat and power ratio for conventional forms of CHP systems and fuel cells CHP systems (Data from reference [16]).

In order for a SPFC CHP scheme to achieve similar system performance to alternative fuel cell technologies (table 3.2), the SPFC system has to be analysed and optimised. System analysis and optimisation of a 40 kWₑ natural gas based SPFC CHP scheme are thus presented. The study details how the components of the system can be
Table 3.1: Calculated SPFC system efficiencies of system with various fuels and fuel processing technologies.

<table>
<thead>
<tr>
<th>FUEL PROCESSOR</th>
<th>HYDROGEN</th>
<th>METHANOL</th>
<th>Natural Gas (METHANE)</th>
<th>DIESEL</th>
<th>GASOLINE</th>
<th>ETHANOL</th>
<th>PROPANE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Type</td>
<td>None</td>
<td>None</td>
<td>Steam</td>
<td>PoX</td>
<td>Steam</td>
<td>PoX</td>
<td>PoX</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>800</td>
<td>750</td>
<td>712</td>
<td>878</td>
<td>600</td>
<td>1027</td>
<td></td>
</tr>
<tr>
<td>Pressure Bar(a)</td>
<td>200</td>
<td>3</td>
<td>2</td>
<td>3</td>
<td>20</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>Ratio (S/C)</td>
<td>20</td>
<td>2.5</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>1</td>
<td>1.3</td>
</tr>
<tr>
<td>Ratio (O/C)</td>
<td>-</td>
<td>81.5%</td>
<td>83.0%</td>
<td>80.0%</td>
<td>80%</td>
<td>90.10%</td>
<td></td>
</tr>
<tr>
<td>Efficiency</td>
<td>Tanks</td>
<td>Tanks</td>
<td>Pd M</td>
<td>CB/SR</td>
<td>CB/SR</td>
<td>CB/SR</td>
<td>Pd M</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>FUEL CELL</th>
</tr>
</thead>
<tbody>
<tr>
<td>Efficiency (LHV)</td>
</tr>
<tr>
<td>Power (kW)</td>
</tr>
<tr>
<td>Current Density (A/cm²)</td>
</tr>
<tr>
<td>Fuel Utilisation</td>
</tr>
<tr>
<td>Voltage (Volts)</td>
</tr>
<tr>
<td>Anode Stoichiometry</td>
</tr>
<tr>
<td>Cathode Stoichiometry</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>COMpressor/EXPander</th>
</tr>
</thead>
<tbody>
<tr>
<td>Expander Efficiency</td>
</tr>
<tr>
<td>Compressor Efficiency</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ANCILLARY SYSTEMS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power Condition Efficiency</td>
</tr>
<tr>
<td>Pumps Efficiency</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>SYSTEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Overall Efficiency</td>
</tr>
<tr>
<td>Electrical Efficiency (LHV)</td>
</tr>
<tr>
<td>Heat Efficiency</td>
</tr>
</tbody>
</table>

| REFERENCE NUMBER | 6 | 14 | 6 | 7 | 12 | 15 | 15 | 14 | 13 | 8 | 11 | 14 |

configured to build a CHP scheme. The performance of integrated system is optimised via usage of necessary components and varying operating conditions of these components. The system includes a methane steam reformer and associated fuel processing equipment, a fuel cell stack, an air compression/expander and a condensing heat recovery economiser. The use of heat exchangers and condensers are also incorporated to achieve the best overall system efficiency. Figure 3.1 shows a schematic presentation of this system. (Hardware illustrated with the dashed lines are optional and only used when required).

Table 3.2: Comparison of CHP system efficiencies

<table>
<thead>
<tr>
<th>CHP Systems</th>
<th>Overall Efficiency</th>
<th>Electrical Efficiency</th>
<th>Heat Efficiency</th>
<th>Heat:Power Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas Turbine</td>
<td>85%</td>
<td>26%*</td>
<td>59%</td>
<td>2.26</td>
</tr>
<tr>
<td>Gas Engine</td>
<td>85%</td>
<td>36%*</td>
<td>49%</td>
<td>1.36</td>
</tr>
<tr>
<td>PACF</td>
<td>85%</td>
<td>45%+</td>
<td>40%</td>
<td>0.89</td>
</tr>
<tr>
<td>SOFC</td>
<td>85%</td>
<td>55%+</td>
<td>30%</td>
<td>0.55</td>
</tr>
<tr>
<td>SOFC/GT</td>
<td>85%</td>
<td>68%+</td>
<td>17%</td>
<td>0.25</td>
</tr>
</tbody>
</table>

Notes: SOFC - Solid Oxide Fuel Cell, GT - Gas Turbine, PAFC - Phosphoric Acid Fuel Cell
* Typical Efficiency, + Maximum Efficiency

A steady state model of a 40 kW<sub>e</sub> SPFC CHP system was used to investigate the impact of varying the parameters of various components and thermal integration on the overall performance of the system. The following investigations were carried out:

1) Effect of preheating the reformer and burner reactants.

2) Use of condensers and/or pre-heater for the fuel cell exhausts gases.

3) Variation of fuel cell parameters
   3.1) The stack loading (10-40 kWe).
   3.2) The stack operating pressure (1-3.25 bar(a)).
   3.3) Cathode stoichiometry (1.2-2.5).

4) Effect of varying the compressor and expander isentropic efficiency.
Figure 3.1: Schematic representation of a 40kW_e SPFC CHP system
CHAPTER 3 - NATURAL GAS BASED SPFC CHP SYSTEM

3.2 FUEL CELL CHP SYSTEM SPECIFICATION

In this section the data used in the system analysis is explained and the choice of operating conditions used in a number of the sub-systems are justified. The SPFC CHP system is divided into two parts, i.e. the power generation system and the waste heat recovery system. The power generation system includes the fuel processor, fuel cell stacks, a compressor and an expander while the waste heat recovery system includes a condensing economiser and network of heat exchangers.

3.2.1 Fuel Processor

The fuel processor is defined as consisting of a methane steam reformer, a high temperature shift (HTS) reactor, a low temperature shift (LTS) reactor and a gas clean-up unit (GCU) which is also well known as a CO preferential oxidation reactor (CO PrOx).

3.2.1.1 Methane Steam Reformer

3.2.1.1.1 Reformer

The natural gas feedstock (North Sea source) has the chemical gas composition shown in Table 3.3. The composition is mainly methane with some light hydrocarbons, nitrogen and a small amount of sulphur [17]. If the reforming catalyst is not tolerant to sulphur then it is necessary to first pass the natural gas through a low and high temperature de-sulfurisation process, whereby the majority of the sulphur is removed (0.1ppb residual) [17]. The processed gas exiting the de-sulfurisation process was assumed to be at 350°C and containing 99.2 % CH₄ and 0.8% N₂. The system analysis were based on this processed gas composition, which has a lower heating value (LHV) of 802 MJ/kmole (methane @ 25°C) [18].

The generation of hydrogen by the steam reformer requires control of thermodynamic and kinetic conditions. The steam reforming of methane is an endothermic reaction, whose conversion is favoured by a high steam to carbon ratio, high temperature and
low pressure. Hence, the critical process variables affecting the performance of the steam reformer are the steam to carbon ratio, reformer operating temperature and pressure [19-23]. To study the effect of these variables and to establish the operating conditions for the steam reformer, a reformer model was developed using the ASPEN PLUS™ software package [24]. The model also calculates the methane conversion efficiency (%) and the reformed gas composition (% by volume (%vol.)) exiting the reformer reactor based on thermodynamic equilibrium conditions and chemical reactions.

<table>
<thead>
<tr>
<th>Component</th>
<th>Percent</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH$_4$</td>
<td>94.84</td>
</tr>
<tr>
<td>C$_2$H$_6$</td>
<td>3.90</td>
</tr>
<tr>
<td>i-C$<em>4$H$</em>{10}$</td>
<td>0.15</td>
</tr>
<tr>
<td>N$_2$</td>
<td>0.79</td>
</tr>
<tr>
<td>S (ppm)</td>
<td>4.0</td>
</tr>
</tbody>
</table>

The operating pressure of the reformer is normally similar to the system pressure. The system pressure in turn is determined by the required fuel cell operating pressure. The fuel cell operating pressure is normally in the range between 1.0 and 4.0 bar absolute (bar(a)). The conversion efficiency of the processed gas in the reformer over pressure range was found to be almost constant, as can be seen in figure 3.2. An operating pressure of 3.0 bar(a) for the reformer was assumed for all the system analysis.

The purpose of the methane steam reformer is to extract the maximum quantity of hydrogen held in water and methane. In order to achieve the maximum conversion of methane, correct water to methane molar ratio needs to be determined. The two reactions, which are responsible for production of hydrogen, are the reforming reaction (3.1) and the water shift reaction (3.2). Reaction (3.1) is more dominant at high temperature while the exothermic shift reaction (3.2) is favoured at lower temperature [25].

\[ \text{CH}_4 + \text{H}_2\text{O} \leftrightarrow \text{CO} + 3\text{H}_2 \quad \cdots (3.1) \]
\[
\text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2 \quad \ldots (3.2)
\]

The obvious ratio to select at higher temperature would be the stoichiometric ratio, which is 1.0 according to the reformer reaction (3.1). However, in practice the reformer is operated at much higher ratio of approximately 3.0-3.5 in order to avoid carbon formation and destruction of the catalyst bed. Nevertheless, there are economical disadvantages when operating at high ratios and therefore recent trends in reformer design, have sought to operate with lower molar ratios [25]. To determine the H\textsubscript{2}O:CH\textsubscript{4} molar ratio for this study, the molar ratios were varied between 0.5 to 3.5 at various temperatures and at a constant pressure of 3 bar(a). Figure 3.3 shows the conversion of CH\textsubscript{4} to reformed gases at these ratios and temperatures. From Figure 3.3, it can be observed that the maximum amount of hydrogen was produced at stoichiometric molar ratio of 1.0 and higher temperatures, as expected from reformer equation (3.1). However, a molar ratio S:C of 1.5 was chosen for this system analysis.
Figure 3.3: Conversion of processed gas at various molar ratios and temperatures.
This ratio, which supplies 50% extra steam into the reformer, was a trade off between the protection of the reformer catalyst bed and economical benefit of higher hydrogen yield and lower energy use to raise steam [25].

In order to determine the optimal operating temperature of the reformer, the temperature was varied between 350 and 2000 °C at a molar ratio H₂O:CH₄ of 1.5 and pressure of 3 bar(a). From figure 3.4, it was evident that between the temperatures of 850 and 1000°C, the maximum amount of hydrogen was produced. To minimise the amount of energy expended in the reformer, a sensible operating temperature of 850°C was chosen.

**Figure 3.4: Composition of reformed gas at various operating temperatures.**

Hence, the operating conditions for the reformer were determined to be 850°C, 3 bar(a) and a S:C molar ratio of 1.5. Under these conditions, the reformer equilibrium conversion efficiency was found to be 93% and the reformed gas consists of following proportions of gases (vol. %):

<table>
<thead>
<tr>
<th>Gas</th>
<th>Vol. %</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td>66.50%</td>
</tr>
<tr>
<td>CO</td>
<td>18.60%</td>
</tr>
<tr>
<td>CO₂</td>
<td>2.70%</td>
</tr>
<tr>
<td>H₂O</td>
<td>10.40%</td>
</tr>
<tr>
<td>N₂</td>
<td>0.20%</td>
</tr>
<tr>
<td>CH₄</td>
<td>1.60%</td>
</tr>
</tbody>
</table>
To calculate the heat of reformation, reaction (3.1) and (3.2) were considered. There are other reactions, which are responsible for production of H$_2$, but when dealing with equilibrium relationships these equations were not considered to be of significant importance. However, it should be noted that when dealing with the kinetic relationships, then the choice of equations is significant [20].

Methane is converted into hydrogen and carbon monoxide at 850°C (1123 K) and the heat of reformation is given by equation (3.3)

$$\text{CH}_4 + \text{H}_2\text{O} \leftrightarrow \text{CO} + 3\text{H}_2 \quad \Delta H_{1123 \text{ K}} = 22.99 \text{ kJ/mole} \quad ... (3.3)$$

The CO reacts further via the water shift reaction to produce more H$_2$ and CO$_2$ and the enthalpy of reaction at 850°C is given by equation (3.4)

$$\text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2 \quad \Delta H_{1123 \text{ K}} = -33.47 \text{ kJ/mole} \quad ... (3.4)$$

### 3.2.1.1.2 Reformer Burner

The burner is an integral part of the reformer and is supplied with the fuel cell stack exhaust gases, de-sulphurised natural gas and air from the compressor. The amount of energy required by the burner was determined by performing a heat balance on the reformer and maintaining the reformer's temperature at 850°C. The supply temperatures of various reactants of the burner were varied according to system configuration and availability of heat energy from the network of heat exchangers. The burner was supplied with 1% excess air to ensure complete combustion. The burner generated heat at 880°C, 30°C higher than the reformer's operating temperature to ensure good heat transfer. The flue gases exited the reformer at 880°C.

### 3.2.1.2 HTS and LTS Reactors

The HTS and LTS reactors convert CO to CO$_2$ and in the process yield more H$_2$ via the water gas shift reaction shown in the chemical equation (3.5). The HTS reactor is usually operated at a temperature of 400°C and typically reduces CO concentrations in
the gas stream down to 2-4%. The LTS reactor is operated at a lower temperature of approximately 200°C and reduces CO concentrations further down to 1-0.3% [26].

\[ \text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2 \]  \hspace{1cm} (3.5)

However, there are other reactions, which are also favourable at these temperatures, especially the low temperature of LTS reactor. The methanation reactions are very thermodynamically favourable at this temperature as seen from reaction (3.6) and (3.7) [26].

\[
\begin{align*}
\text{CO} + 3\text{H}_2 &\leftrightarrow \text{CH}_4 + \text{H}_2\text{O} \hspace{1cm} \Delta H = -206.2 \text{ kJ/mole} \hspace{1cm} (3.6) \\
\text{CO}_2 + 4\text{H}_2 &\leftrightarrow \text{CH}_4 + 2\text{H}_2\text{O} \hspace{1cm} \Delta H = -164.9 \text{ kJ/mole} \hspace{1cm} (3.7)
\end{align*}
\]

These reactions if allowed to take place in the reactor would consume most of the hydrogen and reverse the reforming process. To avoid the methanation reactions, suitable catalysts have to be used in the reactors whose selectivity favours water shift reactions rather than the methanation reactions. In industrial reactors chromia-supported iron based catalysts are used in the HTS reactor while copper and zinc oxide catalysts are used in the LTS reactor [26].

In this study, the HTS and LTS reactors temperature were chosen as 400°C and 200°C respectively, as most of the literature have stated as most favourable temperatures for the reactors [17,22,23,26]. ASPEN PLUS™ software package was also used to model the HTS and LTS reactors. With the temperature of the HTS and LTS fixed at 400°C and 200°C respectively, the reactors were optimised to give maximum conversion of CO to H\textsubscript{2} by varying the S:C molar ratio. The optimum ratio was found to be 0.5, which was equivalent to H\textsubscript{2}O:CO molar ratio of about 1.2. At this operating condition 18.6% CO from the reformer was reduced to 7.3% in the HTS and subsequently reduced to 0.7% in the LTS reactor. The reactor also produced 70% and 77% of H\textsubscript{2} (vol. %) from the HTS and LTS reactors respectively. The reformate gas composition from the outlet of the HTS and LTS reactors are shown below (vol. %):
Under steady state conditions, the exothermic reactions in both the HTS and LTS reactors and thermal energy in the feed, supplied the reactors heat duty and maintained the desired operating temperature of both the reactors. The excess thermal energy was not used in the waste heat recovering system.

### 3.2.1.3 Gas Clean-Up Unit (GCU)

The performance of SPFC can be drastically reduced by the presence of CO in the fuel anode stream. The decrease in the SPFC electrochemical performance is brought about by the preferential adsorption of the CO rather than H$_2$ onto the platinum electrocatalytic sites at the anode. To avoid CO anode poisoning with Platinum electrocatalysts, it is desirable that the CO concentration in the reformed gas is less than 10 ppm (0.001%). (However, some manufactures are now quoting a much higher tolerance levels in the region of several hundred ppm). There are several possible methods for removing CO from the reformed gas. Such methods include palladium membranes, methanation, pressure swing adsorption and catalytic selective oxidation [28]. However, the method selected for analysis here was selective oxidation. Since it has the advantages of fast reaction kinetics, low-pressure drop and relatively low temperature operation [27,28].

The model used in this study incorporates the characteristics of the GCU developed by the Fuel Cell Group at Loughborough University. The GCU unit is designed to reduce CO concentrations to ppm level using a Platinum Ruthenium (Pt-Ru) based catalyst, supported upon a high surface area aluminium heat exchanger. CO oxidation reaction is related to both the operating temperature (120°C-200°C) and O$_2$:CO molar
ratio (1-4). The unit is capable of reducing CO level of less than 15 ppm (<5ppm with dry gases) [27].

The GCU reactor preferentially oxidises the CO to CO₂ over a heterogeneous catalyst at a temperature of about 160°C via the chemical equation (3.8).

\[
\text{CO} + \frac{1}{2} \text{O}_2 \leftrightarrow \text{CO}_2 \quad \Delta H_{298.15 \text{K}} = -283 \text{ kJ/mole} \quad \text{(3.8)}
\]

For this study, the operating condition of the GCU unit were chosen to be 160°C and a O₂:CO molar ratio of 2.5. At these operating conditions, CO was assumed to be reduced to ≤ 10 ppm and the rest of the oxygen was used in H₂ combustion. The clean reformate from the GCU unit had the following gas composition (vol. %):

<table>
<thead>
<tr>
<th>Component</th>
<th>GCU Gas Composition (vol. %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td>69.33%</td>
</tr>
<tr>
<td>CO</td>
<td>0.001%</td>
</tr>
<tr>
<td>CO₂</td>
<td>18.20%</td>
</tr>
<tr>
<td>CH₄</td>
<td>0.94%</td>
</tr>
<tr>
<td>H₂O</td>
<td>5.16%</td>
</tr>
<tr>
<td>N₂</td>
<td>6.36%</td>
</tr>
</tbody>
</table>

3.2.1.4 Air Bleed

To further reduce the CO concentration in the clean reformate from the GCU reactor, 1% air bleed (equal to 1% Hydrogen in the reformat) was mixed with reformate prior to the fuel cell anode inlet [29]. It was assumed that in the anode, all the CO was combusted and any excess oxygen was used to combust hydrogen.
3.2.2 SPFC Stack

The SPFC stack operating conditions has major impact upon the performance of the overall system performance. The variation of these operating conditions also effects the actual performance of the fuel cell. The performance of the fuel cell in terms of operating conditions such as electrical load, pressure, temperature, cathode stoichiometry is described in this section. Data presented is based on a 200 cm$^2$ cell developed by Advanced Power Sources Ltd.

3.2.2.1 SPFC Stack Electrical Loading

For a fixed number of cells in a stack, the performance of the stack is a function of current or the power drawn from the stack. As the current on the fuel cell changes, the fuel cell voltage and efficiency changes. Usually a polarisation curve (a plot of cell voltage versus the current density for a particular operating condition (figure 3.5)) is used to illustrate change in cell voltage as the current changes. A fuel cell stack is generally designed to operate at a particular point on the polarisation curve. If the stack is operated at part load, the cell voltage increases and accordingly the voltage ($\eta_v$) and thermal ($\eta_{th}$) efficiencies (defined in Appendix I) increase, unlike IC engines [30]. This is a unique characteristic of fuel cell and has significant impact upon the overall system efficiency.

This study considers a SPFC stack with 560 cells of 200 cm$^2$ active area operating at a voltage of 0.730 volts per cell and a current density of 0.489 A/cm$^2$. At this design point, the stack delivers a power of 40 kW$e$. Figure 3.5 shows the cell polarisation and power curves at a pressure of 3 bar(a) and 80°C and the operating voltage of the cell at 100%, 75%, 50% and 25% power load. Table 3.4 shows the voltage ($\eta_v$) and thermal ($\eta_{th}$) efficiencies at these loads. The operating points, shown in table 3.4, will be used to analyse the effects of stack loading on the electrical and overall system efficiencies.
Figure 3.5: Polarisation and power curves at 3 bar(a) and 80°C.

Table 3.4: Fuel cell performance at different power loads

<table>
<thead>
<tr>
<th></th>
<th>% Power Load</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>25%</td>
</tr>
<tr>
<td>Cell Voltage (volts)</td>
<td>0.831</td>
</tr>
<tr>
<td>Current Density (A/cm²)</td>
<td>0.108</td>
</tr>
<tr>
<td>Thermal Efficiency, η_Th (LHV)*</td>
<td>66.26%</td>
</tr>
<tr>
<td>Voltage Efficiency, η_V (LHV)*</td>
<td>70.38%</td>
</tr>
</tbody>
</table>

Notes: * Definitions in Appendix I
3.2.2.2 SPFC Operating Pressure

The performance levels of the fuel cell are enhanced when increasing the operating pressure of the cell, especially the cathode pressure. The increase in pressure at the cathode increases the oxygen reaction rate and reducing polarisation losses at the cathode and hence improves the performance of the cell. However, operating at high pressure requires additional energy to compress the gases, which negates the efficiency gains achieved in the cells.

The effect of increasing pressure on the performance of the cell is evident in figure 3.6. The figure shows the polarisation curves for a cell on hydrogen and air at a temperature of 80°C, anode and cathode stoichiometric of 1.5 and 2.0 respectively and pressure range of 1 - 3.25 bar(a). The figure also shows the 40 kW_e power line and the operating points at different pressure is where this line intersects the polarisation curves. The performance of the SPFC at these points on the different pressure curves is shown in the Table 3.5. These operating points are also used to analyse the effect of pressure on the electrical and overall system efficiencies.

Figure 3.6: Polarisation curves for 200 cm² SPFC at different pressures
Table 3.5: 40 kW<sub>e</sub> SPFC performance at different operating pressures

<table>
<thead>
<tr>
<th>Operating Pressure (bar(a))</th>
<th>1.0</th>
<th>1.25</th>
<th>1.50</th>
<th>1.75</th>
<th>2.0</th>
<th>2.25</th>
<th>2.50</th>
<th>2.75</th>
<th>3.0</th>
<th>3.25</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell Voltage (Volts)</td>
<td>0.565</td>
<td>0.678</td>
<td>0.695</td>
<td>0.705</td>
<td>0.715</td>
<td>0.719</td>
<td>0.724</td>
<td>0.728</td>
<td>0.730</td>
<td>0.735</td>
</tr>
<tr>
<td>Current Density (A/cm&lt;sup&gt;2&lt;/sup&gt;)</td>
<td>0.632</td>
<td>0.527</td>
<td>0.514</td>
<td>0.507</td>
<td>0.500</td>
<td>0.497</td>
<td>0.493</td>
<td>0.491</td>
<td>0.489</td>
<td>0.486</td>
</tr>
<tr>
<td>Number of Cells</td>
<td>560</td>
<td>560</td>
<td>560</td>
<td>560</td>
<td>560</td>
<td>560</td>
<td>560</td>
<td>560</td>
<td>560</td>
<td>560</td>
</tr>
<tr>
<td>Anode Exhaust Relative Humidity&lt;sup&gt;+&lt;/sup&gt; (%)</td>
<td>24.12</td>
<td>30.15</td>
<td>36.18</td>
<td>42.21</td>
<td>48.24</td>
<td>54.27</td>
<td>60.30</td>
<td>66.33</td>
<td>72.37</td>
<td>78.40</td>
</tr>
<tr>
<td>Cathode Exhaust Relative Humidity&lt;sup&gt;+&lt;/sup&gt; (%)</td>
<td>40.13</td>
<td>50.16</td>
<td>60.19</td>
<td>70.22</td>
<td>80.26</td>
<td>90.29</td>
<td>100.32</td>
<td>110.35</td>
<td>120.38</td>
<td>130.42</td>
</tr>
<tr>
<td>Efficiency η&lt;sub&gt;Th&lt;/sub&gt; (LHV) &lt;sup&gt;+&lt;/sup&gt; (%)</td>
<td>45.08</td>
<td>54.06</td>
<td>55.45</td>
<td>56.25</td>
<td>57.05</td>
<td>57.35</td>
<td>57.75</td>
<td>58.05</td>
<td>58.25</td>
<td>58.64</td>
</tr>
<tr>
<td>Maximum Heat from the Fuel Cell&lt;sup&gt;+&lt;/sup&gt; (kW)</td>
<td>48.73</td>
<td>34.00</td>
<td>32.13</td>
<td>31.11</td>
<td>30.12</td>
<td>29.75</td>
<td>29.27</td>
<td>28.91</td>
<td>28.68</td>
<td>28.21</td>
</tr>
</tbody>
</table>

Notes: * + Definitions in Appendix I, Relative Humidity < 100 => Water in Vapour Phase
3.2.2.3 SPFC Operating Temperature

The operating temperature of the SPFC is currently limited within the temperature range of between 60-90°C. At temperatures greater than 90°C, the dehydration of commercially available ion-conducting polymeric membranes (e.g. Nafion) takes place, which leads to a reduction in ionic conductivity. The operating temperature of SPFC for this study was chosen as 80°C [31].

3.2.2.4 Cathode Stoichiometry

The performance of the SPFC is influenced to a greater extent by the cathode stoichiometry than the anode stoichiometry. The cell performance is significantly limited by the mass transport of oxygen to active sites at the cathode. This is due to the presence of product water from the oxygen reduction reaction and transport of water across the membrane from the anode, which hinders the access of oxygen into the porous structure of the electrode. Increasing the cathode stoichiometry does not only provide excess oxygen to the cathode, but also helps in removing the excess water from the cathode [31]. However, operating the fuel cell at higher cathode stoichiometry imposes a parasitic load on the fuel cell system, which undermines the achievement gained in fuel cell efficiency.

To study the effect of cathode stoichiometry on the overall system efficiency, the stoichiometry was varied between 1.2 to 2.5. Figure 3.7 shows the polarisation curves for different stoichiometry at 3 bar(a), 80°C and anode stoichiometry of 1.5. The figure also shows the 40 kWₑ power line, which will determine the operating points to be used in the system analysis. Table 3.6 shows the performance of the 40 kWₑ SPFC stack at these operating points.
3.2.3 Compressor and Expander

In accordance with electrochemical theory, fuel cells exhibit improved performance when the fuel and oxidant are supplied at increased pressure. Air is usually supplied to the cathode at elevated pressure by a compressor. In most fuel cell systems, the power required to drive the compressor corresponds to a parasitic load of approximately 20-25% of the fuel cells stack power [32,33]. The parasitic load does not only depend upon the fuel cell stack operating conditions e.g. pressure and cathode stoichiometry, but also on the design of the compressor and its efficiency. Besides operating at optimal point to minimise the parasitic load, the compressor should also be adaptable to change in fuel cell stack and air quality demand. The compressor should also have the capability to handle changes in the airflow at an approximately constant pressure ratio and of delivering uncontaminated air in one stage compression.
Table 3.6: 40 kW<sub>e</sub> SPFC Performance at a range of cathode stoichiometries

(No. Of Cells = 560 cell & Active Cell Area = 200 cm<sup>2</sup>).

<table>
<thead>
<tr>
<th>Cathode Stoichiometry</th>
<th>1.2</th>
<th>1.3</th>
<th>1.4</th>
<th>1.5</th>
<th>1.6</th>
<th>1.7</th>
<th>1.8</th>
<th>1.9</th>
<th>2.0</th>
<th>2.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell Voltage (Volts)</td>
<td>0.307</td>
<td>0.508</td>
<td>0.602</td>
<td>0.650</td>
<td>0.680</td>
<td>0.698</td>
<td>0.709</td>
<td>0.715</td>
<td>0.721</td>
<td>0.732</td>
</tr>
<tr>
<td>Current Density (A/cm&lt;sup&gt;2&lt;/sup&gt;)</td>
<td>1.003</td>
<td>0.606</td>
<td>0.511</td>
<td>0.473</td>
<td>0.452</td>
<td>0.441</td>
<td>0.434</td>
<td>0.430</td>
<td>0.427</td>
<td>0.420</td>
</tr>
<tr>
<td>Anode Exhaust Relative Humidity&lt;sup&gt;+&lt;/sup&gt; (%)</td>
<td>72.37</td>
<td>72.37</td>
<td>72.37</td>
<td>72.37</td>
<td>72.37</td>
<td>72.37</td>
<td>72.37</td>
<td>72.37</td>
<td>72.37</td>
<td>72.37</td>
</tr>
<tr>
<td>Cathode Exhaust Relative Humidity&lt;sup&gt;+&lt;/sup&gt; (%)</td>
<td>188.69</td>
<td>176.19</td>
<td>165.25</td>
<td>155.58</td>
<td>146.99</td>
<td>139.29</td>
<td>132.36</td>
<td>126.09</td>
<td>120.38</td>
<td>98.17</td>
</tr>
<tr>
<td>Efficiency η&lt;sub&gt;TH&lt;/sub&gt; (LHV)&lt;sup&gt;+&lt;/sup&gt; (%)</td>
<td>24.47</td>
<td>40.53</td>
<td>48.03</td>
<td>51.87</td>
<td>54.26</td>
<td>55.69</td>
<td>56.57</td>
<td>57.05</td>
<td>57.53</td>
<td>58.41</td>
</tr>
<tr>
<td>Maximum Heat from SPFC&lt;sup&gt;+&lt;/sup&gt; (kW)</td>
<td>112.94</td>
<td>51.58</td>
<td>36.64</td>
<td>30.37</td>
<td>26.71</td>
<td>24.43</td>
<td>22.88</td>
<td>21.81</td>
<td>20.75</td>
<td>17.43</td>
</tr>
</tbody>
</table>

Notes: Notes: * + Definitions in Appendix I, Relative Humidity <100 ⇒ Water in Vapour Phase
At the present no such commercial compressors exist which are suitable to supply oil free air to the fuel cell efficiently. However, efforts are being made to design and develop small efficient compressors such as the sliding vane \[34\] and screw-type \[33\] for automotive fuel cell applications.

In this steady state study of the SPFC system, the compressor supplies the air to the fuel processor and the fuel cell. The compressor model assumes air as an ideal working fluid and uses isentropic efficiency as a measure of its performance. The model also assumes that the compressor delivers air in one stage compression and its characteristics are matched precisely to the system needs. The required compressor power is dependent on the flow rate, pressure ratio and isentropic efficiency. The model calculates a temperature \(T_2\) equivalent of the compressor work for specified pressure ratio and efficiency by the following equation \(3.9\) \[35\]:

\[
T_2 = \frac{T_a}{\eta_c} \left( \frac{P_2}{P_a} \right)^{\left( \frac{\gamma - 1}{\gamma} \right)} - 1 + T_a
\]

Where

- \(T_a\) is the air inlet temperature (K)
- \(\eta_c\) is the isentropic efficiency
- \(P_2\) is the compressor outlet pressure (Bar)
- \(P_a\) is the compressor air inlet pressure (Bar)
- \(\gamma = 1.4\) for air

In order to understand the effect of compressor on the electrical and overall system efficiency, the compressor isentropic efficiency was varied from 10%-100%. Where the compressor efficiency was not varied (in other case studies), the compressor isentropic efficiency has been taken as 80%, to reflect possible future performances of a compressor in a fuel cell system.
To reduce the parasitic load drain on the system, the chemical energy contained within the burner fuel and anode exhaust gas can be utilised in an expander, to supply the power to the compressor and system. The measure of the expander’s performance in this study is also modelled by the isentropic efficiency. The burner exhaust gases (flue gases) are fed to the inlet of the expander, which generates the power for the compressor. The expander power is calculated using flue gas flow rate, pressure ratio and isentropic efficiency. The model calculates a temperature ($T_4$) equivalent of the expander work for specified pressure ratio and efficiency by the following equation (3.10):

$$T_4 = T_3 - \eta_I T_3 \left[1 - \left(\frac{P_4}{P_3}\right)^{\left(\frac{\gamma - 1}{\gamma}\right)}\right]$$

...(3.10)

Where

- $T_3$ is the flue gas inlet temperature (K)
- $\eta_I$ is the isentropic efficiency
- $P_4$ is the expander outlet pressure (Bar)
- $P_3$ is the expander flue gases inlet pressure (Bar)
- $\gamma = 1.33$ for burner flue gases

The expander power was supplied to the compressor via a mechanical shaft, with a transmission efficiency ($\eta_m$) of 98%. The model assumes that the working envelope of the expander matches that of the compressor, and excess power from the expander generator was supplied to the system load. An electrical motor was also coupled to the compressor/expander shaft to balance the compressor/expander power. (The motor was modelled with a constant efficiency of 90%). Similar to the compressor, the expander efficiency was also varied from 10%-100%, in order to study the effect on the electrical and overall system efficiency. Where the expander efficiency was not varied (in other case studies), the expander efficiency has been taken as 80%.
3.2.4 Waste Heat Recovery System

In this study, the aim was to recover the thermal energy from the burner flue gases, fuel processor equipment and fuel cell stack, for either pre-heating reactants and/or providing hot water for space heat (high-grade) and hot water supply (low-grade). The recovery was via a condensing economiser and network of heat exchangers. The operating conditions are dependent upon optimisation of the overall system, in order to achieve the desired heat to power ratio and overall system efficiency. The thermal energy from the fuel processor and fuel cell stack was recovered by number of heat exchangers. For the heat exchangers, only the inlet and outlet conditions of the working fluid streams were considered and 1% energy loss was assumed from the surface. The thermal energy of the flue gas was first used in the expander and then to preheat the reformer and burner reactants. The condensing economiser then recovered the remaining energy of the flue gases.

The performance of the economiser is dependent upon the inlet and outlet temperatures of the flue gases, the exit temperature of the condensate and economiser's casing losses. The exit temperature of the flue gases and the condensate were kept fixed at 40°C and 35°C respectively. The casing losses were assumed to be 1.5% [1]. The efficiency of the condensing economiser was calculated by varying the flue gases inlet temperature. Figure 3.8 shows the performance of the economiser for a range of flue gases inlet temperatures. The high-grade heat values shown in the figure 3.8 were also calculated for a range of flue gases inlet temperatures. Figure 3.9 shows a typical schematic representation of waste heat recovery system.
Figure 3.8: Condensing economiser performances at range of flue gases inlet temperature
Figure 3.9: Schematic representation of waste heat recovery system

- **HOT WATER TANK**
- **CONDENSATE @ 35°C**
- **FLUE GASES (VARYING TEMPERATURE)**
- **FLUE GASES EXIT @ 40°C**
- **COOLING WATER**
- **Anode 80°C**
- **Cathode**
- **VARYING THERMAL ENERGY & TEMPERATURE**
- **HEX 2**
- **HEX 3**
- **HEX 4**
- **HEX 5**
3.3 STEADY STATE MODEL CALCULATIONS

In this section, the steady state model calculations are illustrated and the subsystem efficiencies defined. The model employs the data and the operating conditions described in the previous section. The model performs steady state heat and mass balances on individual components of the system, in order to determine the performance and efficiency of the component at set point operating conditions. The calculations are based on a net fuel cell output of 40 kW\textsubscript{e}, lower heating value (LHV) of the methane (802 MJ/kmole @ 25°C) \cite{18} and in addition to other system assumptions. The analysis was carried out for a SPFC CHP system depicted in figure 3.10, which operated at 3 bar(a) and the fuel cell stack exhaust gases were condensed rather than preheated. The effect of preheating the fuel cell stack exhaust gases prior to feeding these exhaust gases to the burner is dealt with in section 3.4.

3.3.1 System Assumptions

The model in its calculations made the following assumptions:

1. All calculations were made relative to a datum temperature of 25°C.
2. The pressure drop over the various components of the system has been neglected.
3. The energy used in the desulfurisation process is not accounted for.
4. 1\% reformer surface losses.
5. Electrical requirement for all the ancillary equipment was not considered.
6. Methane in the reformed gas from the reformer is not consumed in the HTS, LTS, GCU and SPFC.
7. All heat exchangers are assumed to have 1\% surface losses.
8. 1\% excess air is used in the burner and the burner efficiency is assumed to be 100\%.
9. 100\% water is removed from the gas stream in the condenser.
10. 40\% water vapour remains in the flue gases exit \cite{1}.
Figure 3.10: Schematic representation of a 40kW$_e$ SPFC CHP system (with condensers) at 3 bar(a)
3.3.2 Fuel Processor

3.3.2.1 Methane Steam Reformer and Burner

The reformer reactants were first preheated to a temperature of 350°C and passed through a desulfurisation process. The processed natural gas (99.2% CH₄, 0.8% N₂) and the steam were further preheated to 800°C and fed to the reformer. The burner was supplied with the fuel cell stack exhaust gases (25°C), processed natural gas and air from the compressor (preheated to 350°C). The amount of supplementary processed natural gas supplied to the burner was determined by performing a heat balance on the reformer and maintaining the reformer's temperature at 850°C. 1% excess air was also supplied to ensure complete combustion and it was assumed that the burner supplied the heat to the catalyst bed at 880°C. The reformer efficiency and power required for the reformer reaction were also determined by heat balance. Figure 3.11 shows the result of the heat balance for the reformer at 3 bar(a).

![Heat Balance Diagram](image)

**Figure 3.11: Reformer heat balance at 3 bar(a)**

| Processed Gas | 40.00 kW | 20.37 % |
| Compressed Air | 1.73 kW | 0.88 % |
| Exhaust Gases | 39.06 kW | 19.90 % |
| Total | 80.79 kW | 41.15 % |
From the reformer heat balance, the reformer efficiency, $\eta_{\text{Ref}}$, was found to be 69.08% and the power for the reformer reactions at 850°C, $\Delta P_{\text{Ref}}$ (1123 K), was determined to be 20.08 kW. The definition of $\eta_{\text{Ref}}$ and $\Delta P_{\text{Ref}}(1123\text{ K})$ are as following:

$$\eta_{\text{Ref}} = \frac{\text{Power in the reformed gases}}{\text{Total power into the reformer}}$$

$$\Delta P_{\text{Ref}}(1123\text{ K}) = (\text{Total Power into the burner}) - (\text{Flue gases power + Power losses})$$

3.3.2.2 HTS and LTS Reactors

The HTS and LTS reactors were heated to the required operating temperature by a combination of heat content of the reformed gases and the exothermic reaction in the shift rectors. Only the inlet and outlet conditions of the reactants and products are considered for the heat and mass balance. To maintain the HTS and LTS reactors at a operating temperatures of 400°C and 200°C respectively, the amount of heat power to be removed by a cooling system was determined to be 4.95 kW and 3.38 kW for the HTS and LTS reactors respectively.

3.3.2.3 GCU Reactor

For the operating conditions detailed in section 3.2.1.3, a heat and mass balance was carried out to determine the thermal power to be removed from the GCU, in order to maintain a temperature of 160°C. This was calculated to be 4.45 kW. (This heat power also contains thermal energy produced via some combustion of product H$_2$ with excess O$_2$ in the GCU.)

3.3.2.4 Fuel Processor Efficiency

Fuel processor efficiency, $\eta_{\text{FP}}$, is a measure of the fuel processor performance compared to other subsystems. The efficiency is defined as follows:

$$\eta_{\text{FP}} = \frac{\text{LHV of Anode Feed Gas (kW)}}{\text{LHV of the Fuel to the system (kW)}}$$
The fuel processor efficiency, $\eta_{FP}$, for the system presented in figure 3.10 was calculated to be 82%.

3.3.3 SPFC Stack

A heat and mass balance for the fuel cell stack was carried out in order to determine the heat to be removed by a cooling system to maintain the stack temperature of $80^\circ$C. The data for the fuel cell at 3 bar(a) detailed in table 3.5, were used in the heat and mass balance calculation. The anode and cathode stoichiometries were 1.5 and 2 respectively. Figure 3.12 shows the heat balance of the fuel cell at these operating conditions.

From the heat balance, the cooling power required to maintain the stack at $80^\circ$C was determined to be 20 kW. The relative humidities of the anode and cathode exhaust gas streams were also calculated using the partial pressure of the water vapour in these
gas streams. These were found to be 72.4% and 120.4% for anode and cathode outlet streams respectively. The mathematical humidity model is shown in appendix I.

3.3.4 Compressor and Expander

For this steady state analysis the isentropic efficiency of the compressor and expander were taken as 80% respectively. Using equation 3.9 in section 3.2.3, the air temperature at the outlet of the compressor, (at a pressure ratio of 3) was calculated to be 163°C. The corresponding compressor power was determined to be 6.53 kW. Including the mechanical transmission efficiency of the shaft (ηₘ = 98%), the total power required by the compressor at pressure ratio of 3, was determined to be 6.66 kW.

The expander power was also calculated for pressure ratio of 3 and isentropic efficiency of 80%. The flue gases at the temperature of 880°C were expanded resulting in an exit temperature of 658.62°C. The power generated by the expander was 13.31 kW. Additional power (6.65 kW) from the expander was combined via a generator with fuel cell stack power and supplied to the system load.

3.3.5 Heat Exchangers and Condensers

From figure 3.10 it can be seen that seven heat exchangers were used in this system analysis. The heat balances were performed by considering only the inlet and outlet conditions of the fluid streams. Where the outlet temperature of one of the fluid streams was required, a heat balance with an iterative process was used to calculate the temperature to match the thermal energy of the outlet fluid stream. 1% surface thermal loss was also included in these process. Heat exchangers 1, 6 and 7 were used for pre-heating the reformer and burner reactants. Heat exchangers 2, 3, 4 and 5 were used in heating water for the waste recovery system. Table 3.7 shows the performance of these heat exchangers.

Condensers were used to cool down and remove all the water from the anode and cathode exhaust gas streams. The exhaust gas streams were cooled down from 80°C
to 25°C with 100% water recovery from the gas streams. The amount of thermal power and latent heat recovered in the condenser was calculated to be 15.57 kW and 99% of this thermal power was used to heat water in the waste recovery system.

Table 3.7: Performance of the heat exchangers at 3 bar(a)

<table>
<thead>
<tr>
<th>Heat Exchanger No.</th>
<th>T₁in (°C)</th>
<th>T₁out (°C)</th>
<th>T₂in (°C)</th>
<th>T₂out (°C)</th>
<th>Power Loss (kW)</th>
<th>Power Transferred or Available (kW)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>850</td>
<td>400</td>
<td>350</td>
<td>800</td>
<td>0.08</td>
<td>8.06</td>
</tr>
<tr>
<td>2</td>
<td>400</td>
<td>200</td>
<td>-</td>
<td>-</td>
<td>0.04</td>
<td>3.77</td>
</tr>
<tr>
<td>3</td>
<td>200</td>
<td>160</td>
<td>-</td>
<td>-</td>
<td>0.01</td>
<td>0.75</td>
</tr>
<tr>
<td>4</td>
<td>160</td>
<td>80</td>
<td>-</td>
<td>-</td>
<td>0.02</td>
<td>1.48</td>
</tr>
<tr>
<td>5</td>
<td>163</td>
<td>80</td>
<td>25/163</td>
<td>350</td>
<td>0.03</td>
<td>3.36</td>
</tr>
<tr>
<td>6</td>
<td>659</td>
<td>424</td>
<td>25</td>
<td>400</td>
<td>0.14</td>
<td>13.49</td>
</tr>
<tr>
<td>7</td>
<td>424</td>
<td>362</td>
<td>25</td>
<td>400</td>
<td>0.04</td>
<td>3.45</td>
</tr>
</tbody>
</table>

Notes: 1,2 - fluid one (e.g. gas stream) & two (e.g. water or reactants).
* Operating condition not calculated.

3.3.6 Waste Heat Recovery System

Waste heat recovery for the system depicted in figure 3.10, was achieved via the condensing economiser, the network of heat exchangers and cooling systems for the stack and GCU (figure 3.9). The final use of the recovered heat which could be used for hot water supply and space heat was not modelled (as end use of thermal energy was not specified), but the thermal power and the maximum temperature at which this waste heat was available was calculated. The high-grade heat for this particular system was defined as the heat available at a temperature of greater than 200°C while the low grade heat was available at a temperature below 200°C.

High grade heat was available from the condensing economiser, where the waste heat power was available at temperature of approximately 350°C from the flue gases. The flue gas stream from heat exchanger 7 entered the economiser at temperature of 362°C. At this flue gas stream temperature, the efficiency and the thermal power of
the economiser was determined to be 73% and 21.31 kW respectively. This thermal power was delivered to water entering the economiser at 25°C.

The low grade heat was supplied by hot water which received the thermal power from heat exchangers 2, 3, 4, 5, condensers, cooling system of fuel cell and GCU. The cold water at 10°C was used to recover heat from heat exchangers 4, 5, condensers and cooling system of fuel cell at 80°C to a high temperature source of thermal power in heat exchanger 2 at 400°C. The maximum amount of low grade thermal power which could be recovered was calculated to be 49 kW. The final delivery temperature of the low grade thermal power in the supply water was not modelled.

3.3.7 System Efficiency and Heat to Power Ratio

The performance of a CHP scheme is usually measured by the overall system efficiency ($\eta_{\text{overall}}$) and the heat to power ratio ($R_{\text{H/P}}$). The overall efficiency is a sum of the electrical ($\eta_{\text{El Sys}}$) and heat ($\eta_{\text{Ht Sys}}$) system efficiencies while the heat to power ratio is the proportion of these two efficiencies. The electrical and heat system efficiencies are defined as following:

\[
\eta_{\text{El Sys}} = \frac{\text{SPFC Power (kW)} + \text{Expander Power (kW)}}{\text{LHV of the Fuel to the system (kW)}}
\]

\[
\eta_{\text{Ht Sys}} = \frac{\text{High and Low Grade Heat (kW)}}{\text{LHV of the Fuel to the system (kW)}}
\]

Therefore, the overall efficiency and heat to power ratio is defined as:

\[
\eta_{\text{Overall}} = \eta_{\text{El Sys}} + \eta_{\text{Ht Sys}} \quad R_{\text{H/P}} = \frac{\eta_{\text{El Sys}}}{\eta_{\text{Ht Sys}}}
\]

The electric and heat efficiencies for SPFC CHP system (seen in figure 3.10) were determined to be 34.55% and 52.06% respectively. The overall system efficiency and
the heat to power ratio were therefore calculated to be 86.61% and 1.51 respectively. Table 3.8 shows the overall system heat balance and system efficiencies.
Table 3.8: Overall heat balance of the SPFC CHP system

<table>
<thead>
<tr>
<th>Description</th>
<th>POWER INTO THE SYSTEM (kW)</th>
<th>POWER INTO THE SYSTEM (%)</th>
<th>POWER OUT OF THE SYSTEM (kW)</th>
<th>POWER OUT OF THE SYSTEM (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>REFORMER REACTANTS</td>
<td>97.07</td>
<td>72%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>FUEL TO THE BURNER</td>
<td>37.94</td>
<td>28%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>REFORMER SURFACE LOSSES</td>
<td></td>
<td></td>
<td>1.16</td>
<td>0.86%</td>
</tr>
<tr>
<td>HEX1</td>
<td></td>
<td></td>
<td>0.08</td>
<td>0.06%</td>
</tr>
<tr>
<td>HTS LOSSES</td>
<td></td>
<td></td>
<td>4.95</td>
<td>3.67%</td>
</tr>
<tr>
<td>HEX2</td>
<td></td>
<td></td>
<td>3.81</td>
<td>2.82%</td>
</tr>
<tr>
<td>LTS LOSSES</td>
<td></td>
<td></td>
<td>3.28</td>
<td>2.43%</td>
</tr>
<tr>
<td>HEX3</td>
<td></td>
<td></td>
<td>0.76</td>
<td>0.56%</td>
</tr>
<tr>
<td>GCU REACTOR COOLING</td>
<td></td>
<td></td>
<td>4.45</td>
<td>3.30%</td>
</tr>
<tr>
<td>HEX4</td>
<td></td>
<td></td>
<td>1.50</td>
<td>1.11%</td>
</tr>
<tr>
<td>FUEL CELL COOLING</td>
<td></td>
<td></td>
<td>20.00</td>
<td>14.82%</td>
</tr>
<tr>
<td>FUEL CELL ELECTRICAL POWER</td>
<td></td>
<td></td>
<td>40.00</td>
<td>29.63%</td>
</tr>
<tr>
<td>FLUE GASES</td>
<td></td>
<td></td>
<td>6.98</td>
<td>5.17%</td>
</tr>
<tr>
<td>CONDENSER</td>
<td></td>
<td></td>
<td>15.57</td>
<td>11.53%</td>
</tr>
<tr>
<td>COMPRESSOR POWER REQUIRED</td>
<td></td>
<td></td>
<td>0.00</td>
<td>0.00%</td>
</tr>
<tr>
<td>EXTRA EXPANDER POWER</td>
<td></td>
<td></td>
<td>6.65</td>
<td>4.93%</td>
</tr>
<tr>
<td>LOW GRADE HEAT</td>
<td></td>
<td></td>
<td>0.00</td>
<td>0.00%</td>
</tr>
<tr>
<td>HIGH GRADE HEAT</td>
<td></td>
<td></td>
<td>21.31</td>
<td>15.78%</td>
</tr>
<tr>
<td>ECONOMISER LOSSES</td>
<td></td>
<td></td>
<td>0.44</td>
<td>0.32%</td>
</tr>
<tr>
<td>ECONOMISER CONDENSATE</td>
<td></td>
<td></td>
<td>0.40</td>
<td>0.29%</td>
</tr>
<tr>
<td>HEX5</td>
<td></td>
<td></td>
<td>3.39</td>
<td>2.51%</td>
</tr>
<tr>
<td>HEX6</td>
<td></td>
<td></td>
<td>0.13</td>
<td>0.10%</td>
</tr>
<tr>
<td>HEX7</td>
<td></td>
<td></td>
<td>0.03</td>
<td>0.03%</td>
</tr>
<tr>
<td>MOTOR LOSSES</td>
<td></td>
<td></td>
<td>0.00</td>
<td>0.00%</td>
</tr>
<tr>
<td>SHAFT LOSSES</td>
<td></td>
<td></td>
<td>0.13</td>
<td>0.10%</td>
</tr>
<tr>
<td>TOTAL</td>
<td></td>
<td></td>
<td>135.02</td>
<td>100.00%</td>
</tr>
</tbody>
</table>

SPFC CHP System @ 3.0 Bar(a) (With Condensers)

<table>
<thead>
<tr>
<th>Description</th>
<th>kW</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>COMPRESSOR POWER</td>
<td>6.66</td>
<td>80.00%</td>
</tr>
<tr>
<td>EXPANDER POWER</td>
<td>13.31</td>
<td>80.00%</td>
</tr>
<tr>
<td>FUEL CELL POWER</td>
<td>40.00</td>
<td>29.63%</td>
</tr>
<tr>
<td>EXPANDER POWER</td>
<td>6.65</td>
<td>4.93%</td>
</tr>
<tr>
<td>TOTAL POWER</td>
<td>46.65</td>
<td>34.55%</td>
</tr>
<tr>
<td>LOW GRADE HEAT</td>
<td>48.98</td>
<td>36.28%</td>
</tr>
<tr>
<td>HIGH GRADE HEAT</td>
<td>21.31</td>
<td>15.78%</td>
</tr>
<tr>
<td>TOTAL HEAT POWER</td>
<td>70.29</td>
<td>52.06%</td>
</tr>
<tr>
<td>OVERALL SYSTEM EFFICIENCY</td>
<td></td>
<td>86.61%</td>
</tr>
<tr>
<td>HEAT TO POWER RATIO</td>
<td></td>
<td>1.51</td>
</tr>
</tbody>
</table>
3.4 SYSTEM OPTIMISATION - RESULTS AND DISCUSSION

For a SPFC CHP scheme to be competitive against both conventional and other fuel cell total energy schemes (Table 3.2), it should ideally have a heat to power ratio closer to one and overall efficiency of greater than 80% [16]. To achieve such a performance, the SPFC CHP system requires optimisation. The objective of this study in this section is to optimise the performance of the SPFC CHP system by investigating the impact of varying the parameters of various components of the system, and evaluating the significance of integration between different system components. Using the data detailed in section 3.2 and the steady state model described in section 3.3, the following investigation were carried out:

1) Effect of preheating the reformer and burner reactants.
2) Use of condensers and/or pre-heater for the fuel cell exhausts gases.
3) Variation of fuel cell parameters
   3.4) The stack loading (10-40 kW_e).
   3.5) The stack operating pressures (1-3.25 bar(a)).
   3.6) Cathode stoichiometry (1.2-2.5).
4) Variation of the compressor and expander isentropic efficiency.

3.4.1 Effect of preheating the reformer and burner reactants

The advantage of preheating in any total energy system or plant could be to minimise waste heat and in the process, maximise the system or plant efficiency. Usually, waste heat is used to preheat reactants before they are fed into a combustion chamber or a burner. By preheating the reactants, the amount of fuel feedstock is reduced and the performance of the component or system is improved. To illustrate the effect of preheat on the performance of 40 kW_e SPFC CHP system, three case studies were carried out, with the reactants supplied to the reformer and burner at three temperatures i.e. 25°C, 350°C and 800°C. The energy for reactant preheating was supplied by the reformed gas stream at 850°C and the flue gases stream existing the expander (≈ 650°C). In all three case studies, the anode and cathode exhaust gas streams were fed directly to the burner, without either been passed through a condenser or preheater. The remainder of the thermal energy in the flue gases was utilised in the waste heat recovery system.
In the first case study, the reactants were not preheated and fed to the reformer and the burner at datum temperature of 25°C. It was assumed that the natural gas feedstock was already desulfurised and the energy used in the process was not accounted for. The heat exchangers 6 and 1 were not employed in the preheat process, as seen in figure 3.10. In the second case study, the reactants are preheated to 350°C by heat exchanger 6. This preheat of reactants to 350°C, especially natural gas, would be a necessary part of the system design prior to the desulfurisation process. The water for the HTS was also preheated to 400°C by heat exchanger 7. In the final case study the reactants were preheated to 800°C and heat exchanger 1 (850°C), 6 (350°C), and 7 (400°C) were all employed.

The results of the three SPFC CHP system case studies are presented in table 3.9. As the reactants preheat temperature was increased, the fuel processor and the system electrical efficiencies increased, while the heat efficiency decreased as more waste heat was used for this preheat process. This performance was a result of less consumption of processed natural gas by the system and better utilisation of the waste heat power. Lower fuel or processed natural gas consumption increased the electrical efficiency and use of waste heat for reactants preheat decreased the heat efficiency. The overall system efficiency was thus lower at maximum preheat reactant temperature of 800°C and the heat to power ratio improved by a factor of 1.4.

Table 3.9: SPFC CHP system performance at different preheat temperatures

<table>
<thead>
<tr>
<th>System Parameters</th>
<th>Reactants Preheat Temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>25</td>
</tr>
<tr>
<td>Total Fuel Power to the System (kW)</td>
<td>190.17</td>
</tr>
<tr>
<td>Reformers Reaction Power, ΔH_{Ref} (kW)</td>
<td>38.57</td>
</tr>
<tr>
<td>Reformers Efficiency, η_{Ref} (%)</td>
<td>54.65</td>
</tr>
<tr>
<td>Fuel Processor Efficiency, η_{FP} (%)</td>
<td>58.23</td>
</tr>
<tr>
<td>Electrical Efficiency, η_{Ele Sys} (%)</td>
<td>27.71</td>
</tr>
<tr>
<td>Heat Efficiency, η_{Heat Sys} (%)</td>
<td>62.18</td>
</tr>
<tr>
<td>Heat to Power Ratio, R (Ht/P)</td>
<td>2.24</td>
</tr>
<tr>
<td>Overall System Efficiency, η_{Overall} (%)</td>
<td>89.89</td>
</tr>
</tbody>
</table>
Hence, as the preheat temperature increased, the waste heat energy of the system was recovered via the network of heat exchangers and the maximum possible reactant preheat temperature of 800°C was accomplished. At this preheat temperature the best performance was achieved by a SPFC CHP system in this investigation. However, in a practical SPFC CHP system, the system designer has to trade off between system performance and economical benefit of using heat exchangers for the preheat process.

3.4.2 Use of condensers and/or pre-heater for the fuel cell exhausts gases

The anode and cathode exhaust gas streams from the SPFC stack were also fed to the burner, either via the condensers or heat exchanger, or via a combination of both these heat recovery or heat transfer methods. The effect of either condensing the water from the exhaust gases and/or heating the gas streams to the maximum available temperature on the performance of the system overall was investigated. The anode exhaust stream contains excess hydrogen and unused methane, while the cathode provides the burner with excess air not used in the fuel cell stack. The anode and cathode exhaust streams also contain water, which could be either in vapour or liquid phase or a mixture of both. The phase state of the water determines the energy content of the exhaust streams and its subsequent contribution to the reformer burner. Three case studies were used to evaluate the effect of using either condensers and/or preheater on the performance of a 40 kW\text{e} SPFC CHP system. In all three case studies, the operating system pressure was kept at 3 bar(a) and burner and reformer reactants were preheated to 800°C.

In the first case study, the fuel cell exhaust gas streams were passed via the condensers whereby the streams were cooled down to 25°C, and all water in the stream was condensed and removed. The chemical and thermal power of the combined anode and cathode exhaust streams after the condenser was reduced from 54.63 kW to 39.06 kW, i.e. approximately 15.57 kW of thermal energy in water was condensed out. In the second case study, the exhaust streams were preheated by heat exchanger 8 (figure 3.1) to maximum temperature, receiving thermal energy from the flue gases. The exhaust streams were preheated to a maximum available temperature of 400°C, with an increase in thermal power of 20.75 kW. However, the thermal
energy in the flue gases was depleted in the process and the condenser economiser
recovered no waste heat from the flue gases. The flue gases temperature also
decreased to 67°C on exit from heat exchanger 8. In the third case study, both the
condensers and heat exchanger were used to treat the fuel cell exhaust gas streams.
The exhaust gas streams were preheated to a maximum available temperature of
330°C by the heat exchanger 8, after being cooled down to 25°C (and all the water
removed in the condensers). The flue gases temperature and power on the exit of the
heat exchanger 8 were determined to be 48°C and 9.38 kW respectively. The power in
the flue gases was depleted for it to be further use in the condensing economiser.

The results of the three SPFC CHP system case studies are presented in table 3.10.
The results of the three case studies were compared with a SPFC CHP system were
the exhaust gas streams were fed directly to the burner without any treatment i.e. the
third case study of the previous section (3.3.1) and table (3.10). The trend seen in
these studies was that the initial fuel consumption in the system was reduced with use
of the condenser and/or preheater. This improved the heat to power ratio, reformer,
fuel processor and electrical efficiencies, but heat and overall efficiencies were
reduced.

In a SPFC CHP system with condensers, both the electrical and heat efficiencies
improved as less fuel was consumed. Thermal energy contained in the water in the
SPFC stack exhaust streams was recovered by the condensers and the condensing
economiser recovered most of the waste heat in the flue gases. Hence, both high and
low grades of heat power were available. An additional advantage of using the
condensers was that the reformer was supplied with dry exhaust gases, which aids the
combustion in the burner since the presence of condensing water droplets may lead to
flame failure [18]. The use of only preheating the fuel cell exhaust gases results in the
consumption of most of the thermal power in the flue gases and redundancy of the
condensing economiser. Hence, a decrease in both heat and overall system
efficiencies. However, the electrical system efficiency and heat to power ratio
improved by a factor of 1.2 and 2.3 respectively. The use of a combination of both
condensers and preheater achieved the desired heat to power ratio of one with an
overall efficiency of greater than 80%. However, once again the thermal power in the
flue gases was depleted and the condensing economiser made redundant. Therefore, high grade heat was not available.

The choice of either using condensers and/or preheater depends significantly upon the final application of the SPFC CHP system. The system with only preheater will ideally suit power generation application where electrical efficiency was the design factor while for CHP system where both heat and power are design factors then either system in case study 1, 3 or without any condensers and preheater would be ideal. For this investigation, the ideal system for SPFC CHP application in a service industry, would be the one with only condensers. Although this system has the heat to power ratio of 1.5, both high and low grades of heat were available and the overall efficiency of greater than 80% was achieved.
Table 3.10: 40 kW<sub>e</sub> SPFC CHP system performance with fuel cell stack exhaust gas streams condensers and/or preheater

<table>
<thead>
<tr>
<th>System Parameters</th>
<th>Anode &amp; Cathode Exhaust Gases Treatment</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>None</td>
</tr>
<tr>
<td>Power in the Anode Exhaust Gases (kW)</td>
<td>41.60</td>
</tr>
<tr>
<td>Power in the Cathode Exhaust Gases (kW)</td>
<td>13.03</td>
</tr>
<tr>
<td>Total Power in the Exhaust Gases (kW)</td>
<td>54.63</td>
</tr>
<tr>
<td>Total Power After Treatment (kW)</td>
<td>-</td>
</tr>
<tr>
<td>Total Fuel Power to the System (kW)</td>
<td>148.62</td>
</tr>
<tr>
<td>Reformer Efficiency, $\eta_{\text{Ref}}$, (%)</td>
<td>59.53</td>
</tr>
<tr>
<td>Fuel Processor Efficiency, $\eta_{\text{FP}}$, (%)</td>
<td>74.51</td>
</tr>
<tr>
<td>Electrical Efficiency, $\left( \eta_{\text{Ei, Sys}} \right)$, (%)</td>
<td>33.90</td>
</tr>
<tr>
<td>Heat Efficiency, $\left( \eta_{\text{H, Sys}} \right)$, (%)</td>
<td>53.11</td>
</tr>
<tr>
<td>Heat to Power Ratio, $R_{\text{(H/P)}}$</td>
<td>1.57</td>
</tr>
<tr>
<td>Overall System Efficiency, $\left( \eta_{\text{Overall}} \right)$, (%)</td>
<td>87.01</td>
</tr>
</tbody>
</table>
3.4.3 Variation of fuel cell parameters

Having established the optimal system configuration with regards to condensers and heat exchangers, the next stage focused upon the investigation of the effect of varying fuel cell parameters on the performance of the SPFC CHP system. The system configuration shown in figure 3.10 with condensers and the data detailed in section 3.2 were used in this investigation. The effect of varying the following parameters were studied:

1) Stack Electrical loading (10-40 kW<sub>e</sub>).
2) Stack operating pressures (1-3.25 bar(a)).
3) Cathode stoichiometry (1.2-2.5).

3.4.3.1 Stack Electrical Loading

The fuel cell operating voltages and currents given in table 3.4 (section 3.2.2.1) were used to investigate the effect of different stack electrical loading on the system performance. Table 3.11 gives the results of this study. The overall system efficiency at different stack loading remained approximately constant, however, the heat to power ratio increased as more power was demanded from the system. As more power was demanded from the system, the fuel cell efficiency decreased (table 3.4) and consequently the system electrical efficiency also decreased and system heat efficiency increased. The increase in the system heat efficiency and decrease in the system electrical efficiency was proportional, giving no change in the overall system efficiency. Therefore, there was no overall system advantage or disadvantage in operating at partial load, due to the inherent electrochemical characteristics of the SPFC stack, which has high efficiency at part load. However, this particular characteristic of the SPFC CHP system is a major advantage over other conventional CHP schemes or plants.
Table 3.11: 40 kW<sub>e</sub> SPFC CHP system performance at different power levels

<table>
<thead>
<tr>
<th>System Parameters</th>
<th>25%</th>
<th>50%</th>
<th>75%</th>
<th>100%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Fuel Power to the System (kW)</td>
<td>29.67</td>
<td>62.09</td>
<td>97.11</td>
<td>135.02</td>
</tr>
<tr>
<td>Reformer Efficiency, η&lt;sub&gt;Ref&lt;/sub&gt; (%)</td>
<td>69.08</td>
<td>69.08</td>
<td>69.08</td>
<td>69.08</td>
</tr>
<tr>
<td>Fuel Processor Efficiency, η&lt;sub&gt;FP&lt;/sub&gt; (%)</td>
<td>82.02</td>
<td>82.02</td>
<td>82.02</td>
<td>82.02</td>
</tr>
<tr>
<td>Electrical Efficiency, (η&lt;sub&gt;El&lt;/sub&gt; sv), (%)</td>
<td>38.63</td>
<td>37.14</td>
<td>35.82</td>
<td>34.55</td>
</tr>
<tr>
<td>Heat Efficiency, (η&lt;sub&gt;Ht&lt;/sub&gt; sv), (%)</td>
<td>48.02</td>
<td>49.50</td>
<td>50.81</td>
<td>52.06</td>
</tr>
<tr>
<td>Heat to Power Ratio, R&lt;sub&gt;(H/P)&lt;/sub&gt;</td>
<td>1.24</td>
<td>1.33</td>
<td>1.42</td>
<td>1.51</td>
</tr>
<tr>
<td>Overall System Efficiency, (η&lt;sub&gt;Overall&lt;/sub&gt;) (%)</td>
<td>86.65</td>
<td>86.64</td>
<td>86.63</td>
<td>86.61</td>
</tr>
</tbody>
</table>

3.4.3.2 Stack Operating Pressure

The operating pressure of the stack was varied between 1-3.25 bar(a) and the effect of pressure on the system performance was investigated. The SPFC system with condensers shown in figure 3.10 was used in this investigation. The SPFC operating data detailed in section 3.2.2.2 were also used in the investigation. To supply the SPFC stack with reformed gases and air at its operating pressure, the fuel processor and the compressor/expander have to operate at the same pressure. Hence, the operating pressure of the stack established the system pressure. Figure 3.13 shows the performance of different components of the system at different operating pressures.

From Table 3.5 it can be seen that the fuel cell stack performance improved as the pressure was increased from 1 to 3.25 bar(a). Pressure also has an effect upon the relative humidities of the anode and cathode exhaust gas streams and the thermal power generated within the SPFC stack. As the pressure was increased, the relative humidities of both streams increased and approached 100% relative humidity. At a relative humidity of 100% and above, the water in the gas streams is a mixture of vapour and liquid (two phase flow). Therefore, less thermal power is utilised to evaporate the water (i.e. latent heat of vaporisation) and more thermal power is removed by the cooling system (to maintain constant stack temperature). This was evident from the calculated values of thermal power removed by the SPFC stack cooling system at different operating pressures.
Figure 3.13: 40 kWc SPFC CHP system performance at varying pressures.
The relative humidity of the cathode increased from 40% to 100% between the operating pressure of 1 bar(a) and 2.5 bar(a) (Table 3.5) and the thermal power removed by the fuel cell cooling system decreased from 31.20 kW to 18.13 kW. Above the stack operating pressure of 2.5 bar(a), the cathode exhaust relative humidity was greater than 100% (two phase flow) and the thermal power removed via the cooling system increased from 18.13 kW to 20.45 kW. This performance of the fuel cell stack at varying pressure also effected the performance of system and its components.

The reformer efficiency remained constant as the system pressure was increased from 1 to 3.25 bar(a), in accordance with the reasons stated in section 3.2.1.1.1. However, the reformer reaction power and the fuel processor efficiency decreased with increased pressure. This was due to the improvement in fuel cell stack efficiency, which resulted in decreased demand for hydrogen rich reformed gas, and hence less processed natural gas was consumed in the reformer. The compressor power increased as the pressure increased from 1 to 3.25 bar(a). As the pressure increased, the pressure ratio increased and at constant isentropic efficiency of 80%, the compressed air temperature increased from 25°C at 1 bar(a) to 175°C at 3.25 bar(a). Similarly, the expander power also increased as the pressure ratio increased from 1 to 3.25 at constant isentropic efficiency of 80%.

The overall system efficiency (heat & power), ($\eta_{overall}$), increased from 86.54 % at ambient pressure to a maximum efficiency of 86.62 % at 2.25 bar(a), with an efficiency of 86.61% at 3.25 bar(a). Beside these minor changes in the overall system efficiency, the efficiency remained approximately constant over the range of operating pressures (figure 3.13). However, the heat and power ratio decreased substantially from 2.8 to 1.5 as the pressure increased. The reason for the decrease in the efficiency and heat to power ratio was that as the performance of the fuel cell improved, the system becomes more electrically efficient than thermally efficient, and the maximum overall efficiency was achieved in the transition. At lower pressures of between 1 and 2.0 bar(a) the system was converting more of the fuel to thermal energy via the burner, while at higher pressures of between 2.5 and 3.25 bar(a) more electrical power was generated via the fuel cell stack and expander. Furthermore, the
waste heat recovery system recovered more thermal power via heat exchangers, condensers and economiser at lower pressure (64% @ 1 bar(a)) than at higher pressure (52% @ 3.25 bar(a)).

From this investigation, it was evident that the SPFC CHP system can be adaptable to operate at different operating pressures, to meet the change in demand for heat and power. For example, a SPFC CHP system can be designed to operate at 1 bar(a) to fulfil the heat demand, while it can be also be designed to operate at 3.25 bar(a) to accomplish the electrical demand. Since the overall system efficiency was approximately constant, the deciding factor would be the heat to power ratio, which indicates to operate at higher pressure to achieve a ratio closer to one. A SPFC CHP system for service industry application, the choice of the operating pressure would be 3 bar(a) where the overall efficiency of greater than 80% and heat to power ratio closer to one was achieved. There are no advantages of operating at any higher pressure since the improvement in heat to power ratio was very small and the system became less efficient (Figure 3.13).

3.4.3.3 Cathode Stoichiometry

To study the effect of cathode stoichiometry on the overall system efficiency, the cathode stoichiometry was varied from 1.2 to 2.0 in steps of 0.1. The stoichiometry was also increased from 2 to 2.5, in order to study the effect of higher stoichiometry than normally used in the SPFC. The anode stoichiometry and the system pressure were kept at 1.5 and 3 bar(a) respectively. The SPFC system with condensers shown in figure 3.10 and the operating data detailed in section 3.2.2.4 were used in the investigation.

The performance of the fuel cell stack improved with higher cathode air stoichiometry as the thermal power generated within the fuel cell stack reduced from 112.94 kW to 17.43 kW at stoichiometry of 1.1 and 2.5 respectively. Figure 3.14 shows the airflow demand by the fuel cell stack, the burner and the total air demanded by the system. The obvious predication would be that the air demand by the fuel cell stack and the
system would increase with increase in the cathode air stoichiometry. However, this was not the case as seen from figure 3.14, the inefficiency of the fuel cell (table 3.6) at stoichiometry of 1.2 demanded much more air than at stoichiometry of 2 or 2.5 (higher current density at stoichiometry of $1.2 = 1 \text{ A/cm}^2$). At higher stoichiometry (i.e. 2.5), the excess oxygen in the cathode exhaust stream supplied the burner with all the required air and therefore, the air demanded by the burner from the compressor decreased to zero. These trends in the air demanded by the stack and system also affect the performance of the other system components, and hence the overall system performance.

Figure 3.15 shows the performance of the system and its components for different cathode stoichiometries. The reformer efficiency remained approximately constant as the cathode stoichiometry increases from 1.2 to 2.0. At cathode stoichiometry of 2.5, the reformer efficiency decreased by $\approx 2\%$ as more fuel was required by the burner to heat the extra air. The fuel processor efficiency and the power required for the reformer reaction decreased as the SPFC stack became efficient and less hydrogen rich gas was demanded from the fuel processor.

![Figure 3.14: Air demand at different cathode stoichiometries](image-url)
Figure 3.15: SPFC CHP system performance at different cathode stoichiometries
The parasitic load imposed upon the system by the compressor decreased with increase in the cathode stoichiometry. Since pressure ratio and the isentropic efficiency were constant, the compressor power was dependent upon the air flowrate demanded by the system. The air demanded by the system was maximum at lower stoichiometry. This was due to fuel cell stack demanding higher flowrate of air and reformed gas from the compressor and reformer (figure 3.14) under such conditions. As the fuel cell stack performance improved with increased stoichiometry, the stack air demand increased, but the burner air demanded from the compressor decreased as the excess air from the stack supplied the burner. This reduced the total air demand from the compressor and decreased the parasitic load of the compressor. Although the stack supplied all the air to the burner at the stoichiometry of 2.5, the fuel cell stack air flowrate was much higher than normal operating conditions (figure 3.14) and therefore the compressor power increased by 0.52 kW.

The expander power also decreased with increased cathode stoichiometry from 1.2 to 2.0 and increased at stoichiometry of 2.5. The expander power at constant pressure ratio and isentropic efficiency was dependent upon the flowrate of the flue gas from the reformer burner. The flue gas flowrate was maximum at lower stoichiometry as result of increased hydrogen demand by the SPFC stack, which led to more fuel to be burnt in the reformer to provide hydrogen rich gases. Since the fuel cell stack performance increased with increased stoichiometry, less fuel was burnt in the reformer burner resulting in reduced flue gases flowrate and hence decreased the expander power. At cathode stoichiometry of 2.5, the high flowrate of the air from the stack into the burner resulted in increased expander power.

A further investigation was also carried out to study the effect of not having a expander in the SPFC CHP system. The study was carried out using a cathode stoichiometry of 2.0 (compressor power was minimum). Table 3.12 shows the performance of the SPFC CHP system with the cathode stoichiometry of 2.0, with and without an expander. An electrical motor (90% efficiency) supplied the compressor power. The thermal power in the flue gases was recovered via the waste heat recovery system. The systems heat efficiency improved with an equivalent decrease in the system electrical efficiency. Hence, the overall system efficiency remained approximately the same (Table 3.12), but the heat to power ratio increased by a factor
of 1.4 to 2.12. Similar results would be obtained for other cathode stoichiometries, whereby the redistribution of flue gases power would maintain the overall system efficiency at approximately the same level, but the heat to power ratio would increase favouring higher system heat efficiency.

Table 3.12: System performance at cathode stoichiometry of 2.0 with and without an expander.

<table>
<thead>
<tr>
<th>System Parameters</th>
<th>Cathode Stoichiometry of 2.0</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>With Expander</td>
</tr>
<tr>
<td>Total Fuel Power to the System (kW)</td>
<td>136.70</td>
</tr>
<tr>
<td>Fuel Processor Efficiency, $\eta_{FP}$, (%)</td>
<td>82.02</td>
</tr>
<tr>
<td>Electrical Efficiency, $(\eta_{EL Sys})$, (%)</td>
<td>34.19</td>
</tr>
<tr>
<td>Heat Efficiency, $(\eta_{HT Sys})$, (%)</td>
<td>52.42</td>
</tr>
<tr>
<td>Heat to Power Ratio, $R_{(HT/PP)}$</td>
<td>1.53</td>
</tr>
<tr>
<td>Overall System Efficiency, $(\eta_{Overall})$, (%)</td>
<td>86.61</td>
</tr>
</tbody>
</table>

The overall system efficiency ($\eta_{Overall}$) improved by approximately 1% as the cathode stoichiometry increased from 1.2 to 2.5. However, the heat to power ratio ($R_{(HT/PP)}$) decreased from 3.74 to 1.53 as the stoichiometry increased from 1.2 to 2.0 and then increased to 1.6 at cathode stoichiometry of 2.5. The reason for this trend was that as the cathode stoichiometry increased the system became more electrically efficient than heat efficient (figure 4.15), since the performance of the SPFC improved and less fuel was consumed by the system (303 kW of fuel power @ 1.2 to 137 kW of fuel power @ 2.0). The SPFC CHP system performance at lower cathode stoichiometry was mainly due to the heat recovery system (64%), while at higher stoichiometry, both the SPFC stack (29%) and the heat recovery system (52%) were responsible. The contribution from the expander remained constant for both cases (5% of the total fuel power into the system).

At a cathode stoichiometry of 2.5, the overall system efficiency, heat to power ratio and the system heat efficiency increased, but the electrical efficiency decreased. The improvement in the performance of the fuel cell stack was minimal (1.5%) compared to amount of additional air demanded by the fuel cell stack. The extra fuel power was
therefore required to heat the excess air from the stack, which was later recovered as thermal power by the waste heat recovery system, and hence resulted in a higher heat to power ratio. The advantage of using a stoichiometry greater than 2.0 was minimal compared to the performance of the system at stoichiometry ≤ 2.0.

From this cathode stoichiometry study detailed, it is evident that a SPFC CHP system has the flexibility of operating at different cathode stoichiometries, depending upon the demand of either, or both, power and heat. It is also evident that the system performance, especially the heat to power ratio, is very much dependent upon the compressor/expander machinery. A SPFC CHP system with a expander/compressor and operating with cathode stoichiometry 2.0 would ideally be appropriate for a service industry application, where the system design requirements are overall system efficiency of greater then 80% and equal heat and electrical demand. However, for a system where heat is the main demand, then a lower cathode stoichiometry of between 1 and 1.5 would be ideal.

3.4.4 Effect of varying the compressor and expander isentropic efficiency

The effect of varying isentropic efficiency on the overall system performance was investigated for a 40 kWe SPFC CHP system, operating at two different pressures i.e. 1.25 (low) and 3 (high) bar(a). The isentropic efficiencies of the compressor and expander were varied from 30 to 100%. The investigation addressed 3 areas:

1. Effect of varying the isentropic efficiency in a high pressure system.
2. Effect of varying the isentropic efficiency in a low pressure system
3. Comparison of high and low pressure systems using efficiency maps (3-D Graph).

In the first two studies, the same isentropic efficiency for both the compressor and expander as used and varied. In the third study, a range of different isentropic efficiencies was used for both the compressor and expander to generate matrixes of data. The data is subsequently presented in the 3-D maps.
3.4.4.1 Effect of varying the isentropic efficiency in high pressure system

The isentropic efficiency of the compressor and expander was varied from 30% to 100%, using the same efficiency for both machineries. Figure 3.16 shows the performance of the system and its components at varying compressor or expander isentropic efficiencies. At lower efficiencies (30%-50%), the compressor power requirement was substantial and greater than what the expander could provide. Where the compressor power exceeds the expander power, the electric motor (efficiency of 90%) supplied the excess power. As the isentropic efficiency increased, the expander power exceeded the compressor power (≥ 60%) and the excess expander power contributed to the system electrical demand.

The reformer reaction power and fuel processor efficiency remained constant as isentropic efficiency increased from 40% to 100%. At isentropic efficiency of 30%, the fuel processor efficiency increased (by 0.2%) because the compressor supplied the air to the burner at 392°C, which was 42°C higher than normal preheated air supply temperature, and therefore less fuel was required by the reformer burner.

As the compressor and the expander efficiency increased, the system electrical efficiency improved while the system heat efficiency decreased. At lower isentropic efficiency (30%-50%), more fuel was required by the system to supply power to the compressor and therefore more heat was recovered via the waste heat recovery system. As the isentropic efficiency increased above 50%, the expander power supplied the power to the compressor and excess power to the system. The improvement in performance of both the compressor and expander required less fuel by the system, which in turn improved the heat to power ratio, as the system became more electrically efficient. The overall system efficiency varied by only 0.23% (86.53% to 86.76%) as the isentropic efficiency varied from 30% to 100%. The minimum value of the overall system efficiency (86.53%) was achieved between an isentropic efficiency of 50% and 60%. The minimum overall system efficiency was a result of the transition between the burner and the expander supplying the compressor power.
Figure 3.16: High pressure (3 bar(a)) system performance at different compressor or expander isentropic efficiencies.
3.4.4.2 Effect of varying the isentropic efficiency in a low pressure system

Similar to that for the high pressure system, the isentropic efficiency of the compressor and expander was varied from 30% to 100%. Figure 3.17 shows the performance of the system and its components at different compressor or expander isentropic efficiencies. The compressor and expander powers for the low pressure system followed similar trends as observed for the high pressure system. The expander power exceeded the compressor power at an isentropic efficiency of approximately 50%. However, the magnitude of both powers was approximately 4-5 times smaller compared to the high pressure system compressor and expander powers.

The reformer reaction power remained constant as the isentropic efficiency was varied from 30%-100%. However, the fuel processing efficiency decreased with increased isentropic efficiency. This was due to the air bleed temperature, which increased as the compressor efficiency dropped from 100% to 30%. The compressed air temperature increased from 45°C at 100%, to 91°C at 30% isentropic efficiency. This significant rise in the temperature, increased the power in the fuel cell stack anode feed gas, which in turn decreased the fuel processing efficiency from 82% to 81.6% as the compressor became more efficient.

The electrical and heat system efficiencies displayed similar trends to high pressure system. As the compressor and expander efficiency increased, less fuel power was consumed by the system and hence the heat to power ratio and the overall system efficiency improved. The minimum overall system efficiency also occurred at the point where the expander supplied the compressor power.
Figure 3.17: Low pressure (1.25 bar(a)) system performance at different compressor or expander isentropic efficiencies.
4.4.4.3 Comparison of high and low pressure systems using efficiency maps

In the two previous studies, the performance of the SPFC CHP system was investigated for a single isentropic efficiency, (which was varied between 30%-100%). In this study, a range of different isentropic efficiencies were used and varied for both the compressor and the expander to generate a data (results) matrix. A 8x8 (30% -100%) matrix data were generated for the overall, electrical, heat system efficiencies and heat to power ratio for both high (3 bar(a)) and low (1.25 bar(a)) pressure systems. Figures 3.18 to 3.25 shows the efficiency maps and heat to power ratio maps for both the high and the low systems.

Most of the trends observed in the graphs in figures 3.16 and 3.17 were also observed in maps 3.18-3.25. It should be note that, the purpose of these maps was to illustrate how the high and low pressure systems were dependent upon compressor and expander performance. Also, since no manufacturing data for the compressor and expander were available, these maps indicate how the system would perform for a range of efficiencies. It was immediately apparent from these maps that high pressure system performance was significantly dependant upon the performance of the compressor/expander, whereas for the low pressure system, the flatter shape indicated that the performance was much less dependant upon the compressor/expander. The dependency of the high pressure system on the compressor/expander was apparent from Table 3.13, which shows the maximum and minimum values of the system performance parameters and the variation between these values.

For both the high (3 bar(a)) and low (1.25 bar(a)) pressure SPFC CHP systems, the performance improved as the compressor and the expander became more efficient. However, the improvement in performance in the lower pressure system was not greatly dependent upon the performance of the compressor/expander. The overall system efficiency for both systems was very similar at lower isentropic efficiencies (30-50%). At these lower isentropic efficiencies, the inefficiency of the compressor/expander was recovered via the waste heat recovery system while at higher isentropic efficiencies (≥ 60%) the system electrical efficiency improved with decreases in system heat efficiency.
Table 3.13: The maximum and minimum system performance parameters for a high and low pressure systems at varying isentropic efficiencies.

<table>
<thead>
<tr>
<th>System Performance Parameters</th>
<th>η_{Overall}</th>
<th>η_{EL Sys}</th>
<th>η_{HT Sys}</th>
<th>R (_{(H/P)})</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>High pressure System</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Maximum</td>
<td>86.76%</td>
<td>37.97%</td>
<td>59.86%</td>
<td>2.23</td>
</tr>
<tr>
<td>Minimum</td>
<td>86.43%</td>
<td>26.84%</td>
<td>48.80%</td>
<td>1.29</td>
</tr>
<tr>
<td>Differences</td>
<td>0.33%</td>
<td>11.13%</td>
<td>11.06%</td>
<td>0.94</td>
</tr>
<tr>
<td><strong>Low pressure System</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Maximum</td>
<td>86.61%</td>
<td>29.62%</td>
<td>59.55%</td>
<td>2.20</td>
</tr>
<tr>
<td>Minimum</td>
<td>86.56%</td>
<td>27.06%</td>
<td>56.99%</td>
<td>1.92</td>
</tr>
<tr>
<td>Differences</td>
<td>0.05%</td>
<td>2.56%</td>
<td>2.56%</td>
<td>0.28</td>
</tr>
</tbody>
</table>

From a theoretical design basis, the SPFC CHP system performance can be significantly enhanced by the utilisation of highly efficient compressor/expander technology. However, in a practical system, depending on the availability of compressor/expander machinery, it would be very difficult either to operate at desired design point or to match the working envelope of compressor and expander. The choice of operating efficiency for both compressor and expander would therefore depend on the type of compressors/expander technology available for the SPFC systems and its measured working envelope. The current development in the compressors/expander technology [33,34] for fuel cell application predict high operating efficiency (70%-90%) and therefore the choice of using an isentropic efficiency of 80% for both compressor and expander for this study is conservative.

A SPFC CHP system for a service industry application, with isentropic efficiency of 80% for both the compressor and expander, produced an overall efficiency of greater than 80% for both the high and low pressure systems. Heat to power ratios of approximately 1.5 and 2 were achieved for both the high and low pressure systems. However, The desired heat to power ratio of one could not be achieved, even if the isentropic efficiency of both compressor and expander was 100%.
Figure 3.18: Overall system efficiency map for a high pressure system (3 bar(a))

Figure 3.19: Overall system efficiency map for a low pressure system (1.5 bar(a))
Figure 3.20: Electrical system efficiency map for a high pressure system

![High Pressure System Efficiency Map](image)

Figure 3.21: Electrical system efficiency map for a low pressure system

![Low Pressure System Efficiency Map](image)
Figure 3.22: Heat system efficiency map for a high pressure system (3 bar(a))

Figure 3.23: Heat system efficiency map for a low pressure system (1.5 bar(a))
Figure 3.24: Heat to Power ratio map for a high pressure system (3 bar(a))

Figure 3.25: Heat to Power ratio map for a low pressure system (1.5 bar(a))
Table 3.14: System performances of high and low pressure systems with and without expander and compressor with isentropic efficiency of 80%.

<table>
<thead>
<tr>
<th>System Parameters</th>
<th>High Pressure System (3.00 bar(a))</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>With Expander</td>
<td>Without Expander</td>
<td></td>
</tr>
<tr>
<td>Total Fuel Power to the System (kW)</td>
<td>135.02</td>
<td>142.34</td>
<td></td>
</tr>
<tr>
<td>Fuel Processor Efficiency, $\eta_{FP}$, (%)</td>
<td>82.02</td>
<td>82.02</td>
<td></td>
</tr>
<tr>
<td>Electrical Efficiency, $\eta_{El\ Sys}$, (%)</td>
<td>34.55</td>
<td>28.10</td>
<td></td>
</tr>
<tr>
<td>Heat Efficiency, $\eta_{Ht\ Sys}$, (%)</td>
<td>52.06</td>
<td>58.59</td>
<td></td>
</tr>
<tr>
<td>Heat to Power Ratio, $R_{(Ht/UP)}$</td>
<td>1.51</td>
<td>2.09</td>
<td></td>
</tr>
<tr>
<td>Overall System Efficiency, $\eta_{Overall}$, (%)</td>
<td>86.61</td>
<td>86.70</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>System Parameters</th>
<th>Low Pressure System (1.25 bar(a))</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>With Expander</td>
<td>Without Expander</td>
<td></td>
</tr>
<tr>
<td>Total Fuel Power to the System (kW)</td>
<td>145.48</td>
<td>146.87</td>
<td></td>
</tr>
<tr>
<td>Fuel Processor Efficiency, $\eta_{FP}$, (%)</td>
<td>81.62</td>
<td>81.62</td>
<td></td>
</tr>
<tr>
<td>Electrical Efficiency, $\eta_{El\ Sys}$, (%)</td>
<td>28.88</td>
<td>27.50</td>
<td></td>
</tr>
<tr>
<td>Heat Efficiency, $\eta_{Ht\ Sys}$, (%)</td>
<td>57.71</td>
<td>59.61</td>
<td></td>
</tr>
<tr>
<td>Heat to Power Ratio, $R_{(Ht/UP)}$</td>
<td>2.0</td>
<td>2.2</td>
<td></td>
</tr>
<tr>
<td>Overall System Efficiency, $\eta_{Overall}$, (%)</td>
<td>86.60</td>
<td>87.10</td>
<td></td>
</tr>
</tbody>
</table>

A further investigation was performed to study the effect of removing the expander from the SPFC CHP system (isentropic efficiency =0). This investigation was carried out for a high and low pressure system with the compressor operating at isentropic efficiency of 80% and the electrical motor supplying the power operating at efficiency of 90%. The results of the study are presented in Table 3.14.

Without the expander, the performance of both the high and low pressure system were substantially affected. The system electrical efficiency decreased while the heat efficiency and the heat to power improved. The overall system efficiency for both the high and low pressure systems was improved by 0.09% and 0.5% respectively. This was due to the redistribution of the flue gases thermal power from the expander to waste heat recovery system, with the latter having less power loss.

This investigation indicates that to achieve a heat to power ratio of one, then the presence of the compressor/expander is crucial, unless the performance of other system components, for example fuel cell stack, are improved to compensate for the contribution of the expander.
3.4.5 A Future SPFC CHP system

SPFC CHP system was analysed in terms of various system configurations, interactions and components parameters. The optimal configurations and operating points of the components were found to achieve either a heat to power ratio of one and an overall system efficiency of greater than 80%. A SPFC CHP system where the SPFC stack exhaust streams were condensed and preheated (table 3.10), achieved a heat to power ratio of approximately one and an overall system efficiency of greater than 80%. However, for this SPFC CHP system the high grade heat from the condenser economiser was not available. The variation of component parameters also did not yield the desired system performance and therefore emphasis would be to improve the actual performance of components in the future. With both the fuel processor and compressor/expander possibly operating at the best present and future performance, the likely system component to improve its performance in the future would be the SPFC stack.

Improvements in the performance of the SPFC in the future is inevitable since the technology continues to attract substantial investment worldwide, particularly in research and development of SPFC stack components [36]. These new components, such as improved MEA's (membrane electrode assembly), catalyst materials and bipolar plates are being designed primarily to reduce the inefficiency of fuel cell operation (activation, ohmic and mass transport overpotentials) [37-40].

If the SPFC stack performance were to be improved by approximately 10-15%, with these new stack components, then the polarisation curves seen in figure 3.6 would be elevated vertically by approximately 0.1 of a volt. These new polarisation curves would generate new operating points for a 40 kW_e power curve at different operating pressures (figure 3.6). A voltage improvement of 0.1 volt for the fuel cell would yield a new operating point for a SPFC operating at 3 bar(a) of 0.85 volts at 0.42 Amps/cm^2. At this new operating point, the thermal efficiency, \( \eta_{\text{th}} \) (LHV) of the cell would be improved from 58% to 68% and the maximum heat from SPFC would be reduced from 20 kW to 11 kW.
A 40 kW<sub>e</sub> SPFC CHP system operating at 3 bar(a) and using the "future" fuel cell operating point was analysed using the steady state model described in section 3.3. Since the anode stoichiometry has a lesser influence on the performance of the fuel cell [30] than the cathode stoichiometry, it was reduced from 1.5 to 1.2. Other operating conditions e.g. temperature and cathode stoichiometry were unchanged for the analysis. (The compressor and the expander isentropic efficiency remained at 80%). The reactants were preheated to 800°C and fuel cell stack exhaust streams were passed through the condensers prior to being fed into the burner.

Table 3.15 shows the comparison of the performance of current and future SPFC CHP systems with condensers. The fuel processor efficiency was reduced as less fuel was consumed, since the stack required less hydrogen rich reformed gas. The improvement in the fuel cell stack efficiency increased the electrical system efficiency and decreased the system heat efficiency. Although the "future" system did not achieve the desired heat to power ratio of one, both overall system efficiency and heat to power ratio further improved. With further improvement in the fuel cell, the desired system performance for the service industry application could easily be achieved. The Sankey diagram (Figure 3.26) displays the power flows through the SPFC CHP system. The diagram also illustrates where the fuel power was utilised and thermal power recycled and recovered.

Table 3.15: The present and future 40 kW<sub>e</sub> SPFC CHP system with condenser performance.

<table>
<thead>
<tr>
<th>System Parameters</th>
<th>SPFC CHP SYSTEM</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Present</td>
</tr>
<tr>
<td>Total Fuel Power to the System (kW)</td>
<td>135.02</td>
</tr>
<tr>
<td>Fuel Processor Efficiency, η&lt;sub&gt;FP&lt;/sub&gt;, (%)</td>
<td>82.02</td>
</tr>
<tr>
<td>Electrical Efficiency, η&lt;sub&gt;Ei Sys&lt;/sub&gt;, (%)</td>
<td>34.55</td>
</tr>
<tr>
<td>Heat Efficiency, η&lt;sub&gt;Ht Sys&lt;/sub&gt;, (%)</td>
<td>52.06</td>
</tr>
<tr>
<td>Heat to Power Ratio, R&lt;sub&gt;Ht/P&lt;/sub&gt;</td>
<td>1.51</td>
</tr>
<tr>
<td>Overall System Efficiency, η&lt;sub&gt;Overall&lt;/sub&gt;, (%)</td>
<td>86.61</td>
</tr>
</tbody>
</table>
Figure 3.26: Sankey diagram for a future 40 kW$_e$ SPFC CHP system with condensers and operating at 3 bar(a).
The optimisation study of the SPFC CHP system indicated that with improved system configuration, integration and efficient system components, the system could achieve the desired system performance. The study also showed that the system designer has the flexibility and choice of using various components to achieve or fulfil the design criteria when designing the SPFC CHP system for a particular industrial or residential application. However, the designer has to trade off between the system performance and economical, social and environmental benefits. To design the best practical and a competitive SPFC CHP system, then both economical and emission models must be include in the design processes.

3.5 SUMMARY OF RESULTS

1. The steam reformer operating condition were established as 850°C, 3 bar(a) and S:C ratio of 1.5. Under these conditions, the reformer equilibrium conversion efficiency was 93% and the reformed gas contained 66.5% hydrogen on a wet basis (vol. %). The reformer ($\eta_{\text{Ref}}$) and fuel processor ($\eta_{\text{FP}}$) efficiencies were determined to be 69.08% and 82% respectively for a thermally integrated SPFC CHP system.

2. Other component performance data or efficiencies were also specified. The following data and efficiencies were used in the steady state system analysis:

**SPFC Stack**
- Current Density (Amp/cm^2) = 0.489 (Active area = 200 cm^2)
- Cell Voltage (volts) = 0.730
- Thermal Efficiency, $\eta_{\text{Th}}$ (LHV) = 58%
- Anode and cathode stoichiometries of 1.5 and 2 respectively

**Compressor & Expander**
- Isentropic Efficiency = 80%

**Waste Heat Recovery System**
- Heat Exchanger Losses = 1%
- Condensing Economiser = 73% @ flue gas temperature of 362°C
3. The effect of pre-heating the reformer and burner reactants to temperatures of 350°C and 800°C on the system performance was investigated. The best system performance ($\eta_{\text{overall}} = 87\%$ and $R_{(H/U)} = 1.57$) was achieved with the maximum possible reactant preheat temperature of 800°C. The electrical ($\eta_{\text{EL Sys}}$) and heat ($\eta_{\text{Hc Sys}}$) efficiencies for this system were determined to be 34% and 53% respectively.

4. A system where the combination of condensers and pre-heaters were used to treat the stack exhaust streams, the system achieved the $\eta_{\text{overall}}$ of 82% and $R_{(H/U)}$ of 1.1. However, a system with only condensers achieved the highest overall efficiency of 87% ($R_{(H/U)} = 1.5$). Although the best heat to power ratio of 0.7 was achieved by a system with only pre-heaters for the exhaust streams, the overall efficiency was poor (69%).

5. The $\eta_{\text{overall}}$ remained approximately constant at different power levels, but the $R_{(H/U)}$ varied as the stack power level increased from 25% to 100%, with the best ratio ($R_{(H/U)}$) of 1.24 being achieved at 25%. This was due to improved SPFC efficiency at lower power level.

6. The system performance improved with increased operating pressure. The $\eta_{\text{overall}}$ improved from 86.54% at ambient pressure to a maximum efficiency of 86.62% at 2.25 bar(a). The $\eta_{\text{overall}}$ decreased to 86.61% at 3.25 bar(a). The $R_{(H/U)}$ improved significantly from 2.8 to 1.5 as the pressure increased from 1 to 3 bar(a). The compressor power (at constant isentropic efficiency = 80%) demand increased from 1.26 kW at 1.25 bar(a) to 7.19 kW at 3.25 bar(a). Over the same pressure range (1.25-3.25 bar(a)), the expander power also increased from 3.25 kW to 7.19 kW.

7. The cathode stoichiometry was varied from 1.2 to 2.0. The $\eta_{\text{overall}}$ improved by approximately 1% as the cathode stoichiometry increased from 1.2 to 2.0. The $R_{(H/U)}$ also improved from 3.74 to 1.53 over the same stoichiometry range. The $\eta_{\text{overall}}$ remain approximately constant, but the $R_{(H/U)}$ increased to 1.6 from 1.53 at cathode stoichiometry of 2.5.
8. The system performance improved as the compressor and the expander became more efficient. However, at high pressure (3 bar(a)), both the system electrical (27%-38%) and heat (60%-49%) efficiencies varied significantly as the isentropic efficiency varied from 30% to 100% compared to a system operating at low (1.25 bar(a)) pressure (27%-30% & 60%-57% respectively). Conversely, for both high and low pressure systems, the overall system efficiency remained approximately constant (86.50% to 86.90%). The minimum value of the overall system efficiency was also achieved between 50%-60%. The desired heat to power ratio of one could not be achieved, even if the isentropic efficiency of both compressor and expander were 100%.

9. In the absence of an expander (isentropic efficiency =0), it was found that both the system electrical and heat efficiencies and hence the heat to power ratio were greatly effected, especially in the high pressure system. For a high pressure, the electrical efficiency decreased to 28% (35% with expander) without an expander in the SPFC CHP system.

10. A SPFC CHP system (figure 3.10) was investigated with a predicted future fuel cell efficiency (\(\eta_{fcb}\)) improvement of 15%-18% and reduced anode stoichiometry (1.5 to 1.2). The improvement in the SPFC stack efficiency from 58% to 68%, improved the electrical system efficiency from 35% to 42% and decreased the system heat efficiency from 52% to 47%. The overall system efficiency and the heat to power ratio also improved from 86.6% to 88% and 1.51 to 1.1 respectively.

11. A 40 kWp SPFC CHP system operating at a pressure of 3 bar(a) achieved the optimal performance of \(\eta_{\text{Overall}}\) of 87% and \(R_{\text{H/P}}\) of 1.1 with the following system configurations and performance of various components:

   - The reformer reactants preheated to 800°C.
   - The stack exhaust gas (anode & cathode) streams condensed before feeding them to the burner (25°C).
   - Fuel processor efficiency = 72%
SPFC Stack efficiency ($\eta_{Fr}$) = 68%
Anode and cathode stoichiometry of 1.2 and 2 respectively.
Compressor and expander isentropic efficiency = 80%
Electrical Efficiency, ($\eta_{El\_sys}$) = 42%
Heat Efficiency, ($\eta_{H\_sys}$), (%) = 47%
3.6 REFERENCES


29. US Patent 4, 910, 099


4. ANALYSIS OF A 50 kW_e INDIRECT METHANOL SPFC SYSTEM FOR TRANSPORTATION APPLICATION

4.1 INTRODUCTION

Due to the global commercialisation of the internal combustion engines (ICEs), the transportation sector has become largely dependent on the petroleum industry. This has now resulted in transportation becoming a major contributor to urban air pollution and also a significant contributor to greenhouse gas, CO₂ [1]. The consequence of both petroleum dependency and impact upon the environment has intensified the transportation sector's search for an alternative technology ICE during the last three decades. The search for an alternative technology has subsequently revived the interest in electric traction as a viable and environmental friendly replacement for the ICE. Fuel cells, with their promise of a clean and efficient power source, have the potential to supply the power for the traction in an electric vehicle.

The renaissance of the solid polymer fuel cell (SPFC) as a potential power source for both stationary and transportation has gained increasing momentum over the last two decades. The high performance (efficiency and power density), low operating temperature (60-90°C) and the physical nature of the electrolyte are a number of the characteristics, which make the SPFC a major contender for a vehicle application [1,2].

Historically, other fuel cell types have also been utilised in both terrestrial and extraterrestrial motive applications. In 1960, a 1.5 kW_e H₂/O₂ alkaline electrolyte fuel cells were used in the NASA Apollo mission [2]. The fuel cell plant for the mission weighed ≈ 150 kg/kW, which corresponded to 1.6 kWh/kg for the 240-hour mission [3]. The first practical fuel cell (alkaline) terrestrial vehicle application was a 20 horsepower (14.91 kW) tractor, which was demonstrated by the Allis-chalmers manufacturing company in the USA [3]. In 1967 General Motors (G.M.) converted a van to operate on Union Carbide H₂-O₂ alkaline fuel cells. The G.M. Electrovan consisted of 32 fuel cell modules, which provided an open circuit voltage of 520 Volts and a peak power output of 160 kW_e (32 kW_e continuous power). At this peak power,
the G.M. Electrovan, consumed 86 g/kWh (H₂) and achieved an overall thermal efficiency of 30% [4].

During the early 1970s, the focus was on the research and development of fuel cell-battery hybrid vehicles. The fuel cells in the hybrid power source solved the problem of low energy density of the battery, while the battery solved the problem of the low power density of the alkaline and phosphoric acid fuel cells. In 1971, a hybrid city (fuel cell/battery) car was constructed by Union Carbide and tested for 4 years covering approximately 21,000 km. The city car consisted of 15 modules of alkaline fuel cell (AFC (120 cells)) and 150 kg of lead acid battery. This hybrid power plant provided the car with continuous and peak power of 7.5 kWₑ and 20 kWₑ respectively and a calculated efficiency of 58% was also achieved [4,5].

The first SPFC vehicle was developed and demonstrated in 1993 by Ballard power systems. The 32-foot light duty transit bus was the first SPFC zero-emission vehicle (ZEV) and seated 20 passengers. The bus engine was powered by 90 kW of SPFCs (MK 5 - 5 kW modules), with the battery used for only initial start up. Hydrogen and air were supplied from compressed tanks and the compressor respectively. The bus achieved a range of 160 km [6,7]. After successfully demonstrating that a SPFC power plant was capable of providing the entire power requirement of the prototype bus, Ballard Power Systems undertook a four phase bus development programme. The objective of the second and third phases of the bus programme was to develop and produce two or three small fleets for testing a SPFC commercial bus engine, which would perform the same as the replaced diesel engine and also occupy the same engine volume. The engine of these commercial buses would consist of Ballard’s second (MK 513 -13 kW modules) and third (MK 7 -32 kW modules) generation fuel cell stacks [8]. The third generation fuel cell stacks where developed jointly by Ballard and Daimler-Benz, and were to meet the power density (1 kW/l, 0.8 kW/kg) targets identified by automarkers the U.S. Partnership for a New Generation Vehicle (PNGV) program. The commercial transit bus will be available in year 2001/2002 and the bus will be powered by 200 kW (275 HP), third generation fuel cell stacks. The bus will have a range of 560 km on compressed hydrogen (tanks) and maximum speed of approximately 95 km/h [5,10].
Table 4.1: Overview of some of the SPFC vehicles built and demonstrated between 1967 and 2001.

<table>
<thead>
<tr>
<th>VEHICLE TYPE &amp; YEAR</th>
<th>FUEL CELL TYPE</th>
<th>FUEL</th>
<th>BATTERY PACK</th>
<th>PROPULSION (MOTOR SIZE &amp; TYPE) POWER (kW)</th>
<th>TOP SPEED (km/h)</th>
<th>RANGE (km)</th>
<th>SIZE (m) OR WEIGHT (kg)</th>
<th>REF.</th>
</tr>
</thead>
<tbody>
<tr>
<td>General Motors (GM) Electronvan (1967)</td>
<td>GM 160 kW AFC</td>
<td>H₂ (l) &amp; O₂ (l) tanks</td>
<td>None</td>
<td>93 kW Induction Motor (4-pole, 3-phase)</td>
<td>105-112</td>
<td>160-240</td>
<td>3230</td>
<td>4,5</td>
</tr>
<tr>
<td>Union Carbide Hybrid City Car (1970)</td>
<td>6 kW AFC</td>
<td>H₂ (g) tanks &amp; Air Blower</td>
<td>150 kg of Lead Acid</td>
<td>DC series motor with 7.5 kW cont. and 20 kW peak power</td>
<td>80</td>
<td>770</td>
<td>181 (Power source)</td>
<td>4,5</td>
</tr>
<tr>
<td>Ballard Power System Transit Bus (1993-2002)</td>
<td>Ballard MK 5 205 kW SPFC</td>
<td>Compressed H₂ Gas (CHG)</td>
<td>220 Ah Lead Acid (For Starting)</td>
<td>Brushless dc, liquid-cooled (93%), Power Output (Cont.) 160 kW</td>
<td>95</td>
<td>400-560</td>
<td>32-40 ft long</td>
<td>5,6,7,8,9</td>
</tr>
<tr>
<td>Daimler-Benz NeCar 2 (1996)</td>
<td>Ballard MK 7 50kW SPFC</td>
<td>CHG -2x140 lit tanks</td>
<td>For Starting</td>
<td>Three phase asynchronous motor 33 kW cont., 45 kW peak</td>
<td>110</td>
<td>250</td>
<td>2600</td>
<td>5,9,11</td>
</tr>
<tr>
<td>Toyota RAV4 EV (1997)</td>
<td>25 kW SPFC (400 cells)</td>
<td>Methanol</td>
<td>Ni-MH &quot;Buffer Battery&quot;</td>
<td>50 kW (peak) synchronous permanent magnet motor</td>
<td>125</td>
<td>500</td>
<td>approx. 4x1.7x2.4 (L,W,H)</td>
<td>5,11</td>
</tr>
<tr>
<td>Daimler-Benz NeCar 3 (1997)</td>
<td>Ballard MK 7 50kW SPFC</td>
<td>Methanol</td>
<td>For Starting</td>
<td>Three phase asynchronous motor 33 kW cont., 45 kW peak</td>
<td>120</td>
<td>400</td>
<td>1750</td>
<td>5,11</td>
</tr>
<tr>
<td>Mazda passenger Car (1997)</td>
<td>20 kW SPFC</td>
<td>H₂ in Metal hydride tank (33lits)</td>
<td>20 kW Ultracapacitor</td>
<td>AC synchronised motor with 40 kW peak power</td>
<td>90</td>
<td>170</td>
<td>approx. 4x1.7x1.5 (L,W,H)</td>
<td>5</td>
</tr>
<tr>
<td>Daimler-Benz NeCar 4 (1999)</td>
<td>Ballard MK 7 70kW SPFC</td>
<td>Liquid H₂ Tanks</td>
<td>For Starting</td>
<td>ECOSTAR asynchronous motor with 55 kW peak</td>
<td>145</td>
<td>450</td>
<td>1750</td>
<td>5,11</td>
</tr>
<tr>
<td>Ford Motor Co. P2000 FC EV (1999)</td>
<td>Ballard 75 kW SPFC</td>
<td>CHG 1.4 kg two tanks</td>
<td>Service Battery</td>
<td>ECOSTAR 67kW traction drive</td>
<td>145</td>
<td>160</td>
<td>1514</td>
<td>5</td>
</tr>
<tr>
<td>General Motors &quot;Precept&quot; (2000)</td>
<td>GM 100 kW SPFC (400 cells)</td>
<td>H₂ in Hydride tank (4.9 kg of H₂)</td>
<td>3 kWh Ni-MH &amp; 3 kWh Li-Poly</td>
<td>Electro motor 85 kW peak, 35kW cont.(liquid Cooled)</td>
<td>190</td>
<td>800</td>
<td>1243 (Curb) 1616 (GVM)</td>
<td>5</td>
</tr>
<tr>
<td>Peugeot Hydro -Gen (2001)</td>
<td>Air Liquide 30 kW SPFC</td>
<td>CHG (350 Bar) 140 l = 3.3 kg</td>
<td>10 Ah Ni-MH Battery</td>
<td>Motor 20 kW nominal. 33kW peak power</td>
<td>95</td>
<td>300</td>
<td>1800</td>
<td>5</td>
</tr>
</tbody>
</table>
Further to the successful demonstration of the SPFC technology in bus applications, SPFC systems have also been developed and demonstrated by automotive manufactures for passenger car applications. Many partnerships between SPFC developers and automobile companies have been accomplished, these partnerships and numerous demonstration vehicles have illustrated the feasibility of the fuel cell technology for transportation applications. Table 4.1 gives an the overview of some of the SPFC vehicles built and demonstrated by the many different coalitions of automobile companies, government departments, research organisations and SPFC developers. Although most of the vehicles overviewed in table 4.1 are either using compressed hydrogen gas or liquid H₂ to supply the hydrogen to the fuel cell stack, there are a number of passenger prototype cars which are demonstrating the technology of generating hydrogen on-board using different fuels. The demonstration of on board hydrogen generation technology is essential for the fuel cell vehicle to be competitive and successful against internal combustion engine (ICE) vehicles. It is also vital for the fuel cell vehicle to perform similar to or better than ICE vehicle, whilst utilising conventional fuel and supply infrastructures. Furthermore, the lack of hydrogen supply and storage infrastructures and the inferior volumetric energy density of the both liquid and gaseous hydrogen compared to other fuels (Table 2.2), has also driven the development of vehicles with on board hydrocarbon reformers.

Today, stringent targets have been set for integrated fuel cell systems for transport applications in order for them to be competitive against conventional vehicles. Table 4.2 shows the ambitious targets set for a fuel cell system for vehicles by the US PNGV [12]. For a fuel cell vehicle to use a conventional fuel and fulfil these stringent targets, the fuel cell system manufactures will have to design and develop system components, which are compact, responsive, environmentally friendly and highly efficient.

The choice of fuel and reformer type is crucial when designing an integrated fuel cell power system to satisfy the targets set for fuel cell vehicle technology. Liquid fuels represent a more attractive method of carrying hydrogen than compressed hydrogen itself. Using conventional liquid fuels such as gasoline or diesel, enables the present fuel infra-structure to be used. However, reforming of these fuels on-broad a vehicle presents a number of challenges including system complexity, weight, performance
and SPFC efficiency (due to the presence of inert gases and impurities in the reformate [13]). Alternatively, using liquid fuels such as methanol, which can be a renewable fuel, can provide 75% hydrogen rich reformate (steam reforming) with a much less complex system, higher efficiency and a more compact system for vehicle application [1,13,14].

Table 4.2: PNGV targets for the integrated fuel cell power system (including fuel processor)

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>PNGV Targets</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy Efficiency @ 25% peak power</td>
<td>48%</td>
</tr>
<tr>
<td>Power Density</td>
<td>300 W/l</td>
</tr>
<tr>
<td>Specific Power</td>
<td>300 W/kg</td>
</tr>
<tr>
<td>Cost</td>
<td>$50/kW</td>
</tr>
<tr>
<td>Start-up to full power</td>
<td>0.5 min</td>
</tr>
<tr>
<td>Transient response (from 10 to 90% power)</td>
<td>10 sec</td>
</tr>
<tr>
<td>Emissions</td>
<td>&lt;Tier 2</td>
</tr>
<tr>
<td>Durability</td>
<td>5000 hours</td>
</tr>
</tbody>
</table>

Notes: All Data from reference [13]

Methanol is considered to be an attractive fuel for on-board generation of hydrogen, since it provides an acceptable compromise in terms of efficiency, renewable fuel advantage and cost. Methanol processing can be approached either through a partial oxidation or steam reforming or a combination of both of these processes i.e. autothermal reforming. Steam reforming of methanol is the most developed and popular reformer technology used today. The low temperature operation, high hydrogen yield and better integration of the reactor with fuel cell system favours steam reforming over partial oxidation. Advances and proven experience with steam reforming technology in the last three to four decades has encouraged some of the world's leading automotive manufacturers (DaimlerChrysler, Toyota and Ford) to develop a SPFC vehicle system using a methanol steam reformer. However, the exothermic process of partial oxidation does offer the benefits of a smaller reactor size, faster start-up and a rapid response to change in demand [13,15]. Johnson Matthey's HotSpot reactor combines the best features of both the steam and partial
oxidation reactors to produce high yield of hydrogen with fast start-up time and a high steady state reactor efficiency of 95.4% [15].

For the fuel cell vehicle to be successful and competitive in the automobile industry, a fuel cell system with an on-board fuel processor has to have higher efficiency (pre-drivetrain) and lower or ultra low emissions than the current internal combustion (IC) engines or the recently developed engine hybrids. The overall efficiency (Carnot limited efficiency) of internal combustion (IC) engine is approximately between 30-33%, i.e. % of the fuel energy delivered by the engine to the drivetrain [16,17]. The current fuel-to-wheel or the vehicle efficiency for the medium sized passenger cars, is approximately 18%. With current advances in internal combustion engine technology (direct injection, lean-burn operation or variable valve timing), the fuel-to-wheel efficiency has the potential to increase to greater than 23% [17]. The recent development of hybrid electric vehicles, such as the Toyota Prius [18], with its small ICE and battery pack have claimed to improve the fuel to wheel efficiency to 36% [17,18].

The electric efficiency (pre-drivetrain) of future fuel cell vehicle system has to be greater than 45% to be competitive with the future IC and hybrid engines, (assuming the drivetrain losses of approximately 5-10%, giving the vehicle efficiency of ≈ 35-40%). The steady state electric efficiency of a methanol fuelled SPFC system has been reported to be 44% (steam reformer) and 36.5% (partial oxidation) for a fuel cell efficiency of 55% and fuel utilisation of 70% [19]. In order to achieve system electrical efficiency of greater than 45%, a SPFC system with a methanol steam reformer has to be analysed, optimised and thermal integrated.

A steady state model of a 50 kW_e SPFC system, incorporating, a methanol steam reformer was developed to analyse the overall system performance of an integrated system. Figure 4.1 shows the schematic representation of a 50 kW_e SPFC system for a transport application. The initial aim of the study was to achieve electrical system efficiency ≥ 45%, using the steady state model calculations and the optimised operating conditions for each component described in section 3.3 and 3.4 respectively. The second aim of this study was to assess the performance of a real fuel cell hybrid
van drive train using realistic drive patterns i.e. "Brass-Board" project. The "Brass-Board" project was a research project (1993-1995) funded in part by The Commission of the European Communities, under the framework of the Joule II-programme. The objective of the project was to develop the technology needed to integrate key components of a reformer / fuel cell / battery hybrid vehicle [20,21].

4.2 SPFC SYSTEM SPECIFICATION (FOR TRANSPORTATION APPLICATION)

A SPFC system for transportation application consists of essentially of two main components, the power generator and the electric drivetrain (figure 4.1). The power generator includes a fuel processor (methanol reformer and a gas clean-up unit), a SPFC stack, a compressor and an expander and network of heat exchangers. The drivetrain of the electric vehicle generally includes the electric motor, vehicle controllers (DC/DC converter & inverter) and the transmission. In this section, the data and the operating conditions of each component of the system are specified for use in the system analysis.

4.2.1 Fuel Processor

The on board vehicle fuel processor incorporates a methanol steam reformer and a gas clean up unit (CO preferential oxidation reactor).

4.2.1.1 Methanol Steam Reformer

The methanol steam reformer consists of the burner and the steam reformer. The vaporisation of the reformer (methanol and water) and burner (methanol) reactants, is also an integral part of the fuel processor and is discussed in section 4.3.
Figure 4.1: Schematic representation of the SPFC system for transport application (without any thermal integration)
4.2.1.1 Steam Reformer

Steam reforming of methanol to produce hydrogen is a well established and proven industrial technology. In industry, methanol is used to produce high purity hydrogen at high temperature and pressure for hydrogenation processes [22]. However, for fuel cell vehicle applications, further desired features for a methanol reformer include rapid start-up, good dynamic response, small size and weight and high fuel conversion [23]. A methanol reformer operating at low temperature and pressure would fulfil most of these desired features. A low temperature methanol reformer for the production of hydrogen for a fuel cell system was investigated during 1970’s by the US Army [22]. The Reformer utilised a CuO/ZnO based catalyst. Subsequently, the thermodynamic, mechanisms and kinetics of the reformer process have been extensively studied and a number of laboratory and commercial reactors have been developed for automobile applications.

Methanol is a favourable source of hydrogen for fuel cell applications since it has a high hydrogen density (high H/C ratio). The absence of carbon-carbon bond in methanol implies that methanol can be reformed at relatively low temperature and has a lower tendency for carbon formation compared to other higher hydrocarbons [15,24]. Methanol can also be a renewable and clean fuel that can be produced from any source of carbon and hydrogen. Natural gas is largely the main source of methanol in industry today, but Methanol can also be made from numerous other feedstocks such as coal, wood waste, municipal sewage and household garbage [24].

Reforming methanol to hydrogen involves a reaction of gaseous methanol and steam on heterogeneous catalytic surfaces. The reaction proceeds in two steps, the first being the decomposition of methanol to hydrogen

\[ \text{CH}_3\text{OH} \rightarrow \text{CO} + 2 \text{H}_2 \]  
\[ \ldots(1) \]

and the second step is the water shift reaction

\[ \text{CO} + \text{H}_2\text{O} \leftrightarrow \text{CO}_2 + \text{H}_2 \]  
\[ \ldots(2) \]
The combination of these two reactions gives an overall reaction for methanol steam reformation [23]:

For Gaseous reactants

\[
\text{CH}_3\text{OH} (\text{g}) + \text{H}_2\text{O} (\text{g}) \leftrightarrow \text{CO}_2 (\text{g}) + 3\text{H}_2 (\text{g}) \quad \Delta H_{298} = +49.48 \text{ kJ/mol} \quad (3)
\]

For Liquid reactants

\[
\text{CH}_3\text{OH} (\text{l}) + \text{H}_2\text{O} (\text{l}) \leftrightarrow \text{CO}_2 (\text{g}) + 3\text{H}_2 (\text{g}) \quad \Delta H_{298} = +130.99 \text{ kJ/mol} \quad (4)
\]

A methanol steam reformer with suitable catalyst and ideal operating conditions should achieve nearly 100% equilibrium conversion of methanol. A typical theoretical equilibrium proportions of 74/24/2 by volume for H$_2$/CO$_2$/CO respectively can be achieved within the temperature range of 200-300°C, pressure of between 3-5 atmospheres and molar ratio of steam to methanol of greater than one [22,25].

Steam reforming of methanol has been studied over various copper based catalysts at both high (250°C-400°C) and low (150°C-250°C) temperatures. However, the most commonly employed catalysts in the steam reformer are the low temperature copper-based shift catalysts [26,27]. The two most widely used and studied catalysts are the Cu/ZnO/Al$_2$O$_3$ and CuO/ZnO/Al$_2$O$_3$ [22,27,28]. These catalysts have been shown to have the highest activity and conversions at lower temperature, with thermal stability and little deactivation over period of time. The optimal operating temperature with these catalysts was established to be in the range of 170-260°C. Since the performance of the reformer is intrinsically dependent upon the rate at which the required heat of reaction can be transferred to the catalyst (rather than reaction rate). The operating pressure of the reactor has significantly less effect on the performance of the reformer [19]. Hence, the operating pressure of the reformer has been reported as high as 20 bar(a) to as low as the atmospheric pressure [22,26,29].

The choice of feed ratio of H$_2$O:CH$_3$OH or (the steam to carbon ratio) is also important for achieving high yields of hydrogen from the reformer. The problem of carbon formation on the reformation catalyst, especially at elevated temperature, is related to choice of steam to carbon ratio and can be prevented by using higher than
stoichiometric requirement of steam. Although, methanol steam reforming is carried out at reduced temperatures compared to other higher hydrocarbons, a molar ratio of steam to methanol of >1 is required. Many studies report using steam to methanol ratios of between 1.1 -1.5 [19,22,25,29].

The are two possible main mechanism by which methanol is believed to reform to hydrogen. In the first mechanism, it is believed that methanol is first decomposed into CO and H₂ via reaction (1) and then followed by the water gas shift reaction (2), where the CO is oxidised by steam to produce more hydrogen and CO₂ [30]. While in the second mechanism it is assumed that methanol first reduces an active site on the catalyst by taking away the oxygen and producing CO₂ and H₂. The reduced catalyst site is then oxidised by water to produce H₂ [23].

The reactor’s operating temperature and pressure and the molar steam to methanol ratio also considerably influence the performance of the steam reforming. Steam reforming of methanol is an endothermic process and therefore is favoured by high temperature (1 & 3) while the water gas shift reaction (2) is exothermic and is favoured by low temperature. As reported by Amphlett et al. [22] that the selectivity of the catalyst for reaction (3,4) is reduced and the rate of production of CO increases relative to the rate of production of H₂ as the temperature increases. Therefore, an optimal operating temperature has to be chosen, so that the production of hydrogen is maximised and production of CO is minimised. Similar to temperature, the reactor pressure has an effect on the conversion rate of the reformer reactors. The conversion rate of reaction (1) and (3) decreases with increase in reactor pressure. According to Amphlett et al. [25], the rate of reaction (3) decreases more rapidly than reaction (1), which implies that at higher pressure more CO is produced. The steam to methanol ratio also has a considerable influence on the establishment of the thermodynamic equilibrium. According to reaction (3), the ideal ratio to use would be a stoichiometry ratio of one. However, without adding excess water the reformed gas would be rich in CO, as less CO will be consumed via reaction (2). Therefore, to achieve a maximum conversion of methanol to CO₂ & H₂, a molar ratio of greater than one should be used. However, an optimal ratio should be chosen as a much higher ratio increases the heating requirement for vaporisation of the excess water in the feed.
In this study, a reformer model was developed using the ASPEN PLUS™ software package [31]. The reformer model was used to study the effect of the various reformer variables such as temperature, pressure, molar ratio etc and to establish the operating conditions for the steam reformer. The model also calculates the methanol conversion efficiency (%) and the reformed gas composition (% by volume (%vol.)) exiting the reformer reactor based upon thermodynamic equilibrium conditions and chemical reactions.

The operating pressure of the reformer was determined by the system pressure, which in turn was determined by the fuel cell operating pressure. Based upon the SPFC systems operating at 3.0 bar(a), the reformer pressure was thus established to be 3.0 bar(a) for this system analysis. The steam to methanol molar ratio for this study was chosen on the criteria that the ratio would give a methanol conversion rate of greater than 95% and the CO content (% vol.) of less than 1% should be achieved. The effect of the molar ratio was optimised in the reformer model (ASPEN PLUS™) and the result is shown in Figure 4.2. It is evident from Figure 4.2 that the high rate of the conversion of methanol and low CO content was achieved at molar ratios of between 1 and 5. However, the hydrogen content decreases over this range. To keep the molar ratio to its minimum (low heat of vaporisation) and achieve the desired high methanol conversion (>95%) and low CO content (<1%), a molar ratio of 1.3 was chosen for this study. At this molar ratio the methanol conversion was greater than 99% and the % by volume content of CO and H₂ was 0.82% and 68.82% respectively.

The effect of temperature on the performance of the reformer was also study at pressure of 3 bar(a) and molar ratio of 1.3. Figure 4.3 shows the equilibrium composition of the product gas at a range of different temperatures. From figure 4.3 it is evident that high level of hydrogen content was achieved between the temperature of 175°C and 215°C and the nearly 100% conversion of methanol was attained at temperature greater than 190°C. On the basis of the thermodynamic equilibrium calculations, chemical and previous published practical studies, the reformer operating temperature was chosen as 200°C.
Figure 4.2: Equilibrium gas compositions for range of steam to methanol ratios

Figure 4.3: Equilibrium gas compositions for range of different temperatures
The operating condition of the methanol steam reforming for the SPFC vehicle system analysis were chosen as 200°C, 3 bar(a) and a molar steam to methanol ratio of 1.3. At this operating condition the methanol conversion rate was established as 99.92% and the reformed gas equilibrium gas composition (by volume) was 68.82% (H₂), 22.39% (CO₂), 7.89% (H₂O), 0.82% (CO) and 0.08% (CH₃OH).

4.2.1.1.2 Reformer Burner

The burner is an integral part of the reformer since the performance of the reformer is intrinsically related to the rate at which the required heat of reaction can be transferred to the catalyst rather than reaction rate. The burner was supplied with the fuel cell stack exhaust gases, methanol and air from the compressor to produce the thermal power for the endothermic methanol steam reforming process. The amount of energy required by the burner was determined by performing a heat balance on the reformer and maintaining the reformer's temperature at 200°C. The supply temperatures of various reactants of the burner are varied according to system configuration and availability of heat energy from the network of heat exchangers. The burner was supplied with 1% excess air to ensure complete combustion (if the oxygen from the cathode exhaust stream was insufficient). The burner generates heat at 230°C, 30°C higher than the reformer's operating temperature to ensure good heat transfer. The flue gases exits the reformer at 230°C.

4.2.1.2 Gas Clean-Up Unit (GCU)

The GCU model and data used in this study remains as described in the natural gas SPFC system studied in chapter 3. The operating condition of the GCU unit (section 3.2.1.3) were chosen to be 160°C and a O₂:CO molar ratio of 2.5. At these operating conditions, CO was assumed to be reduced to ≤ 10 ppm with the remainder of the oxygen was used in CH₃OH and H₂ combustion. The clean reformate from the GCU unit had the following gas composition (vol. %):
**CHAPTER 4 - METHANOL BASED SPFC VEHICLE SYSTEM**

### Component Composition (vol. %)

<table>
<thead>
<tr>
<th>Component</th>
<th>GCU Gas Composition (vol. %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td>55.65%</td>
</tr>
<tr>
<td>CO</td>
<td>0.001%</td>
</tr>
<tr>
<td>CO₂</td>
<td>20.58%</td>
</tr>
<tr>
<td>H₂O</td>
<td>12.28%</td>
</tr>
<tr>
<td>N₂</td>
<td>11.48%</td>
</tr>
</tbody>
</table>

### 4.2.1.3 Air Bleed

To further reduce the CO concentration in the clean reformate from the GCU reactor, a 1% air bleed (equal to 1% Hydrogen in the reformat) was mixed with the reformate prior to the fuel cell anode inlet (reference in section 3.2.1.4).

### 4.2.2 SPFC Stack

A 50 kWₑ SPFC stack was used in this vehicle system analysis, to provide the electric power to the drivetrain. The stack design was based on a predicted future fuel cell performance data detailed in section 3.4.5 and the optimised operating condition studied in section 3.4. Table 4.4 shows the present and future fuel cell performance. The SPFC stack had 700 cells and operated at 3 bar(a) and 80°C. The stack also used anode and cathode stoichiometries of 1.2 and 2 respectively.

#### Table 4.4: The present and future SPFC Performance

<table>
<thead>
<tr>
<th>SPFC Performance</th>
<th>Present</th>
<th>Future</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell Voltage (volts)</td>
<td>0.730</td>
<td>0.850</td>
</tr>
<tr>
<td>Current Density (Amp/cm²)</td>
<td>0.489</td>
<td>0.420</td>
</tr>
<tr>
<td>Thermal Efficiency, $\eta_{th}$ (LHV)</td>
<td>58.25%</td>
<td>67.82%</td>
</tr>
<tr>
<td>Voltage Efficiency, $\eta_V$ (LHV)</td>
<td>61.86%</td>
<td>72.00%</td>
</tr>
</tbody>
</table>
4.2.3 Compressor and Expander

From the optimisation study in the previous chapter (Section 3.4.4), the compressor and expander isentropic efficiency for this system analysis was taken as 80%, to reflect possible future performances of a compressor in a fuel cell system. The expander power was supplied to the compressor via a mechanical shaft, with a transmission efficiency ($\eta_t$) of 98%. The model assumes that the working envelope of the expander matches that of the compressor, and excess power from the expander generator was supplied to the system load, i.e. the drivetrain.

4.2.4 Heat Exchangers and Condensers

In this study, the heat exchangers were used to recover the thermal energy from the burner flue gases, fuel processor equipment and the fuel cell stack, for pre-heating reformer reactants. For the heat exchangers, only the inlet and outlet conditions of the working fluid streams were considered and 1% energy loss was assumed from the surface. The thermal energy of the flue gas was first used in the expander and then to preheat the reformer and burner reactants. Condensers were used to cool down and remove water from the anode and cathode exhaust gas streams. The exhaust gas streams were cooled down from 80°C to 25°C.

4.2.5 Electric Vehicle Drivetrain or Powertrain

The drivetrain of the electric vehicle for this analysis includes the electric motor, DC/DC converter, inverter and the transmission (figure 4.1).

4.2.5.1 Electric Motor

The function of the motor in an electric drivetrain is to convert electrical energy into mechanical energy. There are many different types of motor available in industry today such as the brushless dc motors (permanent magnet synchronous), induction motors (asynchronous) and dc brushed motors, which can be used in the electric vehicle drivetrain. For an electric vehicle application, the choice of the motor will depend on the weight, cost, compactness, peak and continuous power, high electrical and mechanical efficiency and above all the capability of the motor to operate as a
generator for regenerative braking. Today, Ecostar Electric Drive Systems (Ecostar), a joint venture between Ford, Ballard Power Systems and DaimlerChrysler is focused on developing advanced electric drive systems for fuel cell, hybrid electric and battery-powered vehicles [32]. The high speed induction motors developed by Ecostar can achieve high mechanical efficiencies of between 95-97% and is also capable of a wide range of operating speeds. The integrated transmission (gearbox) with its wide range of gear ratio has also been developed by Ecostar and has a high efficiency of between 95-98% [32].

4.2.5.2 DC/DC converter and inverter

A DC/DC converter converts the fuel cell stack voltage into a regulated voltage corresponding to battery voltage or dc link voltage. This is an electronic power supply also that takes high voltage DC power from the fuel cell stack or battery pack and provides an isolated 12 volt output to power standard vehicle accessories. This process includes a small power loss of usually between 1-2% [32]. The role of the inverter is to convert dc power to ac power and is the interface between the dc-link and the electric motor (figure 4.1). The inverter also provides motor and vehicle control. The modern power electronics in the inverter offer a high efficiency of > 97% [32].

To calculate the fuel-to-wheel or the vehicle efficiency in this system analysis, the efficiency of various components of the drivetrain were considered. To reflect the future performance of these components the following efficiencies were used in the steady state system analysis:

- DC/DC converter efficiency = 98%
- Motor electric efficiency = 95%
- Inverter efficiency = 98%
- Transmission losses = 1% (99% efficient)
4.2.5.3 Battery

Battery is an integral part of the SPFC Vehicle system and usually used for starting up process, peak power sharing (hybrid concept) and storing energy via regenerative braking. However, in this steady state analyse, the battery was not employed and battery energy was not consumed.

4.2.6 Ancillary System

The ancillary system accounts for the power supplied to the fuel processor, fuel cell system and vehicle system auxiliaries such as fuel tanks, flowrate control valves, pumps and vehicle climatic control and lighting. The typical load range of the ancillary system that would supply power to all conventional electric power consuming items of the 12 volts on board dc link, was calculated to be between 1-5 kW for a passenger car with air conditioning system (BMW 750hL) [33].

For this fuel cell vehicle study (without air conditioning system), the ancillary load of 1.5 kW of electric power or 3% of the fuel cell power was demanded from the dc-link.

4.3 SPFC VEHICLE SYSTEM ANALYSE

In this section, a steady state model of a 50 kW<sub>e</sub> methanol SPFC system was used to analyse the system performance and thermal integration of various system components in order to achieve the desired electric system efficiency (pre-drive train) of greater than 45%. The analyses used the steady state model calculations illustrated and efficiency definitions stated in section 3.3. The model also utilised the data and operating conditions specified in section 4.2.

The performance of the SPFC vehicle system depicted in figure 4.1 was first analysed and a number of efficiencies were calculated including the overall electric system efficiency. The second part of the SPFC vehicle system analysis was to optimise the system performance by integrating the thermal power with a network of heat
exchangers and condensers. The analyses were based on a net fuel cell output of 50 kW\(_e\) and a lower heating value (LHV) for methanol of 630 MJ/kmole @ 25°C [34].

### 4.3.1 STEADY STATE CALCULATIONS

The steady state model used the data and the operating conditions described in the previous section. Steady state heat and mass balance on individual component of the system were performed, to determine the performance and efficiency of the components at their operating conditions. The analysis was based on SPFC vehicle system (figure 4.1) in which the reformer and burner reactants were not pre-heated and the fuel cell stack exhaust gases were neither condensed nor pre-heated. (Hardware illustrated with the dashed lines was optional and only used when required).

#### 4.3.1.1 System Assumptions

The model in its calculations made the following assumptions:

1. All calculations were made relative to a datum temperature of 25°C.
2. The pressure drop over the various components of the system has been neglected.
3. 1% reformer surface losses.
4. Electrical requirement for all the ancillary equipment was not considered.
5. Unreacted methanol in the reformed gas from the reformer was completely oxidised in the GCU.
6. All heat exchangers are assumed to have 1% surface losses.
7. Where required, 1% excess air was used in the burner and the burner efficiency was assumed to be 100%.
8. 100% water was removed from the gas stream in the condenser.
9. No energy from the battery was consumed for the steady state analyses.
4.3.1.2 Fuel Processor

4.3.1.2.1 Reformer Reactants Flowrate

For 50 kW_e power from the SPFC stacks and an anode stoichiometry of 1.2, the hydrogen demand from the fuel processor was calculated to be 0.366 mol/s (491.70 SLPM). The equivalent methanol flowrate to satisfy the hydrogen demanded from the SPFC stacks was determined to be 0.132 mol/s (0.319 LPM @25°C). With molar ratio of steam to methanol of 1.3, the water flowrate was calculated to be 0.172 mol/s (0.186 LPM @25°C).

4.3.1.2.2 Methanol Steam Reformer and Burner

The reformer reactants were fed to the reformer at a temperature of 25°C. The burner was supplied with the fuel cell stack exhaust gases (80°C) and methanol from the tank. The oxygen demand by the burner was fulfilled by the cathode exhaust stream, which supplied ≈ 50% excess oxygen than required by the burner. However, there was option for supplying excess air, if it was required from the compressor (163°C). The amount of supplementary methanol supplied to the burner was determined by performing a heat balance on the reformer and maintaining the reformer's temperature at 200°C. The burner supplied the heat to the catalyst bed at 230°C to ensure adequate heat transfer. The power required for the reformer reaction was determined from the overall heat of reaction (equation 4) at 200°C [35]. For a methanol flowrate of 0.132 mol/s and a conversion efficiency of 99.7%, the power required to reform methanol at 200°C was calculated to be 7.7 kW.

\[
\text{CH}_3\text{OH} (\text{g}) + \text{H}_2\text{O} (\text{g}) \leftrightarrow \text{CO}_2 (\text{g}) + 3\text{H}_2 (\text{g}) \quad \Delta H_{473} = +58.4 \text{ kJ/mol} \quad \ldots(4)
\]
Figure 4.4: Reformer heat balance at 3 bar(a) and 200°C

From the reformer heat balance, the reformer efficiency, $\eta_{\text{Ref}}$, was found to be 69.61% and the power for the reformer reactions at 200°C, $\Delta P_{\text{Ref}(473\,\text{K})}$, was determined to be 26.41 kW (including the power required to heat the reactants to 200°C). The definition of $\eta_{\text{Ref}}$ and $\Delta P_{\text{Ref}(473\,\text{K})}$ are as following:

$$\eta_{\text{Ref}} = \frac{\text{Power in the reformed gases}}{\text{Total power into the reformer}}$$

$$\Delta P_{\text{Ref}(473\,\text{K})} = (\text{Total Power into the burner}) - (\text{Flue gases power} + \text{Power losses} + \text{Reaction Power})$$
4.3.1.2.3 GCU Reactor

For the operating conditions detailed in section 4.2.1.2, a heat and mass balance was carried out to determine the thermal power to be removed from the GCU, in order to maintain a temperature of 160°C. This was calculated to be 5.03 kW. (This heat power also contains thermal energy produced via combustion of all remaining CH₃OH and loss H₂ with excess O₂ in the GCU).

4.3.1.2.4 Fuel Processor Efficiency

The fuel processor efficiency defined in section 3.3.2.4, \( \eta_{FP} \), for the system presented in figure 4.1 was calculated to be 82.38%.

4.3.1.3 SPFC Stack

A heat and mass balance for the fuel cell stack was carried out in order to determine the heat to be removed by a cooling system, to maintain the stack temperature of 80°C. The fuel cell data detailed in table 4.4, was used in the heat and mass balance calculation. The anode and cathode stoichiometries were 1.2 and 2 respectively. Figure 4.5 shows the heat balance of the fuel cell at these operating conditions. From the heat balance, the cooling power required to maintain the stack at 80°C was determined to be 15 kW. The relative humidities (Appendix I) of the anode and cathode exhaust gas streams were also calculated using the partial pressure of the water vapour in these gas streams. These were found to be 138.83% and 120.40% for anode and cathode outlet streams respectively.

4.3.1.4 Compressor and Expander

For this steady state analysis, the isentropic efficiency of the compressor and expander were both taken as 80%. Using equation 3.9 (section 3.2.3), the air temperature at the outlet of the compressor, (at a pressure ratio of 3) was calculated to be 163°C.
Figure 4.5: SPFC heat balance at 3 bar(a) and 80°C

The corresponding compressor power was determined to be 6.23 kW. Including the mechanical transmission efficiency of the shaft ($\eta_s = 98\%$), the total power required by the compressor at pressure ratio of 3, was found to be 6.35 kW. The expander power was also calculated for pressure ratio of 3 and isentropic efficiency of 80%. The flue gases at the temperature of 230°C were expanded to a temperature of 125.34°C. The power generated by the expander was 6.09 kW at pressure ratio of 3. Additional power (0.26 kW) for the compressor was supplied via the dc-link (figure 4.1).
4.3.1.5 Heat Exchangers and Condensers

From figure 4.1 it can be seen that four heat exchangers were used in this system analysis. The performance of the heat exchanger was determined by considering only the inlet and outlet conditions of the fluid streams. Since in this study the reformer and burner reactants are not preheated, the excess thermal power from the heat exchangers was not used. However, the excess thermal power of these heat exchangers will be used in the system thermal integration study. Heat exchanger 1 and 2 were used to cool down the reformed gases from 200°C to 160°C and then eventually down to 80°C, before being fed into the SPFC stack. Heat exchanger 3 was used to cool down compressed air from 163°C to 80°C, while heat exchanger 4 was optional and not utilised in this particular study. Table 4.5 shows the performance of these heat exchangers. Condensers were not used in this study and the SPFC stack exhaust gases were fed directly into the burner at 80°C.

Table 4.5: Performance of the heat exchangers at 3 bar(a)

<table>
<thead>
<tr>
<th>Heat Exchanger No.</th>
<th>Properties (°C) &amp; (kW)</th>
<th>Power Available</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Tin</td>
<td>Tout</td>
</tr>
<tr>
<td>1</td>
<td>200</td>
<td>160</td>
</tr>
<tr>
<td>2</td>
<td>160</td>
<td>80</td>
</tr>
<tr>
<td>3</td>
<td>163</td>
<td>80</td>
</tr>
</tbody>
</table>

4.3.1.6 Electric Vehicle Drivetrain and Ancillary system

In this study, the performance of the individual drivetrain components were modelled by their efficiency. Using the efficiencies of different components of the drivetrain stated in section 4.2.5, overall drivetrain efficiency ($\eta_{\text{dr}}$) was determined to be 90.33%. The corresponding power loss was calculated as 4.83 kW. An ancillary load of 1.5 kW was also demanded from the system to support auxiliary components. This ancillary load of 1.5 kW corresponded to ancillary system efficiency ($\eta_{\text{anc}}$) of 96.94%.
Table 4.6 shows the individual component efficiency and power losses incurred by these components of the drivetrain and ancillary system.

Table 4.6: Drivetrain and ancillary system efficiencies and losses

<table>
<thead>
<tr>
<th>Component</th>
<th>Efficiency</th>
<th>Power loss (kW)</th>
</tr>
</thead>
<tbody>
<tr>
<td>DC-DC Converter</td>
<td>98.00%</td>
<td>1.00</td>
</tr>
<tr>
<td>Inverter</td>
<td>98.00%</td>
<td>0.95</td>
</tr>
<tr>
<td>Motor</td>
<td>95.00%</td>
<td>2.33</td>
</tr>
<tr>
<td>Transmission</td>
<td>99.00%</td>
<td>0.44</td>
</tr>
<tr>
<td>Ancillary Load</td>
<td>96.94%</td>
<td>1.50</td>
</tr>
<tr>
<td>Overall</td>
<td>87.56%</td>
<td>6.22</td>
</tr>
</tbody>
</table>

4.3.1.7 Overall system heat balance and System efficiencies

An overall system heat balance of a vehicle system (figure 4.1) was carried out to determine the electrical system efficiency and vehicle efficiency (fuel to wheel efficiency). Table 4.7 shows the overall system heat balance of the vehicle system and number of system efficiencies. The electrical ($\eta_{\text{El Sys}}$) and vehicle ($\eta_{\text{Veh}}$) system efficiencies are defined as following:

$$\eta_{\text{El Sys}} = \frac{\text{SPFC Power (kW)} + \text{Expander Power (kW)}}{\text{LHV of the Fuel to the system (kW)}}$$

$$\eta_{\text{Veh}} = \eta_{\text{El Sys}} \times \eta_{\text{O dt}} \times \eta_{\text{anc}}$$
### Table 4.7: Overall heat balance of the vehicle system

<table>
<thead>
<tr>
<th>Component</th>
<th>Power Into the System (kW)</th>
<th>Power into the System (%)</th>
<th>Power Out of the System (kW)</th>
<th>Power out of the System (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>REFORMER REACTANTS</td>
<td>83.36</td>
<td>73.01%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>FUEL TO THE BURNER</td>
<td>30.52</td>
<td>26.73%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>REFORMER LOSSES</td>
<td></td>
<td></td>
<td>8.53</td>
<td>7.47%</td>
</tr>
<tr>
<td>HEX1</td>
<td></td>
<td></td>
<td>0.75</td>
<td>0.65%</td>
</tr>
<tr>
<td>GCU REACTOR COOLING</td>
<td></td>
<td></td>
<td>5.03</td>
<td>4.41%</td>
</tr>
<tr>
<td>HEX2</td>
<td></td>
<td></td>
<td>1.44</td>
<td>1.26%</td>
</tr>
<tr>
<td>SPFC STACK COOLING</td>
<td></td>
<td></td>
<td>15.04</td>
<td>13.18%</td>
</tr>
<tr>
<td>SPFC STACK ELECTRICAL POWER</td>
<td></td>
<td></td>
<td>50.00</td>
<td>43.80%</td>
</tr>
<tr>
<td>FLUE GASES</td>
<td></td>
<td></td>
<td>29.59</td>
<td>25.92%</td>
</tr>
<tr>
<td>COMPRESSOR POWER REQUIRED</td>
<td>0.29</td>
<td>0.26%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>EXTRA EXPANDER POWER</td>
<td></td>
<td></td>
<td>0.00</td>
<td>0.00%</td>
</tr>
<tr>
<td>HEX3</td>
<td></td>
<td></td>
<td>3.63</td>
<td>3.18%</td>
</tr>
<tr>
<td>MOTOR LOSSES</td>
<td></td>
<td></td>
<td>0.03</td>
<td>0.02%</td>
</tr>
<tr>
<td>SHAFT LOSSES</td>
<td></td>
<td></td>
<td>0.13</td>
<td>0.11%</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>114.17</strong></td>
<td><strong>100.00%</strong></td>
<td><strong>114.17</strong></td>
<td><strong>100.00%</strong></td>
</tr>
<tr>
<td><strong>COMPRESSOR POWER</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>EXPANDER POWER</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>SPFC VEHICLE SYSTEM</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>FUEL CELL POWER</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>EXPANDER POWER</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>DRIVETRAIN &amp; ANCILLARY SYSTEM</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DC/DC CONVERTER LOSSES</td>
<td>1.00</td>
<td>2.00%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ANCILLARY LOAD</td>
<td>1.50</td>
<td>3.06%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>INVERTER LOSSES</td>
<td>0.95</td>
<td>2.00%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MOTOR LOSSES</td>
<td>2.33</td>
<td>5.00%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TRANSMISSION LOSSES</td>
<td>0.44</td>
<td>1.00%</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>ELECTRICAL POWER</strong></td>
<td>50.00</td>
<td>43.80%</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>THERMAL POWER AVAILABLE</strong></td>
<td>64.16</td>
<td>56.20%</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>POWER TO WHEELS</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>VEHICLE EFFICIENCY</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*SPFC Vehicle System @ 3.0 Bar(a) (Without Preheat & Condensers)*
4.3.1.8 Results of steady state calculations

Table 4.8 shows the summary of the results of the steady state study of a methanol fuelled SPFC vehicle system (figure 4.1) with no reactant pre-heat and without the use of condensers. The analysis did not achieve the desired electric system efficiency, \( \eta_{\text{El Sys}} \), (pre-drivetrain) of greater than 45%. To improve the electric system efficiency and hence the vehicle efficiency, the total fuel to the system has to be reduced. The reduction of the fuel to the system can be achieved by pre-heating the reactants by utilising the thermal power within the system. This requires the integration of the thermal power with use of a network of heat exchangers and condensers.

Table 4.8: Summary of results from the study of the SPFC vehicle system

<table>
<thead>
<tr>
<th>System Parameters</th>
<th>SPFC Vehicle System (@3 bar(a))</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>No Preheat &amp; Condensers</td>
</tr>
<tr>
<td>Total Fuel Power to the System (kW)</td>
<td>114.17</td>
</tr>
<tr>
<td>Fuel Processor Efficiency, ( \eta_{\text{FP}} ), (%)</td>
<td>82.38%</td>
</tr>
<tr>
<td>Electrical Efficiency, ( \eta_{\text{El Sys}} ), (%)</td>
<td>43.80%</td>
</tr>
<tr>
<td>Drivetrain, ( \eta_{\text{Dt}} ), (%)</td>
<td>90.33%</td>
</tr>
<tr>
<td>Ancillary Efficiency, ( \eta_{\text{anc}} ), (%)</td>
<td>96.94%</td>
</tr>
<tr>
<td>Power to the wheels, (kW)</td>
<td>43.78</td>
</tr>
<tr>
<td>Vehicle Efficiency, ( \eta_{\text{Veh}} ), (%)</td>
<td>38.35%</td>
</tr>
</tbody>
</table>
4.4 OPTIMISATION OF SYSTEM PERFORMANCE

The system performance of the SPFC vehicle system was optimised by integrating the thermal power with the use of a network of heat exchangers and condensers. Two case studies were carried out:

1) Effect of pre-heating the reformer and burner reactants.
2) Use of condensers for the fuel cell exhausts gases.

The investigations used the data detailed in section 4.2 and the steady state calculation described in section 4.3.

4.4.1 Effect of preheating the reformer and burner reactants

In this case study the reformer and the burner reactants are pre-heated to the maximum possible temperature. Heat exchangers 1,3,4 and the GCU reactor were used in the reactants pre-heat process. Figure 4.6 shows the result of thermal integrating and pre-heating processes on the heat exchangers and system performance. The step change in the efficiencies and thermal power in heat exchanges seen in figure 4.5 was due to the methanol and water changing its phase from liquid to vapour (i.e. the influence of latent heat of vaporisation). Heat exchanger 4 (HEX 4) was used to transfer the maximum thermal power from the flue gases at 125°C to reformer and burner reactants. The reformer reactants (methanol and water) and burner methanol were heated to a temperature of 120°C in HEX 4. The flue gases temperature was decreased to ≈ 60°C and 7.7 kW of the thermal power was used in this heating process. The reformer and burner methanol was further heated to 160°C by HEX 1. The methanol water was also further heated to 160°C by combination of HEX 3 and the GCU reactor. Figure 4.7 shows the thermally integrated SPFC Vehicle system and the heat treatment received by the reactants via various heat exchanges and the GCU reactor. The reason for heating the reactants prior to feeding them into the respective components was to reduce the amount of fuel consumed in the system and hence improve the system electrical and the overall vehicle efficiencies. Table 4.9 shows the system performance after the thermal integration process.
Table 4.9: Summary of results after thermal Integration process

<table>
<thead>
<tr>
<th>System Parameters</th>
<th>SPFC Vehicle System (@3 bar(a))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Fuel Power to the System (kW)</td>
<td>96.66</td>
</tr>
<tr>
<td>Fuel Processor Efficiency, ( \eta_{FP} ), (%)</td>
<td>96.65%</td>
</tr>
<tr>
<td>Electrical Efficiency, ( \eta_{EI , sys} ), (%)</td>
<td>51.73%</td>
</tr>
<tr>
<td>Drivetrain, ( \eta_{O , dt} ), (%)</td>
<td>90.33%</td>
</tr>
<tr>
<td>Ancillary Efficiency, ( \eta_{anc} ), (%)</td>
<td>96.94%</td>
</tr>
<tr>
<td>Power to the wheels, (kW)</td>
<td>43.78</td>
</tr>
<tr>
<td>Vehicle Efficiency, ( \eta_{Veh} ), (%)</td>
<td>45.30%</td>
</tr>
</tbody>
</table>

4.4.2 Use of condensers for the fuel cell exhausts gases

The use of condensers to cool and remove the water from the SPFC stack anode and cathode exhaust gases was also investigated. The SPFC stack exhaust gases were cooled down from 80°C to 25°C and the power in the gases (thermal and chemical) was reduced from 31.6 kW to 14.8 kW i.e. 16.8 kW extracted via the condensers. Figure 4.8 shows the thermally integrated SPFC Vehicle system with condensers. The consequence of using the condensers was that the power to the burner and the power in the flue gases were both reduced. Reduced power in the flue gases leads to less power being recovered via the expander and also less power being available for the reactants heating process. However, the advantage of using condensers is that the amount of water fed to the burner or combustion chamber was reduced, and hence less power was required to heat it to the burner temperature of 230°C. The effect of using less fuel in the system led to higher system electrical efficiency and hence improved vehicle efficiency.

For heating the reactants to 160°C the process was configured differently since the thermal power in the flue gases was not enough to heat both water and methanol to 120°C. The reformer and burner methanol was heated to 100°C by HEX 4 and to 200°C by HEX 1. Nearly 68% of the thermal power was utilised in HEX1 compared to 47% in SPFC Vehicle system without condensers (section 4.4.1). The flue gas temperature was decreased from 125°C to 26°C and thermal power was reduced from
Figure 4.6: Result of thermal integrating and heating process on heat exchangers and system performance.

- System Electrical Efficiency
- Fuel Processor Efficiency
- Refiner Efficiency
- Refiner Reaction Power
- Flue Gases (@ 125 C)
- GCU Reactor (@ 160 C)
- HEX 1 (@ 200 C)
- HEX 3 (@ 163 C)

Electrical System Efficiency (%) & Fuel Processor (%)

Reformer Efficiencies (%) & Refomer Power (kW)

Thermal Power in Heat Exchangers, Flue gases & GCU reactor

Reformer & Burner Reactants Preheat Power (kW)
Figure 4.7: Schematic representation of the thermally integrated SPFC vehicle system
9 kW to 3 kW. The water was heated to 160°C via the HEX 3 and GCU reactor and 97% of thermal power from both these components was utilised. The total fuel to the system was reduced by approximately 1% and the electrical system efficiency was improved from 51.73% to 52.24%. The vehicle efficiency was also improved by 1% to 45.74%.

**4.5 RESULTS AND DISCUSSION**

The results of the steady state study carried out in section 4.3 and the two investigations of the SPFC vehicle system carried out in section 4.4 are summarised in table 4.10.

**Table 4.10: Summary of results of steady state analyses of the methanol fuelled SPFC vehicle system.**

<table>
<thead>
<tr>
<th>System Parameters</th>
<th>SPFC Vehicle System (@3 bar(a))</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>None</td>
</tr>
<tr>
<td>Total Fuel Power to the System (kW)</td>
<td>114.17</td>
</tr>
<tr>
<td>Fuel Processor Efficiency, $\eta_{FP}$, (%)</td>
<td>82.38%</td>
</tr>
<tr>
<td>Electrical Efficiency, $\eta_{ElSys}$, (%)</td>
<td>43.80%</td>
</tr>
<tr>
<td>Drivetrain, $\eta_{dt}$, (%)</td>
<td>90.33%</td>
</tr>
<tr>
<td>Ancillary Efficiency, $\eta_{anc}$, (%)</td>
<td>96.94%</td>
</tr>
<tr>
<td>Power to the wheels, (kW)</td>
<td>43.78</td>
</tr>
<tr>
<td>Vehicle Efficiency, $\eta_{veh}$, (%)</td>
<td>38.35%</td>
</tr>
</tbody>
</table>

**4.5.1 Steady State Calculations**

In the first steady state study, where the reactants were not preheated and fed to the reformer and burner at 25°C, and the fuel cell operating at pressure of 3 bar(a)
Figure 4.8: Schematic representation of the thermally integrated SPFC vehicle system with condensers
and 0.85 volts ($\eta_{\text{Th}} = 68\% \text{ (LHV)}$) to envisaged future performance, the electric system efficiency ($\eta_{\text{EL,sys}}$) of 43.8% was achieved. It was evident from the heat balance shown in table 4.7, that the waste heat arising mainly from inefficiency of the stack (13%) and flue gases (26%) was determined to be 56.2%. After accounting for component losses and unusable waste heat (10%), only 78% of this waste heat (43.74%) was available further to be used in the system to reduce fuel energy in order to maximise system efficiency. The quality and quantity of this waste heat power varied from 80°C (stack cooling system) to 200°C (reformer) and from 0.25 kW to 30 kW respectively.

Hence, a SPFC vehicle system (figure 4.1) without any thermal integration achieved vehicle efficiencies 38.4% and an overall power balance (pre-drivetrain) of power/coolant/exhaust = 44/44/12%, compared to an ICE’s =33/33/33% (current ICE performance) [36]. The (power/coolant/exhaust) power balance representing % electrical power for mechanical work, % coolant power removed by the heat exchangers or cooling system and % exhaust power removed from the system as unusable power. The 44% coolant or waste heat power has to be utilised to optimise the system performance and attain the desired electrical system efficiency of > 45% in order to be competitive with the future ICE and hybrid version thereof.

**4.5.2 Effect of Preheat**

When using thermal integration the performance of the SPFC vehicle system (figure 4.7) was optimised to achieve an improvement of approximately 18% in both the electrical and vehicle efficiencies. This improvement in efficiency was achieved by both preheating the methanol and water to a maximum possible temperature of 160°C and minimising the total fuel power to the system to 96.6 kW from 114.2 kW. Around 15 kW of thermal power was required to pre-heat the reactants to 160°C and majority of the power coming from flue gases at 120°C, GCU reactor at 160°C and heat HEX 3 at 163°C. However, the consequence of burning less fuel in the burner was that less power was recovered via the expander from the flue gases and hence, an extra 2% compressor power was demanded from the DC link. A thermally integrated SPFC vehicle system also achieved an electric system efficiency, $\eta_{\text{EL,sys}}$, (pre-drivetrain) of
51.7% and a competitive vehicle efficiency of 45%. The overall power balance of this system was determined to be power/coolant/exhaust = 51.7/33.3/15%. Compared to the system without any thermal integration, the electrical efficiency and exhaust power increased while the coolant power was reduced. The majority of the coolant power was of low grade thermal power at 80°C from the fuel cell stack cooling system and the depleted flue gas power (60°C). The exhaust power mostly included low quality thermal power from the various heat exchangers and inefficiencies of various components of the system. Hence, although the desired electrical efficiency of > 45% was achieved, a large amount of low grade heat power and poor quality exhaust power was unusable.

4.5.3 Use of Condensers

The second investigation was to model the effect of using condensers to cool and condense all of the water out of the anode and cathode gas streams. The advantages of using condensers in a SPFC vehicle system (figure 4.8) are firstly to dry the anode and cathode streams before feeding the gases into the burner and secondly, to recycle the condensed water back to the fuel cell stack system. The effects of condensing the water out of the stack exhaust gases were that the total fuel to the system was reduced by approximately 1% and the thermal power of the flue gases was reduced from 33 kW to 14 kW, for a system with condensers. This reduction in the quantity of the thermal power led to reconfiguration of preheating the reactants to 160°C (section 4.4.2). The reduction of total amount of fuel going into the system improved the system electrical efficiency from 51.73% to 52.24%. Improvement in the electrical efficiency also improved the vehicle efficiency by 1% to 45.74%. The overall power balance of this vehicle system was determined to be power/coolant/exhaust = 52.2/31.4/16.4%. Compared to the previous system the thermal power of the water in the anode and cathode streams was available coolant power at 80°C from the condensers. The flue gases thermal power was completely depleted (26°C) and became part of the exhaust power, which was increased from 15% to 16.4%.

From the results presented in table 4.10 and detailed above, it is evident that the more thermal power recuperated, via the recovery apparatus, the better the performance of the system. The thermal integration study was focused on achieving the highest
possible temperature for the system reactants using only the thermal power available in the system. However, in many similar studies [19,29] the methanol and water are usually heated and superheated up to the reformer operating temperature by electric heaters.

4.5.4 General Discussion

There are other critical and important issues related to fuel cell vehicles in which are not investigated in this analysis but require a reference mentioning. Some of these issues which were not discussed in this analysis were stack size, operating pressure of the system and vehicle emissions.

4.5.4.1 Stack Size

One way of increasing the system electrical efficiency and reduce coolant thermal load is by increasing the stack size. Increasing the stack size equates to operating the stack at a lower electrical loading i.e. at higher voltage and lower current density. If the number of cells were doubled to 1400 in the vehicle system the 50 kW electrical power from the fuel cell system becomes a partial load (with the full load being 100 kW). Operating the stack at partial load will improve the fuel cell efficiency and reduce thermal load (Section 3.4.3.1), but the increase in system cost and size would be much greater than the benefit achieved by the system in its performance [36]. Another method of increasing the stack size is to increase the stack area or active area. This lowers the current density and improves the stack efficiency for equivalent output power. However, it has been reported [36] that doubling the active area increase the stack cost in excess of 50% and stack volume by 60%. Hence, an optimum stack size has to be chosen based on system performance, size and cost.
4.5.4.2 Operating Pressure

Choosing the appropriate operating pressure of a fuel cell system is critical, especially for a vehicle system, since it is very important to minimise any paratactic losses and maximise the vehicle efficiency. The optimal operating pressure from the study carried out in section 3.4.3.2 was found to be 3 bar(a) and was chosen as the operating pressure for the SPFC vehicle system analysis. However, to study the effect of operating at lower pressure on the compressor/expander system, thermal integration and hence vehicle efficiency, a low pressure system investigation was carried out. The investigation used operating pressure of 1.25 bar(a) and the operating conditions of the SPFC stack at 1.25 bar(a) were used (section 3.2.2.2). The performance of other subsystems like fuel processor, compressor/expander were kept the same. The fuel cell voltage of 0.678 volts at a current density of 0.527 A/cm² was used. This corresponded to thermal ($\eta_{Th}$) efficiency of the SPFC of 54%.

Table 4.11: Effect of pressure on the performance of SPFC vehicle system

<table>
<thead>
<tr>
<th></th>
<th>SPFC Vehicle System with Preheating &amp; Condensers</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.25 Bar(a)</td>
</tr>
<tr>
<td>Cell Voltage (volts)</td>
<td>0.678</td>
</tr>
<tr>
<td>Current Density (Amp/cm²)</td>
<td>0.527</td>
</tr>
<tr>
<td>Thermal Efficiency, $\eta_{Th}$ (LHV)</td>
<td>54.06%</td>
</tr>
<tr>
<td>Compressor Power (kW)</td>
<td>1.40</td>
</tr>
<tr>
<td>Expander Power (kW)</td>
<td>1.35</td>
</tr>
<tr>
<td>Total Fuel Power to the System (kW)</td>
<td>127.79</td>
</tr>
<tr>
<td>Fuel Processor Efficiency, $\eta_{FP}$, (%)</td>
<td>89.85%</td>
</tr>
<tr>
<td>Electrical Efficiency, ($\eta_{El Sys}$), (%)</td>
<td>39.13%</td>
</tr>
<tr>
<td>Drivetrain, ($\eta_{O, dt}$), (%)</td>
<td>90.33%</td>
</tr>
<tr>
<td>Ancillary Efficiency, ($\eta_{ane}$), (%)</td>
<td>96.94%</td>
</tr>
<tr>
<td>Power to the wheels, (kW)</td>
<td>43.78</td>
</tr>
<tr>
<td>Vehicle Efficiency, ($\eta_{veh}$), (%)</td>
<td>34.26%</td>
</tr>
</tbody>
</table>

Table 4.11 compares the results of this investigation with a vehicle system operating at 3 bar(a). The effect of operating pressure was more pronounced with the compressor and expander system. The compressor power and expander power were reduced by 22% and 29% respectively as the pressure was reduced from 3 to 1.25
bar(a). Although the parasitic load on the system was reduced at lower pressure, the electrical system efficiency and hence, the vehicle efficiency, was also decreased. The superior fuel cell efficiency at high pressure compensated for the high parasitic load by demanding less hydrogen from the fuel processor and hence less fuel was used in the high pressure system. The fuel demand for the low pressure system was also high because the quality and quantity of the thermal power was inadequate for the reactants pre-heat process to the same temperature as the high pressure system. The lower dew point or boiling point at lower pressure increased the thermal power demand for the pre-heat process and so the water could only be heated to 100°C and methanol to 160°C.

The overall power balance for the lower pressure system was calculated to be power/coolant/exhaust = 39.1/42.2/18.7%. Compared to the high pressure system (52.2/31.4/16.4%), nearly 61% of the fuel power was converted to thermal power. Most of this thermal power was available as low grade heat at 80°C from the fuel cell cooling system and condensers. The inferior fuel cell efficiency at lower pressure was mainly responsible for the large percentage of coolant power. The exhaust thermal power was mainly poor quality thermal power in the flue gases at 38°C. Hence, the advantages gained by operating at high pressure are considered more superior than those achieved by a vehicle system operating at lower pressure.

4.5.4.3 Vehicle Emissions

Fuel cells generate electric power with zero emission by electrochemically reacting hydrogen and oxygen to produce high purity water and waste heat. However, this zero emission characteristic of the fuel cell does not exist when hydrocarbon fuels are used. When onboard fuel processing is considered then the emissions from a fuel cell system have to be considered, measured and comply to the standards set by the legislative bodies.

In a fuel cell system with an onboard fuel processor, the burner is a major source of nitrogen oxides (NOₓ), CO, unburnt hydrocarbons (HC) and particulate emissions. In addition to these emissions, CO₂, N₂ and water also form part of the exhaust gases
Compared to ICEs, the emission from a SPFC vehicle system (i.e. local vehicle emissions) are extremely low. Some of the reasons for low emissions from a SPFC vehicle with an onboard fuel processor are:

1) The high fuel cell system efficiency increases the fuel economy or (lowers fuel consumption), which leads to lower CO₂ production per mile. Also some of the fuels used to power the vehicle have high H:C ratios (CH₄ & CH₃OH) which would also help to reduce CO₂ emissions. [17,38].

2) The low temperature operation (NOₓ), the catalytic based processes (HC, CO) and the purification stages of reformed gas (HC, CO) would nearly eliminate all the local emission [17].

3) NOₓ, HC, CH₄ and particulate emissions levels are also reduced by using low temperature and high pressure catalytic burners or the low NOₓ burners. Furthermore, using lean fuel like the anode off-gas helps in reducing NOx levels [37,39].

Beside the local vehicle emissions from a SPFC vehicle, the emissions released and energy consumed during the process of extraction, production and delivery of both the primary and secondary fuels also has to be considered. It is estimated that a fuel cell vehicle using either methanol or other hydrocarbon fuel has the potential to halve so called “well-to-wheels” CO₂ emissions [17]. A typical small to medium ICEs vehicle sold today has a “well-to-wheels” CO₂ emission of between 90-220 g/km (small-medium) while a modern hybrid engine has “well-to-wheels” CO₂ emissions of around 110 g/km. The production and distribution energy efficiency for methanol (produced from methane) is around 63% (<60% for hydrogen) [17].

In another study where the steady state emissions from the on-board reformer (methanol and natural gas) were used to compare the emissions from conventional cars (petrol & diesel), it was estimated that the emissions (CO, SOₓ, NMHC (no methane HC), NOₓ and Particulate) were down by one to two orders of magnitude and the CO₂ emissions for the methanol fuel cell car was 62% less than that of the petrol car [39]. It was also concluded that most of the emissions occurs higher up the fuel
supply chain i.e. in the process of extraction, production and delivery of fuel [39]. The steady state emissions from a gasoline POX (partial oxidation) fuel processor show that HC and NOx emission levels were < 20% and CO levels were under 0.5% of what is allowed by ULEV (ultra low emission vehicle) standard [38].

In this steady state analysis of the SPFC vehicle system there was no model to predict any emissions from the system. However, it was evident from the measured steady state emission and other emission studies that a fuel cell system with on-board fuel processor has the potential to meet the emission targets or standards set by legislative bodies (figure 4.9) and to be beneficial to the environment. Nevertheless, it should be remembered that fuel cell vehicle with on-board fuel processor still has to undergo the transient operation required by the standard driving cycle used to evaluate ULEV compliance.

Figure 4.9: American and Europe Emissions Standards
(Data from references [39] & [40])
4.6 SUMMARY OF RESULTS

1. Each component of the system was modelled and its performance data or efficiency was specified. The following data and efficiency were used in the steady state system analysis:

**Fuel Processor**
Reformer Temperature = 200°C
Reformer Pressure = 3 bar(a)
S:C ratio = 1.3
Methanol conversion efficiency = 99.92% (H₂ = 68.82% (Vol. %))
Reformer efficiency (\(\eta_{\text{Ref}}\)) = 69.61% (without thermally integration)
Fuel processor efficiency (\(\eta_{\text{FP}}\)) = 82.38% (without thermally integration)

**SPFC Stack**
Current Density (Amp/cm²) = 0.420 (Active area = 200 cm²)
Cell Voltage (volts) = 0.850
Thermal Efficiency, \(\eta_{\text{Th}}\) (LHV) = 67.8%
Voltage Efficiency, \(\eta_{\text{V}}\) (LHV) = 72%
Anode and cathode stoichiometries of 1.2 and 2 respectively.

**Compressor & Expander**
Isentropic efficiency = 80%,

**Drivetrain Components & Ancillary load**
DC/DC converter efficiency = 98%
Motor electric efficiency = 95%
Inverter efficiency = 98%
Transmission losses = 1% (99% efficient)
Ancillary Load = 1.5 kWₑ (3% of SPFC Stack power)

2. A SPFC vehicle system (figure 4.1) without any thermal integration achieved electric system efficiency (\(\eta_{\text{ELSys}}\)) (pre-drivetrain) and vehicle efficiency (\(\eta_{\text{Veh}}\)
of 43.8% and 38.4% respectively. The analysis did not achieve the desired vehicle efficiency \( \eta_{\text{veh}} \geq 45\% \). The overall power balance (pre-drivetrain) of this system was determined to be power/coolant/exhaust = 44/44/12\%.

3. A thermally integrated SPFC vehicle system achieved an electric system efficiency, \( \eta_{\text{El Sys}} \) (pre-drivetrain) of 51.7\% and a competitive vehicle efficiency of 45.3\%. The fuel processor efficiency for this system was improved from 82\% to 97\%. The overall power balance of this system was determined to be power/coolant/exhaust = 51.7/33.3/15\%.

4. The effect of using condensers (for the anode and cathode gas streams (figure 4.8)) in a thermally integrated system also improved the vehicle efficiency by \( \approx 1\% \) to 45.74\%. The overall power balance of this vehicle system was power/coolant/exhaust = 52.2/31.4/16.4\%.

5. The vehicle efficiency was decreased from 45.74\% to 34.26\% as the pressure was reduced from 3 (\( \eta_{\text{Th}} = 68\% \)) to 1.25 (\( \eta_{\text{Th}} = 54\% \)) bar(a). The overall power balance for the lower pressure system was calculated to be power/coolant/exhaust = 39.1/42.2/18.7\%. Compared to the high pressure system (52.2/31.4/16.4\%), nearly 61\% of the fuel power was converted to thermal power.
4.7 BRASS-BOARD INTEGRATION OF A REFORMER /SPFC /BATTERY/ ELECTRIC MOTOR SYSTEM FOR ELECTRIC TRACTION

4.7.1 INTRODUCTION

The brass-board integration of a reformer/SPFC/battery/electric motor system for electric traction was a system integration project, which developed an electric traction system for a 4.6 tonne delivery van. This was termed as "Brass-Board" project. The "Brass-Board" project was (1993-1995) funded in part by The Commission of the European Communities, under the framework of the Joule II-programme. The objective of the project was to develop the technology needed to integrate key components of a reformer/fuel cell/battery hybrid vehicle, as well as to assess the performance of the system using realistic drive patterns [20,21].

In the framework of the Joule II-programme, the "Brass-Board" project work was divided between the partners; ECN (NL), Holec Ridderkerk (NL), TNO (NL), TECNARS (IT) and Loughborough University (UK). Each of the five European partners was responsible for different tasks and the Loughborough University tasks are summarised as following:

- Specify components for the brass-board after undertaking model calculations based on actual vehicle duty data.
- Instrument internal combustion engine vehicles in order to record test data.
- Identify and develop (in conjunction with TECNARS) the operations necessary for fuel gas purification and successful integration of reformer with fuel cell.
- Use single cell systems to test effectiveness of the gas clean up process.
- Contribute to brass-board component integration and testing.
- To validate the model by comparison with actual brass-board performance.

In this section the work carried out to fulfil the Loughborough University modelling task is detailed. The brass-board hybrid van system model is explained, specified and the performance of the hybrid system under various duty cycles is compared with actual brass-board system performance under identical duty cycles.
4.7.2 Brass-Board System Description and Specification

The brass-board hybrid van system consisted of two major parts, the power generator and the electric drivetrain. The power generator consisted of a methanol steam reformer, gas clean-up unit, air compressor and SPFC system. The drivetrain consisted of up-chopper (dc/dc converter), battery pack, electric motor system (motor, controller & inverter) and vehicle controller (supervisory control unit & control strategy). Figure 4.10 shows the schematic representation of the 4.6 tonne brass-board hybrid system. The maximum mechanical power specified for the brass-board system was 60 kW, of which the generator could provide a maximum of 16 kW_e.

4.7.2.1 Methanol Steam Reformer

Tecnars were responsible for the design and construction a methanol steam reformer. The reformer was to produce 20 m^3/hr of hydrogen (equivalent to 20 kW_e fuel cell power) at normal condition (273 K and 1 bar) with a minimum of CO (=1-2% vol.) in the fuel gas or reformed gas.

4.7.2.2 GCU

It was the task of Loughborough University to construct and evaluate the performance of a gas clean unit (GCU). The GCU would be integrated with a methanol reformer to form the fuel processor for the brass-board system. The GCU would facilitate the supply of a hydrogen rich fuel stream containing 20 ppm CO to the fuel cell stacks. The best performance of < 20 ppm CO output from the GCU was achieved with three Pt/Rh catalysed metallic monoliths in series with oxygen stoichiometry of 4.5% (O_2: H_2) and optimum operating temperature in the region of 120 -130°C.
Figure 4.10: The Schematic Representation Of A 4.6 Tonne Brass-Board Hybrid System
4.7.2.3 SPFC System

Four Ballard MK-5 stacks were procured based upon criteria of delivery time, fuel cell performance and cost. Each stack was rated 5 kWₑ on pure H₂ and air, which would give the gross power from the stacks of 20 kWₑ. For operation on reformate (75%H₂, 25% CO₂) the total stack power was measured to be 16-17 kWₑ with 2% air bleed. Each stack had 36 cells and a maximum current of 200 A. Each cell had an active area of 250 cm² and hence maximum current density of 0.8 A/cm². The operating pressure and temperature of the stack was 3 bar(a) and 75-80°C respectively.

The fuel cell system was constructed by ECN and it consisted of all the hardware for system controls, heat management, air compression and water management. The four stacks were arranged electrically in series. The water in the anode and cathode exhaust gases was condensed and recycled while the gases were expelled into the atmosphere via the pressure regulator valves. Upon integration with a steam reformer, these gases would be fed into the burner. The maximum heat transfer capacity of the heat exchanger for the fuel cell cooling system was 30 kW at cooling water flowrate of 40 l/min.

4.7.2.4 Air Compressor

The air compressor was responsible for supplying compressed air to the fuel cell stack at a pressure of 3 bar(a). The air has to be clean, oil-free and the temperature of the compressed air should not exceed 80°C. The maximum flowrate of the compressor was determined to be 1250 l/min under normal conditions (273 K and 1 bar). An air compressor meeting these specifications was not available in the commercial market and therefore modifications were necessary to adapt a standard compressor for the application.

The compressor selected by ECN for the brass-board system was a water injected screw compressor. Water was used both for lubrication and cooling. The compressed oil free air delivered by the compressor was cooled to the 80°C. A water injected
screw compressor which was designed for a delivery pressure of 8-10 bars(a) was modified to supply air at 3 bar(a). The compressor power (parasitic power loss) was determined to be 5 kW at maximum SPFC stack power (16 kWe) which accounted for the shaft power inefficiency of the motor and pressure losses. A turbo-charger for energy recovery from the exhaust gases was also investigated but no efficient turbo-charger was found for this size of system.

4.7.2.5 Up-Chopper (DC/DC Converter)

The up-chopper was developed by HOLEC and was used to convert 20 kW_e from the fuel cell stack to the DC-link voltage of system. The up-chopper was DC current controlled and was designed to accept maximum input current of 250 A. The current of the up-chopper was in turn controlled in relation with the gas flows through the power generator. Analysis of the up-chopper indicated that the losses should reach a maximum of approx. 1 kW when operating at full power.

4.7.2.6 Battery Pack

Batteries were used on the brass-board system as both as energy buffer and main power supply for electric traction. The Battery pack was selected and tested by TNO. In order to select and purchase an optimum battery pack, a number of traction battery performance specifications were studied both by TNO and Loughborough University. The brass-board vehicle simulation programme (section 4.7.3), developed by Loughborough University, was used to simulate acceleration, speed and range tests for the brass-board hybrid van with the different battery packs. From this study it was concluded that the chosen battery pack should not only exhibit both a high specific power (W/kg) and energy density (Wh/kg), it should also fulfil the following the technical criteria [20]:

- Continuous discharge power (½ hr): 30 kW
- Peak discharge power (20% SoC, 30 sec): 45 kW
- Energy capacity (½ hr rate): 15 kWh
After considering the battery pack weight, cost, maintenance level (sealed & unsealed battery), the delivery time of a complete system and the requirements of other brass-board components, Daug-Hoppecke nickel-cadmium (Ni-Cd) battery type FNC H100 (100 Ah) were selected for the application. The battery pack consisted of 180 cells in series with nominal voltage of 216 Volts. The energy capacity of the battery pack was determined to be 15 kWh (2C rate) and the maximum discharge and charge power was 55 kW (peak, <30 sec) and 15 kW (continuous) respectively. The battery pack had a mass of 500 kg. The Daug-Hoppecke H100 battery system also included controller, temperature management, inner trays and charger.

Subsequent to testing of 60 FNC H100 batteries, the following conclusions were made:

- The specifications for a peak discharge power of 15 kW at 20% SoC, 13.5 kW for continuous power (2.5 C at 0.9 V/cell) and maximum peak power of 18.9 kW (3.5C at 0.9 V/cell) were proved.
- During a repeated acceleration test, the battery could meet the power requirement and the temperature rise was below the tolerated 43°C (maintained to ≤ 29°C).
- The battery also met the range test, which was to drive with 100 kph (km/hr) for 26 minutes. The SoC of the battery pack was 32% and the temperature rise below the tolerated 43°C after the test.
- The battery system was able to meet the most demanding part of the Leicester urban drive cycle (section 4.7.5) and the temperature of the battery remained within the specified range during a drive cycle of nearly 8 hours.

In summary, the battery pack fulfilled the requirements of the brass-board system and in a number of tests, the performance specifications were exceeded.

4.7.2.7 Electric Motor

The electric drive motor was provided under contract by Magnetic Systems Technologies (MST). The motor was a brushless dc type, which was torque controlled to provide the driver with the same sensation of acceleration as with a normal ICE
vehicle. The motor provided a continuous power rating of 60 kW, with a base torque of 150 Nm and a maximum speed of ≈12000 RPM. An efficiency of >90% was achieved at the best operating condition. Furthermore, the motor was capable of recovering energy through regenerative braking. The mass and volume of the motor and controller were approx. 70 kg and 0.1 m³ respectively.

4.7.2.8 Vehicle Controller

The vehicle controller consisted of supervisory control unit in conjunction with the control strategy of the brass board system.

4.7.2.8.1 Supervisory Control Unit (SCU)

The supervisory control unit, which was located in a centralised computer, interacted with local subsystems controller via a CAN-network. The SCU was responsible for operating the energy management system and the safety measures of the brass-board system, by providing the local controllers with the set points. The data acquisition system (DAS) was also integrated into the central computer and was responsible for collecting and logging the most important parameters of the system.

4.7.2.8.2 Control Strategy

The control strategy was implemented in the SCU and consisted of energy management, drive control and system monitoring processes.

- The objective of the energy management process was to achieve control of the systems operating procedures, powering up and down sequences and setting the generator to full or standby power depending upon system conditions. The strategy was to operate the generator, either on full or standby power (depending on the state of charge (SoC) of the battery) and use the generator more or less as a battery charger. This was due to the fuel reformer response times (≈ 60 sec). Within the energy management, processes also included mechanisms to protect
additional subsystems from damage by imposing limits on power or current drawn and/or delivered to a subsystem.

- Drive control calculates torque set points for acceleration and braking by considering driver torque requests, and power limitations imposed by the energy management.

- System monitoring process monitors system behaviour and produces event messages, which are sent to the DAS. If a serious error was detected then the system monitoring process would initiate a system shut-down event.

4.7.3 Brass-Board System model and Simulation

A brass-board simulation programme was developed by Loughborough University to model each component of the Brass-Board system using measured data (where available) in order to [41]:

- Determine the component sizes to fulfil the performance specification of the van, which were:
  - The van should accelerate from rest to 60 km/hr (kph) in no greater than 17 seconds.
  - The van should maintain its maximum cruising speed (100kph) for between 20 and 30 minutes. This was equivalent to a range of between 33.3 km and 50 km at this maximum speed.

- To predict the performance of the Brass-Board hybrid van and its components on various drive schedules. The predicted performance was then compared to the actual brass-board system (without the fuel processor) performance, on the various drive schedules. (The electrical testing of the actual brass-board system used the calculated speed from simulation as the input to the system).
The working of the simulation program was based on the "backward calculation method" whereby the simulation program determined the amount of energy required per second for predefined drive schedule. The simulation program was written in Turbo Pascal for Windows and used Windows as its user interface. The next part of this section summarises the modelling of each subsystem and the relevant measured data used in the models.

4.7.3.1 Vehicle Model

The Mercedes 410D panel van was chosen to be the brass-board model vehicle. The van has GVW (Gross Vehicle Weight) of 4.6 tonnes. Coastdowns tests were performed on this van to estimate the aerodynamic characteristic [42]. The drag coefficients were calculated from the coastdowns analysis to be \( A_d = 0.008 \) and \( C_d = 0.59 \). However, the value for \( C_d \) coefficient was chosen to be 0.4 in order to reflect the aerodynamic shape of a future vehicle. The following van characteristics were specified for the brass-board vehicle model:

\[
\begin{align*}
A_d &= 0.008 \\
B_d &= 0.000 \text{ (to reflect the future vehicle)} \\
C_d &= 0.400 \text{ (to reflect the future vehicle)} \\
\text{Frontal Area} &= 4.2 \text{ m}^2 \\
\text{Wheel Radius} &= 0.315 \text{ m} \\
\text{Fixed Vehicle Structure Mass (GVW)} &= 4600.00 \text{ kg}
\end{align*}
\]

The brass-board vehicle was simulated with three of the five gearbox ratios supplied with Mercedes 410D panel van, these ratios were:

- First: 25.31
- Second: 12.94
- Third: 7.16
The gearbox model was used to find a suitable gear so as to operate the motor in an efficient area. The gearshift time was taken as 1 second. The transmission efficiency for the vehicle was taken to be a constant percentage loss of 10%. The gears were changed according to the speed (RPM) of the motor and was done as following

\[
IF \quad (Motor \ Speed > 11455) \quad THEN \quad (Change \ to \ Higher \ gear) \\
IF \quad (Motor \ Speed < 2000) \quad THEN \quad (Change \ to \ Lower \ gear)
\]

These vehicle and transmission characteristics were used in the transmission model to calculate the motor speed and the motor torque.

### 4.7.3.2 Motor Model

The motor model used the motor speed and torque from the vehicle system to calculates the motor mechanical power. The motor mechanical power and the motor efficiency are then used in the motor controller model to calculate the motor loss power and motor electrical power. Motor efficiency was obtained from a two dimension look up table by linear interpolation. Figure 4.11 shows the predicted efficiencies for the MST 60kW Brushless DC Motor and inverter.

### 4.7.3.3 Battery Model

The battery model which included the battery charging model was based upon the traction battery model shown in figure 4.12 [43]. Battery characteristics such as cell voltage, charge and discharge resistances were obtained from the manufacturing data by interpolation of the charge and discharge characteristics at constant current, for a range of capacity values. The resistance and voltage values are obtained from these characteristics and stored as function of state of charge. (The resistance and voltage values as function of temperature were not calculated, as data for this was not available). Table 4.12 shows these values as a function of SoC (%) for a Ni-Cd FNC H100 battery pack with 180 cells and a de-rated capacity of 85 Ah (15% de-rated to provide a acceptable life).
Figure 4.11: Predicted Efficiencies for MST 60 kW Brushless DC Motor and Inverter
Figure 4.12: The traction battery model

Table 4.12: Ni-Cd FNC H100 Data for the Battery model

<table>
<thead>
<tr>
<th>SoC (%)</th>
<th>Cell Voltage (Volts)</th>
<th>Charge Resistance (mΩ)</th>
<th>Discharge Resistance (mΩ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0%</td>
<td>0.88</td>
<td>3.85</td>
<td>3.85</td>
</tr>
<tr>
<td>10%</td>
<td>1.20</td>
<td>3.38</td>
<td>3.38</td>
</tr>
<tr>
<td>20%</td>
<td>1.22</td>
<td>1.53</td>
<td>1.53</td>
</tr>
<tr>
<td>30%</td>
<td>1.22</td>
<td>1.33</td>
<td>1.33</td>
</tr>
<tr>
<td>40%</td>
<td>1.22</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>50%</td>
<td>1.23</td>
<td>0.86</td>
<td>0.86</td>
</tr>
<tr>
<td>60%</td>
<td>1.24</td>
<td>0.83</td>
<td>0.83</td>
</tr>
<tr>
<td>70%</td>
<td>1.25</td>
<td>0.77</td>
<td>0.77</td>
</tr>
<tr>
<td>80%</td>
<td>1.27</td>
<td>0.73</td>
<td>0.73</td>
</tr>
<tr>
<td>90%</td>
<td>1.28</td>
<td>0.67</td>
<td>0.67</td>
</tr>
<tr>
<td>100%</td>
<td>1.36</td>
<td>0.54</td>
<td>0.54</td>
</tr>
</tbody>
</table>

Side Voltage (volts)  
1.72

Side Resistance (mΩ)  
5
4.7.3.4 Ancillary Model

The ancillary model accounts for supply of power to low power systems and the parasitic load. The low power system was set to a value of 1.35 kW, this accounted for a climatic control power of 1 kW and ancillary power of 0.35 kW. The parasitic load accounts for the power supply to the air compressor system. The parasitic power supply was modelled as function of the fuel cell power. From preliminary data available for the air compressor system, the parasitic load was modelled as 20% of the fuel cell power, with a maximum parasitic load of 3.24 kW at maximum SPFC stack power (16 kW_e). However, from experimental evaluation of the compressor, the maximum parasitic load was measured to be 5 kW (31.25% of maximum SPFC Stack power). The ancillary model was subsequently modified and the various brass-board tests were repeated (section 4.7.4).

4.7.3.5 Vehicle controller Model

The vehicle controller model managed the power flow between different sub-systems and arrested the simulation if the power supply from either the fuel cell or the battery was less then power demanded by the motor, ancillary and the battery models. The charge power was calculated from the current required to maintain the batteries fully charged (99% SoC). If the power demanded was negative i.e. the motor was regenerating power then the excess power was used in charging the battery. The vehicle controller model also set the operating point of the power generator according to the control strategy set for the brass-board system. The control strategy of the brass-board was to avoid the fuel cell from rapidly fluctuating between the maximum and minimum value, and use the power generator as battery charger. The control strategy was implemented on the simulation program as following:

IF SoC > 90% THEN GENERATOR SET POINT= 4kW (Standby Power)
IF SoC < 70% THEN GENERATOR SET POINT= 16kW (Full Power)
4.7.3.6 Power Generator Model

The generator model consisted of the Up-Chopper, SPFC model, GCU and methanol steam reformer models.

4.7.3.6.1 Up-Chopper Model

The up-chopper model was based on data provided by HOLEC. The maximum up-chopper power loss was approximately 0.8 kW at maximum SPFC stack power. The up-chopper power consumption data was modelled as a function of up-chopper power output (%) in a look up table.

4.7.3.6.2 SPFC Stack Model

The four Ballard fuel cell stacks utilised, produced 20 kW electrical power when using hydrogen and air. However, on reformate, the fuel cell stacks produced 16 kW. In the fuel cell model, the fuel cell stacks were designed to operate at 80°C, 3 bar and produce 16 kW maximum. The stacks had 144 cells and an area of 250 cm². Generic fuel cell data was used before the actual measured data of the SPFC stack became available. The actual measured polarisation curve was implementing as a lookup table. At maximum stack power, the operating cell voltage and current density of each cell were 0.62 volts and 0.717 A/cm² respectively. The SPFC stack model was designed to follow the capability of the methanol reformer since the dynamic of the fuel processor was slower than the stack. The fuel cell stack model responded to change in power demand in 60 (step up in power demanded) and 15 (step down in power demand) seconds respectively. The corresponding reformer step up and step down time constants were 15 and 3 seconds respectively.

4.7.3.6.3 Methanol Reformer and GCU Model

Since the actual data for the reformer was not available, the reformer model used a constant methanol to hydrogen conversion rate of 5.333 (mass ratio) and reformer
efficiency of 84.5% (HHV). This ratio and efficiency were used to calculate the amount of methanol that was required to fulfil the hydrogen demand by the SPFC stack. It was also assumed that the reformer produced an exit gas composition of 74% H₂, 24% CO₂, and 1% CO. The 1% CO in the reformed gas was further reduced to less than 20 ppm in the GCU, prior to feeding into the fuel cell. The maximum amount of the methanol, which could be stored on the brass-board van, was 56kg. The size of the fuel tank was based on the existing Mercedes 410D tank.

4.7.4 Brass-Board Test Programme

The aim of the test programme was to assess the brass-board system integration of the SPFC stack (power generator), up-chopper, battery pack and electrical motor/inverter and to check whether the brass broad system could fulfil the performance specification of the van stated in 4.7.3. These brass-board performance specifications were translated in the test programme. The test programme consisted of the following duty cycles:

- Functionality test
- Constant speed test
- Acceleration test
- Deceleration test
- ECE 1504 drive cycle test
- Leicester drive cycle test
- New drive cycle test

The simulation programme was used to calculate the vehicle speed for these duty cycles and the vehicle speed for each cycle were used as the input to the actual brass-board system. The objective, duration and characteristic of these drive cycle tests will be stated with the results, from both the simulation programme and the actual brass-board system test under these drive cycles in the result and discussion section (4.7.5).
4.7.5 Results and Discussion

The simulation program was used to predict the performance of the brass-board system and its component behaviour under seven drive cycle tests (4.7.4). The vehicle speed-time profile of each test from the simulation results was used as the input load signal to the actual integrated brass-board system (minus the fuel processor).

The models in the simulation program were modified to adapt to change in the performance data (section 4.7.3) of some of components after the actual results of the seven drive cycle tests were compared with initial simulation results. The two significant changes were made to the simulation program before re-simulating the seven drive cycle tests. These were:

- The compressor model was changed so that the compressor power demand was 5 kW at maximum SPFC stack power (31.25% of max. SPFC stack power).

- An actual polarisation curve was used in the SPFC model, such that the correct voltage and current were used at maximum SPFC stack power. In addition, the dynamic model was modified so that SPFC model followed the compressor capability (8-10 minutes) rather than the capability of the reformer (1 minute).

In this section, the results from both the simulation program and actual brass-board system of the seven drive cycle tests are presented, compared and discussed.
4.7.5.1 Functionality Test

The functionality test checks the correct functioning of the brass board system, by switching the generator on and off several times.

Objectives: To gain confidence in the control of the system and in energy flow through the system.

Characteristics: The test applies a constant mechanical output load of 5 kW on the generator and the test starts with 90% SoC of battery and generator on standby power.

Duration: One cycle (i.e. the SoC goes from 90% to 70% and back to 90%) took 112 minutes (1.87 hours), and this cycle was repeated until the functionality was proven or for a maximum of 8 hours.

4.7.5.1.1 Functionality test results

The functionality test results are shown in figures 4.13 and 4.14. From these figures, it can be observed that the measured and calculated results correlated very well. The compressor power and the response time of the fuel cell were increased and hence the charging current of the battery was decreased from 15 to 6 Amps. This decrease in the charging rate of the battery and increased the duration of the functionality test to ≈ 3 hours for one cycle (i.e. the SoC goes from 90% to 70% and back to 90%).
Figure 4.13: Measured and calculated results for the Functionality test
(Motor electrical, Battery, SPFC stack & Compressor powers)
Figure 4.14: Measured and calculated results for the Functionality test

(SoC, Battery current & voltage, Generator (SPFC stack) current & voltage)
4.7.5.2 Constant Speed Test

Objective: To verify the capability of the brass board vehicle to maintain cruising speed of 100 kph for 20 minutes.

Characteristics: The vehicle was accelerated to 100 kph in 2 minutes and this speed was maintained for 20 minutes. The test starts with 100% SoC of the battery and generator on standby power. This produces a continuous power output sufficient for driving 100 kph for 20 minutes. After 20 minutes the vehicle decelerates to a halt in 2 minutes. Then the batteries are charged to 90% SoC. This cycle was repeated twice. (100%- 90%-90%).

Duration: The test took 4.35 hours (15655 seconds) to complete two cycles.

4.7.5.2.1 The constant speed test results

The constant speed test results are shown in figures 4.15 and 4.16. The main difference between the actual brass-board system results and simulation results was that the constant speed test on the brass-board system could not be completed. This was due to the battery temperature increasing beyond its maximum operating limit of 43°C during the acceleration part of the constant speed (100 kph in 2 minutes). To protect the battery from over heating, the control strategy reverted the SPFC stack to standby power i.e. 4 kWₑ. Therefore, the battery did not recharge back to 90% SoC for the second cycle of the constant speed to begin. Although the actual brass-board system could not comply with the constant speed test due to the limitations imposed by the battery thermal management, it can be concluded that the control system and control strategy were implemented correctly and functioned to protect the components of the system.
Since the battery thermal model was not included in the simulation program, the constant speed test in the simulation program was completed. The results from the simulation programme for the first part of the constant speed (approx. the first hour) correlated very well with the measured results. The total duration of the constant speed test was about 4 hours, which involved three cycles (SoC- 100%-90%-90%) and charging the battery back to 90% Soc.

### 4.7.5.3 Acceleration Test

**Objective:**
To verify the capability of brass board vehicle to accelerate from 0 to 60 kph within 17 seconds.

**Characteristics:**
The test produces maximum power output during the acceleration of the vehicle from 0 to 60 kph. The test starts with 100% SoC of the battery and generator (SPFC stack) on standby power. The acceleration of the vehicle was repeated every 2 minutes until the battery SoC was ≤ 70% and generator at full power.

**Duration:**
The test took 53 minutes (3180 seconds) to complete and included 25 accelerations before the battery SoC was ≤ 70% and generator at full power.
Figure 4.15: Measured and calculated results for the Constant Speed test

(Motor electrical, Battery, SPFC stack & Compressor powers)
Figure 4.16: Measured and calculated results for the Constant Speed test
(SoC, Battery current & voltage, Generator (SPFC stack) current & voltage)
4.7.5.3.1 The acceleration test results

The acceleration test results are shown in figures 4.17 and 4.18. From these figures, it can be observed that the measured and calculated results correlated very well. However, in the actual brass-board system the acceleration test terminated before the SoC was \( \leq 70\% \). This was due to the actual system was using the calculated vehicle speed (of initial simulation results) as input and hence, the acceleration test terminated when the simulated test finished. The duration of the acceleration test (with modified models and data) was increased to 58 minutes and included 27 accelerations before SoC of the battery attained 70\%. The generator power changes from standby power to full power towards the end of the test. A similar observation would have been noted if the acceleration test on the actual brass-board system was run for further 6-8 minutes (figure 4.17).

4.7.5.4 Deceleration Test

Objective: To verify the regenerative braking capability

Characteristics: This test verified energy management with regenerative braking. The test starts with 90\% SoC of the battery and the generator on standby power. The vehicle was accelerated to 60 kph in 60 seconds and then decelerated to a halt in 60 seconds to use 1/3 of the maximum regenerative braking capacity. After 2 minutes the vehicle was again accelerated to 60 kph in 60 seconds and decelerated to a halt in 40 seconds to use 2/3 of the maximum regenerative braking capacity. After 2 minutes the vehicle was again accelerated to 60 kph in 60 seconds and decelerated to a halt in 20 seconds to use the maximum regenerative braking capacity.

Duration: The test took 9 minutes (540 seconds) to complete.
Figure 4.17: Measured and calculated results for the Acceleration test
(Motor electrical, Battery, SPFC stack & Compressor powers)
Figure 4.18: Measured and calculated results for the Acceleration test
(SoC, Battery current & voltage, Generator (SPFC stack) current & voltage)
4.7.5.4.1 The deceleration test results

The results of the deceleration test are shown in figures 4.19 and 4.20. From these figures, it can be observed that the measured and calculated results correlated very well. However, in the actual brass-board system, the generator power (SPFC stack) fluctuated between the standby power of 4 kW and 0 kW at certain periods during the test. This was due to an error in the generator control program, which was responsible for the stack power management. The duration of the deceleration test remained the same (9 minutes to complete).

4.7.5.5 ECE 1504 Drive Cycle Test

Objective: To test the vehicle first on this friendly drive cycle for its standardised driving characteristic.

Characteristics: The test started with 90% SoC of the battery and generator on standby power. The drive cycle was repeated until the battery were charged back to 90% SoC and the generator on standby power.

Duration: The test took 2 hours and 17 mins (8222 seconds) to complete.

4.7.5.5.1 The ECE 1504 drive cycle test results

The results of ECE 1504 drive cycle test are shown in figures 4.21 and 4.22. The test was successfully completed with the brass-board system and the calculated results correlated very well with the measured results. The duration of the ECE 1504 drive cycle test was calculated to be 2 hours and 15 minutes.
Figure 4.19: Measured and calculated results for the deceleration test
(Motor electrical, Battery, SPFC stack & Compressor powers)
Figure 4.20: Measured and calculated results for the deceleration test

(SoC, Battery current & voltage, Generator (SPFC stack) current & voltage)
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Figure 4.21: Measured and calculated results for the ECE 1504 drive cycle test

(Motor electrical, Battery, SPFC stack & Compressor powers)
Figure 4.22: Measured and calculated results for the ECE 1504 drive cycle test

(SoC, Battery current & voltage, Generator (SPFC stack) current & voltage)
4.7.5.6 Leicester (UK) Drive Cycle Test

The Leicester drive cycle was recorded around Leicester City centre using the Mercedes 410D panel van. The average speed of the cycle was 19.14 kph and 3656 seconds (approx. 1 hr) long.

Objective: To verify the capability of the vehicle to drive on actual measured drive cycle.

Characteristics: The test started with 90% SoC of the battery and generator on standby power. The drive cycle was repeated until the battery are charged back to 90% SoC and the generator on standby power.

Duration: The test took 2.26 hours (8152 seconds) to complete, that was approximately 2 drive cycles.

4.7.5.6.1 The Leicester (UK) drive cycle test results

The Leicester drive cycle test was the most demanding cycle for the brass-board system, due to the many acceleration and deceleration peaks. The results of Leicester drive cycle test are shown in figures 4.23 and 4.24. From these figures, it can be observed that the Leicester drive cycle test was not successfully completed with actual brass-board system. However, the system functioned without problems during the first hour in which the SoC dropped from 90% to 70% and the measured results correlated very well with the calculated results. The high battery voltage, attained in the actual brass-board system, terminated the test. In the simulation, the test was completed since the high current and voltage was not reached. The duration of the Leicester drive cycle was calculated to be 2 hours and 20 minutes.
Figure 4.23: Measured and calculated results for the Leicester drive cycle test
(Motor electrical, Battery, SPFC stack & Compressor powers)
Figure 4.24: Measured and calculated results for the Leicester drive cycle test

(SoC, Battery current & voltage, Generator (SPFC stack) current & voltage)
4.7.5.7 New Drive cycle Test

The new drive cycle was derived from both the London and Leicester drive cycles. The cycle was made of two main parts. The London drive cycle recorded within the city centre while delivering Royal Post Office parcels with a van with GVW of 4.6 T. Since the London drive cycle included many stops, it did not demonstrate the hybrid character of the system. This was due to the total distance driven and the associated energy consumption being too low to make efficient use of the on board charger. Therefore, it was decided to create a new drive cycle, which would include parts of both the London and Leicester (without any stops) drive cycles. The drive cycle was made up of ABBBA formation, where part A was from the London drive cycle and Part B was from Leicester drive cycle. Figure 4.25 shows the configuration of the new drive cycle and its parameters. The statistical analysis of the drive cycle showed that the new drive cycle was an average cycle of both the London and Leicester drive cycle and the length of the new drive cycle was 1.82 hours.

Figure 4.25: Configuration and parameters of the New drive cycle.

<table>
<thead>
<tr>
<th>Drive Cycle Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Time - 1.82 hours i.e. 6535 seconds</td>
</tr>
<tr>
<td>(2 * PART A &amp; 3 * PART B) = (ABBBA)</td>
</tr>
<tr>
<td>Delivery stopping time - 1351 Seconds</td>
</tr>
<tr>
<td>Traffic Stopping time - 1111 Seconds</td>
</tr>
<tr>
<td>No. of Stops - 6 delivery + 40 traffic = 46</td>
</tr>
<tr>
<td>No. of Stops per km - 1.32</td>
</tr>
<tr>
<td>% Stopping time - 37.67 %</td>
</tr>
<tr>
<td>Driving time - 4073 Seconds (v&gt;1.0)</td>
</tr>
<tr>
<td>Average Driving Speed - 30.76 kph</td>
</tr>
<tr>
<td>Average Speed - 19.21 kph</td>
</tr>
<tr>
<td>Distance - 34.8 km</td>
</tr>
</tbody>
</table>
Objective: To verify the capability of the vehicle to drive on actual measured drive cycle.

Characteristics: The test started with 90% SoC and generator on standby power. The drive cycle was repeated until the battery pack was charged back to 90% SoC and the generator on standby power.

Duration: The test took 3.75 hours (13504 seconds) to complete.

5.6.5.7.1 The new drive cycle test results

The results of new drive cycle test are shown in figures 4.26 and 4.27. The new drive cycle test was successfully completed with the actual brass-board system. The test on the simulation test took similar time (2.13 hrs) as the actual brass-board system to completed and the measured and calculated results correlated well.
Figure 4.26: Measured and calculated results for the New drive cycle test
(Motor electrical, Battery, SPFC stack & Compressor powers)
Figure 4.27: Measured and calculated results for the New drive cycle test

(SoC, Battery current & voltage, Generator (SPFC stack) current & voltage)
4.7.6 SUMMARY OF RESULTS

1. Each component of the system was modelled and their performance data were specified. The following configuration for the Brass-board hybrid van was used in the simulation program to perform the seven drive cycle tests:

**Vehicle:-**
- Mass = 4600 kg
- Ad = 0.008
- Bd = 0.00
- Cd = 0.4
- Frontal Area = 4.2 m\(^2\)
- Wheel Radius = 0.3 m
- Transmission Efficiency = 90%

**Motor:-**
- Type: MST 60kW Brushless DC Motor
- Max. Torque = 150 Nm
- Max. Speed = 11459 rpm
- Efficiency = Data array for Efficiency Map

**SPFC Stack:-**
- Max. Power = 16 kW\(_e\)
- Cell Voltage at Max. Power = 0.850 V/Cell @ 0.712 A/cm\(^2\)
- Active area = 250 cm\(^2\)
- Number of cells = 144 (4 stacks @ 36 cells)

**Methanol Reformer:-**
- Constant methanol to hydrogen conversion rate = 5.333 (mass ratio)
- Reformer efficiency = 84.5% (HHV)

2. All tests except the constant speed and Leicester drive cycle tests, were successfully completed with the actual brass-board system. The constant speed on the actual brass-board system was not completed due to battery overheating (>43°C). The Leicester drive cycle was prematurely terminated because the
supervisory control unit (SCU) had failed to react when some parameters reached their maximum values (battery temperature and voltage).

3. Table 4.13 shows the comparison of the duration of the seven tests after there were re-simulated with changes made to the models in the simulation program. The difference in the duration between the simulated and measured results was due to decrease in the charging rate of the battery due to higher compressor power and longer respond time of the stack power.

Table 4.13: Comparison of the duration of the seven brass-board system tests

<table>
<thead>
<tr>
<th>Type of test</th>
<th>Duration of the Brass-Board System Simulation Programme</th>
<th>Duration of the Actual Brass-board System</th>
</tr>
</thead>
<tbody>
<tr>
<td>Functionality</td>
<td>3 hrs (SoC 90%-70%-90%)</td>
<td>2 hrs 45 mins (SoC 90%-70%-80%)</td>
</tr>
<tr>
<td>Constant Speed</td>
<td>6 hrs (Completed)</td>
<td>1 hrs 30 mins (Incomplete)</td>
</tr>
<tr>
<td>Acceleration</td>
<td>58 mins (27 accelerations)</td>
<td>53 mins (25 accelerations)</td>
</tr>
<tr>
<td>Deceleration</td>
<td>9 mins (Completed)</td>
<td>9 mins (Completed)</td>
</tr>
<tr>
<td>ECE 1504 drive cycle</td>
<td>2 hrs 15 mins (Completed)</td>
<td>2 hrs 16 mins (Completed)</td>
</tr>
<tr>
<td>Leicester drive cycle</td>
<td>2 hrs 3 mins (Completed)</td>
<td>2 hrs 1 mins (Incomplete)</td>
</tr>
<tr>
<td>New drive cycle</td>
<td>2 hrs 10 mins (Completed)</td>
<td>2 hrs 13 mins (Completed)</td>
</tr>
</tbody>
</table>

4. The results for the seven drive cycle tests from the simulation tool correlated to within 2-3% compared to results from actual brass-board integration of a methanol reformer/SPFC/battery/electric motor system for the hybrid van.
4.7.7 RECOMMENDATIONS

The following recommendations were suggested:

- Improve the battery model by including the thermal characteristic of the battery pack and also include the temperature, voltage and current limits in the vehicle controller.

- Improve the compressor model by including the actual compressor operating characteristics i.e. efficiency, pressure ratio, temperature, pressure drop and dynamics.

- Improve the fuel processor model with either actual measured results or theoretical thermodynamic data for both reformer and GCU unit.

- Repeat the seven tests on the actual brass-board system with new results from the simulation program, since calculated results vehicle speed was used as the input via the load unit.

- Repeat the tests with a motor coupled to the system, rather than using the load unit to simulate the motor and vehicle input.

- Finally, analyse the system performance and losses by carrying out an energy efficiency study under certain duty cycle.
4.8 REFERENCES

20. A. Brunia et al., 27th ISATA, 94ELO42, 1994, Germany, pages 183-188.
5. INDIRECT DIESEL SPFC SYSTEM FOR MARINE APPLICATION

5.1 INTRODUCTION

Interest in using the fuel cell technology in marine applications was initiated in the 1960's. A major driving force behind the interest was the defence industry searching for a clean and silent power source to replace gasoline or diesel driven auxiliary power sources. For marine application in the defence industry, the SPFC offered the advantages of not only high efficiency, but also low detectability (i.e. low noise and thermal signal) and modular flexibility. Thus, the SPFC was attractive for both use as the main propulsion power source and also as an auxiliary power source [1,2,3]. The use of SPFC systems for marine vehicle applications ranges from supplying emergency power and generating electricity in environmentally friendly harbours through to powering an all-electric surface or sub-surface marine vehicles (naval & military applications).

For naval and military ship applications, the small thermal and acoustic signatures of the SPFC system helps in the low detectability while for a merchant ship or ferry applications the low noise levels aid in precision measurement and residential comfort. It is reported that the noise level are reduced by over 30 dB (A) in the engine room and 15 dB (A) in the cabins when diesel engines (110 dB (A) & 65 dB (A)) are replaced by fuel cell system [4]. The modular characteristics of the SPFC system offer design flexibility of the entire propulsion system, which would lead to decrease in ship volume and size [4,5]. Additional advantages of fuel cell technology over diesel engines or gas turbines for marine vehicles include reduction in fuel consumption of around 25-30% [5] and reduced pollutants in the exhaust gases discharged into the atmosphere [4].

At present the application of SPFC system for merchant or surface ships has primarily been in the feasibility studies or at the demonstration stage. This is due to high cost of the system and unavailability of an established SPFC system including a suitable hydrocarbon on board fuel processor [6]. Conversely, a pure hydrogen and air SPFC
system has been employed on board boats to demonstrate the SPFC technology. In 1998, a boat in Italy was modified to take hybrid propulsion system with a 40 kW\textsubscript{e} SPFC system, liquid hydrogen storage and a 100 Ah lead acid battery. The boat had a capacity for carrying 90 passengers and a range of 300 km [6]. As a project for Expo 2000, an excursion boat was also fitted with a 10 kW\textsubscript{e} SPFC propulsion system with two metal hybrid hydrogen storage tanks with total hydrogen capacity of 54 m\textsuperscript{3} at standard condition [6].

For naval surface ships, many feasibility studies have been performed to evaluate the use of SPFC system as either replacement for the conventional diesel power generator or integrated electric energy production and distribution system for propulsion, sensors, weapons and general ship's network (All-electric-ship (AES) concept) [6]. In U.K., the Defence Evaluation and Research Agency (DERA) were evaluating the use of SPFC to provide electric power of about 1-2 MW for ship's network during harbour and anchored operation [6,7]. This evaluation study has also led to building an AES research vessel. In the USA, a three phase program by the Office of Naval Research aims to demonstrate that commercially developed fuel cell technologies can be operated in naval sphere using naval fuels [6].

The interest of use of SPFC system for air independent propulsion (AIP) in submarines was initiated in early 1980's, when Siemens began to develop a 34 kW\textsubscript{e} SPFC module for the German Ministry of Defences [8,9]. The Siemens's AIP system has been developed and integrated into both class 212 and 214 submarines by the German ship company HDW. The AIP system developed for the class 212 submarine consisted of nine Siemens SPFC modules (35-50 kW\textsubscript{e}), a metal hydride storage system for hydrogen and liquid oxygen tanks [6].

For fuel cell technology to be successfully integrated on board a surface marine vessel, the technology should use conventional fuels and the existing fuel storage infrastructure both on board the vessel and in the worldwide ports. The most widely used and acceptable fuel in both commercial and defence marine vessels is diesel. Diesel is available in most international ports and exists in most Navy fuels inventory [2]. However, diesel has to be processed and reformed to produce the H\textsubscript{2} for SPFC system. The naval diesel fuel contains a sulphur concentration up to about 1%. Both
conventional reforming catalysts and the electrocatalysts used in the SPFC are extremely sensitive to sulphur and therefore a sulphur desulphurisation is necessary [10]. The diesel reformation process includes partial oxidation or steam reforming or autothermal reforming to produce hydrogen rich gas which is further processed to minimise CO and sulphur contaminants before being used as fuel for the fuel cell system.

Although at present the SPFC system using hydrogen and oxygen has been demonstrated, integrated and implemented on board submarines, the SPFC systems with diesel fuel processors for marine application currently remain in the research and development phase. Many diesel fuel processors are currently being developed and the research in the laboratory is focused on optimising the reactors size, weight and performance. The SPFC systems with diesel fuel processor are also in the design phase and the performance of these systems are being evaluated using either steady state models or dynamic simulations.

In this chapter a SPFC hybrid system with a diesel fuel processor and battery pack was analysed as an auxiliary power source for the ship hotel load. A dynamic simulation of the SPFC hybrid system was developed using Matlab/Simulink to study the component interactions between a 1.5 MW SPFC system, diesel fuel processor and 8448 kWh (C5 rate) battery pack. The performance of the hybrid system was analysed using the hotel load duty cycle. Figure 5.1 shows the schematic representation of a SPFC hybrid system as an auxiliary power source for a marine application. A steady state model was also developed at peak fuel cell stack power to determine the overall system performance of an integrated system. However, in this study the aim was not to optimise the system performance by thermal integration with the use of network of heat exchangers.
Figure 5.1: Schematic representation of a SPFC hybrid system for a marine application (without thermal integration)
5.2 SPFC SYSTEM SPECIFICATION (FOR MARINE APPLICATION)

Similar to the SPFC system designed for a transportation application, the system for the marine application consists of mainly of two main parts, i.e. the power generator and the electric drivetrain (figure 5.1). The power generator includes a fuel processor (diesel partial oxidation reactor, HTS reactor, LTS reactor and a gas clean-up unit), a SPFC system, a compressor, a burner, an expander and network of heat exchangers. The electric drivetrain includes DC/DC converter, battery pack and the system load. In this section, the data and the operating conditions of each component of the system are specified and how they are implemented in the dynamic simulation program and used in the system analysis.

5.2.1 Diesel Fuel Processor

The on board vehicle fuel processor incorporates a diesel partial oxidation, HTS, LTS reactors and a gas clean-up unit (CO preferential oxidation reactor).

5.2.1.1 Diesel Thermal Partial Oxidation (PoX) Reactor

The complete oxidation or combustion of hydrocarbons produces CO$_2$ and H$_2$O. The partial oxidation process avoids the complete combustion of the reactants by limiting the supply of oxygen (in air) and the products are CO and H$_2$. However, in practical applications the partial oxidation process can not avoid the conversion of a certain percentage of reactants and/or products to complete combustion products. Usually, the partial oxidation process is carried out without the presence of a catalyst. However, it should be noted that recently catalytic partial oxidation reactors have been considered and are in the research and development phase [19]. The use of a catalyst in the partial oxidation process can inhibit the complete combustion of the hydrocarbon and accelerates (at relatively low temperatures) the reaction paths to the desired products [11].
Some of the advantages of a non catalyst partial oxidation (PoX) reactor over the steam reformer or catalyst PoX reactor are:

- The fuel feedstock with sulphur content can be used directly in the reactor
- The reactor has potentially better transient response and the over system is much simpler.

However, the main problem with PoX reactor is the formation of particulate carbon in the reactor and impurities such as HCN, H₂S, NOₓ, benzene can be present in the exit gas [12,13]. The level of these impurities in the reformed gas depends upon type of fuel feedstock and operating condition of the reactor.

Since diesel is the most widely used and available fuel in the marine industry, the use of a fuel processor for the production of hydrogen rich gas using diesel as a feedstock has recently been researched and developed. Although diesel fuel has a much higher energy density than methanol (Table 4.2), it is a complex mixture of many different hydrocarbons. Hence, diesel fuel processing to H₂ is much more complicated and requires much higher temperatures [14]. A simulation study of a SPFC system with a diesel steam reformer and high pressure hydrogen purifier (Pd membrane) by Amphett et al. estimated the fuel processor efficiency of 80% (LHV) and the reformer produced 47% (vol.) hydrogen on wet basis. The study further concluded that diesel reforming results in a high parasitic load and net system efficiency was higher at lower reforming temperature and high system pressure [15]. Recently an autothermal reformer (ATR) was developed by the U.S. Department of Energy in conjunction with commercial partners to reform a marine diesel fuel (NATO F-76) with 1% sulphur by weight. The ATR with catalyst developed by Catalytica Advanced Technologies showed increased sulphur tolerance, high catalyst activity and minimal carbon deposition problem. The ATR also exhibited a flatter temperature profile and lower temperature peak [16]. A F³P (catalytic ATR) fuel processing system developed by Hydrogen Burner Technology has successfully reformed many fuels and achieved fuel processing efficiency of 73% (LHV H₂ / LHV Fuel) for reforming diesel. The F³P operates between 760- 870 °C and 41-42% of H₂ (dry Vol.) was produced from the reactor [17]. A similar ATR reformer developed at the DaimlerChrysler AG
reformers different hydrocarbon fuels with reasonable efficiencies of between 80-85%. It was found that diesel fuel was most difficult to reform and vaporise [18].

The generation of hydrogen by partial oxidation (PoX) reforming of a hydrocarbon can be represented as [19,20]

\[ C_nH_m + x(O_2 + 3.76 \text{ N}_2) + (2n-2x)\text{H}_2\text{O} \rightarrow n\text{CO}_2 + (2n-2x + \frac{1}{2}m)\text{H}_2 + 3.76\text{N}_2 \]

where \( x \) is the oxygen to fuel ratio. The value of \( x \) is a critical as it determines the amount of water required to convert CO to CO\(_2\) and hydrogen yield. The PoX reactor should be operated in such a manner that the above reaction is exothermic and an optimal value of \( x \) should be used for high conversion efficiency and minimal carbon or soot formation [20,21]. Beside the O:C ratio, the other process parameters which effect performance of the PoX reactor are temperature, pressure and H\(_2\)O:C ratio. From both kinetic and equilibrium study, it is found that above 800°C the conversion efficiency of an uncatalysed PoX reactor, reforming hydrocarbon, is close to equilibrium conversion and independent of temperature while at temperature below 800°C the efficiency decreases [20,21]. The conversion efficiency of the PoX reactor is also favoured with lower O:C ratio ( \( \approx 1 \) ). A reasonable H\(_2\)O:C ratio (\( \geq 1 \)) also improves the conversion efficiency and inhibits soot or carbon formation [21]. In another steam reforming thermodynamic study of diesel fuel it was established that maximum hydrogen was yield at S:C ratio of between 1.1-1.3 and at pressure below 5 bar [22].

In this study, an uncatalysed PoX reactor was model in the ASPEN PLUS\textsuperscript{TM} software package [23], since no experimental and kinetic data were available to model the reactor. The PoX model was use to study the effect of various reformer variables such as temperature, pressure, molar ratio etc and to establish the operating conditions for the PoX reactor. The diesel fuel composition used in the model consisted of 90% \( \text{C}_{12}\text{H}_{22} \) (Bicyclohexyl) and 10% \( \text{C}_{12}\text{H}_{18} \) (M-diisopropylbenzene) [13, 15, 23] and the lower heating value (LHV) of the fuel was taken as 41.5 (MJ/kg) [15]. The average molecular weight and specific heat capacity of the fuel also used in this study were 165.90 g/mol [23] and 2.05 kJ/ kg K [24] respectively.
To simplify the model, it was also assumed that there was no sulphur present in the diesel fuel. The operating pressure of the reactor was chosen to be the same as the operating pressure of the SPFC system, i.e. 3 bar(a), since lower pressure favours the production of hydrogen and inhibits carbon formation [21,22]. A study of the O:C ratio in the PoX reactor model operating at 800°C, 3 bar(a) and a H$_2$O:C ratio of 1 (Table 5.1) showed that the hydrogen yield was higher at lower O:C ratios. However, the heat duty (power) required per mole of the fuel was very high at the lower ratios. As the O:C was increased, more fuel was consumed in the reactor to provide the power to heat the reactor to its operating temperature and hence the hydrogen yield was decreased. An optimal O:C ratio has to be chosen, such that some of the fuel is used in the PoX reaction and some fuel is used to generate power within the reactor via the combustion process. The choice of O:C ratio can also be influenced by pre-heating the reactants via the other components of the system. From a literature review [13,20] and results from the PoX model, an O:C ratio of 1 was chosen for the PoX reactor model in this SPFC system analysis.

Table 5.1: Effect of O:C ratio on PoX reactor performance
(800°C, 3 Bar(a), H$_2$O:C=1)

<table>
<thead>
<tr>
<th>O:C ratio</th>
<th>PoX Reactor Heat Duty (kW)</th>
<th>Hydrogen Yield (% Vol.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.25</td>
<td>2374.49</td>
<td>47.95</td>
</tr>
<tr>
<td>0.50</td>
<td>1894.09</td>
<td>39.74</td>
</tr>
<tr>
<td>0.75</td>
<td>1336.47</td>
<td>32.39</td>
</tr>
<tr>
<td>1.00</td>
<td>748.21</td>
<td>26.10</td>
</tr>
<tr>
<td>1.25</td>
<td>148.21</td>
<td>20.77</td>
</tr>
<tr>
<td>1.50</td>
<td>-456.18*</td>
<td>16.24</td>
</tr>
<tr>
<td>1.75</td>
<td>-1062.16</td>
<td>12.37</td>
</tr>
<tr>
<td>2.00</td>
<td>-1668.58</td>
<td>9.02</td>
</tr>
</tbody>
</table>

*Negative value implies extra power from the reactor.

With the O:C ratio established, the H$_2$O:C ratio for the PoX reactor was also studied in the PoX model. The H$_2$O:C ratio was varied between 0.25 and 2 at 800°C, 3 bars and an O:C ratio of 1. Figure 5.2 shows the results of this study. It was observed from figure 5.2 that the maximum amount of hydrogen was produced at H$_2$O:C ratio of 1 and therefore, this ratio was selected for the PoX reactor model.
In order to determine the operating temperature of the PoX reactor, the temperature was varied between 25 and 1200°C at a molar ratio O:C of 1, H₂O:C of 1 and pressure of 3 bar(a). Figure 5.3 shows the result of this study. From figure 5.3, it was evident that between the temperatures of 700 and 800°C, the maximum amount of hydrogen was produced. These gas compositions at different reactor temperatures were incorporated into the dynamic simulation as a look-up table.

5.2.1.2 HTS and LTS Reactors

Similarly, the HTS and LTS reactors (section 3.2.1.2) were also modelled using ASPEN PLUS™ software package and the exit gas compositions of each reactor at respective temperature were also implemented into the dynamic simulation as a look-up table. The steam to carbon ratio (H₂O:C) used in the model was 1.5. Table 5.2 shows the gas composition from the HTS and LTS reactor at their best operating temperature of 400°C and 200°C respectively. It was assumed that the catalysts used in these reactors favoured the water shift reaction and therefore the methane from the PoX reactor was not consumed in the HTS and LTS reactors (section 3.2.1.2).
Figure 5.3: Equilibrium gas composition for range of different temperatures

Table 5.2: Performance of the HTS and LTS reactors at 400°C and 200°C respectively. (3 Bar(a), H₂O:C=1.5)

<table>
<thead>
<tr>
<th>Component</th>
<th>HTS Gas Composition (vol. %)</th>
<th>LTS Gas Composition (vol. %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td>28.67</td>
<td>29.93</td>
</tr>
<tr>
<td>CO</td>
<td>1.34</td>
<td>0.08</td>
</tr>
<tr>
<td>CO₂</td>
<td>14.53</td>
<td>15.79</td>
</tr>
<tr>
<td>CH₄</td>
<td>0.07</td>
<td>0.07</td>
</tr>
<tr>
<td>H₂O</td>
<td>25.40</td>
<td>24.14</td>
</tr>
<tr>
<td>N₂</td>
<td>29.99</td>
<td>29.99</td>
</tr>
</tbody>
</table>

5.2.1.3 Gas Clean-Up Unit (GCU)

The GCU model and data used in this study was identical to the model used in the natural gas SPFC system described in chapter 3. The operating conditions of the GCU (section 3.2.1.3) were chosen to be 160°C and a O₂:CO molar ratio of 2.5. At these operating conditions, it was assumed that the CO was reduced to ≤10 ppm and the remainder of the oxygen was used in H₂ combustion. These operating conditions were implemented in the dynamic simulation. The clean reformate from the GCU, at peak SPFC stack power (1.5 MWₑ), had the following gas composition (vol. %):
5.2.1.4 Air Bleed

To further reduce the CO concentration in the clean reformate from the GCU reactor, 1% air bleed (equal to 1% Hydrogen in the reformat) was mixed with the reformate prior to the fuel cell anode inlet (section 5.2.1.4). It was assumed that all the CO was consumed with the oxygen in the air bleed and the additional oxygen reacted with the hydrogen. The air bleed was also incorporated in the dynamic simulation and 1% of hydrogen was consumed with extra oxygen at peak SPFC stack power (1.5 MW_e).

5.2.2 SPFC Stack

A parametric model of the SPFC [25,26] was used to predict the performance of the SPFC as a function of many variables such as temperature, pressure, \((H_2, O_2)\) concentrations etc. The fuel cell voltage was calculated using the following equation:

\[
V = E + \eta_{\text{act}} + \eta_{\text{ohmic}}
\] ... (5.1)

Where

\(E, \eta_{\text{act}}, \eta_{\text{ohmic}}\) are the thermodynamic equilibrium potential (volts), overvoltage due to activation loss (volts) and overvoltage due to ohmic resistance (volts) respectively.

These overvoltages are defined as

\[
E = E^o - (RT/nF)\ln[P_H_2(P_O_2)^{\frac{1}{2}}], \text{ where } E^o = E^0 + (T-T_o)(\Delta S^o/nF)
\]

\[
\eta_{\text{act}} = \xi_1 + \xi_2T + \xi_3T(\ln[O_2]^*) + \xi_4T(\ln(i))
\]
\[ \eta_{\text{ohmic}} = -i \times R, \text{ where } R = r_1 + r_2 \times T + r_3 \times i \]

Also where:

- \( E^0 \) - reference potential (volts)
- \( E^\circ \) – standard state reference potential =1.229 V (@ 298 K and 1 atmosphere)
- \( R \) – gas constant = 8.3143 J/mol K
- \( n \) – number of electrons transferred
- \( F \) – Faraday’s constant = 96,487 C/mol
- \( P_{H_2}, P_{O_2} \) – partial pressure of components
- \( T, T_0 \) – operating and datum temperature, K
- \( \Delta S^0 \) – standard state entropy change, kJ/mol
- \([O_2]^*\) - concentration of species, mol/cm³
- \( i \) – current, Amps

The values of \( \xi_{1-4} \) and \( r_{1-3} \) are manipulated to fit the resulting polarisation curve from equation (5.1) to measure empirical data. For the dynamic simulation, the parameter values of \( \xi_{1-4} \) and \( r_{1-3} \) were estimated to fit the resulting polarisation curve to experimental polarisation curve for a SPFC operating at 3 bar(a) and cell area of 200 cm² (figure 3.6). The estimated parameter values are shown in table 5.3. Figure 5.4 shows the calculated and experimental polarisation curve. These values and equation 5.1 were implemented into the dynamic simulation and the SPFC voltage was estimated for different cell operating conditions.

Table 5.3: Parameter values used in the SPFC model

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \xi_1 )</td>
<td>-1.00</td>
</tr>
<tr>
<td>( \xi_2 )</td>
<td>3.106E-03</td>
</tr>
<tr>
<td>( \xi_3 )</td>
<td>8.700E-05</td>
</tr>
<tr>
<td>( \xi_4 )</td>
<td>-2.800E-05</td>
</tr>
<tr>
<td>( r_1 )</td>
<td>1.598E-02</td>
</tr>
<tr>
<td>( r_2 )</td>
<td>-4.211E-05</td>
</tr>
<tr>
<td>( r_3 )</td>
<td>1.000E-08</td>
</tr>
</tbody>
</table>
Figure 5.4: The calculated and experimented polarisation curve

5.2.3 Compressor and Expander

Similar to the natural gas and methanol SPFC systems studied in chapters 3 and 4, the compressor and expander isentropic efficiency for dynamic simulation was taken as 80%. This value reflects possible future performances of a compressor in a fuel cell system. Since the PoX fuel processing system has no burner, a separate burner was included to combust the SPFC stack anode and cathode exhaust gases and provide the flue gas to the expander at the system operating pressure. The expander power was supplied to the compressor via a mechanical shaft, with a transmission efficiency ($\eta_t$) of 98%. The model assumes that the working envelope of the expander matches that of the compressor, and excess power from the expander generator was supplied to the system load.

5.2.4 SPFC Exhaust Gases Burner

SPFC stack exhaust gases (anode and cathode exit gases) were burned in a combustion chamber to provide flue gases at higher temperature to the expander. The water from the exhaust gases was removed via the condensers and supplied dry to the
chamber. Since the cathode and anode stoichiometries were constant at 2 and 1.5 respectively, the molar fraction of various gases in the anode and cathode stream remained the same over different operating points on the polarisation curve (i.e. voltage & current density). Table 5.4 shows the percentage dry gas composition (vol. %) of the anode and cathode streams.

Table 5.4: Gas composition of the anode and cathode streams

<table>
<thead>
<tr>
<th>Component</th>
<th>Anode Gas Composition (vol. %)</th>
<th>Cathode Gas Composition (vol. %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H₂</td>
<td>16.82</td>
<td>-</td>
</tr>
<tr>
<td>CH₄</td>
<td>0.12</td>
<td>-</td>
</tr>
<tr>
<td>CO₂</td>
<td>27.61</td>
<td>-</td>
</tr>
<tr>
<td>N₂</td>
<td>55.45</td>
<td>11.73</td>
</tr>
<tr>
<td>O₂</td>
<td>-</td>
<td>88.27</td>
</tr>
</tbody>
</table>

The exit temperature of the flue gases was estimated by assuming that the combustion process was adiabatic (heat loss Q = 0) and at constant volume. This implies that all the chemical energy is transformed into sensible internal energy, resulting in a rise in temperature. This maximum temperature remains constant for a given fuel to air ratio [27]. Since the fuel (H₂ & CH₄) and oxygen ratio remained the same at different operating points on the polarisation curve, the estimated temperature of the flue gases remained same. The temperature of the flue gases (i.e. combustion product) was estimated by performing a heat balance on the combustion chamber. The heat balance is represented by the following equation:

\[ \sum n_p (H_{PT} - H_{P298}) + \Delta H_{298} + \sum n_r (H_{RT1} - H_{P298}) = 0 \]

Where, 
\[ \sum n_p (H_{RT1} - H_{P298}) \] - is the thermal power in the reactants (R) at inlet temperature (T1). 
\[ \Delta H_{298} \] - is the enthalpy of reaction of the fuel (\( \Delta H_{298} \)) at datum temperature (298 K). 
\[ \sum n_r (H_{PT} - H_{P298}) \] - is the thermal power of the products at final product temperature.
The final product temperature was estimated by iterating the above equation with different temperature (PT) until the heat balance equalled to zero. For the SPFC stack with polarisation curve shown in figure 5.4, the product temperature was estimated to be 746 K (473°C). This product temperature was used in the dynamic simulation. The flue gases with temperature of 473°C and pressure of 3 bar(a) were fed into the expander at varying flowrates depending on the performance of the SPFC stack.

5.2.5 Lead Acid Battery

In this system study of marine applications, batteries were used on board the vehicle as an energy buffer, peak power sharing and for starting up process. High temperature lead acid batteries (Type 8400) were used. Battery characteristics such as the cell voltage, charge and discharge resistances were obtained from the manufacturing data, by interpolation of the charge and discharge characteristics at constant current for a range of capacity values. The resistance and voltage values obtained from these characteristics are stored as function of state of charge. The charge and discharge values used in this study were calculated using charge and discharge curves for the lead acid battery at 450°C and 500°C. These resistance and voltage values as function of state of charge are used in the dynamic simulation as a lookup table.

The battery pack consisted of 80 dockyard exchange modules (DEM). Each module had 480 cells (20 series x 24 parallel) and each cell had a capacity of 50 Ah and nominal voltage of 1.5 volts, giving total energy per module of 36 kWh. These 80 modules were arranged in 20 (series) by 4 (parallel) configuration. This configuration yielded a battery pack capacity of 4800 Ah and nominal voltage of 600 volts (2.88 MWh). The DEM had an energy density of 80 Wh/kg, which gave the total weight of the battery pack of 36 tonnes.

5.2.6 DC/DC converter

A DC/DC converter was used in the SPFC marine system to convert the fuel cell stack voltage into a regulated voltage corresponding to battery voltage or bus-bar voltage (dc link voltage). In this system analysis (and in the dynamic simulation of the
system) a constant efficiency of 98% was assumed for the DC/DC converter (section 4.1.5.2).

5.3 DYNAMIC SIMULATION OF THE SPFC HYBRID SYSTEM

A dynamic simulation of a SPFC marine hybrid system (figure 5.1) was developed in a Matlab/Simulink environment, to study the component interactions between a diesel fuel processor, a 1.5 MW SPFC system, a compressor/expander system and a lead acid battery pack. The integration of the overall marine system and the performance of this system were investigated under a duty cycle, representative of a ship hotel load [7]. In this section, the models developed in the Matlab/Simulink environment (using the data specified in section 5.2) are described and the results from the simulation of the SPFC marine system under a ship hotel load, are presented and discussed. The results of steady state calculations at peak SPFC stack power of 1.5 MW_e are also presented. Figure 5.5 shows the representation of a SPFC marine hybrid system in a Matlab/Simulink environment.
Figure 5.5: Dynamic Simulation of the SPFC marine hybrid system in a Matlab/Simulink Environment

Diesel Fuel Processor
- Fuel_FR (kg/s)
- Ref_FR (mol/s)
- Fuel_MFR (kg/s)
- Fuel_Left (kg)
- CO_PPM

System Control & Strategy
- FR (kg/s)
- SPFC_SP (MW)
- Net_Load (MW)
- Eff = (FC_P/Fuel_P)
- SoC (%)

SPFC System
- [H2O,CO,H2,N2,CH4,CO2]
- 13.44
- 0.0005537
- 16.26
- 16.89
- 0.03845
- 8.717

Burner
- FC_AEX (mol/s)
- FC_CEXT (mol/s)
- FC_AEX (mol/s)
- FC_CEX (mol/s)
- FC_Volt

DC_Link
- L_Sources
- Exp_P (W)
- FCS_AIR (mol/s)
- Cell_Volt
- FCS_CE (mol/s)
- FCS_AEX

Air Compressor
- Comp_Power (MW)
- FCS_AIR (mol/s)
- Exp_Power (W)
- C_E_Net_P (MW)

Lead Acid Battery
- SoC
- BB_V
- BB_I
- BB_P (MW)
- DC_J_Out

Hotel Load
- L_Load
- I_Load
- I_Sources
- C_E_Net_P (MW)
- A_Load_P (MW)
- L_Out

Clock
- Hr
- Sec
- 3240.00
- 29.86
- 1
- 19609.80
- 10

DOUBLE-CLICK to send Simulation Results data to Excel Sheet - File Name in the Setup file. (Note: Excel File Must be OPEN before sending the data)
5.3.1 Diesel Fuel Processor

In the Matlab/Simulink environment the diesel fuel processor was represented by Tank model, Flowrate, PoX Reactor Model, HTS Reactor model, LTS Reactor model and GCU Reactor model blocks. Figure 5.6 shows the fuel processor representation in the Matlab/Simulink environment.

![Figure 5.6: Diesel Fuel Processor in the dynamic simulation]

5.3.1.1 Fuel Processor Reactants Flowrate

In the dynamic simulation, the diesel flowrate was determined by the system control and strategy block (figure 5.5) and this flowrate was then fed into the tank model block, which checks if there was sufficient fuel in the tank to supply the flowrate demand. The flowrate was then passed into the flowrate block to calculate the air and water flowrates for the partial oxidation and shift reactors.
5.3.1.2 Diesel Thermal Partial Oxidation (PoX) Reactor

Figure 5.7: PoX reactor model in the dynamic simulation

![PoX reactor model diagram]

Figure 5.7 shows the PoX reactor model in the Matlab/Simulink environment. The thermal model of the reactor was represented by first order lag and a PID controlled reactor temperature. The mole fractions of the various reformed gases from the reactor were calculated via a look up table for different reactor temperatures. The warm up period of the reactor, modelled by the thermal lag, was approximately $\frac{1}{2}$ hour. The flowrate supplied from the flowrate block was used to calculate the flowrate of the reformed gases at the reactor’s temperature and supplied to the HTS reactor.

5.3.1.3 HTS and LTS Reactors

A similar model to the PoX reactor model was used in both HTS and LTS reactors, with the set point temperature of the reactors being 400°C and 200°C respectively. The warm up period or the response time of the reactors was identical to PoX reactor. The HTS and LTS reactors were heated to the required operating temperature by a combination of the heat content of the reformed gases, the exothermic reaction in the shift reactors and pre-heated shift reactor water (250°C @ steady state condition).
5.3.1.4 Gas Clean-Up Unit (GCU)

Figure 5.8 illustrates the GCU reactor model in the Matlab/Simulink environment. The thermal model of the reactor was represented by first order lag, with a set point temperature of 160 °C. The O₂:CO ratio and amount of CO to burn to achieve the desired ppm of CO in the reformed gas stream were also included in the model. The values of these variables were set in a variable set up file, which was initiated at the beginning of the simulation.

Figure 5.8: GCU reactor model in the dynamic simulation

5.3.2 SPFC Stack

Translation of the SPFC parametric model (section 5.2.2) into the dynamic simulation is shown in Figure 5.9. This model was used to calculate the cell voltage for a given hydrogen flowrate, received from the fuel processor block. The reformed gases from the fuel processor were only inputted to the stack if the CO level was ≤ 10 ppm, otherwise reformed gases were either fed back to the burner, or vented. The estimated parameter values, shown in table 5.3, were used in the model to simulate the polarisation curve shown in figure 5.4.
Figure 5.9: SPFC model in the dynamic simulation
Figure 5.10: Compressor model in the dynamic simulation
5.3.3 Compressor and Expander

The compressor and expander models in the dynamic simulation are shown in figure 5.10 and 5.11 respectively. These models include the data specified in section 5.2.3 and the equations 3.9 and 3.10 given in section 3.2.3. In the compressor model, the shaft and motor efficiency were also included. The motor was used during start up and when expander power was less than the required compressor power. The motor power or excess expander power was either added or subtracted from the total system load. The resulting net load (power) was then taken from the SPFC system and/or battery pack.

**Figure 5.11: Expander model in the dynamic simulation**
5.3.4 SPFC Exhaust Gases Burner

Figure 5.12: Burner model in the dynamic simulation

Figure 5.12 shows the burner model in the Simulink/Matlab environment. The constant burner temperature (section 5.2.4) was used to calculate the thermal power in the flue gases at a pressure of 3 bar(a). The total thermal power of the flue gases and the burner temperature were fed into the expander block to calculate the expander exit flue gases temperature and expander power.
Figure 5.13: Lead Acid battery model in the dynamic simulation
5.3.5 Lead Acid Battery

The lead acid battery model was developed in the Matlab/Simulink environment using the data specified in section 5.2.5 and the traction battery model shown in figure 4.10. Figure 5.13 shows the lead acid battery model used in the dynamic simulation. The mathematics of the traction battery model are detailed in Appendix I. For the steady state study, the battery power was not included. However, the dynamic simulation of marine system does include results from the battery pack.

5.3.6 DC/DC Converter

Figure 5.14 shows the DC/DC converter model in the Matlab/Simulink environment, using the data specified in section 5.2.6. The DC link voltage was kept constant and equal to the nominal 600 V of the battery pack. The DC/DC converter matches the SPFC voltage to the DC link voltage. The SPFC power was used to calculate the DC/DC converter current at the DC link voltage. Some of the power was lost in the converter to reflect the 98% efficiency of the device. For the steady state study, the DC/DC converter losses were not included. However, the dynamic simulation of marine system does account for the losses from the converter.
5.3.7 Marine Hotel Load

The marine hotel load profile was constructed to reflect the electricity usage on board a typical marine vessel. The profile was based on load profiles in the electrical supply market in U.K. [28], where the maximum electrical power demanded was in early morning (6-10 a.m.) and evening (6-10 p.m.). The marine hotel load has maximum and minimum loads of 2 MW_e and 1 MW_e respectively. The load profile was designed to demand 2 MW_e at peak hours (8-10 A.M. & 6-9 P.M.) and minimum power demanded from 11 P.M. to 5 A.M. and 2 P.M. to 5 P.M. In between these times the load profile demanded, average power of 1.5 MW_e. Figure 5.15 shows the hotel load profile (three repeated profiles) and its implementation in the dynamic simulation.

Figure 5.15: Hotel Load model in the dynamic simulation

5.3.8 System Control and Strategy

The control strategy used in the system study employed the SPFC stack as a battery changer. The state of charge (SoC) of battery was maintained ≥ 80%. This chosen strategy protected the fuel cell stack and its performance from high and variable levels of CO concentration, which would result from cyclic operation of fuel processor. To implement this strategy, the control system has to control the diesel flowrate of the fuel processor by first minimising the difference between the actual SoC and set point
SoC (80-90%). Secondly, the strategy minimised the error between the net system load demand and SPFC stack power. A first order lag and a PID controller were used in the feedback control system to determine the PoX reactor diesel flowrate. A limiter was used to regulate the flowrate for a maximum SPFC stack power. Figure 5.16 shows the control system implementation in the Matlab/Simulink environment.

Figure 5.16: Control system model in the dynamic simulation

5.4 RESULTS AND DISCUSSION

5.4.1 Dynamic Simulation Results

The results presented in this section describe a SPFC marine system operating under a ship hotel load. The objective of this simulation study was to investigate if an average power delivered from the SPFC stack, i.e. 1.5 MW was capable of maintaining the battery SoC ≥ 80%, during and at the end of the duty cycle. Therefore, the simulation was run for more than 24 hrs or until the SoC was ≥ 80%, after the normal period of the cycle (24 hrs). The second objective was also to analyse the system component integration and interaction between various sub-systems and the effect of the control system and strategy on the performance of the individual components of the system.
The dynamic simulation of the SPFC marine system under a ship hotel load was simulated with the following set-up:

**TIME:** 108000 Sec (30-hrs with time step of 20 Sec)

**LOAD:** Marine Hotel Load (24-hrs duty cycle -repeated)

**SYSTEM VARIABLES:**
- Pressure = 3 bar (a)
- Datum Temperature = 298 K

**FUEL PROCESSOR:**

**Fuel Type:** Diesel (41.47 MJ/kg @ 298 K)

**Fuel Tank:** 20 tonnes

**Fuel Flow Limit:** 0.1205 kg/s (for 1.5 MW SPFC Stack)

**Reactor Type:** Diesel Thermal Partial Oxidation (PoX)
- PoX Temperature: 800 °C
- O: C ratio: 1
- S: C ratio: 1

**Reactor Type:** High Temperature Shift (HTS)
- HTS Temperature: 400 °C
- S: C ratio: 1.5

**Reactor Type:** Low Temperature Shift (LTS)
- LTS Temperature: 200 °C

**Reactor Type:** Gas Clean-up Unit (GCU)
- GCU Temperature: 160 °C
- O2: CO ratio: 2.5
- CO PPM: ≤10

**Air Bleed:** 1% (of hydrogen in the reformate)
CHAPTER 5 - DIESSEL BASED SPFC MARINE SYSTEM

SPFC STACK SYSTEM:

- Power: 1.5 MW (0.7277 Volts/cell @ 0.5 A/cm²)
- No of Cells: 20500
- Anode Stoichiometry: 1.5
- Cathode Stoichiometry: 2.0
- Active Cell Area: 200 cm²
- Temperature: 80 °C

COMPRESSOR & EXPANDER:

- Burner Temperature: 745.92 K
- Expander efficiency: 80%
- Compressor efficiency: 80%
- Shaft transmission losses: 2%
- Motor efficiency: 90%
- Motor transmission losses: 2%

BATTERY:

- Type: Lead Acid (80 Dockyard exchange modules, DEM)
- Capacity: 50 Ah/Cell
- Nominal Voltage: 1.5 V/Cell
- Mass: 36 tonnes (80Wh/Kg per DEM)
- No. Of Cells: 38400
- Energy Capacity: 2.88 MWh
- Initial SoC: 80%
- Final SoC: 85%

DC/DC CONVERTER & DC-LINK:

- Efficiency: 98%
- Voltage: 600 volts (Battery nominal voltage)
Figure 5.17 shows the SPFC stack power (1.5 MW<sub>e</sub>), battery power and SoC response to the load demand. The duration of the simulation was 30 hours i.e. one and quarter hotel load cycle and during this period, the battery SoC varied from initial 80% to 24% at peak demand and was > 80% at end of the 30 hrs. However, at the end of 24 hours i.e. one day load cycle, the SoC of the battery was down to 45% and not > 80%, as anticipated by the control strategy. Nevertheless, during the first two hours of the next duty cycle the SoC of the battery was > 80% and the hybrid power source of the SPFC stack and battery was sufficient to meet the remainder of second day’s hotel load demand. Although the SPFC stack power and battery energy combination were adequate to supply the necessary power for the ship hotel load, in a practical terms the daily discharging the battery to < 25% SoC may compromise the life expectancy of the battery. Consequently, to avert this problem either a larger SPFC stack or battery pack may be required.

Since the space or the volume for the battery pack on board a marine vessel would be constrained, the only other possibility of improving the hybrid power source would be to increase the SPFC stack power. This was achieved by either increasing the stack size or decreasing the SPFC voltage efficiency i.e. operation at higher current density. In this simulation study, the latter method of increasing the current density was adopted. By increasing the current density or lowering the operating cell voltage from 0.728 volts (\(\eta_{\text{Th}} = 58\%\)) to 0.703 volts (\(\eta_{\text{Th}} = 56\%\)), the stack power was increased from 1.5 MW<sub>e</sub> to 1.7 MW<sub>e</sub>. Figure 5.18 shows the results of the simulation with increased SPFC stack power (1.7 MW<sub>e</sub>).

From figure 5.18, it can be observed that with increased stack power, the battery did not discharge below 50% at the peak load demanded and the SoC of the battery was > 80% at the end of the first hotel load cycle. Hence, the increase in stack power achieved the desired SoC of > 80% at the end of every hotel load profile (24 hrs). However, the SPFC electrical efficiency ((SPFC Power)/(Total Diesel Fuel Power)) decreased by 1% from 30% to 29% at peak SPFC stack power.
Figure 5.17: Results from the Dynamic Simulation for 1.5 MWₑ Stack Power (Load, SoC, Stack power & Battery power)
Figure 5.18: Results from the Dynamic Simulation for 1.7 MW\textsubscript{e} Stack Power (Load, SoC, Stack power & Battery power)
Since a SPFC stack power of 1.7 MW_e was adequate to supply power to the marine system without compromising the battery’s life expectancy, it was chosen as the peak power of the stack in the dynamic simulation. The flowrate of the diesel fuel was regulated in the control system to achieve this maximum stack power and hence, the control system determined the SPFC stack power via the diesel flowrate set-point to the fuel processor, according to the electrical load demand and SoC of the battery. The dynamic simulation results presented in figures 5.19 to 5.22 are for the 1.7 MW_e SPFC stack. These results also illustrate component integration, subsystems interaction and also the effect of the control system on the performance of system components. Figures 5.19 and 5.20 show the current and voltage characteristics of both SPFC and battery respectively. Figure 5.21 shows the compressor power, expander power and system electrical efficiency ((SPFC Power) / (Total Diesel Fuel Power)). Finally, figure 5.22 shows the diesel fuel, air and hydrogen flowrates during the simulation period.

The effect of warm-up period (= ½ hrs) of the fuel processor and its effect on the performance of the system is also shown in these figures (5.19-5.22). The battery supplied all the power demanded during this warm-up period and therefore discharging rapidly to SoC of approx. 50%. The battery also supplied the parasitic power load of the compressor, which was approx. 0.1 MW. However, some of the power demand by the marine vessel system during the warm-up period could have been supplied via the burner/expander system by combusting the unusable reformed gases. However, in this simulation study it was assumed that the reformed gases during the warm-up period were vented to the atmosphere rather than combusted in the burner.

Subsequent to the warm-up period, the SPFC system and the expander supplied the majority of the system power demand. The expander power supplied 100% compressor power and any excess expander power was used to overcome the system load (Figure 5.21). Figure 5.19 shows the performance and response of the SPFC stack to the load demand. It can be seen in figure 5.19 that the SPFC stack was used at three different power levels (i.e. 1,1.5 & 1.7 MW_e).
Figure 5.19: Results from the Dynamic Simulation

(Load, SPFC Stack power, Cell Current and Cell Voltage)
Figure 5.20: Results from the Dynamic Simulation

(Load, Battery power, Current and Voltage)
Figure 5.21: Results from the Dynamic Simulation

(Load, Compressor power, Expander power & Electrical Efficiency)

Electrical System Efficiency

Expander Power

Compressor Power

Ship Hotel Load
Figure 5.22: Results from the Dynamic Simulation

(Load, Diesel, Air & Hydrogen Flowrate)
5.4.2 Steady State System Analysis

A steady state analysis of the marine SPFC system was performed for the average system power of 1.5 MW_e. However, the estimated values of the overall system electrical efficiency for the 1.7 MW_e system will also be described and compared with the 1.5 MW_e system. The aim of this study was to estimate the system electrical efficiency, fuel processor efficiency and to investigate if the system had sufficient thermal power to supply the system with pre-heat, such that it was self-sufficient from the energy supplied by the diesel fuel. This investigation was important since the dynamic simulation has no thermal integration and assumes no extra power was required for steady state conditions. However, battery power was available to supply the transient power requirements.

5.4.2.1 Diesel Fuel Processor

For 1.5 MW_e of electrical power from the SPFC stacks and an anode stoichiometry of 1.5, the hydrogen demand from the fuel processor was calculated to be 15.94 mol/s (21,424 SLPM). The equivalent diesel flowrate to satisfy the hydrogen demanded from the SPFC stacks was determined to be 0.730 mol/s (8.24 LPM @25°C). With molar ratio of H_2O: C of 1.0 and O: C ratio of 1, the water and the air flowrate were calculated to be 8.76 mol/s and 20.86 mol/s respectively. The H_2O: C ratio of 1.5 was also used for the HTS and LTS reactor water and the flowrate of water for these reactors was calculated to be 13.14 mol/s.

5.4.2.1.1 Diesel Thermal Partial Oxidation (PoX) Reactor

For the reactor steady state calculations at 800°C, all the diesel was partially oxidised (conversion efficiency of 100%) and the proportion of hydrogen produced in the PoX reactor was 26%. From the PoX reactor heat balance, the reactor efficiency, η_{Ref}, was found to be 99.11% (heat losses from the surface) and the power required for the reformer reactions at 800°C, ΛP_{Ref,(873K)}, was determined to be 508 kW (includes the power required to heat the reactants to 800°C).
The definition of $\eta_{\text{Ref}}$ and $\Delta P_{\text{Ref}(1073 \text{ K})}$ are as following:

$$\eta_{\text{Ref}} = \frac{\text{Power in the reformed gases}}{\text{Total power into the PoX}}$$

$$\Delta P_{\text{Ref}(1073 \text{ K})} = (\text{Total Power into the PoX}) - (\text{Power losses} + \text{Reaction Power})$$

5.4.2.1.2 HTS and LTS Reactors

For the steady state calculation, only the inlet and outlet conditions of the reactants and products were considered for the heat and mass balance. To maintain the HTS and LTS reactors at an operating temperature of 400°C and 200°C respectively, the amount of heat power to be removed by the cooling system was determined to be 321.38 kW and 57.57 kW for the HTS and LTS reactors respectively.

5.4.2.1.3 Gas Clean-Up Unit (GCU)

For the operating conditions detailed in section 5.2.1.3, a heat and mass balance was carried out to determine the thermal power to be removed from the GCU, in order to maintain a temperature of 160°C. This was calculated to be 49.3 kW. (This heat power also contains thermal energy produced via the combustion of $H_2$ with excess $O_2$ in the GCU.)

5.4.2.1.4 Fuel Processor Efficiency

The fuel processor efficiency defined in section 3.3.2.4, $\eta_{\text{FP}}$, for the system presented in figure 5.1 was calculated to be 87% at steady state condition and 1.5 MW $e$ SPFC stack power.
5.4.2.2 SPFC Stack

A heat and mass balance for the fuel cell stack was carried out to determine the heat to be removed by the cooling system to maintain the stack temperature of 80°C. The fuel cell data detailed in table 5.5, were used in the heat and mass balance calculation. The anode and cathode stoichiometries used in this calculation were 1.5 and 2 respectively. Figure 5.23 shows the heat balance of the fuel cell at these operating conditions. From the heat balance, the cooling power required to maintain the stack at 80°C was determined to be 847 kW.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell Voltage (Volts)</td>
<td>0.7277</td>
</tr>
<tr>
<td>Current Density (A/cm²)</td>
<td>0.5</td>
</tr>
<tr>
<td>Number of Cells</td>
<td>20500</td>
</tr>
<tr>
<td>Anode Exhaust Relative Humidity (%)</td>
<td>192.31%</td>
</tr>
<tr>
<td>Cathode Exhaust Relative Humidity (%)</td>
<td>120.4%</td>
</tr>
<tr>
<td>Efficiency $\eta_{\text{th}}$ (LHV) (%)</td>
<td>58.06%</td>
</tr>
</tbody>
</table>

Table 5.5: SPFC performance used in the steady state study

Figure 5.23: SPFC heat balance at 3 bar(a) and 80°C
5.4.2.3 Compressor and Expander

For the steady state analysis, the isentropic efficiency of the compressor and expander were both taken as 80% respectively. Using equation 3.9 (section 3.2.3), the compressor air outlet temperature, (at a pressure ratio of 3) was calculated to be 163°C. The corresponding compressor power was determined to be 296.82 kW. Including the shaft mechanical transmission efficiency ($\eta_s = 98\%$), the total power required by the compressor was determined to be 302.88 kW. The expander power was also calculated for pressure ratio of 3 and isentropic efficiency of 80%. The burner flue gases (473°C) were expanded to a temperature of 329.7°C. The power generated by the expander was 356.8 kW at a pressure ratio of 3. Additional power (53.92 kW) was used to supply the hotel load.

5.4.2.4 Heat Exchangers and Condensers

In the study, the heat exchangers 1 and 6 (figure 5.1) were used to recover the thermal energy for pre-heating the PoX reactor and HTS reactor reactants respectively. For the heat exchangers, only the inlet and outlet conditions of the working fluid streams were considered (and 1% energy loss was assumed from the surface). From figure 5.1 it can be seen that six heat exchangers were used in this system analysis. Heat exchanger 1 was used to cool down the reformed gases from 800°C to 400°C. The thermal power recovered from cooling of the reformed gases was used to pre-heat the PoX reactor reactants (diesel fuel and water). The diesel fuel and PoX water were heated to a temperature of 250°C and these reactants provided the heat duty of 508 kW required by the PoX reactor. Heat exchanger 6 was also used to preheat water for the HTS reactor to 250°C. The thermal power in the flue gases were used to heat the HTS reactor water and consequently in the process the flue gases were cooled down from 330°C to 42°C.

The remaining heat exchangers (2,3,4,5) were used to cool the gas streams to the respective reactors operating temperatures. Heat exchanger 2, 3 and 4 were used to cool the reformed gases from 400°C to 160°C and then to 80°C, before the reformate was introduced into the SPFC stack. Heat exchanger 5 was used to cool the
compressed air from 163°C to 80°C. The thermal power recovered via the heat exchanger network were not used in the system, and was available as low grade heat. Table 5.6 shows the thermal power available from the heat exchangers.

Condensers were used to cool down and remove all the water from the anode and cathode exhaust gas streams. The exhaust gas streams were cooled down from 80°C to 25°C with 100% water recovery from the gas streams. The amount of thermal power and latent heat recovered in the condenser was calculated to be 868 kW. 99% of this thermal power was available as low grade heat.

5.4.2.5 Overall System Power Balance and System Efficiency

An overall system power balance of a marine system (figure 5.1) was carried out to determine the electrical system efficiency. Table 5.6 shows the overall system heat balance of the marine system and system electrical efficiency. The electrical (\( \eta_{\text{El, Sys}} \)) system efficiency was defined as following:

\[
\eta_{\text{El, Sys}} = \frac{\text{SPFC Power (kW) + Expander Power (kW)}}{\text{LHV of the Fuel to the system (kW)}}
\]

A similar steady state analysis for 1.7 MW_e marine SPFC system was also performed. Table 5.7 summaries the results of both the 1.5 and 1.7 MW_e systems.

**Table 5.7: Results of the steady state analysis of the Marine SPFC Systems**

<table>
<thead>
<tr>
<th>System Parameters</th>
<th>Marine SPFC Systems</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1.5 MW_e</td>
</tr>
<tr>
<td>Total Fuel Power to the System (MW)</td>
<td>5.01</td>
</tr>
<tr>
<td>Fuel Processor Efficiency, ( \eta_{\text{FP}} ) (%)</td>
<td>87</td>
</tr>
<tr>
<td>Electrical Efficiency, ( \eta_{\text{El, Sys}} ) (%)</td>
<td>30.84</td>
</tr>
</tbody>
</table>
Table 5.6: Overall power balance of the 1.5 MW<sub>e</sub> SPFC marine system

<table>
<thead>
<tr>
<th>Component</th>
<th>POWER INTO THE SYSTEM (MW)</th>
<th>POWER INTO THE SYSTEM (%)</th>
<th>POWER OUT OF THE SYSTEM (MW)</th>
<th>POWER OUT OF THE SYSTEM (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PoX REACTANTS</td>
<td>5.01</td>
<td>100.00%</td>
<td>0.05</td>
<td>1.00%</td>
</tr>
<tr>
<td>PoX REACTOR LOSSES</td>
<td></td>
<td></td>
<td>0.06</td>
<td>1.17%</td>
</tr>
<tr>
<td>HEX1</td>
<td></td>
<td></td>
<td>0.32</td>
<td>6.41%</td>
</tr>
<tr>
<td>HTS REACTOR</td>
<td></td>
<td></td>
<td>0.37</td>
<td>7.46%</td>
</tr>
<tr>
<td>HEX2</td>
<td></td>
<td></td>
<td>0.06</td>
<td>1.15%</td>
</tr>
<tr>
<td>LTS REACTOR</td>
<td></td>
<td></td>
<td>0.07</td>
<td>1.36%</td>
</tr>
<tr>
<td>HEX3</td>
<td></td>
<td></td>
<td>0.05</td>
<td>0.98%</td>
</tr>
<tr>
<td>GCU REACTOR COOLING</td>
<td></td>
<td></td>
<td>0.36</td>
<td>7.16%</td>
</tr>
<tr>
<td>SPFC STACK COOLING</td>
<td></td>
<td></td>
<td>0.85</td>
<td>16.90%</td>
</tr>
<tr>
<td>SPFC STACK ELECTRICAL POWER</td>
<td></td>
<td></td>
<td>1.49</td>
<td>29.76%</td>
</tr>
<tr>
<td>FLUE GASES</td>
<td></td>
<td></td>
<td>0.27</td>
<td>5.47%</td>
</tr>
<tr>
<td>CONDENSERS</td>
<td></td>
<td></td>
<td>0.87</td>
<td>17.31%</td>
</tr>
<tr>
<td>COMPRESSOR POWER REQUIRED</td>
<td>0.00</td>
<td>0.00%</td>
<td>0.00</td>
<td>0.00%</td>
</tr>
<tr>
<td>EXTRA EXPANDER POWER</td>
<td></td>
<td></td>
<td>0.05</td>
<td>1.08%</td>
</tr>
<tr>
<td>HEX5</td>
<td></td>
<td></td>
<td>0.13</td>
<td>2.53%</td>
</tr>
<tr>
<td>HEX6</td>
<td></td>
<td></td>
<td>0.01</td>
<td>0.14%</td>
</tr>
<tr>
<td>MOTOR LOSSES</td>
<td></td>
<td></td>
<td>0.00</td>
<td>0.00%</td>
</tr>
<tr>
<td>SHAFT LOSSES</td>
<td></td>
<td></td>
<td>0.01</td>
<td>0.12%</td>
</tr>
<tr>
<td>TOTAL</td>
<td>5.01</td>
<td>100.00%</td>
<td>5.01</td>
<td>100.00%</td>
</tr>
</tbody>
</table>

Compressor power: 0.303 MW, 6.04%
Expander power: 0.357 MW, 7.12%
Net compressor/expander power: 0.05 MW, 1.08%
Fuel cell power: 1.49 MW, 29.76%
System electrical power: 1.55 MW, 30.84%
Thermal power available: 2.72 MW, 54.33%
Overall system efficiency: 4.27 MW, 85.17%
From the steady state analysis, the electrical system efficiency ($\eta_{\text{EL,sys}}$) for the 1.5 MW$_e$ and 1.7 MW$_e$ SPFC marine system were calculated to be 29.86% and 28.85% respectively. With 1% decrease in electrical system efficiency, the SPFC stack delivered $\approx 13\%$ more stack power and improved the system performance in overcoming the marine hotel load. This operational flexibility and modular design of the fuel cell would meet the specific requirements of the marine vessel in terms of replacing the current diesel power source on board a vessel.

The SPFC marine system has also low grade thermal power available (54%), which could be used on board a vessel. If the low grade thermal power was recuperated through a network of heat exchangers, then the overall system (combined heat and power) efficiency of 85% could be achieved. Beside the high system efficiency of the SPFC system, the marine SPFC system also offers many further advantages over the internal combustion engines. Some of these advantages of the SPFC system as previously mentioned are high efficiency, lower emissions, low noise and thermal signal, modular flexibility and potential of using a multiple fuel processor to supply the hydrogen.

5.5 SUMMARY OF RESULTS

1. The operating condition for the diesel thermal Partial Oxidation (PoX) reformer were established as 800°C, 3 bar(a), O:C ratio of 1 and S:C ratio of 1. At these operating conditions, the PoX reformer produced 26% hydrogen (on a wet basis) and the reactor efficiency, $\eta_{\text{Ref}}$, of 99.11%. The fuel processor efficiency ($\eta_{\text{FP}}$) was calculated to be 87% at 1.5 MW$_e$ SPFC stack power.

2. A parametric model of the SPFC was used to predict the performance of the SPFC as a function of many variables such as temperature, pressure, ($H_2$, $O_2$) concentrations etc. At 1.5 MW$_e$ SPFC stack power, the operating conditions for the stack were determined as (Anode and cathode stoichiometry of 1.5 and 2 respectively):
Cell Voltage = 0.727 Volts/cell
Current Density = 0.5 A/cm²
Number of Cells = 20500
SPFC Stack efficiency ($\eta_{Th}$) = 58%

1. The isentropic efficiency of the compressor and expander were both taken as 80% respectively.

2. A traction battery model was used to predict the performance of a high temperature Lead Acid battery. The battery pack consisted of 80 dockyard exchange modules (DEM) and had an energy density of 80 Wh/kg. The total weight of the batter pack was 36 tonnes.

3. An adiabatic model was used to estimate the exit temperature of the flue gases from a burner combusting SPFC stack exhaust (anode & cathode) gases. The exit temperature of the flue gases was estimated to be 746 K (473°C).

4. The simulation was run for 30 hrs and at the end of 24 hrs i.e. one day load cycle, the SoC of the battery was down to 45% and not > 80%, as anticipated by the control strategy. The battery had also discharged to a minimum SoC of 24% during the first 24 hrs cycle.

5. To protect the battery from discharging to SoC of <25% daily, the SPFC Stack operating point was changed to supply 1.7 MWₑ at system peak demanded. With increased stack power (i.e. lowering of $\eta_{Th} = 58\%$ to 56%), the battery did not discharge below 50% at the peak load demanded and the SoC of the battery was > 80% at the end of the first hotel load cycle. However, the system electrical efficiency ($\eta_{El,Sys}$) decreased by 1% from 31% to 30% at peak SPFC stack power.

6. During the warm-up period (= ½ hrs) the battery supplied all the power demanded during this warm-up period and therefore discharging rapidly to SoC of approx. 50%. The battery also supplied the parasitic power load of the compressor, which was approx. 0.1 MW.
7. For a 1.5 MW SPFC system with a diesel fuel processor, the electrical system efficiency was calculated to be 31%. (30% for 1.7 MW_e SPFC system). This system had the following system configurations and components performance:

- The reformer reactants and the HTS reactor's water were pre-heated to 250°C.
- The stack exhaust gas (anode & cathode) streams condensed before feeding them to the burner (25°C).
- Fuel processor efficiency = 87%
- SPFC Stack efficiency ($\eta_{th}$) = 58%
- Anode and cathode stoichiometry of 1.5 and 2 respectively.
- Compressor and expander isentropic efficiency = 80%
5.6 REFERENCES

23. ASPEN PLUS™ (chemical engineering modelling software package), Aspen Technology Inc. (Aspen Tech), Release 9.3-1, 1996, 10 Canal Park, Cambridge, MA 02141, USA.


25. Amphelt 1

26. Amphelt 2


6. CONCLUSIONS AND RECOMMENDATIONS

6.1 CONCLUSIONS

➢ A detailed study of solid polymer fuel cell (SPFC) power system for transport and stationary applications has been carried out. This work has shown the importance of system configuration and thermal integration to achieve the desired optimal system performance. The study has also revealed the significance of understanding how the various components of a SPFC power system interact and that system optimisation requires a systematic analysis of many parameters.

➢ Steady state models of a natural gas (40 kW_e), methanol (50 kW_e) and diesel (1.5 MW_e) fuelled SPFC power system have been developed and employed to analyse and optimise the performance of these systems for stationary and transport applications. A dynamic simulation tool of a SPFC power system has also been developed and used to predict the performance of SPFC systems under different control strategies and various load profiles. The tool has the potential to incorporate different fuel processor technologies and hydrogen storage systems. Hence, the dynamic simulation tool can be applied to stationary, transport and portable SPFC systems.

➢ For each system, the fuel processor data was established based on thermodynamic equilibrium models. The process variables, such as steam to carbon ratio, operating pressure and temperature, critical to the performance of the fuel processor were investigated and determined. For other components, where the measured data were not available, realistic values were obtained to reflect possible future performances. However, these values were varied in order to understand the effect on electric and overall system efficiency.

➢ The choice of fuel had significant impact on the performance of the SPFC power system. The analyses of two different SPFC systems with different fuel feedstocks, but similar fuel processing technology (i.e. steam reforming), showed that a methanol fuelled thermally integrated SPFC system achieved a higher
electrical system efficiency ($\eta_{EI_{sys}}$) of 52\% compared to a natural gas fuelled SPFC system ($\eta_{EI_{sys}}=42\%$). The same SPFC thermal ($\eta_{Th}$) and compressor/expander efficiencies, of 68\% and 80\% respectively, were employed in both these analyses. The higher efficiency of the methanol fuel processor $\eta_{FP}=99\%$ ($\eta_{Ref}=82\%$), compared to the natural gas fuel processor of 72\% ($\eta_{Ref}=67\%$) was responsible for achieving a superior electrical system efficiency ($\eta_{EI_{sys}}$).

The type of fuel processor technology used in a SPFC power system had a great influence on the configuration, thermal integration and performance of the system. In a diesel fuelled SPFC system with a partial oxidation reactor, the anode and cathode stack exhaust could not be utilised within the fuel processing process to potentially reduce consumption of fuel feedstock and increase the overall efficiency. However, a separate burner was employed to burn the exhaust gases and use the thermal power of the flue gas to generate electric power via an expander. In a natural gas fuelled SPFC system, the reformer burner was an integral part of the fuel processor and the exhaust gases were burnt to provide the necessary thermal power for the reforming process and waste heat recovery equipments. For the same SPFC stack thermal efficiency ($\eta_{Th}=58\%$), the $\eta_{EI_{sys}}$ for the diesel fuelled system was determined to be 31\%, while a natural gas fuelled system with a steam reformer achieved a $\eta_{EI_{sys}}$ of 35\%. However, a SPFC system with a partial oxidation reactor offered a reduced system complexity and the prospect of faster dynamic response due to the absence of a recycle loop for the spent stack fuel and oxidant gases.

A 40 kW$_e$ natural gas based SPFC combined heat and power (CHP) system maximised the use of thermal power, via waste heat recovery apparatus, to achieve an overall system efficiency of greater than 80\% ($\eta_{EI_{sys}}=42\%$, $\eta_{HI_{sys}}=47\%$). Conversely, in a SPFC vehicle system, the goal of the system designer is to minimise the system size and maximise the electrical system efficiency. A 50 kW methanol based SPFC vehicle system achieved an electrical system efficiency of 52\% with 31\% of the thermal power rejected by the cooling system and 16\% as exhaust heat.
A 40 kW_e natural gas based SPFC combined heat and power (CHP) system was used to investigate the impact of varying the parameters of various components and thermal integration on the overall performance of the system. The main objective of this study was to achieve a heat to power ratio ($R_{\text{HUP}}$) of one, and an overall efficiency ($\eta_{\text{Overall}}$) of greater than 80%. The main conclusions of this investigation are as follows:

1) A SPFC CHP system without thermal integration and reactant (reformer & burner) pre-heating (25°C) achieved electric and heat efficiencies of 27.7% and 62.2% respectively. The overall efficiency and the heat to power ratio were determined to be 89.9% and 2.24 respectively. The fuel processor ($\eta_{\text{FP}}$) and SPFC thermal ($\eta_{\text{Th}}$) efficiencies for this system were 55.2% and 55% respectively. Pre-heating the reactants to 800°C, via thermal integration, improved the electric efficiency to 34% and decreased the heat efficiency to 53%. Although the overall system efficiency decreased to 87%, the heat to power ratio improved to 1.57. The use of waste heat to pre-heat the reactants to 800°C resulted in lower consumption of the processed natural gas and improved the $\eta_{\text{FP}}$ by a factor of $\approx 1.3$ to 74.5%.

2) The effect of either pre-heating or condensing the anode and cathode exhaust gas streams on the SPFC CHP system was also investigated. A thermally integrated SPFC CHP system (i.e. reactants preheated to 800°C) achieved the best heat to power ratio and $\eta_{\text{EL_SYS}}$ of 0.69 and 41% respectively with only pre-heating the exhaust gas streams. However, for this system the overall efficiency was < 80% (69%). The combination of both condensers and heat exchangers (for the pre-heating process) achieved the best system performance of $\eta_{\text{Overall}}$ of 82% and $R_{\text{HUP}}$ of 1. However, the thermal energy in the flue gases was depleted in the process and the condenser economiser recovered no waste heat from the flue gases. For a SPFC CHP system, where the high and low grades of heat are necessary, the system with only condensers for exhaust gas streams was ideal. This system achieved an $\eta_{\text{Overall}}$ of 87% and $R_{\text{HUP}}$ of 1.5 and delivered both high and low grades of heat. The trend seen in this investigation was that the initial fuel consumption in the system was reduced
with use of the condenser and/or pre-heater. This improved the heat to power ratio, fuel processor and electrical efficiencies, but heat and overall efficiencies were reduced.

3) SPFC operating parameters were also varied to study the effect on the overall system performance. The $\eta_{\text{Overall}}$ remained approximately constant, but the $R_{(H/P)}$ improved significantly from 2.8 to 1.5 as the stack operating pressure increased from 1 to 3 bar(a). The SPFC thermal efficiency increased (from 45% to 58%) as pressure increased and hence, the system became more electrically efficient (23% to 34%). The fuel processor efficiency remained approximately constant, while both the compressor and expander power increased (at a constant isentropic efficiency of 80%). The optimal system performance was at 3 bar(a) where the overall efficiency of > 80% and heat to power ratio of 1.53 were achieved.

4) The $\eta_{\text{Overall}}$ improved by approximately 1% as the cathode stoichiometry increased from 1.2 to 2.0. However, the $R_{(H/P)}$ improved from 3.74 to 1.53 as the stoichiometry increased to 2. As the cathode stoichiometry increased (from 1.2 to 2.0) the SPFC stack became more efficient and the fuel processor efficiency decreased. The parasitic load imposed upon the system by the compressor decreased with the increase in the cathode stoichiometry. This was due to inefficiency of the SPFC stack at lower cathode stoichiometry (i.e. low voltage hence higher current), which demanded more air (higher flowrate) from the compressor. The advantage of using a stoichiometry > 2.0 was minimal compared to the performance of the system at stoichiometry ≤ 2.0 (improvement to SPFC performance was marginal compared to the higher parasitic load at stoichiometry of 2.5)

5) For both high (3 bar(a)) and low (1.25 bar(a)) operating pressures, the system performance improved as the compressor and the expander became more efficient. However, at high pressure, both the system's electrical (27%-38%) and heat (60%-49%) efficiencies improved significantly as the isentropic efficiency varied from 30% to 100% compared to a system operating at low
pressure (27%-30% and 60%-57%). Although the overall system efficiency remained approximately constant, the heat to power ratio improved significantly, in particularly for the high pressure system (2.3-1.3). However, the desired heat to power ratio of 1 could not be achieved, even if the isentropic efficiency of both compressor and expander was 100%.

6) The performance of both high and low pressure SPFC CHP system without the expander (expander isentropic efficiency=0, electric motor efficiency=90% and compressor isentropic efficiency=80%) were substantially affected. For a high pressure system, the electrical efficiency decreased by 19% and the heat to power ratio increased to 2 from 1.5. This was due to the redistribution of the flue gas thermal power from the expander to waste heat recovery system. Hence, the presence of compressor/expander in the SPFC CHP system is crucial in achieving a reasonable and competitive performance.

7) A SPFC CHP system was investigated with a predicted future SPFC efficiency ($\eta_{TH}$) improvement of 15%-18% and reduced anode stoichiometry (1.5 to 1.2). The improvement in the SPFC stack efficiency from 58% to 68%, increased the electrical efficiency from 35% to 42% and decreased the heat efficiency from 52% to 47%. The overall system efficiency and the heat to power ratio also improved from 86.6% to 88% and 1.51 to 1.1 respectively. Although the "future" SPFC CHP system did not achieve the desired heat to power ratio of one, both the overall system efficiency and heat to power ratio further improved. With additional improvement in the fuel cell efficiency, the desired performance for the service industry application could easily be achieved.

8) The optimisation study of the SPFC CHP system indicated that with better thermal integration and efficient components, the system could achieve an overall efficiency ($\eta_{Overall}$) of ≥ 80% and heat to power ratio ($R_{(H/P)}$) of one. The study also showed that the system designer has the flexibility and choice of using various components to achieve or fulfil the design criteria when designing the SPFC CHP system for a particular industrial or residential application.
A 50 kW_e methanol fuelled SPFC vehicle system was used to analyse the overall system performance for transport applications. The power generator of the electric vehicle included a fuel processor (methanol steam reformer and a gas clean-up unit), a SPFC stack, a compressor and an expander. The aim of the study was to achieve electrical system efficiency ≥ 45%. The main conclusions of this investigation are:

1) A SPFC vehicle system without any thermal integration achieved an electric system efficiency (\( \eta_{\text{EL,sys}} \)) (pre-drivetrain) and vehicle efficiency (\( \eta_{\text{veh}} \)) of 43.8% and 38.4% respectively. The Fuel processor (\( \eta_{\text{FP}} \)), SPFC thermal (\( \eta_{\text{Th}} \)) and drivetrain efficiencies (\( \eta_{\text{O_d}} \)) for this system were determined to be 82%, 68% (anode stoichiometry = 1.2) and 90% respectively. From the overall power balance (pre-drivetrain) of power/coolant/exhaust = 44/44/12%, it was evident that the 44% coolant or waste heat power had to be utilised to optimise the system performance and attain the desired electric system efficiency. (The power/coolant/exhaust representing % electrical power for mechanical work, % coolant power removed by the cooling system and % exhaust power removed from the system as unusable power).

2) A thermally integrated SPFC vehicle system with condensers achieved an electric system efficiency, \( \eta_{\text{EL,sys}} \), (pre-drivetrain) of 52.24% and a competitive vehicle efficiency of 45.74%. For this thermal integrated system, the fuel processor efficiency (\( \eta_{\text{FP}} \)) was improved from 82% to 99%. This improvement in efficiency was achieved by minimising the total fuel power to the system (95.7 kW from 114.2 kW) via thermal integration. The overall power balance of this system was determined to be power/coolant/exhaust = 52.2/31.4/16.4%. Although the desired electrical efficiency of >45% was achieved, a large amount of low grade heat power and poor quality exhaust power was unusable.

3) A SPFC vehicle system, operating at low pressure (1.25 bar(a)), achieved an electric system efficiency, \( \eta_{\text{EL,sys}} \), of 39.1% (pre-drivetrain) and a vehicle efficiency of 34.26%. The overall power balance for the lower pressure system
was calculated to be power/coolant/exhaust = 39.1/42.2/18.7%. Compared to the high pressure system (52.2/31.4/16.4%), nearly 61% of the fuel power was converted to thermal power. This was due to the inferior SPFC efficiency ($\eta_{Th}$ = 54%) at lower pressure, which was mainly responsible for the large percentage of coolant power.

4) Compared to current ICE (33/33/33%), a methanol fuelled thermally integrated SPFC vehicle system (with condensers) has a superior performance (52.2/31.4/16.4%) and the potential of competing with future IC and hybrid engines. However, for the fuel cell hybrid vehicle to make any impact in the automobile market, the manufacturing cost of the vehicle should be reduced in order to be competitive with IC vehicles and the fuel infrastructure available. Furthermore, the SPFC vehicle system should be well designed and integrated into a vehicle similar in size to current IC automobiles (i.e. the system volume and weight should be minimised).

> A simulation program was developed to specify components (at the design stage) and assess the performance of an electric traction system for a 4.6 tonne delivery hybrid van and compare measured and simulated results. The brass-board hybrid van system consisted of two major parts, the power generator and the electric drivetrain. The power generator consisted of a methanol steam reformer, gas clean-up unit, air compressor and SPFC system. The drivetrain consisted of an up-chopper (dc/dc converter), Ni-Cd battery pack (15 kWh), a 60 kW electric motor system (motor, controller & inverter) and vehicle controller. The maximum mechanical power specified for the brass-board system was 60 kW, of which the SPFC stack could provide a maximum of 16 kW_e.

The hybrid van performance specifications (i.e. acceleration test, constant speed test and drive cycle) were translated into seven duty cycles. The simulation program was used to simulate these seven duty cycles and predict the performance of the Brass-Board hybrid van and its components. The predicted performance was then compared to the actual brass-board system (without the fuel processor)
performance, on the seven drive schedules. The following conclusions are drawn from this simulation study:

1) All tests except the constant speed and Leicester drive cycle tests, were successfully completed with the actual brass-board system. The constant speed on the actual brass-board system was not completed due to battery overheating (>43°C). The Leicester drive cycle was prematurely terminated because the supervisory control unit (SCU) had failed to react when some parameters reached their maximum values (battery temperature and voltage).

2) The models in the simulation tool predicted the operational characteristic of each component very accurately. The results for the seven drive cycle tests from the simulation tool correlated to within 2-3% when compared to results from the actual system.

A dynamic simulation of the SPFC hybrid system was developed using Matlab/Simulink to study the component interactions between a 1.5 MW SPFC system, diesel fuel processor and 8448 kWh (C5 rate) battery pack. The objective of this simulation study was to investigate if the power delivered from the SPFC stack was capable of maintaining the battery SoC ≥ 80%, during and at the end of the duty cycle (ship hotel load). A steady state model was also developed to determine the overall system performance of an integrated system at peak fuel cell stack power (i.e. 1.5 MWe). The following conclusions are drawn from both these analyses:

1) In the dynamic simulation study the hotel load profile was designed to demand 2 MWₑ at peak hours (8-10 A.M. & 6-9 P.M.) and minimum power (1 MWₑ), demanded from 11 P.M. to 5 A.M. and 2 P.M. to 5 P.M. The simulation was run for 30 hrs and at the end of 24 hrs (i.e. one day load cycle), the SoC of the battery was down to 45% and not > 80%, as anticipated by the control strategy. However, during the first two hours of the next duty cycle the SoC of the battery was > 80% and the hybrid power source of the SPFC stack and
battery was sufficient to meet the remainder of the second day's hotel load demand.

2) To protect the battery from discharging to an SoC of <25% daily, the SPFC Stack operating point was changed to supply 1.7 MW\textsubscript{e} at system peak demanded. With increased stack power (i.e. lowering of $\eta_{\text{Th}} = 58\%$ to 56%), the battery did not discharge below 50% at the peak load demanded and the SoC of the battery was > 80% at the end of the first hotel load cycle. Hence, the increase in stack power achieved the desired SoC of > 80% at the end of every hotel load profile (24 hrs). However, the system's electrical efficiency ($\eta_{\text{el Sys}}$) decreased by 1% from 31% to 30% at peak SPFC stack power.

3) A 1.5 MW SPFC marine system, with a diesel fuel processor, achieved an electrical system efficiency of 31%. The Fuel processor ($\eta_{\text{FP}}$) and SPFC thermal ($\eta_{\text{Th}}$) efficiencies for this system were 87% and 58% respectively. The compressor and expander isentropic efficiency, used in the analysis, was 80% and the system reactants were pre-heated to 250°C. If the low grade thermal power (54%) was recuperated through a network of heat exchangers, then the overall system (combined heat and power) efficiency of 85% could be achieved. (The electrical efficiency for a 1.7 MW SPFC system was reduced by 1% to 30%).

Finally, table 6.1 summaries the performance of the three different thermal integrated SPFC power systems for stationary and transport applications.

6.2 RECOMMENDED FUTURE WORK

To make a complete assessment of a SPFC power system performance and judge the merits of this performance against conventional and commercially available power systems, the present steady state and dynamic system analysing tools would require development and implementation of additional models. These additional models
would aid in evaluating the environmental and economical benefits of the SPFC system, for both stationary and transport applications.

Table 6.1: Summary of performance of the three different SPFC power systems

<table>
<thead>
<tr>
<th>System Parameters</th>
<th>SPFC Power Systems</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>40 kW Natural Gas</td>
</tr>
<tr>
<td></td>
<td>50 kW Methanol</td>
</tr>
<tr>
<td></td>
<td>1.5 MW Diesel</td>
</tr>
<tr>
<td></td>
<td>based system</td>
</tr>
<tr>
<td>Reform Efficiency, ( \eta_{Ref} ), (%)</td>
<td>69 69</td>
</tr>
<tr>
<td>Fuel Processor Efficiency, ( \eta_{FP} ), (%)</td>
<td>82 72</td>
</tr>
<tr>
<td>SPFC Thermal Efficiency, ( \eta_{Th} ), (%)</td>
<td>58 68</td>
</tr>
<tr>
<td>Cathode Stoichiometry</td>
<td>2 2</td>
</tr>
<tr>
<td>Anode Stoichiometry</td>
<td>1.5 1.2</td>
</tr>
<tr>
<td>Compressor Isentropic Efficiency, (%)</td>
<td>80 80</td>
</tr>
<tr>
<td>Expander Isentropic Efficiency, (%)</td>
<td>80 80</td>
</tr>
<tr>
<td>Electrical Efficiency, ( \eta_{El Sys} ), (%)</td>
<td>35 42</td>
</tr>
<tr>
<td>Heat Efficiency, ( \eta_{Heat Sys} ), (%)</td>
<td>52 47</td>
</tr>
<tr>
<td>Heat to Power Ratio, (R_{H/P})</td>
<td>1.5 1.1</td>
</tr>
<tr>
<td>Overall System Efficiency, ( \eta_{Overall} ), (%)</td>
<td>87 88</td>
</tr>
</tbody>
</table>

Note: A fuel processor efficiency of >100% is possible as they are defined as the ratio of LHV of the anode feed to LHV of the fuel feedstock.

Hence, the following future work is recommended:

1) Development of fuel processor and compressor/expander models with actual component performance data, size, weight and transient and dynamic characteristics.

2) Development of an emission model to predict the transient and steady state emissions of a SPFC power system, including a fuel processor, under realistic duty cycles.

3) Development of an economical appraisal model to assess the viability of the SPFC power system and predict the overall energy cost savings and payback period.
APPENDIX I - Mathematical Models

Electrochemistry of the SPFC — (Thermodynamics & Electrode Kinetics)

A fuel cell is an electrochemical system in which the chemical energy of a fuel is converted directly into electrical energy in the presence of an oxidant. In the SPFC, hydrogen and oxygen (usually from the air) are the reactants. When hydrogen is consumed in the anode side of the SPFC by the following half reaction (figure 2.2):

\[ \text{H}_2 \rightarrow 2\text{H}^+ + 2e^- \quad E^\circ = 0.0 \text{ volts} \quad \cdots (1) \]

From this half reaction equation (1), it can be observed that for each mole of hydrogen consumed results in two moles of electrons, which flows (i.e. current) via the external circuit to the cathode side. Beside the electrons \(2e^-\), the hydrogen ions \(2\text{H}^+\) also flow through the electrolyte to the cathode side, where they combine with oxygen molecules to produce water according to the following half equation:

\[ \frac{1}{2} \text{O}_2 + 2\text{H}^+ + 2e^- \rightarrow \text{H}_2\text{O} \quad E^\circ = +1.23 \text{ volts} \quad \cdots (2) \]

or

\[ \frac{1}{2} \text{O}_2 + 2\text{H}^+ + 2e^- \rightarrow \text{H}_2\text{O} \quad E^\circ = +1.18 \text{ volts} \quad \cdots (3) \]

The standard theoretical reversible cell potential \(E^\circ_{\text{rev}}\) or the e.m.f (electromotive force) of the overall cell reaction (i.e. the potential when there is no flow of current and the cell is operating reversibly) is calculated using the half equations (1,2,3):

For water as the liquid product:

\[ \frac{1}{2} \text{O}_2 + 2\text{H}^+ + 2e^- \rightarrow \text{H}_2\text{O} \quad E^\circ = 1.23 \text{ V} \]

\[ \text{H}_2 \rightarrow 2\text{H}^+ + 2e^- \quad E^\circ = 0.00 \text{ V} \]

\[ \text{H}_2 + \frac{1}{2} \text{O}_2 \rightarrow \text{H}_2\text{O} \quad E^\circ_{\text{rev}} = 1.23 \text{ V} \quad \cdots (4) \]

For water as the vapour product:

\[ \frac{1}{2} \text{O}_2 + 2\text{H}^+ + 2e^- \rightarrow \text{H}_2\text{O} \quad E^\circ = 1.18 \text{ V} \]

\[ \text{H}_2 \rightarrow 2\text{H}^+ + 2e^- \quad E^\circ = 0.00 \text{ V} \]

\[ \text{H}_2 + \frac{1}{2} \text{O}_2 \rightarrow \text{H}_2\text{O} \quad E^\circ_{\text{rev}} = 1.18 \text{ V} \quad \cdots (5) \]
The maximum available electrical energy from a SPFC operating at constant temperature and pressure is given by

\[ W_{\text{elec}} = \Delta G^\circ = n F E_{\text{rev}}^\circ \]

Where,
\[ \Delta G^\circ \] - Gibbs free energy change for the reaction (4) or (5) at 25°C, kJ/mol
\[ n \] - the number of moles of electrons transferred in the reaction (4) or (5), \( n = 2 \)
\[ F \] - Faraday Constant, \( F = 9.64846 \times 10^4 \), C/mol

The change in enthalpies (i.e. the heat of combustion for hydrogen) for one mole of hydrogen reacted in reaction (4) and (5) is given by \( \Delta H^\circ_{\text{HHV}} \) (kJ/mol) and \( \Delta H^\circ_{\text{LHV}} \) (kJ/mol) respectively. (HHV – High heating value & LHV- Lower heating value)

Hence, if all the free energy change in a SPFC is available as electrical energy, then the maximum efficiency for reaction (4) or (5) is given by

\[ \eta_{\text{rev}} = \frac{\Delta G^\circ}{\Delta H^\circ} = \frac{n F E_{\text{rev}}^\circ}{(\Delta H^\circ_{\text{HHV}} \text{ or } \Delta H^\circ_{\text{LHV}})} \]

In addition, not all energy of the fuel is converted into electricity and hence, according to second law of thermodynamics, it can be shown that the heat absorbed (from the surrounding by a fuel cell operating isothermally and at constant pressure) by a reversible cell is equal to

\[ Q_{\text{rev}} = T \Delta S^\circ = \Delta H^\circ - \Delta G^\circ \]

Where,
\[ \Delta S^\circ \] - Entropy change for the reaction at temperature T
\[ \Delta H^\circ \] - Enthalpy change for the reaction, which could be HHV or LHV

Depending on the magnitude and direction of the entropy change (\( \Delta S^\circ \)), the heat flow either is to surrounding or absorbed by the cell. For a practical SPFC, the \( \Delta S^\circ \) is negative and therefore the heat will be released from the fuel cell to the surrounding. The calculated values of \( \eta_{\text{rev}} \) and \( Q_{\text{rev}} \) for reaction (4) and (5) are summarised below:
In practical SPFC, when a net current, I, is drawn, the reversible cell voltage or the open circuit voltage $E_{\text{rev}}^0$ drops and the new cell voltage, $E_{\text{cell}}$, is established at that current. The amount by which the $E_{\text{rev}}^0$ drops depends on amount of current drawn from the cell and the in the cell (activation, concentration and ohmic) losses (section 2.2.1.1). The mathematics model to calculate the cell voltage, $E_{\text{cell}}$, is described in section 5.2.2.

Now, the cell current, I, is directly related to the hydrogen molar flowrate ($\dot{M}_{H_2}$) and the relationship in given the following equation:

$$I = \dot{M}_{H_2} \times L \times 2e = \dot{M}_{H_2} \times F \times 2$$

Where,

$$L = 6.02205 \times 10^{23} \text{ mol}^{-1} \text{ (Avogadro constant)}$$
$$e = 1.60219 \times 10^{-19} \text{ C \ (Electron charge)}$$
$$F = L \times e = 9.64846 \times 10^4 \text{ C/mol \ (Faraday Constant)}$$

The molar flowrate of the oxygen, ($\dot{M}_{O_2}$), from reaction (4) or (5) is given by

$$\dot{M}_{O_2} = \frac{1}{2} \times \dot{M}_{H_2}$$
The electrical power out of the SPFC is calculated by

\[ P_{\text{SPFC}} = I \times E_{\text{cell}} = (\dot{M}_{H_2} \times F \times 2) \times E_{\text{cell}} = \dot{M}_{H_2} \times \Delta G^o \]

For current, \( I \), the hydrogen energy per second (hydrogen power) flowing into the SPFC is calculated by

\[ P_{H_2} = \dot{M}_{H_2} \times \Delta H^o_{\text{LHV}} \text{ or } P_{H_2} = \dot{M}_{H_2} \times \Delta H^o_{\text{HHV}} \]

Hence, the thermal efficiency of the SPFC operating at cell voltage and current of \( E_{\text{cell}} \) and \( I \) respectively, is given by

\[
\eta_{\text{Th}}(\text{LHV}) = \frac{P_{\text{SPFC}}}{P_{H_2}} = \frac{E_{\text{cell}} \times I}{\dot{M}_{H_2} \times \Delta H^o_{\text{LHV}}} = \frac{\dot{M}_{H_2} \times F \times 2 \times E_{\text{cell}}}{\dot{M}_{H_2} \times \Delta H^o_{\text{LHV}}} = \frac{E_{\text{cell}}}{1.25}
\]

\[
\eta_{\text{Th}}(\text{HHV}) = \frac{P_{\text{SPFC}}}{P_{H_2}} = \frac{E_{\text{cell}} \times I}{\dot{M}_{H_2} \times \Delta H^o_{\text{HHV}}} = \frac{\dot{M}_{H_2} \times F \times 2 \times E_{\text{cell}}}{\dot{M}_{H_2} \times \Delta H^o_{\text{HHV}}} = \frac{E_{\text{cell}}}{1.48}
\]

In addition, the SPFC voltage efficiency is also defined as

\[
\eta_{V}(\text{LHV}) = \frac{E_{\text{cell}}}{E_{\text{rev}}^o} = \frac{E_{\text{cell}}}{1.18}
\]

\[
\eta_{V}(\text{HHV}) = \frac{E_{\text{cell}}}{E_{\text{rev}}^o} = \frac{E_{\text{cell}}}{1.23}
\]

The typical operating cell voltage for a practical SPFC system range from 0.6 to 0.85, then the LHV thermal and voltage efficiencies will range from 48% to 68% and 51% to 72% respectively. The rest of energy of the fuel in a practical fuel cell is released as heat, which is much greater than \( Q_{\text{rev}} \). Most of this heat or thermal energy is removed by a cooling system in a practical SPFC. However, a better way to analysis the performance of a practical cell or stack is to perform a heat and mass balance on the
cell or stack. The heat and mass balance analysis shows the actual percentage of the total hydrogen power produced as electrical power, removed in the anode and cathode stream and by the cooling system. An example of heat and mass balance is shown in section 3.3.3.

Relative Humidity Calculations for SPFC

The performance of the SPFC improves with humidification of the feed gases, particularly the cathode feed gas. However, the water management inside the cell also affects the performance of the cell and therefore calculating the relative humidity of both the feed and exhaust gases is crucial in understanding how SPFC performances under these operating conditions.

The relative humidity ($\phi$) is defined as the ratio of the actual partial pressure ($P_a$) of the vapour to the partial pressure ($P_s$) of the vapour when the air (or feed or exhaust gases) is saturated at the same temperature. (Ref: Engineering Thermodynamics...Book by Rogers & Mayhew – 3rd Edition).

$$\phi = \frac{P_a}{P_s}$$

To illustrate how to calculate the relative humidity of either a feed or exhaust gases, the following operating conditions of the SPFC and an example of a cathode exhaust gas (mixture of oxygen, nitrogen & water) will be used:

- **SPFC Operating temperature** $= T_{fc}$ (K)
- **SPFC Operating Pressure** $= P_{fc}$ (Bar)
- **Total Molar flowrate of the Cathode** $= M_t$ (mol/s)
- **Molar flowrate of water in cathode stream** $= M_w$ (mol/s)

Now, the actual partial pressure of the water or vapour in the cathode stream is
Assuming the cathode gases exiting the SPFC at same temperature \( T_{fc} \) as the cell, then the partial pressure \( (P_s) \) of the vapour when cathode exhaust gases is saturated at the SPFC temperature, \( T_{fc} \), is calculated using the Clausius-Clapeyron equation. This equation gives similar values as the steam tables. \( \text{(Ref.: Physical Chemistry Book by P. W Atkins - 3rd Edition).} \)

\[
P_s = P_{ref} \times \text{Exp} \left[ - \left( \frac{\Delta H_{vap}}{R} \right) \times \left( \frac{1}{T_{fc}} - \frac{1}{T_{ref}} \right) \right]
\]

Where,

- \( P_{ref} \) - Reference pressure = 1 atm = 1.01325 bar
- \( T_{ref} \) - Reference temperature = Boiling point of water = 373.15 K
- \( \Delta H_{vap} \) - Standard molar enthalpy of vaporisation = 40.62 kJ/mol
- \( R \) - Gas Constant = 8.3145 J/molK

Hence, the relative humidity of the cathode exhaust gas is then given by

\[
\phi = \frac{P_a}{P_s} = \frac{\left( \frac{M_w}{M_t} \right) \times P_{fc}}{P_{ref} \times \text{Exp} \left[ - \left( \frac{\Delta H_{vap}}{R} \right) \times \left( \frac{1}{T_{fc}} - \frac{1}{T_{ref}} \right) \right]}
\]

From this relationship, it can be concluded that, if \( (P_a \geq P_s) \) then the relative humidity \( \phi \geq 100\% \) and gas stream will be mixture of liquid and vapour phase. When the \( \phi < 100\% \) than the gas stream is all in vapour phase. Using the same equation, but different operating conditions, the relative humidity of the anode exhaust, anode and cathode feeds can also be calculated.
From the relative humidity calculation, the phase of the gas stream can be known, however, to calculate the vapour or water content of the gas mixture, a humidity ratio or specific humidity of the mixture is required. Humidity ratio or specific humidity, \( \omega \), is defined as the ratio of the mass of the water vapour (\( m_a \)) to the mass of dry exhaust or feed gases (\( m_g \)) in any given volume \( V \) of the mixture. Hence,

\[
\omega = \frac{m_a}{m_g}
\]

Assuming that both the water vapour and cathode gases are perfect gases and using the ideal gas law (\( PV = nRT \)), then

For given volume, \( V \) and constant temperature \( T_{fc} \),

\[
M_a = \frac{(MW_a P_a V)}{(RT_{fc})} \quad \text{and} \quad M_g = \frac{(MW_g P_g V)}{(RT_{fc})}
\]

Where,

- \( P_g = (P_{fc} - P_s) \) — the partial pressure of the dry cathode gases
- \( MW_a \) — Molecular weight of the actual water or vapour
- \( MW_g \) — Molecular weight of the dry cathode gases (\( O_2, N_2 \))

\[
\omega = \frac{m_a}{m_g} = \frac{MW_a \times P_a}{MW_g \times P_g} = \left( \frac{MW_a}{MW_g} \right) \times \left( \frac{P_s}{P_{fc} - P_s} \right)
\]

Note: Usually for air and vapour this relationship is given as \( \omega = (0.622) \times (P_s/(P-P_s)) \), where 0.622 is ratio of molecular weight of water to that of air (18/29) and \( P_s, P \) are the partial pressure of the vapour and total pressure respectively.

Now, if \( \phi = 100\% \) then

\[
\omega(100\%) = \left( \frac{MW_a}{MW_g} \right) \times \left( \frac{P_s}{P_{fc} - P_s} \right)
\]
If $\phi < 100\%$ (all vapour phase) then

$$\omega_{(<100\%)} = \left( \frac{MW_a}{MW_g} \right) \times \left( \frac{P_s}{P_{fc} - P_s} \right)$$

If $\phi > 100\%$ (vapour & liquid phase) then

For vapour $\omega_{(vap)} = \omega_{(100\%)}$

For Liquid $\omega_{(vap)} = \omega_{(<100\%)} - \omega_{(100\%)}$

> Chemical and Thermal Power Calculations

To perform a heat balance on various components of the SPFC system at steady state condition, chemical and thermal power calculations of each individual inlet and outlet stream need to be carried out. These chemical and thermal power calculations are calculated using the following equations:

Chemical Power of the working fluid – mainly for combustible fuels

$$P_{Ch} = \dot{M} \times \Delta H^\circ$$

Where,

$P_{Ch}$ - Chemical power of the working fluid (kW)
$\dot{M}$ - Molar flowrate of the working fluid in the stream (mol/s)
$\Delta H^\circ$ - Enthalpy of the working fluid, which could be HHV or LHV

Thermal Power of the working fluid

$$P_{Th} = \dot{M} \int_{T_1}^{T_2} Cp \, dT$$

Where,

$Cp = a + bT + c/T^2$ - Molar heat capacity as a function of temperature (kJ/mol K)
$T_1, T_2$ - Absolute temperatures (K) for operating condition 1 & 2
The table below shows values of constant $a$, $b$, $c$ for the molar heat capacity and calculation of $C_{pdT}$ at 353 K (SPFC operating temperature). The enthalpy ($\Delta H$) values for some combustible fuels used in SPFC system analyses are also shown in the table below.

<table>
<thead>
<tr>
<th>Fluids</th>
<th>$a$ (J/Kmol)</th>
<th>$b$ (J/K$^2$mol)</th>
<th>$c$ (JK/mol)</th>
<th>Temp (K)</th>
<th>$C_{pdT}$ (J/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_2$</td>
<td>2.73E+01</td>
<td>3.26E-03</td>
<td>5.00E+04</td>
<td>3.53E+02</td>
<td>1580.582</td>
</tr>
<tr>
<td>CO</td>
<td>2.84E+01</td>
<td>4.10E-03</td>
<td>-4.60E+04</td>
<td>3.53E+02</td>
<td>1606.984</td>
</tr>
<tr>
<td>CO$_2$</td>
<td>4.42E+01</td>
<td>8.79E-03</td>
<td>-8.62E+05</td>
<td>3.53E+02</td>
<td>2133.201</td>
</tr>
<tr>
<td>$H_2O$ (V)</td>
<td>3.05E+01</td>
<td>1.03E-02</td>
<td>0.00E+00</td>
<td>3.53E+02</td>
<td>1858.876</td>
</tr>
<tr>
<td>$H_2O$ (L)</td>
<td>7.55E+01</td>
<td>0.00E+00</td>
<td>0.00E+00</td>
<td>3.53E+02</td>
<td>4140.078</td>
</tr>
<tr>
<td>$N_2$</td>
<td>2.86E+01</td>
<td>3.77E-03</td>
<td>-5.00E+04</td>
<td>3.53E+02</td>
<td>1608.879</td>
</tr>
<tr>
<td>CH$_4$</td>
<td>2.36E+01</td>
<td>4.79E-02</td>
<td>-1.92E+05</td>
<td>3.53E+02</td>
<td>2051.266</td>
</tr>
<tr>
<td>CH$_3$OH (L)</td>
<td>3.13E+01</td>
<td>1.50E-01</td>
<td>4.94E+05</td>
<td>3.53E+02</td>
<td>4653.596</td>
</tr>
<tr>
<td>O$_2$</td>
<td>3.00E+01</td>
<td>4.18E-03</td>
<td>-1.67E+05</td>
<td>3.53E+02</td>
<td>1630.919</td>
</tr>
</tbody>
</table>

**STANDARD ENTHALPY VALUES ($\Delta H$)**

<table>
<thead>
<tr>
<th></th>
<th>(LHV) (J/mol)</th>
<th>(HHV) (J/mol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_2$</td>
<td>-241840.00</td>
<td>-284000.00</td>
</tr>
<tr>
<td>CH$_4$</td>
<td>-802310.00</td>
<td>-890800.00</td>
</tr>
<tr>
<td>CH$_3$OH</td>
<td>-645500.00</td>
<td>-726000.00</td>
</tr>
<tr>
<td>Diesel</td>
<td>-6867432.00</td>
<td>-7038000.00</td>
</tr>
</tbody>
</table>

**Condensing Economiser**

A condensing economiser, which may be incorporated into the design of a boiler, is an additional heat exchanger in the flue passage and uses energy in the flue gas to preheat the feed water before it enters the main boiler.
To determine the boiler efficiency, a heat balance is carried out on the economiser. Hence,

**Power in the inlet streams:**

(1) Power in the Flue gas Inlet, with mixture of $i$ gases and water vapour:

$$P_{FG,\text{In}} = \sum_i M_i \times \left( \int_{T_d}^{T_{FG,\text{In}}} C_{p_i} dT \right) + \left( M_w \times \left( \int_{T_d}^{T_{dew}} C_{p(w)} dT + \Delta H_{\text{vap}} + \int_{T_d}^{T_{dew}} C_{p(v)} dT \right) \right)$$

Where

- $M_i$ - Molar flowrate of gas (mol/s)
- $C_{p_i}$ - Heat capacity of gas (kJ/mol K)
- $T_d$ - Datum Temperature = 298.15 K
- $T_{FG,\text{In}}$ - Flue gas inlet temperature (K)
- $T_{dew}$ - Dew point temperature of the water at its partial pressure (K).
- $\Delta H_{\text{vap}}$ - Enthalpy of Evaporation at the dew point temperature (kJ/mol)
- $C_{p(w)}$, $C_{p(v)}$ - Heat capacity of water and vapour (kJ/mol K)

(2) Power in the feed water:

$$P_{W,\text{In}} = M_{w,\text{in}} \times \int_{T_d}^{T_{W,\text{In}}} C_{p(w)} dT$$

**Power in the outlet streams:**

(1) Power in the hot water outlet

$$P_{W,\text{Out}} = M_{w,\text{out}} \times \left( \int_{T_d}^{T_{dew}} C_{p(w)} dT + \Delta H_{\text{vap}} + \int_{T_d}^{T_{dew}} C_{p(v)} dT \right)$$
To determine the boiler efficiency, a heat balance is to be performed on the economiser. Hence,

> **Power in the inlet streams:**

(1) Power in the Flue gas Inlet, with mixture of $i$ gases and water vapour:

$$ P_{FG, In} = \left( \sum_i \dot{M}_i \times \int \frac{T_{FG, In}}{T_d} \right) + \left( \dot{M}_w \times \left( \int \frac{T_{dew}}{Cp(w)T_d} + \Delta H_{vap} + \int \frac{T_{FG, In}}{Cp(v)T_{dew}} \right) \right) $$

Where
- $\dot{M}_i$ - Molar flowrate of gas (mol/s)
- $Cp_i$ - Heat capacity of gas (kJ/mol K)
- $T_d$ - Datum Temperature = 298.15 K
- $T_{FG, In}$ - Flue gas inlet temperature (K)
- $T_{dew}$ - Dew point temperature of the water at its partial pressure (K).
- $\Delta H_{vap}$ - Enthalpy of Evaporation at the dew point temperature (kJ/mol)
- $Cp(w), Cp(v)$ - Heat capacity of water and vapour (kJ/mol K)

(2) Power in the feed water:

$$ P_{W, In} = \dot{M}_{w, In} \times \int \frac{T_{W, In}}{Cp(w)T_d} $$

> **Power in the outlet streams:**

(1) Power in the hot water outlet

$$ P_{W, Out} = \dot{M}_{w, out} \times \left( \int \frac{T_{dew}}{Cp(w)T_d} + \Delta H_{vap} + \int \frac{T_{W, Out}}{Cp(v)T_{dew}} \right) $$
(2) Power in flue gas exit

It is assumed in the model that 40% of the water remains in the flue gas and the economiser operates with an exit flue gas temperature ($T_{FG,Out}$) of 40°C.

$$P_{FG,Out} = \left( \sum_i M_i \times \frac{T_{FG,Out}}{T_d} \right) + \left( 0.4 \times \dot{M}_w \times \frac{T_{dew}}{T_d} \left( \int \frac{C_p(w) \, dT}{T_d} + \Delta H_{ap} + \int \frac{C_p(v) \, dT}{T_{dew}} \right) \right)$$

(3) Power in the condensate

It is assumed in the model that the temperature of the condensate ($T_{con}$) is 35°C.

$$P_{Con} = \dot{M}_{con} \times \frac{T_{con}}{T_d} \int \frac{C_p(w) \, dT}{T_d}$$

(4) Casing or surface losses

The casing losses ($P_{Cas}$) are assumed as 1.5% of the total power into the economiser.

$$P_{cas} = 0.015 \times P_{FG,In}$$

**Efficiency of the condensing economiser:**

The condensing economiser efficiency ($\eta_{Ecn}$) is calculated by the following equation:

$$\eta_{Ecn} = 1 - \frac{(P_{FG,Out} + P_{Con} + P_{Cas})}{P_{FG,In}}$$

Figure 3.8 in Section 3.2.4 shows the economiser efficiency as a function of flue gas inlet temperature.
Battery

The battery model is based on the traction battery model shown in the diagram above. From this diagram the following equations are derived:

Now, for $l > 0$, i.e. Battery Discharging

\[
\text{Battery Current, } I, \quad \Rightarrow \quad I = \frac{E_C - V_B}{R_d}
\]

and

\[
\text{Battery Power, } P_B, \quad \Rightarrow \quad P_B = I \times V_B = V_B \times \left( \frac{E_C - V_B}{R_d} \right) = \frac{V_B \times E_C - (V_B)^2}{R_d}
\]

To determine the relationship between battery voltage ($V_B$) and power ($P_B$), then need to solve the following equation, hence,

\[
\frac{V_B \times E_C - (V_B)^2}{R_d} - P_B = 0 \quad \text{or} \quad \frac{-(V_B)^2}{R_d} + \frac{V_B \times E_C}{R_d} - P_B = 0
\]

Now if $A = \frac{-1}{R_d}$ and $B = \frac{E_C}{R_d}$ than
\[-\frac{(V_B)^2}{R_d} + \frac{V_B \times E_c}{R_d} - P_b = 0 \Rightarrow A \times (V_B)^2 + B \times (V_B) + P_B = 0\]

Hence, solving this quadratic equation give the following solutions:

\[V_B = \frac{-B \pm \sqrt{B^2 - 4 \times A \times P_b}}{2 \times A}\]

Considering only the positive square root value, therefore,

\[V_B = \frac{-B + \sqrt{B^2 - 4 \times A \times P_b}}{2 \times A}\]

where \(A = \frac{-1}{R_d}\) and \(B = \frac{E_c}{R_d}\) for discharging battery

and

where \(A = \frac{-1}{R_c}\) and \(B = \frac{E_c}{R_c}\) for charging battery

This equation with values of \(R_d\), \(R_c\) and \(E_c\) from the manufacturing data is implemented into Matlab/Simulink simulation described in chapter 5 (section 5.3.5).

To protect the battery from either overcharging or completely discharging, the battery model also determines the maximum power available from the battery at a particular state of charge (SoC).

Now, at maximum power \(\frac{\partial P_B}{\partial V_B} = 0\), therefore

\[P_B = \frac{V_B \times E_c - (V_B)^2}{R_d} \Rightarrow \frac{\partial P_B}{\partial V_B} = \frac{E_c - 2 \times (V_B)}{R_d} = 0 \Rightarrow V_B = \frac{E_c}{2}\]
Hence, Maximum Battery Power, \( P_{B_{\text{Max}}} = \frac{(Ec)^2}{4 \times R_d} \) or \( \frac{(Ec)^2}{4 \times R_c} \)

For given power demand from the battery, the model also calculates the battery current and SoC.

The current is calculated by the equation:

\[
I = \frac{Ec - V_B}{R_d} \quad \text{or} \quad \frac{Ec - V_B}{R_c}
\]

and SoC is calculated by the equation:

\[
\text{SoC} = \text{Cell Charge} \pm \int I \, dt
\]

All these equations are also implemented in the Matlab/Simulink simulation.
APPENDIX II - List of Publications

➢ Modelling of solid polymer fuel cell system for marine application
   *Fuel Cell Seminar, Palm Springs, California, USA, November 1998, Page 675*

➢ Effect of operating pressure on the system efficiency of a methane-fuelled solid polymer fuel cell power source
   *Journal of Power Sources, Vol.71, March 1998, Page 337*

➢ Efficiency of an indirect fuelled solid polymer fuel cell (SPFC) vehicle

➢ Efficiency and performance assessment of a 4.6 tonne fuel cell van
   *EVS-12, Anaheim, California, USA, December 1994*

➢ Efficiency analysis of Methanol/SPFC and Hydrogen/SPFC traction systems
   *Fuel Cell Seminar, San Diego, California, USA, November 1994, Page 609*